# Higher Order Semiclassical Approximations for Hamiltonians with Operator-Valued Symbols

**Dissertation**

der Mathematisch-Naturwissenschaftlichen Fakultät
der Eberhard Karls Universität Tübingen
zur Erlangung des Grades eines
Doktors der Naturwissenschaften
(Dr. rer. nat.)

vorgelegt von

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Tübingen
2021

Gedruckt mit Genehmigung der Mathematisch-Naturwissenschaftlichen Fakultät
der Eberhard Karls Universität Tübingen.

Tag der mündlichen Qualifikation: 29.04.2021
Dekan: Prof. Dr. Thilo Stehle
1. Berichterstatter: Prof. Dr. Stefan Teufel
2. Berichterstatter: Prof. Dr. Caroline Lasser

# Danksagungen

Zuallererst möchte ich mich bei meinem Doktorvater Stefan Teufel bedanken. Danke, dass du es mir ermöglicht hast, mich mit diesem interessanten Thema zu beschäftigen. Trotz deiner vielen Verpflichtungen hast du dir immer Zeit für mich und meine Fragen genommen. Die interessanten Diskussionen mit dir hatten enormen Einfluss auf meine wissenschaftliche und persönliche Entwicklung. Ohne deine Hilfe und Unterstützung wäre diese Arbeit nicht denkbar gewesen.

Ein großer Dank geht auch an meinen Zweitbetreuer Christian Hainzl: unsere inhaltliche Zusammenarbeit hat sich zwar in Grenzen gehalten, aber du warst immer da wenn ich mal eine Ablenkung benötigt habe.

Motivierend für mich war außerdem die immer nette und produktive Atmosphäre in unserer Arbeitsgruppe: danke an euch alle!

Herzlichen Dank an Caroline Lasser dafür, dass du dich als Zweitgutachterin zur Verfügung gestellt hast. Außerdem bist du eine der Hauptverantwortlichen dafür, dass ich überhaupt eine Promotion in Tübingen begonnen habe, danke auch dafür.

Ferner bedanke ich mich bei der Deutschen Forschungsgemeinschaft und insbesondere beim Graduiertenkolleg 1838 für die finanzielle Förderung meiner Promotion und insbesondere meines Aufenthalts in Chicago.

In diesem Zusammenhang auch ein Dank an Christof Sparber, George Hagedorn und Jianfeng Lu für die Betreuung und interessanten Diskussionen während meines Aufenthaltes in den Vereinigten Staaten.

Außerdem möchte ich mich bei meinen WG-Kollegen Tobi und Peter bedanken: durch euch habe ich mich in Tübingen vom ersten Tag an zuhause gefühlt.

Danke an meine Freunde aus der Heimat: immer wenn ich mit euch zusammen bin, kann ich komplett abschalten und enorme Kraft tanken. Ihr seid die Besten!!

Ein großer Dank geht an meine Familie und besonders meine Eltern Angelika und Walter sowie meine Schwester Eva-Maria: ihr habt mich mein ganzes Leben hindurch unterstützt und wart ein fantastischer Rückhalt. Ohne euch wäre ich niemals so weit gekommen.

In diesem Sinne ein besonderer Dank auch an meine Freundin Laura, die mich fast seit Beginn meiner Promotion begleitet: du hast mich auch in schwierigen Zeiten ausgehalten und mich über die ganze Zeit stets so gut wie möglich unterstützt.

Abschließend möchte ich meinem kleinen Leo danken: du hast vielleicht nicht gerade dabei geholfen meine Dissertation schneller abzuschließen, aber etwas Ablenkung tut ja manchmal auch ganz gut.

# Zusammenfassung

Semiklassische Approximationen spielen eine wichtige Rolle in der mathematischen Physik. Hierbei ist es das Ziel, Eigenschaften geeigneter quantenmechanischer Systeme im Grenzwert $\hbar \to 0$ durch klassisch Hamiltonsche Systeme anzunähern. Im Standardfall wird das quantenmechanische System durch einen selbstadjungierten Hamiltonoperator $\hat{h} = h(x, -\mathrm{i}\,\hbar\,\nabla_x)$ auf dem Hilbertraum $L^2(\mathbb{R}^n)$ repräsentiert. Dann ist das assoziierte klassisch Hamiltonsche System gegeben durch $(T^*\mathbb{R}^n, \omega^0, h)$ wobei die Hamilton-Funktion $h$ das Symbol des Hamiltonoperators $\hat{h}$ und $(T^*\mathbb{R}^n, \omega^0)$ eine $2n$-dimensionale symplektische Mannigfaltigkeit darstellt. Der Phasenraum $T^*\mathbb{R}^n \cong \mathbb{R}^{2n}$ ist das Kotangentialbündel des $\mathbb{R}^n$. Die kanonische symplektische Form $\omega^0$ ist durch ihre Koeffizientenmatrix $\omega^0 = \left(\begin{smallmatrix} 0 & \mathbf{1}_n \\ -\mathbf{1}_n & 0 \end{smallmatrix}\right)$ festgelegt. Die durch semiklassische Methoden approximierten quantenmechanischen Eigenschaften umfassen das Spektrum und die Eigenfunktionen des Hamiltonoperators $\hat{h}$, Lösungen der zeitabhängigen Schrödingergleichung, die unitäre Gruppe $\mathrm{e}^{-\mathrm{i}\,\hat{h}t/\hbar}$, sowie statistische Erwartungswerte $\mathrm{tr}\Big(f(\hat{h})\,\hat{a}\Big)$.

Jedoch verhalten sich in vielen Situationen nur einige physikalische Freiheitsgrade semiklassisch. Das einfachste Beispiel hierzu sind Teilchen mit Spin. Hier nimmt die Wellenfunktion $\psi$ Werte in $\mathbb{C}^l$ an, also ist der Zustandsraum durch $L^2(\mathbb{R}^n, \mathbb{C}^l)$ gegeben. Allgemeiner betrachtet man den Zustandsraum $L^2(\mathbb{R}^n, \mathcal{H}_\mathrm{f})$, wobei $\mathcal{H}_\mathrm{f}$ einen separablen Hilbertraum darstellt. Der Hilbertraum $\mathcal{H}_\mathrm{f}$ wird als Raum der 'gefaserten' oder 'schnellen' Freiheitsgrade bezeichnet. In vielen derartigen Quantensystemen kann der Hamiltonoperator $\hat{H}^\varepsilon$ als Weyl-Quantisierung $\mathrm{op}_\varepsilon(H) = \hat{H}^\varepsilon = H(x, -\mathrm{i}\,\varepsilon\,\nabla_x)$ eines auf dem Phasenraum $T^*\mathbb{R}^n$ definierten Symbols $H(q,p)$ mit Werten in den linearen selbstadjungierten Operatoren auf $\mathcal{H}_\mathrm{f}$ dargestellt werden, also $\hat{H} = \mathrm{op}_\varepsilon(H)$ mit $H : T^*\mathbb{R}^n \cong \mathbb{R}^{2n} \to \mathcal{L}_\mathrm{sa}(\mathcal{H}_\mathrm{f})$. Hierbei kontrolliert der kleine, dimensionslose Parameter $\varepsilon \ll 1$ die Trennung der Skalen. Die physikalische Bedeutung von $\varepsilon$ ist abhängig vom konkreten Anwendungsbeispiel. Der asymptotische Grenzwert $\varepsilon \to 0$ entspricht dem adiabatischem Limes, in welchem sich die 'langsamen' von den 'schnellen' Freiheitsgrade entkoppeln. Gleichzeitig stellt $\varepsilon \to 0$ den semiklassischen Limes der 'langsamen' Freiheitsgrade dar. Für einen Überblick über adiabatische Probleme in der Physik verweisen wir auf das Buch von Bohm, Mostafazadeh, Koizumi, Niu und Zwanziger [Boh+13].

Auch im Zusammenhang adiabatischer Quantensysteme ist die semiklassische Analysis sehr erfolgreich und die Menge an existierenden Arbeiten in diesem Zusammenhang ist enorm. Das Ziel semiklassischer Methoden ist es, quantenmechanische Eigenschaften auf der Skala der 'langsamen' oder 'semiklassischen' Freiheitsgrade zu approximieren. In dieser Arbeit liegt der Fokus auf folgenden Eigenschaften: dem quantenmechanischen Erwartungswert einer Observable $\hat{A}^\varepsilon$ im thermodynamischen Gleichgewicht mit Zustand $f(\hat{H}^\varepsilon)$

$$\mathrm{tr}_{\mathcal{H}}(f(\hat{H}^\varepsilon)\,\hat{A}^\varepsilon)$$

sowie der quantenmechanischen Evolution einer Observable $\hat{A}^\varepsilon$ im Heiseberg-Bild der Quantenmechanik

$$\hat{A}^\varepsilon(t) = \mathrm{e}^{-\mathrm{i}\,\hat{H}t/\varepsilon}\,\hat{A}^\varepsilon\,\mathrm{e}^{-\mathrm{i}\,\hat{H}t/\varepsilon}\,.$$

Hierbei ist die Observable $\hat{A}^\varepsilon$ ein selbst-adjungierter Operator auf dem Hilbertraum $\mathcal{H}$ mit operatorwertigem Symbol $A : T^*\mathbb{R}^n \to \mathcal{L}_{\mathrm{sa}}(\mathcal{H}_\mathrm{f})$.

Es existiert eine Vielzahl an Methoden zur Herleitung solcher semiklassischer Approximationen. Beispiele hierfür sind adiabatische Störungstheorie (siehe z.B. [PST03b; Teu03]), WKB Methoden (siehe z.B. [EW96; Car08; WLY13]), Gaußsche Bündel (siehe z.B. [GRT88; DGR02; JWY08]), kohärente Zustände (siehe z.B. [Hag80; Hag87; Hag89; Hag94; HJ99; HJ01]) oder Wigner-Maße (siehe z.B. [Gér+97; MMP94; Bal+99; BMP01]). Was alle diese Methoden gemeinsam haben, ist die Einschränkung des Zustandsraumes $\mathcal{H}$ auf einen Unterraum, welcher mit einem oder einer Menge an Eigenwerten $e^{(i)}(q,p)$ des Symbols $H(q,p)$ assoziiert ist. Hierbei ist es notwendig, dass der Eigenwert oder die Menge an Eigenwerten $e^{(i)}(q,p)$ eine Lücke zum Rest des Spektrums von $H(q,p)$ aufweisen. Bekanntermaßen kommutiert die Quantisierung $\widehat{P^{(i)}}^\varepsilon$ der Projektion $P^{(i)}$ auf den Eigenraum des Eigenwertes $e^{(i)}(q,p)$ mit dem quantenmechanischen Evolutionsoperator $\mathrm{e}^{-\mathrm{i}\,\hat{H}t/\varepsilon}$ bis auf Fehler der Ordnung $\varepsilon\,(1+|t|)$, siehe z.B. [Teu03, Abschnitt 2.2]. Somit bleibt der Unterraum $\widehat{P^{(i)}}^\varepsilon\,\mathcal{H}$ bis auf Fehler der Ordnung $\varepsilon\,(1+|t|)$ invariant unter der quantenmechanischen Zeitevolution. Hierbei ist zu bemerken, dass, im Gegensatz zu $\mathrm{e}^{-\mathrm{i}\,\hat{H}t}$, der unitäre Operator $\mathrm{e}^{-\mathrm{i}\,\hat{H}t/\varepsilon}$ den Zeitevolutionsoperator auf der Skala der 'langsamen' Freiheitsgrade darstellt. Außerdem ist bekannt, dass für eine semiklassische Observable $\hat{a}^\varepsilon$ der quantenmechanische Erwartungswert im thermodynamischen Gleichgewicht, sowie die quantenmechanische Evolution der Observablen $\hat{a}^\varepsilon$, eingeschränkt auf den

Raum $\widehat{P^{(i)}}^{\varepsilon}\mathcal{H}$, durch die klassischen Analoga zum Hamiltonschen System $(\mathbb{R}^{2n}, \omega^0, e^{(i)})$ bis auf Fehler der Ordnung $\varepsilon$ approximiert werden. Es gilt:

$$\mathrm{tr}_{\mathcal{H}}\Big(f(\hat{H}^{\varepsilon})\,\hat{A}^{\varepsilon}\,\widehat{P^{(i)}}^{\varepsilon}\Big) = (2\pi\varepsilon)^{-n}\int_{\mathbb{R}^{2n}} f(h)\,a\,\lambda^0 + \mathcal{O}\Big(\varepsilon^{1-n}\Big) \tag{1}$$

sowie

$$\Big\|\widehat{P^{(i)}}^{\varepsilon}\Big(\hat{A}^{\varepsilon}(t) - \mathrm{op}_{\varepsilon}\Big(a(\Phi_0^t)\Big)\Big)\,\widehat{P^{(i)}}^{\varepsilon}\Big\| \leq \mathcal{O}\Big(\varepsilon\Big)\,, \tag{2}$$

wobei $\lambda^0 = \mathrm{d}q\,\mathrm{d}p$ das Liouville-Maß der kanonischen symplektischen Form $\omega^0$ und $\Phi_0^t$ den Fluss der Hamiltonschen Bewegungsgleichungen darstellen.

Basierend auf der Arbeit von Helffer und Sjöstrand [HS90a] bereiteten Nenciu und Sordoni [NS04] mit der Herleitung der fast-invarianten oder super-adiabatischen Projektion $\hat{\Pi}^{\varepsilon} = \widehat{P^{(i)}}^{\varepsilon} + \mathcal{O}(\varepsilon)$ den Weg für semiklassische Approximationen höherer Ordnung in $\varepsilon$. Die fast-invariante Projektion $\hat{\Pi}^{\varepsilon}$ kommutiert mit dem Hamiltonoperator $\hat{H}^{\varepsilon}$ und somit auch mit dem unitären Zeitevolutionsoperator $\mathrm{e}^{-\mathrm{i}\hat{H}t/\varepsilon}$ bis auf Fehler welche asymptotisch kleiner als jede Potenz von $\varepsilon$ sind. Somit bleibt der sogenannte fast-invariante Unterraum $\hat{\Pi}^{\varepsilon}\mathcal{H}$ bis auf Fehler beliebiger Ordnung in $\varepsilon$ invariant unter der quantenmechanischen Zeitevolution.

Aber wie verhalten sich quantenmechanische Systeme, wenn man den Zustandsraum auf den fast-adiabatischen Unterraum $\hat{\Pi}^{\varepsilon}\mathcal{H}$ einschränkt? Welches klassisch Hamiltonsche System kann mit einem solchen Quantensystem assoziiert werden? Oder anders gefragt: Welchen Einfluss hat die Störung der Eigenprojektion $P^{(i)}$ auf die Geometrie des klassischen Phasenraums und die Hamiltonfunktion? Können der quantenmechanische Erwartungswert im thermodynamischen Gleichgewicht und die quantenmechanische Evolution von Observablen eingeschränkt auf den fast-adiabatischen Unterraum $\hat{\Pi}^{\varepsilon}\mathcal{H}$ auf höhere Ordnungen in $\varepsilon$ semiklassisch approximiert werden? Und was ist mit Observablen mit operatorwertigen Symbolen? All diese Fragen können bisher nur teilweise oder gar nicht beantwortet werden. Ziel dieser Arbeit ist es eine vollständige Antwort auf alle obigen Fragen zu liefern.

Im Folgenden werden wir unsere Ergebnisse vorstellen, wobei wir auf technische Details verzichten. Wir betrachten einen Hamiltonoperator $\hat{H}^{\varepsilon}$ auf dem Hilbertraum $\mathcal{H} = L^2(\mathbb{R}^n, \mathcal{H}_{\mathrm{f}})$ mit Symbol $H : \mathbb{R}^{2n} \to \mathcal{B}_{\mathrm{sa}}(\mathcal{H}_{\mathrm{f}})$, welches Werte in den beschränkten, selbst-adjungierten Operatoren auf dem separablen Hilbertraum $\mathcal{H}_{\mathrm{f}}$ annimmt. Weiters sei $e_0 : \mathbb{R}^{2n} \to \mathbb{R}$ ein isolierter, nicht-entarteter Eigenwert von $H(q,p)$, der glatt von $(q,p)$ abhängt. Die Eigenprojektion zum Eigenwert $e_0(q,p)$ wird mit $P_0(q,p)$, und die mit $e_0(q,p)$ assoziierte super-adiabatische Projektion mit $\hat{\Pi}^{\varepsilon}$ bezeichnet. Für die genauen Voraussetzungen siehe Abschnitt 2.3.

In Abschnitt 3.2 zeigen wir, dass für jeden geeigneten Weyl-Operator $\hat{B}^{\varepsilon}$ mit operatorwertigem Symbol $B : \mathbb{R}^{2n} \to \mathcal{B}(\mathcal{H}_{\mathrm{f}})$ ein fast-eindeutiger semiklassischer Operator $\hat{b}^{\varepsilon}$ existiert, welcher die Wirkung des Operators $\hat{B}^{\varepsilon}$ eingeschränkt auf den fast-invarianten Unterraum $\hat{\Pi}^{\varepsilon}\mathcal{H}$ bis auf Fehler beliebiger Ordnung in $\varepsilon$ approximiert. Der Begriff fast-eindeutig bedeutet hier und im Folgenden, dass der Operator und sein Symbol eindeutig bis auf Fehler beliebiger Ordnung in $\varepsilon$ sind.

*Effektive Operatoren (cf. Satz 3.6)*
Sei $B : \mathbb{R}^{2n} \to \mathcal{B}(\mathcal{H}_{\mathrm{f}})$ ein geeignetes operatorwertiges Symbol und die Koeffizienten $b_i(z)$ rekursiv gegeben durch

$$b_0 = \mathrm{tr}_{\mathcal{H}_{\mathrm{f}}}\,(B\,P_0)$$

und

$$b_{j+1} = \mathrm{tr}_{\mathcal{H}_{\mathrm{f}}}\,(\beth_{j+1}\,P_0) \quad \text{für} \quad j \geq 0\,,$$

wobei $\beth_{j+1}$ als $j+1$-ter Koeffizient der asymptotischen Entwicklung $\pi \,\#\, (B - b^{(j)}\mathbf{1}_{\mathcal{H}_{\mathrm{f}}}) \,\#\, \pi \asymp \sum_{i=0}^{\infty} \varepsilon^i\, \beth_i$ mit $b^{(j)} = \sum_{i=0}^{j} \varepsilon^i\, b_i$ gegeben ist. Weiters sei das skalarwertige Symbol $b : \mathbb{R}^{2n} \to \mathbb{C}$ gegeben als Resummation der asymptotischen Entwicklung $\sum_{i=0}^{\infty} \varepsilon^i\, b_i(z)$.
Dann gilt

$$\pi \,\#\, B \,\#\, \pi - \pi \,\#\, b \,\#\, \pi = \mathcal{O}(\varepsilon^{\infty})$$

und

$$\left\| \hat{\Pi}^{\varepsilon}\, \hat{B}^{\varepsilon}\, \hat{\Pi}^{\varepsilon} - \hat{\Pi}^{\varepsilon}\, \hat{b}^{\varepsilon}\, \hat{\Pi}^{\varepsilon} \right\| = \mathcal{O}(\varepsilon^{\infty}).$$

Außerdem gilt für $\hat{B}^{\varepsilon}$ Spurklasse und beliebiges $N \in \mathbb{N}_0$, dass

$$\mathrm{tr}_{\mathcal{H}}\left(\left(\hat{B}^{\varepsilon} - \widehat{b^{(N)}}^{\varepsilon}\right)\hat{\Pi}^{\varepsilon}\right) = \mathcal{O}\left(\varepsilon^{N+1-n}\,\|B\|^{\varepsilon}_{L^1}\right).$$

Im Folgenden nennen wir $\hat{b}^{\varepsilon}$ den effektiven Operator von $\hat{B}^{\varepsilon}$ und $b(z)$ das entsprechende effektive Symbol. Beachte, das effektive Symbol $b$ ist reellwertig, falls das Symbol von $\hat{B}^{\varepsilon}$ Werte in den selbst-adjungierten Operatoren auf $\mathcal{H}_{\mathrm{f}}$ annimmt. Die Koeffizienten der asymptotischen Entwicklung $b(z) \asymp \sum_{i=0}^{\infty} \varepsilon^i\, b_i(z)$ sind explizit gegeben in Abhängigkeit vom Symbol $B(z)$, dem Symbol des Hamiltonoperators $H(z)$, dem Eigenwert $e_0(z)$, der Eigenprojektion $P_0(z)$ sowie deren Ableitungen.

Damit existiert ein fast-eindeutiger semiklassischer Operator $\hat{h}^{\varepsilon}$ mit $\varepsilon$-abhängigem Symbol $h : \mathbb{R}^{2n} \to \mathbb{R}$, welcher die Wirkung des Hamiltonoperators $\hat{H}^{\varepsilon}$ eingeschränkt auf den fast-invarianten Unterraum $\hat{\Pi}^{\varepsilon}\mathcal{H}$ auf beliebige

Ordnung in $\varepsilon$ approximiert, siehe Korollar 3.8. Die asymptotische Entwicklung von $h$ ist von der Form

$$h(z) \asymp e_0(z) + \sum_{i=1}^{\infty} \varepsilon^i M_i(z) .$$

Für den expliziten Ausdruck von $h$ inklusive der Korrektur zweiter Ordnung in $\varepsilon$, siehe (3.65). Das skalarwertige Symbol $h$ stellt die klassische Hamiltonfunktion des zum adiabatischen Quantensystem assoziierten klassisch Hamiltonschen Systems dar.

Dies ist die erste Arbeit, in welcher effektive Operatoren im obigen Sinne hergeleitet werden. Bisher war nicht bekannt und wurde noch nicht einmal vermutet, dass im Allgemeinen semiklassische Operatoren existieren, welche die Wirkung des Hamiltonoperators $\hat{H}^{\varepsilon}$ im fast-invarianten Unterraum $\hat{\Pi}^{\varepsilon}\mathcal{H}$ auf Fehler höherer Ordnung als $\varepsilon^2$ approximieren, siehe [ST13, Kapitel 3]. Hingegen ist die Existenz eines solchen effektiven Hamiltonoperators zu erster Ordnung schon bekannt, siehe zum Beispiel [ST13, Kapitel 3]. Die Korrektur erster Ordnung $M_0(z)$ zum Eigenwert $e_0(z)$ ist bekannt als 'M', 'no-name' oder Rammal-Wikinson-Term. Die Verallgemeinerung auf beliebige operatorwertige Symbole ist unseres Wissens auch für die Approximation zu Fehlern zweiter Ordnung in $\varepsilon$ eine Neuerung.

Es ist beachtlich, dass die Wirkung der 'schnellen' Freiheitsgrade im fast-adiabatischen Unterraum bis auf Fehler beliebiger Ordnung in $\varepsilon$ durch Korrekturen der semiklassischen Operatoren eingefangen werden kann. Dies ist eines der Hauptergebnisse dieser Arbeit, da es die Grundlage für die semiklassischen Approximationen in dieser Arbeit ist. Wir werden uns hier auf die Anwendung dieser effektiven Operatoren zur Herleitung semiklassischer Approximationen höherer Ordnung unter der Verwendung von Weyl-Calculus beschränken. Gleichwohl erwarten wir, dass mithilfe der effektiven Hamiltonfunktion $h$, durch Erweiterung der Methode von Emmrich und Weinstein [EW96], bessere WKB-Approximationen hergeleitet werden können.

Nachdem wir mit $h(z)$ die zugehörige Hamiltonfunktion des auf den fast-invarianten Unterraum eingeschränkten Quantensystems gefunden haben, beantworten wir im nächsten Schritt die Frage des Einflusses der Einschränkung auf den fast-invarianten Unterraum auf die Geometrie des Phasenraumes $\mathbb{R}^{2n}$. Hierzu zeigen wir in Proposition 3.2 die Existenz einer fast-eindeutigen Rang-1 Projektion $\mathcal{P}^{\varepsilon}(\varepsilon, z) = P_0(z) + \mathcal{O}(\varepsilon)$ welche, bis auf die

$P_0$-diagonale Korrektur $\varepsilon\,\tilde{\pi}(\varepsilon, z)$, mit dem Symbol $\pi(\varepsilon, z)$ der adiabatischen Projektion $\hat{\Pi}^{\varepsilon}$ übereinstimmt, es gilt

$$\pi(\varepsilon, z) = \mathcal{P}^{\varepsilon}(\varepsilon, z) + \varepsilon\, P_0(z)\,\tilde{\pi}(\varepsilon, z)\,P_0(z) + \varepsilon\, P_0^{\perp}(z)\,\tilde{\pi}(\varepsilon, z)\,P_0^{\perp}(z).$$

Die Familie von Rang-1 Projektionen $\mathcal{P}^{\varepsilon}(\varepsilon, z)$ induziert eine symplektische Form $\omega^{\varepsilon}$ auf dem Phasenraum $T^*\mathbb{R}^n$. Hierbei betrachtet man das Hilbertbündel $E : T^*\mathbb{R}^n \times \mathcal{H}_{\mathrm{f}} \overset{P_E}{\to} T^*\mathbb{R}^n$ mit $P_E$ der Projektion auf die erste Komponente und versehen mit dem kanonisch flachen Zusammenhang $\nabla$, wobei für $\phi \in \Gamma(E)$ und $X \in \Gamma(T(T^*\mathbb{R}^n))$ gilt, dass $(\nabla_X \phi)(z) = X^j\,\partial_j \phi(z)$. Das Symbol $H : T^*\mathbb{R}^n \to \mathcal{B}(\mathcal{H}_{\mathrm{f}})$ kann als Schnitt im Endomorphismenbündel von $E$ betrachtet werden, das heißt $H \in \Gamma(\mathrm{End}(E))$ wirkt auf Schnitte $\phi \in \Gamma(E)$. Nun wird mit der Rang-1 Projektion $\mathcal{P}^{\varepsilon} \in \Gamma(\mathrm{End}(E))$ das Vektorbündel $L^{\varepsilon} := \{(z, \phi)\,|\,\phi(z) \in \mathcal{P}^{\varepsilon}(\varepsilon, z)\,\mathcal{H}_{\mathrm{f}}\}$ von $E$ assoziiert. Durch Projektion des Zusammenhangs $\nabla$ auf $E$ wird nun ein Zusammenhang auf $L^{\varepsilon}$ induziert, also $\nabla^{\varepsilon}_X\,\phi := \mathcal{P}^{\varepsilon}\nabla_X\,\phi$ für $\phi \in \Gamma(L) \subset \Gamma(E)$ und $X \in \Gamma(T(T^*\mathbb{R}^n))$. Der resultierende Zusammenhang $\nabla^{\varepsilon}$ wird im Folgenden als modifizierter Berry-Zusammenhang bezeichnet. Die Krümmungsform $R^{\varepsilon}$ des modifizierten Berry-Zusammenhangs $\nabla^{\varepsilon}$, genannt modifizierte Berry-Krümmung, ist gegeben durch $\frac{1}{2} R^{\varepsilon}_{ij}\,\mathrm{d}z^i \wedge \mathrm{d}z^j$, wobei

$$R^{\varepsilon}_{ij} = \mathrm{tr}_{\mathcal{H}_{\mathrm{f}}}(\mathcal{P}^{\varepsilon}\,[\partial_i \mathcal{P}^{\varepsilon}, \partial_j \mathcal{P}^{\varepsilon}]),$$

siehe Proposition 3.9.

Die modifizierte Berry-Krümmung induziert eine symplektische Form $\omega^{\varepsilon}$ über dem klassischen Phasenraum $T^*\mathbb{R}^n$ durch $\omega^{\varepsilon} := \omega^0 - \varepsilon\,\mathrm{i}\,R^{\varepsilon}$, siehe Proposition 3.10. Somit definiert $\omega^{\varepsilon}$ eine $2n$-dimensionale symplektische Mannigfaltigkeit $(T^*\mathbb{R}^n, \omega^{\varepsilon})$ über dem Phasenraum $T^*\mathbb{R}^n$. Es stellt sich also heraus, dass die Einschränkung auf den fast-invarianten Unterraum $\hat{\Pi}^{\varepsilon}\mathcal{H}$ eine Krümmung der kanonischen symplektischen Mannigfaltigkeit $(T^*\mathbb{R}^n, \omega^0)$ induziert, welche durch die symplektische Form $\omega^{\varepsilon}$ dargestellt wird.

Des Weiteren ist die Koeffizientenmatrix der modifizierten Berry-Krümmung $R^{\varepsilon}$, bis auf einen Faktor $\mathrm{i}$, gegeben als Imaginärteil des modifizierten quantengeometrischen Tensors

$$\mathcal{T}^{\varepsilon}_{ij} := 2\,\mathrm{tr}_{\mathcal{H}_{\mathrm{f}}}(\mathcal{P}^{\varepsilon}\,\partial_i \mathcal{P}^{\varepsilon}\,\partial_j \mathcal{P}^{\varepsilon})\,.$$

Der Realteil des modifizierten quantengeometrischen Tensors $\mathcal{T}^\varepsilon$ definiert eine Fubini-Study-Metrik $g^\varepsilon$ auf dem Phasenraum $T^*\mathbb{R}^n$. Die Fubini-Study-Metrik $g^\varepsilon = g^\varepsilon_{ij}\,\mathrm{d}z^i \otimes \mathrm{d}z^j$ auf $T^*\mathbb{R}^n$ ist dann geben durch

$$g^\varepsilon_{ij} = \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\mathcal{P}^\varepsilon\,[\partial_i \mathcal{P}^\varepsilon, \partial_j \mathcal{P}^\varepsilon]_+)\,,$$

wobei $[\cdot,\cdot]_+$ den Anti-Kommutator darstellt.

Zusammen mit der klassischen Hamiltonfunktion $h$ definiert die symplektische Form $\omega^\varepsilon$ ein klassisch Hamiltonsches System $(T^*\mathbb{R}^n, \omega^\varepsilon, h)$. Durch die Hamiltonschen Gleichungen $\omega^\varepsilon(X^\varepsilon_h, \cdot) = \nabla h$ ist das Hamiltonsche Vektorfeld durch $X_h^{(\varepsilon,j)} = -(\omega^\varepsilon)^{-1}_{ji}\,\partial_i h$ gegeben. Dadurch ergeben sich die klassischen Bewegungsgleichungen

$$\begin{pmatrix} \dot{q} \\ \dot{p} \end{pmatrix} = -\omega^\varepsilon(q,p)^{-1} \begin{pmatrix} \partial_q h(q,p) \\ \partial_p h(q,p) \end{pmatrix} .$$

Wir sehen in weiterer Folge, dass, analog zu (1) und (2), quantenmechanische Gleichgewichtserwartungswerte, sowie die quantenmechanische Evolution von Erwartungswerten approximiert werden durch die zum klassisch Hamiltonschen System $(T^*\mathbb{R}^n, \omega^\varepsilon, h)$ zugehörigen, klassischen Analoga. Dabei müssen für semiklassische Approximationen höherer Ordnung Quantenkorrekturen der Ordnung $\varepsilon^2$ berücksichtigt werden.

Analog zur Herleitung des modifizierten Berry-Zusammenhangs $\nabla^\varepsilon$ induziert die führende Ordnung der Projektion $\mathcal{P}^\varepsilon$, die Eigenprojektion $P_0$, ein Vektorbündel $L := \{(z,\phi)\,|\,\phi(z) \in P_0(z)\,\mathcal{H}_\mathrm{f}\}$ von $E$, das sogenannte Eigenbündel. Der mit dem Eigenbündel assoziierte Zusammenhang $\nabla^{\mathrm{Berry}} = P_0\,\nabla$ ist bekannt als Berry-Zusammenhang. Der Berry-Zusammenhang ist eine wichtige Größe in der Festkörperphysik und allgemein im Zusammenhang mit adiabatischen Problemen. Die Holonomiegruppe des Berry-Zusammenhangs, die Berry-Phase, spielt eine wichtige Rolle in der Erforschung von Bloch-Elektronen und vielen verwandten Themen, wie schon in vielen wichtigen physikalischen und mathematischen Arbeiten untersucht [ST13; PST03b; MMP94; WLY13; CMS04; DL11; Bus87]).

Die mit der Eigenprojektion $P_0$ assoziierte Fubini-Study-Metrik $g_0$ auf dem Phasenraum $T^*\mathbb{R}^n$ ist unter anderem bekannt als Quantenmetrik. Im Vergleich zur Berry-Krümmung ist die Quantenmetrik nicht sehr gut erforscht, hat aber zuletzt reges Interesse in der Festkörperphysik geweckt, siehe [Pié+16; GYN14; GYN15; Tan+19; Roy14; PG18]. Wir werden sehen, dass die Quantenmetrik eine entscheidende Rolle in der semiklassischen

Approximation von quantenmechanischen Erwartungswerten im thermodynamischen Gleichgewicht spielt.

Unseres Wissens ist dies die erste Arbeit, in welcher, mit dem modifizierten Berry-Zusammenhang $\nabla^\varepsilon$ und der Fubini-Study-Metrik $g^\varepsilon$, allgemeine Korrekturen zum bekannten Berry-Zusammenhang $\nabla^{\mathrm{Berry}}$ und der Quantenmetrik $g_0$ herleitet werden. Durch Einführung eines Zusatzschrittes ergibt sich die Projektion $\mathcal{P}^\varepsilon$ auf natürliche Weise aus der Konstruktion der super-adiabatischen Projektion $\hat{\Pi}^\varepsilon$, siehe Lemma 3.1. Daher ist der Beweis von Existenz und Eindeutigkeit der Projektion $\mathcal{P}^\varepsilon$ relativ einfach, vorausgesetzt man ist vertraut mit der Konstruktion der super-adiabatischen Projektion $\hat{\Pi}^\varepsilon$. Die Hauptschwierigkeit und der Fortschritt liegen hier in der Entdeckung einer natürlichen Definition für $\mathcal{P}^\varepsilon$, sodass das damit assoziierte klassisch Hamiltonsche System $(T^*\mathbb{R}^n, \omega^\varepsilon, h)$, bis auf Quantenkorrekturen, quantenmechanische Gleichgewichtserwartungswerte sowie die quantenmechanische Evolution von Erwartungswerten approximiert. Für den Spezialfall von Bloch-Elektronen in einem uniformen elektromagnetischen Feld haben Gao, Yang und Niu [GYN14; GYN15] einen modifizierten Bloch-Zustand hergeleitet, welcher eng mit der Entwicklung zur ersten Ordnung der Projektion $\mathcal{P}^\varepsilon = P_0 + \varepsilon\, P_1 + \mathcal{O}(\varepsilon^2)$ verwandt ist, für weitere Details hierzu siehe Abschnitt 1.2.

Für ein Hamiltonsches System $(T^*\mathcal{M}, \omega, h)$ ist der Ensemble-Mittelwert einer Observable $a(z)$ im thermodynamischen Gleichgewicht mit Dichteverteilung $f(h(z))$ gegeben durch das Phasenraummittel

$$\langle a \rangle_{f(h)} := \int_{T^*\mathcal{M}} \rho(h)\, a\, \lambda\,,$$

wobei die Volumenform oder das Liouville-Maß der symplektischen Mannigfaltigkeit $(T^*\mathcal{M}, \omega)$ durch

$$\lambda := \tfrac{(-1)^{n(n-1)/2}}{n!}\, \omega^{\wedge n} = \tfrac{(-1)^{n(n-1)/2}}{n!}\, \underbrace{\omega \wedge \cdots \wedge \omega}_{n\text{-times}} \tag{3}$$

gegeben ist. Um quantenmechanische Erwartungswerte mit klassischen Erwartungswerten im thermodynamischen Gleichgewicht vergleichen zu können, ist es notwendig, die Lebesgue-Dichte $\nu^\varepsilon$ des Liouville-Maßes $\lambda^\varepsilon$ zur symplektischen Form $\omega^\varepsilon$ zu berechnen. Die Dichte $\nu^\varepsilon$ is verwandt mit der Pfaffschen Determinante $\mathrm{pf}(\omega^\varepsilon)$ der Koeffizientenmatrix $\omega^\varepsilon_{ij}$ der symplektischen Form $\omega^\varepsilon$ durch

$$\lambda = (-1)^{n(n-1)/2}\, \mathrm{pf}(\omega)\, \mathrm{d}q^1 \wedge \cdots \wedge \mathrm{d}p^n\,. \tag{4}$$

Des Weiteren nimmt die, aus der modifizierten Berry-Krümmung $R^\varepsilon$ resultierende, symplektische Form $\omega^\varepsilon$ die spezielle Form $\omega^\varepsilon = \omega^0 + \varepsilon\,\Omega^\varepsilon$ an. In diesem Zusammenhang zeigen wir zwei Spurformeln: Eine für die Dichte $\nu$ einer beliebigen symplektischen Form $\omega$ (Satz 2.9) und eine weiter Spurformel für die Entwicklung in $\varepsilon$ der Dichte $\nu^\varepsilon$ des Liouville-Maßes $\lambda^\varepsilon$ zur symplektischen Form $\omega^\varepsilon = \omega^0 + \varepsilon\,\Omega^\varepsilon$ (Proposition 2.7). Es ist bemerkenswert, dass die Spurformel zu allgemeinen symplektischen Formen direkt aus der $\varepsilon$-Entwicklung der Dichte $\nu^\varepsilon$ folgt, die umgekehrte Richtung ist hingegen schwierig zu zeigen. Daher ist unsere Strategie in Abschnitt 2.2, zuerst die Spurformel für die Entwicklung von $\nu^\varepsilon$ zu zeigen und die allgemeine Spurformel dann direkt daraus zu folgern. Der Beweis von Proposition 2.7 ist überaus technisch und nicht trivial.

*Spurformel für Liouville-Maße (cf. Satz 2.9)*
Sei $\Omega = \frac{1}{2}\sum_{i,j\in\{1,\dots,2n\}} \Omega_{ij}\,\mathrm{d}z^i \wedge \mathrm{d}z^j$ eine symplektische Form. Dann kann das Liouville-Maß $\lambda$ von $\Omega$ definiert durch (3) dargestellt werden als

$$\lambda = \sum_{\substack{\alpha\in\mathbb{N}_0^n,\\ \sum_{i=1}^n i\,\alpha_i = n}} \left(-\tfrac{1}{2}\right)^{|\alpha|} \prod_{j=1}^n (j^{\alpha_j}\,\alpha_j!)^{-1}\,\mathrm{Tr}_{2n}\Big((\omega^0\,\Omega)^j\Big)^{\alpha_j}\,\mathrm{d}q^1 \wedge \cdots \wedge \mathrm{d}p^n\,. \tag{5}$$

Kürzlich und unter Verwendung eines anderen Ansatzes zeigte Krivoruchenko in [Kri16], dass für zwei schiefsymmetrische Matrizen $A, B \in \mathbb{R}^{2n\times 2n}$ gilt:

$$\mathrm{pf}(A)\,\mathrm{pf}(B) = \sum_{\substack{\alpha\in\mathbb{N}_0^n,\\ \sum_{i=1}^n i\,\alpha_i = n}} \left(-\tfrac{1}{2}\right)^{|\alpha|} \prod_{j=1}^n (j^{\alpha_j}\,\alpha_j!)^{-1}\,\mathrm{Tr}_{2n}\Big((A\,B)^j\Big)^{\alpha_j}\,.$$

Dies ist eine Verallgemeinerung unserer Spurformel (5), da diese direkt aus obiger Formel, dem Zusammenhang zwischen dem Liouville-Maß und der Pfaffschen Determinante (4), sowie dem Fakt $\mathrm{pf}(\omega^0) = (-1)^{n(n-1)/2}$ folgt.

Jedoch wird für unsere Zwecke eine Formel für die $\varepsilon$-Entwicklung des Liouville-Maßes $\lambda^\varepsilon$ für semiklassische symplektische Formen $\omega^0 + \varepsilon\,\Omega$ benötigt. Unseres Wissens ist dies die erste Arbeit, welche eine solche Spurformel angibt und beweist.

*Spurformel für semiklassische Liouville-Maße (cf. Proposition 2.7)*
Sei $\omega^\varepsilon = \omega^0 + \varepsilon\,\Omega^\varepsilon$ eine $\varepsilon$-abhängige symplektische Form. Dann ist das Liouville-Maß $\lambda^\varepsilon$ von $\omega^\varepsilon$ gegeben durch

$$\lambda^\varepsilon = \sum_{k=0}^n \varepsilon^k\,\lambda_k^\varepsilon = \Big(1 + \sum_{k=1}^n \varepsilon^k\,\nu_k^\varepsilon\Big)\,\mathrm{d}q^1 \wedge \cdots \wedge \mathrm{d}p^n$$

mit

$$\nu_k^\varepsilon = \sum_{\substack{\alpha\in\mathbb{N}_0^k,\\ \sum_{i=1}^k i\,\alpha_i = k}} \left(-\tfrac{1}{2}\right)^{|\alpha|} \prod_{j=1}^{k} (j^{\alpha_j}\,\alpha_j!)^{-1}\,\mathrm{Tr}_{2n}\Big((\omega^0\,\Omega^\varepsilon)^j\Big)^{\alpha_j} \quad \text{für } 1\le k\le n\,.$$

Die Formel der Dichte $\nu^\varepsilon$ zur zweiten Ordnung in $\varepsilon$ ist gegeben durch

$$\nu^\varepsilon = 1 - \tfrac{1}{2}\,\varepsilon\,\mathrm{Tr}_{2n}(\omega^0\,\Omega^\varepsilon)) + \tfrac{1}{8}\,\varepsilon^2\,\mathrm{Tr}_{2n}(\omega^0\,\Omega^\varepsilon)^2 - \tfrac{1}{4}\,\varepsilon^2\,\mathrm{Tr}_{2n}(\omega^0\,\Omega^\varepsilon\,\omega^0\,\Omega^\varepsilon) + \mathcal{O}(\varepsilon^3)\,,$$

siehe Korollar 2.8.

Eines der Hauptziele dieser Arbeit ist die Herleitung semiklassischer Approximationen von quantenmechanischen Erwartungswerten für thermodynamische Gleichgewichtszustände. Hierbei ist der wichtigste und schwierigste Schritt, welcher auch den Großteil von Kapitel 4 ausmacht, die Herleitung der effektiven Operatoren von Gleichgewichtszuständen $f(\hat{H}^\varepsilon)$ eingeschränkt auf den fast-invarianten Unterraum $\hat{\Pi}^\varepsilon\mathcal{H}$. Hier ist zu bemerken, dass vor dieser Arbeit die Existenz semiklassischer Operatoren, welche die Wirkung von Gleichgewichtszuständen $f(\hat{H}^\varepsilon)$ im fast-invarianten Unterraum $\hat{\Pi}^\varepsilon\mathcal{H}$ auf Fehler der Ordnung höher als $\varepsilon^2$ approximieren, unbekannt war, auch auf heuristischer Ebene.

*Effektive stationäre Zustände (cf. Proposition 4.3)*
Sei $f:\mathbb{R}\to\mathbb{R}$ eine geeignete Verteilungsfunktion. Dann existieren $\varepsilon$-abhängige skalare Symbole $f^{\mathrm{sc}}(h)$ und $f^{\mathrm{adi}}(\pi,h)$, sodass

$$\Big\|\,\hat{\Pi}^\varepsilon\,\Big(f(\hat{H}^\varepsilon) - \mathrm{op}_\varepsilon\,(f^\varepsilon(h,\pi))\Big)\,\hat{\Pi}^\varepsilon\,\Big\| = \mathcal{O}(\varepsilon^\infty)$$

mit

$$f^\varepsilon(h,\pi) = f(h) + \varepsilon^2\,f^{\mathrm{sc}}(h) + \varepsilon^2\,f^{\mathrm{adi}}(\pi,h)\,.$$

Die explizite Konstruktion von $f^{\mathrm{sc}}(h)$ und $f^{\mathrm{adi}}(\pi,h)$ ist im Beweis von Proposition 4.3 dargestellt. Die asymptotische Entwicklung von $f^{\mathrm{sc}}(h)$ und $f^{\mathrm{adi}}(\pi,h)$ beginnt mit

$$\begin{aligned} f^{\mathrm{sc}}(h) &= -\tfrac{1}{24}\,f'''(e_0)\,\langle\,\omega^0\,\nabla e_0\,,\,\nabla^2 e_0\,\omega^0\,\nabla e_0\,\rangle \\ &\qquad + \tfrac{1}{16}\,f''(e_0)\,\mathrm{Tr}_{2n}(\omega^0\,\nabla^2 e_0\,\omega^0\,\nabla^2 e_0) + \mathcal{O}(\varepsilon) \\ &= -\tfrac{1}{24}\,\mathrm{Tr}_{2n}\Big(\omega^0\,\nabla(f''(e_0)\,\nabla^2 e_0\,\omega^0\,\nabla e_0)\Big) \\ &\qquad + \tfrac{1}{48}\,f''(e_0)\,\mathrm{Tr}_{2n}\Big((\omega^0\,\nabla^2 e_0)^2\Big) + \mathcal{O}(\varepsilon) \end{aligned}$$

und

$$f^{\mathrm{adi}}(h,\pi) = -\tfrac{1}{4}\,f''(e_0)\,\|\omega^0\,\nabla e_0\|_{g_0}^2 + \mathcal{O}(\varepsilon)\,.$$

Hierbei ist $g_0$ die Quantenmetrik, also die führende Ordnung der modifizierten Quanten-Metrik $g^\varepsilon$. Die führende Ordnung der Quantenkorrektur $f^{\mathrm{sc}}(h)$ stimmt mit der Korrektur überein, welche von Wigner [Wig32] für den Fall einer Boltzmann-Verteilung und semiklassischem Hamiltonoperator hergeleitet wurde, siehe (1.4). Im Gegensatz dazu stammt die Korrektur $f^{\mathrm{adi}}(\pi, h)$ von der adiabatischen Approximation, also von den 'schnellen' Freiheitsgraden.

Bis zu diesem Zeitpunkt gibt es in der Literatur keine systematische semiklassische Betrachtung von Gleichgewichtserwartungswerten, welche über die erste Ordnung in $\varepsilon$ hinausgeht. Insbesondere im Fall von nicht-trivialisierbaren Eigenbündeln sind keine semiklassischen Approximationen höherer Ordnung von quantenmechanischen Erwartungswerten im thermodynamischen Gleichgewicht bekannt, weder in speziellen Anwendungen, noch auf heuristischer Ebene. Bevor wir tiefer in die Thematik nicht-trivialer Eigenbündel eingehen, präsentieren wir eines der Hauptergebnisse dieser Arbeit: die semiklassische Approximation von Gleichgewichtserwartungswerten zu beliebiger Ordnung in $\varepsilon$.

*Erwartungswerte im thermodynamischen Gleichgewicht (cf. Satz 4.4)*
Sei $A : \mathbb{R}^{2n} \to \mathcal{B}_{\mathrm{sa}}(\mathcal{H}_{\mathrm{f}})$ das operatorwertige Symbol einer geeigneten Observable $\hat{A}^\varepsilon$. Dann gilt für jedes $N \in \mathbb{N}_0$, dass

$$\begin{aligned}\mathrm{tr}_{\mathcal{H}}\Big(f(\hat{H}^\varepsilon)\,\hat{A}^\varepsilon\,\hat{\Pi}^\varepsilon\Big) =&(2\pi\varepsilon)^{-n}\int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_{\mathrm{f}}}(\pi)\,\#\,f^\varepsilon(h,\pi)\,a^{(N)}\,\mathrm{d}z\\ &-\mathrm{i}\,\varepsilon\,(2\pi\varepsilon)^{-n}\int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_{\mathrm{f}}}(\pi\,\#\,\tfrac{\mathrm{i}}{\varepsilon}\,[\,f^\varepsilon(h,\pi)\,,\pi\,]_{\#})\,a^{(N)}\,\mathrm{d}z\\ &+\mathcal{O}\Big(\varepsilon^{-n+N+1}\,\|A\|^\varepsilon_{L^1}\Big)\,.\end{aligned}$$

Hierbei ist $a^{(N)} = \sum_{j=0}^N \varepsilon^j\,a_j(z)$ die asymptotische Entwicklung zur $N$-ten Ordnung des effektiven Symbols $a : \mathbb{R}^{2n} \to \mathbb{R}$ von $A(z)$, definiert durch (3.26).

Für Approximationen zu Fehlern der Ordnung $\varepsilon^3$ kann obiges Resultat umformuliert werden zu

$$\begin{aligned}\mathrm{tr}_{\mathcal{H}}\Big(f(\hat{H}^\varepsilon)\,\hat{A}^\varepsilon\,\hat{\Pi}^\varepsilon\Big) = (2\pi\varepsilon)^{-n}\Big(\int_{\mathbb{R}^{2n}} f^\varepsilon(h,\pi)\,a^{(2)}\,\lambda^\varepsilon + \varepsilon^2\int_{\mathbb{R}^{2n}} Q(e_0,g_0)\,a_0\,\mathrm{d}z\Big)\\ +\mathcal{O}\Big(\varepsilon^{3-n}\,\|A\|^\varepsilon_{L^1}\Big)\,,\end{aligned}$$

wobei $\lambda^\varepsilon$ das Liouville-Maß (3.74) zum Hamiltonschen System $(T^*\mathbb{R}^n, \omega^\varepsilon, h)$ darstellt. Der explizite Ausdruck der Quantenkorrektur $Q(e_0, g_0)$ ist gegeben durch

$$Q(e_0,g_0) = \tfrac{1}{2}\,\mathrm{Tr}_{2n}(\omega^0\,\nabla(f'(e_0)\,g_0\,\omega^0\,\nabla e_0)\,)\,.$$

In Satz 4.4 wird die erste rigorose und systematische Herleitung der semiklassischen Approximation quantenmechanischer Gleichgewichtserwartungswerte zu Ordnungen höher als $\varepsilon^2$ angegeben. Für den allgemeinen Fall von Observablen $\hat{A}^\varepsilon$ mit operatorwertigen Symbolen $A(z)$ ist uns kein vergleichbares Ergebnis bekannt, auch nicht für Approximationen erster Ordnung in $\varepsilon$. Wir weisen darauf hin, dass die Quantenkorrekturen zweiter Ordnung neben der Bandenergie $e_0$ und der Verteilungsfunktion $f$ nur von der Quanten-Metrik $g_0$ abhängen. Dies bekräftigt die allgemeine Bedeutung der Quanten-Metrik. Das $\varepsilon$-abhängige Hamiltonsche System $(T^*\mathbb{R}^n, \omega^\varepsilon, h)$ schließt große Teile der semiklassischen Approximation von Gleichgewichtserwartungswerten zu zweiter Ordnung ein. Obwohl wir annehmen, dass dies auch für beliebig hohe Ordnungen gilt, wird dies in dieser Arbeit nicht bewiesen.

Fast alle bestehenden Methoden zur Herleitung semiklassischer Approximationen für Quantensysteme mit operatorwertigen Symbolen basieren auf Eigenfunktionen $\phi_0(z)$ von $H(z)$ zum Eigenwert $e_0(z)$, also einer Trivialisierung des Eigenbündels $L := \{(z,\phi)\,|\,\phi(z) \in P_0(z)\,\mathcal{H}_\mathrm{f}\}$. Dies ist ein essenzieller Unterschied zu unserer Methode, sowie der Methoden in [ST13] und [EW96], welche sich auf die Verwendung der Eigenprojektion $P_0(z)$ stützen. Die wesentlichen Probleme bei der Verwendung von Eigenfunktionen sind einerseits die Uneindeutigkeit der Eigenfunktion $\phi(z)$, da mit $\phi(z)$ auch $\mathrm{e}^{\mathrm{i}\,b(z)}\,\phi(z)$ für reellwertiges $b : \mathbb{R}^{2n} \to \mathbb{R}$ eine Eigenfunktion von $H(z)$ darstellt. Andererseits gibt es Anwendungen bei welchen das Eigenbündel nicht trivialisierbar ist, also aus geometrischen Gründen keine glatte Wahl von $\phi(z)$ existiert. Natürlich ist $\mathbb{R}^{2n}$ kontrahierbar, was die Trivialisierbarkeit des Eigenbündels impliziert. Jedoch muss Weyl-Calculus für die Anwendbarkeit in bestimmten Applikationen erweitert werden, was dazu führen kann, dass die Trivialisierbarkeit des Eigenbündels nicht mehr gegeben ist. Ein Beispiel hierfür sind magnetische Bloch-Bänder, siehe Kapitel 6. Hier muss Weyl-Calculus für sogenannte $\tau$-equivariante Symbole erweitert werden, siehe [Teu03][Appendix B]. Dies führt dazu, dass Eigenbündel mit nichtverschwindender Chern-Zahl nicht trivialisierbar sind.

Als Nächstes diskutieren wir die semiklassische Approximation der quantenmechanischen Evolution von Observablen im Heisenberg-Bild der Quantenmechanik, auch bekannt als Satz von Egorov. Es existieren bereits Egorov-artige Ergebnisse zu beliebiger Ordnung in $\varepsilon$. Zum Beispiel liefert die raumadiabatische Störungstheorie solche Ergebnisse, siehe [Teu03]. Aber auch hier haben alle bestehenden Ergebnisse die Gemeinsamkeit, dass sie von der Trivialisierbarkeit des Eigenbündels abhängig sind. Außerdem muss in vielen Herleitungen von Ergebnissen des Egorov-Typs viel Arbeit in die Transformation zu eichinvarianten Resultaten gesteckt werden. In dieser Arbeit leiten wir semiklassische Approximationen der Evolution von Observablen her, welche, anstatt auf Eigenfunktionen, auf Eigenprojektionen basieren. Daher sind unsere Resultate per definitionem eichinvariant und können auch im Fall von nicht-trivialen Eigenbündeln angewandt werden. Weiters zeigen wir, mindestens für Approximationen zu Fehlern der Ordnung $\varepsilon^3$, dass die klassische Evolution des modifizierten Hamiltonschen Systems $(T^*\mathbb{R}^n, \omega^\varepsilon, h)$ die quantenmechanische Evolution, bis auf Quantenkorrekturen, approximiert.

*Satz von Egorov (cf. Satz 5.2)*
Sei $A : \mathbb{R}^{2n} \to \mathcal{B}_{\text{sa}}(\mathcal{H}_\text{f})$ das operatorwertige Symbol einer geeigneten Observable $\hat{A}^\varepsilon$ mit quantenmechanischer Zeitevolution

$$\hat{A}^\varepsilon(t) := \mathrm{e}^{\mathrm{i}\hat{H}^\varepsilon t/\varepsilon}\hat{A}^\varepsilon \mathrm{e}^{-\mathrm{i}\hat{H}^\varepsilon t/\varepsilon}\,.$$

Des Weiteren sei $\Phi^t_\varepsilon$ der Fluss des Hamiltonschen Systems $(T^*\mathbb{R}^n, \omega^\varepsilon, h)$ und $a(\Phi^t_\varepsilon)$ die klassische Zeitevolution des effektiven Symbols von $\hat{A}^\varepsilon$. Dann existiert ein $\varepsilon$-abhängiges semiklassisches Symbol $\mathfrak{A}(t) : \mathbb{R}^{2n} \to \mathbb{R}$, sodass:

$$\left\|\hat{\Pi}^\varepsilon \left(\hat{A}^\varepsilon(t) - \mathrm{op}_\varepsilon \left(a(\Phi^t_\varepsilon) + \varepsilon^2\, \mathfrak{A}(t)\right)\right) \hat{\Pi}^\varepsilon\right\| \leq \mathcal{O}\Big(\varepsilon^{N+1} \sum_{j=0}^{N+3} |t|^j\Big)$$

für jedes $N \in \mathbb{N}$.

Das semiklassische Symbol $\mathfrak{A}(t) : \mathbb{R}^{2n} \to \mathbb{R}$ hat eine asymptotische Entwicklung $\mathfrak{A}(t) \asymp \sum_{j=0}^\infty \varepsilon^{2j}\, \mathfrak{A}^N_{2j}(t)$ mit $\mathfrak{A}^N_{2j}(t) : \mathbb{R}^{2n} \to \mathbb{R}$ induktiv gegeben durch

$$\mathfrak{A}^N_0(t) := \int_0^t \mathfrak{A}^{c,N}_{h,\varepsilon}(a(\Phi^\tau_\varepsilon)) \circ \Phi^{t-\tau}_\varepsilon \,\mathrm{d}\tau$$

und

$$\mathfrak{A}^N_{2j}(t) := \int_0^t \mathfrak{A}^{c,N}_{h,\varepsilon}(\mathfrak{A}^N_{2(j-1)}(\tau)) \circ \Phi^{t-\tau}_\varepsilon \,\mathrm{d}\tau \quad \text{für } j \geq 1\,.$$

Zur Konstruktion des $\varepsilon$-abhängigen Symbols $\mathfrak{A}^{c,N}_{h,\varepsilon}(a)(z) : \mathbb{R}^{2n} \to \mathbb{R}$ siehe Proposition 5.1, insbesondere (5.14). Der explizite Ausdruck von $\mathfrak{A}^N_0(t)$ zu Fehlern der Ordnung $\varepsilon^3$ ist gegeben durch

$$\begin{aligned}\mathfrak{A}^2_0(t) = {} & 2\,\mathrm{i} \int_0^t \{e_0\,, a_0(\Phi^\tau_\varepsilon)\}_3 \circ \Phi^{t-\tau}_\varepsilon \,\mathrm{d}\tau \\ & - \tfrac{1}{2} \int_0^t \mathrm{tr}_{\mathcal{H}_\text{f}}(\{\{e_0\,, P_0\}\ , \{a_0(\Phi^\tau_\varepsilon)\,, P_0\}\}) \circ \Phi^{t-\tau}_\varepsilon \,\mathrm{d}\tau + \mathcal{O}(\varepsilon)\,.\end{aligned}$$

Folglich gilt für die quantenmechanische Zeitevolution des Erwartungswertes eines nicht-stationären Zustandes $\rho(t) = \mathrm{e}^{-\mathrm{i}\hat{H}^\varepsilon t/\varepsilon}\,\rho_0\,\mathrm{e}^{\mathrm{i}\hat{H}^\varepsilon t/\varepsilon}$ mit Anfangszustand $\rho_0 = \hat{\Pi}^\varepsilon \rho_0\, \hat{\Pi}^\varepsilon$, dass

$$\begin{aligned}\mathrm{tr}_{\mathcal{H}}(\rho(t)\,\hat{A}^\varepsilon) &= \mathrm{tr}_{\mathcal{H}}(\rho_0\,\hat{\Pi}^\varepsilon\,\hat{A}^\varepsilon(t)\,\hat{\Pi}^\varepsilon)\\ &= \mathrm{tr}_{\mathcal{H}}\Big(\rho_0\,\mathrm{op}_\varepsilon\Big(a(\Phi^t_\varepsilon) + \varepsilon^2\,\mathfrak{A}(t)\Big)\Big) + \mathcal{O}(\varepsilon^\infty)\,.\end{aligned}$$

Aufgrund der Darstellung unseres Egorov Theorems scheint die klassische Evolution des modifizierten Hamiltonschen Systems $(T^*\mathbb{R}^n, \omega^\varepsilon, h)$ große Teile der semiklassischen Approximation der Quanten-Evolution von Observablen beliebiger Ordnung zu umfassen. Obwohl wir dies annehmen, werden wir diese Aussage nur für semiklassische Approximationen zu Fehlern der Ordnung $\varepsilon^3$ beweisen. Zu diesem Zeitpunkt besteht auch die Möglichkeit, dass das Hinzunehmen der Terme höherer Ordnung des modifizierten Hamiltonschen Systems $(T^*\mathbb{R}^n, \omega^\varepsilon, h)$ zu zusätzlichen Korrekturen führt.

In Abschnitt 5.2 werden wir ein Schema zur Herleitung numerischer Approximationen der Zeitevolution quantenmechanischer Erwartungswerte $\mathrm{tr}_{\mathcal{H}}(\hat{\rho}^{\psi_t}\,\hat{A}^\varepsilon)$ mit initialer Wellenfunktion $\psi_0 \in \hat{\Pi}^\varepsilon\mathcal{H}$ zu beliebiger Ordnung in $\varepsilon$ herleiten. Hierzu formulieren wir die Korrekturen $\mathfrak{A}^N_j(t)$ für festes $N \in \mathbb{N}_0$ um. Es gilt:

$$\mathfrak{A}^N_j(t,z) = \sum_{j=0}^{N} \varepsilon^j \sum_{k=0}^{l_j} \Gamma_{j,k}(t, z, D^{m_{j,k}} a \circ \Phi^t_\varepsilon(z))\,,$$

wobei jedes

$$\Gamma_{j,k}(t,z) : \mathbb{R}^{\overbrace{2d \times \cdots \times 2d}^{m_{j,k}\ \text{times}}} \to \mathbb{R}$$

eine explizite, von dem effektiven Symbol $a$ unabhängige, lineare Abbildung vom Raum der $m_{j,k}$-Tensoren in die reellen Zahlen darstellt. Als Nächstes leiten wir ein System von Anfangswertproblemen erster Ordnung für die Komponenten von $\Gamma^{j,k}(t,z)$ her, sodass die Vektorisierung des Systems dargestellt werden kann als

$$\frac{\partial}{\partial t}\vec{\Gamma}(t,z) = N(t,z)\,\vec{\Gamma}(t,z) + b(t,z)\,.$$

Hierbei sind die Komponenten der Matrix $N(t,z)$ und des Vektors $b(t,z)$ explizit gegeben in Abhängigkeit von der Hamiltonfunktion $h$, dem Symbol der adiabatischen Projektion $\pi$, sowie deren Ableitungen, ausgewertet entlang des klassischen Flusses $\Phi^t_\varepsilon$. Somit kann die in [GL14] entwickelte, auf Wignermaße basierende Phasenraummethode direkt angewendet werden.

Das Resultat ist ein sehr effektiver Algorithmus zur Approximation der Zeitevolution von quantenmechanischen Erwartungswerten. In Abschnitt 7.4 validieren wir die Genauigkeit und Effektivität des numerischen Algorithmus, indem wir diesen auf ein einfaches Quantensystem des Born-Oppenheimer-Typs mit matrixwertigem Potential

$$V(x) = \begin{pmatrix} \tanh(x) & \delta \\ \delta & -\tanh(x) \end{pmatrix}, \qquad \delta > 0\,,$$

anwenden.

In Kapitel 6 wenden wir unsere Ergebnisse auf ein Gas von nicht-wechselwirkenden Fermionen in der Tight-Binding-Approximation auf dem Gitter $\mathbb{Z}^2$ und unter Einfluss eines starken konstanten magnetischen Feldes und eines zusätzlichen elektromagnetischen Feldes mit langsam variierenden Potentialen, genannt Hofstadter-Modell, an. Hier ist zu bemerken, dass bei nicht-verschwindendem starkem Magnetfeld $\mathbf{B} = \left(\begin{smallmatrix} 0 & B_0 \\ -B_0 & 0 \end{smallmatrix}\right)$, $B_0 = 2\pi\frac{p}{q}$ die assoziierten Eigenbündel im Allgemeinen nicht-trivialisierbar sind. Dies führt dazu, dass die meisten Methoden zur Herleitung semiklassischer Approximationen in diesem Fall nicht anwendbar sind.

Wir leiten in dieser Anwendung die Bewegungsgleichungen der sogenannten Hofstadter-Elektronen her und geben diese bis zu Fehlern der Ordnung $\varepsilon^3$ explizit an, siehe Abschnitt 6.1. Außerdem applizieren wir Satz 5.2 auf dieses Modell und erhalten damit zum ersten Mal eine semiklassische Approximation der quantenmechanischen Zeitevolution von Observablen zu Fehlern der Ordnung $\varepsilon^3$ für magnetische Bloch-Bänder.

Des Weiteren wenden wir Satz 4.4 an, um die freie Energie von Hofstadter-Elektronen unter Einfluss starker magnetischer Felder $\mathbf{B} = \left(\begin{smallmatrix} 0 & B^\varepsilon \\ -B^\varepsilon & 0 \end{smallmatrix}\right)$, $B^\varepsilon = 2\pi\frac{p}{q} + \varepsilon\, b$, $b \in \mathbb{R}$, $p \in \mathbb{Z}$, $q \in \mathbb{N}$ ungerade, auf Fehler der Ordnung $\varepsilon^3$ zu approximieren. Mithilfe der semiklassischen Approximation der freien Energie berechnen wir die Suszeptibilität $\mathcal{S}(B^\varepsilon, \beta, \mu) = \partial^2_{B^\varepsilon} p(B^\varepsilon, \beta, \mu)$. Hierbei ist die Approximation zu höherer Ordnung entscheidend, da jede Approximation zu Fehlern der Ordnungen kleiner $\varepsilon^3$, mit Null, ein falsches Ergebnis für die Suszeptibilität liefert.

Es ist zu bemerken, dass die Anwendung auf magnetische Bloch-Bänder eine Hauptmotivation für diese Arbeit ist. Semiklassische Approximationen zweiter Ordnung und insbesondere die Suszeptibilität von Bloch-Elektronen haben zuletzt starkes Interesse im Bereich der Festkörperphysik geweckt, wie bestätigt durch die große Anzahl jüngster Arbeiten [GYN14; GYN15; LZZ15; OF15; Oga16; Rao+15; Pié+16]. Auch diese Arbeiten basieren jedoch auf Eigenfunktionen und sind daher nicht anwendbar, sobald die Eigenbänder nicht-trivialisierbar sind. Dies ist aber bei Betrachtung starker Magnetfelder im Allgemeinen der Fall (Chern-Zahl $\neq 0$). Daher liefern diese Methoden nur im Fall $B^\varepsilon = \varepsilon\, b$ Ergebnisse. Für die Suszeptibilität können auf Eigenfunktionen basierende Methoden im Allgemeinen nur Ergebnisse für ein verschwindendes Magnetfeld liefern. Für eine ausführlichere Einführung in Bloch-Elektronen sowie einen detaillierteren Vergleich mit existierender Literatur verweisen wir auf Abschnitt 1.2, beziehungsweise Kapitel 6.

Zu guter Letzt betrachten wir das Paradebeispiel für adiabatische Quantensysteme, nämlich Hamiltonoperatoren vom Born-Oppenheimer-Typ, Kapitel 7. Also betrachten wir einen Hamiltonoperator

$$\hat{H}^\varepsilon = \tfrac{\varepsilon^2}{2}(-\mathrm{i}\,\nabla_x - A(x))^2 + V(x)$$

auf dem Hilbertraum $\mathcal{H} = L^2(\mathbb{R}^n) \otimes \mathcal{H}_\mathrm{f}$ mit magnetischem Vektorpotential $A : \mathbb{R}^n \to \mathbb{R}^n$ und operatorwertigem Potential $V(x) \in \mathcal{B}_\mathrm{sa}(\mathcal{H}_\mathrm{f})$. Moleküle unter Einfluss elektromagnetischer Felder werden von Hamiltonoperatoren von obiger Form beschrieben. Daher ist die effektive Beschreibung von Born-Oppenheimer-Typ Systemen von großer Wichtigkeit in der Chemie sowie der theoretischen Physik.

Auch in diesem Zusammenhang basieren die meisten bekannten Methoden auf der Verwendung von Eigenfunktionen mit dem Nachteil, dass die Resultate oft von der Eichung abhängen. Des Weiteren sind die Eigenwerte des elektronischen Hamiltonoperators $V(x)$ im nuklearen Konfigurationsraum $\mathbb{R}^n$ im Allgemeinen nur lokal isoliert. In diesen Fällen ist man gezwungen sich auf Lösungen der Schrödingergleichung zu beschränken, deren Träger initial in $\Lambda \subset \mathbb{R}^n$ ist und in diesem Gebiet bleibt, wobei $\Lambda \subset \mathbb{R}^n$ die Region darstellt in welcher der betrachtete Eigenwert $e_v(x)$ die 'Gap'-Bedingung erfüllt. Dann definiert die entsprechende Eigenfunktion $P_0 : \Gamma \to \mathcal{B}(\mathcal{H}_\mathrm{f})$ ein Vektorbündel, das im Allgemeinen nicht-trivialisierbar ist. Nichtsdestotrotz werden wir uns in dieser Arbeit auf den Fall mit global-isoliertem Eigenband beschränken.

Wir leiten die Bewegungsgleichungen für die 'langsamen' Freiheitsgrade, die Atomkerne, her und geben diese bis zu Fehlern der Ordnung $\varepsilon^3$ explizit an, siehe Abschnitt 7.1. Durch Anwendung von Satz 4.4 leiten wir, unseres Wissens zum ersten Mal, eine semiklassische Approximation von quantenmechanischen Erwartungswerten im thermodynamischen Gleichgewicht her, Abschnitt 7.2. Außerdem applizieren wir Satz 5.2 und erhalten damit die explizite semiklassische Approximation der quantenmechanischen Zeitevolution von Observablen zu Fehlern der Ordnung $\varepsilon^3$, Abschnitt 7.3.

# Contents

# 1 Introduction

Semiclassical approximations play a significant role in mathematical physics. Here, the goal is to approximate properties of quantum mechanical systems in the limit $\hbar \to 0$ using an appropriate classical Hamiltonian system. Typically, a semiclassical quantum system is represented by a self-adjoint Hamiltonian operator $\hat{H} = H(x, -\mathrm{i}\,\hbar\,\nabla_x)$ acting on the Hilbert space $\mathcal{H}$. Then, the associated classical Hamiltonian system is of the form $(T^*\mathbb{R}^n, \omega, h)$ where $(T^*\mathbb{R}^n, \omega)$ is a symplectic $2n$-dimensional manifold and the classical Hamiltonian $h$ is a smooth function on phase space $T^*\mathbb{R}^n$ with values in the reals. The phase space $T^*\mathbb{R}^n \cong \mathbb{R}^{2n}$ is the cotangent bundle of the $n$-dimensional space $\mathbb{R}^n$. The range of properties approximated by semiclassical methods includes the spectrum and eigenfunctions of the Hamiltonian operator $\hat{H}$, solutions to the time-dependent Schrödinger Equation, the full unitary group $\mathrm{e}^{-\mathrm{i}\,\hat{H}t/\hbar}$ as well as statistical expectation values $\mathrm{tr}\big(f(\hat{H})\,\hat{a}\big)$.

An essential tool in semiclassical analysis is pseudodifferential calculus. Here, a classical function on phase space $a : \mathbb{R}^{2n} \to \mathbb{C}$ is linked directly to a quantum operator on $L^2(\mathbb{R}^n)$ through a quantization rule. We denote the function $a(q,p)$ on phase space as symbol of the quantized operator $\hat{a}^\varepsilon = a(x, -\mathrm{i}\,\hbar\,\nabla_x)$. The most commonly used quantization rule is the Weyl quantization where one of the main arguments for this particular quantization rule is that it maps classical observables to quantum observables, i.e. it maps real valued functions to essentially self-adjoint operators on $L^2(\mathbb{R}^n)$. For a more detailed introduction and a selection of known results from Weyl calculus, see Section 2.1.

In a quantum mechanical system the time evolution of an initial state $\psi_0 \in \mathcal{H}$ is governed by the underlying Schrödinger equation

$$\mathrm{i}\,\hbar\,\partial_t \psi_t = \hat{H}\,\psi_t$$

or equivalently by the action of the unitary evolution operator, i.e.

$$\psi_t = \mathrm{e}^{-\mathrm{i}\hat{H}t/\hbar}\,\psi_0\,.$$

In the Heisenberg picture of quantum mechanics, rather than considering a time-dependent wave function $\psi_t$ one considers time-dependent observables $\hat{a}(t)$ whose time-evolution is given by

$$\hat{a}(t) = \mathrm{e}^{\mathrm{i}\hat{H}t/\hbar}\, \hat{a}\, \mathrm{e}^{-\mathrm{i}\hat{H}t/\hbar}\,.$$

The quantum mechanical expectation with respect to an observable $\hat{a}$ is equal in both pictures since

$$\begin{aligned} \langle \psi_t\,,\, \hat{a}\,\psi_t \rangle_{\mathcal{H}} &= \left\langle \mathrm{e}^{-\mathrm{i}\hat{H}t/\hbar}\,\psi_0\,,\, \hat{a}\,\mathrm{e}^{-\mathrm{i}\hat{H}t/\hbar}\,\psi_0 \right\rangle_{\mathcal{H}} \\ &= \left\langle \psi_0\,,\, \mathrm{e}^{\mathrm{i}\hat{H}t/\hbar}\,\hat{a}\,\mathrm{e}^{-\mathrm{i}\hat{H}t/\hbar}\,\psi_0 \right\rangle_{\mathcal{H}} = \langle \psi_0\,,\, \hat{a}(t)\,\psi_0 \rangle_{\mathcal{H}}\,. \end{aligned}$$

On the contrary, the classical Hamiltonian function $h \in C^\infty(T^*\mathcal{M})$ defines the so called Hamiltonian vector field $X_h$ by $\omega(X_h, \cdot) = \mathrm{d}h$. The flow $\Phi^t$ generated by the Hamiltonian vector field $X_h$ is known as the Hamiltonian flow associated to the Hamiltonian system $(T^*\mathcal{M}, \omega, h)$. The classical time-evolution of an observable $a \in C^\infty(T^*\mathcal{M})$ is governed by the Hamiltonian flow $\Phi^t$, we have $a(t) = a(\Phi^t)$.

The standard system of semiclassical analysis is a Hamiltonian $\hat{h}^\varepsilon$ acting on $L^2(\mathbb{R}^n)$ where $\hat{h}^\varepsilon$ is the Weyl quantization of a real-valued function $h : T^*\mathbb{R}^n \cong \mathbb{R}^{2n} \to \mathbb{R}$. Then, using Weyl calculus and a standard Duhamel argument one can show that the quantum mechanically evolved observable $\hat{a}^\varepsilon(t)$ is approximated by the Weyl quantization of the classically evolved symbol $a(\Phi^t)$. Here, $\Phi^t$ is the flow of the classical Hamiltonian system $(\mathbb{R}^{2n}, \omega^0, h)$ where $\omega^0$ is the canonical symplectic form with coefficient matrix $\left(\begin{smallmatrix} 0 & \mathbf{1}_n \\ -\mathbf{1}_n & 0 \end{smallmatrix}\right)$. This result is usually referred to as Egorov's theorem and has first been formulated in [Ego69]. More precisely, one gets for any $N \in \mathbb{N}_0$ that

$$\left\| \mathrm{e}^{\mathrm{i}\,\hat{h}^\varepsilon\, t/\hbar}\, \hat{a}^\varepsilon\, \mathrm{e}^{-\mathrm{i}\,\hat{h}^\varepsilon\, t/\hbar} - \mathrm{op}_\varepsilon\left(a(\Phi^t)\right) - \sum_{j=1}^{N} \hbar^{2j}\, \mathrm{op}_\varepsilon\left(a_j(t)\right) \right\| = \mathcal{O}(\hbar^{2N+1}) \qquad (1.1)$$

holds uniformly on bounded time intervals where the higher order corrections are given explicitly in terms of the symbols $a, h$ and their derivatives. For a proof of the above result and refined error estimates within the context of semiclassical microlocal analysis, see e.g. [Rob87; BR02; Zwo12]. Note here, using the above result one can approximate the quantum evolution of observables up to arbitrary order in terms of the classical counterparts $h$ and $a$ to the Hamiltonian $\hat{h}^\varepsilon$ and observable $\hat{a}^\varepsilon$. Here, one shall keep that the classical evolution yields an approximation to errors of order $\hbar^2$. The higher order corrections can not be expressed as classical Hamiltonian system.

Another important application of semiclassical analysis that will be of big importance throughout this thesis is the approximation of quantum statistical expectation values. For a thermodynamic equilibrium state $f(\hat{H})$ the expectation value with respect to a trace-class observable $\hat{a}$ is given by

$$\langle \hat{a}^{\varepsilon} \rangle_{f(\hat{H})} := \operatorname{tr}\Big(f(\hat{H})\,\hat{a}\Big)\,.$$

For a classical Hamiltonian system $(T^*\mathcal{M}, \omega, h)$ the average of an observable $a(z)$ in thermodynamic equilibrium with distribution $f(h(z))$ is given by the phase space average

$$\langle a \rangle_{f(h)} := \int_{T^*\mathcal{M}} \rho(h)\, a\, \lambda \tag{1.2}$$

where the volume form or Liouville measure of the symplectic space $(T^*\mathcal{M}, \omega)$ is given by

$$\lambda := \tfrac{(-1)^{n(n-1)/2}}{n!}\, \omega^{\wedge n} = \tfrac{(-1)^{n(n-1)/2}}{n!} \underbrace{\omega \wedge \cdots \wedge \omega}_{n\text{-times}}\,. \tag{1.3}$$

In the standard case of a purely semiclassical system, i.e. a Hamiltonian $\hat{h}^{\varepsilon}$ given as Weyl quantization of a real-valued function $h(q,p)$, it is well known that the expectation value of a thermodynamic equilibrium distribution $f(\hat{h}^{\varepsilon})$ with respect to a trace-class observable $\hat{a}^{\varepsilon}$ is approximated by its classical counterpart, i.e.

$$\left| \operatorname{tr}\Big(f(\hat{h}^{\varepsilon})\,\hat{a}^{\varepsilon}\Big) - \tfrac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^{2n}} f(h(z))\, a(z)\, \mathrm{d}z \right| = \mathcal{O}(\hbar^{2-n})\,.$$

In his famous paper 'On the Quantum Correction for Thermodynamic Equilibrium' [Wig32] Wigner derived the second order correction to the classical phase space average for the special case of Boltzmann distributed particles subject to an external potential. Herein, the importance of the second order quantum correction as first correction to the classical evolution was pointed out. Using Weyl calculus, Wigner's result can be generalized to

$$\left| \operatorname{tr}\Big(f(\hat{h}^{\varepsilon})\,\hat{a}^{\varepsilon}\Big) - \tfrac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^{2n}} \Big(f(h(z)) + \hbar^2\, f^{\mathrm{sc}}(h)(z)\Big)\, a(z)\, \mathrm{d}z \right| = \mathcal{O}(\hbar^{4-n}) \tag{1.4}$$

where

$$\begin{aligned} f^{\mathrm{sc}}(h)(z) = &-\ \tfrac{1}{24}\, f'''(h(z))\, \Big\langle \omega^0\, \nabla h(z)\,,\, \nabla^2 h(z)\, \omega^0\, \nabla h(z) \Big\rangle_{\mathbb{C}^{2n}} \\ &+ \tfrac{1}{16}\, f''(h(z))\, \mathrm{Tr}_{\mathbb{C}^{2n}}\Big(\omega^0\, \nabla^2 h(z)\, \omega^0\, \nabla^2 h(z)\Big) \end{aligned}$$

with $\omega^0$ the coefficient matrix of the canonical symplectic form.

Moreover, the above result extends to semiclassical approximations to arbitrary order in $\hbar$, see [DS99, Chapter 8].

To summarize, in the special case of a semiclassical system one can approximate the evolution of observables as well as expectation values in thermodynamic equilibrium to errors or order $\varepsilon^2$ by the classical counterparts. Moreover, there are explicit expressions in terms of the operator's symbols and their derivatives to approximate those quantities to arbitrary order in $\varepsilon$.

Nonetheless, the above results hold only for very specific systems where all degrees of freedom behave semiclassically but there are many examples of quantum mechanical systems where only some degrees of freedom behave semiclassically. The simplest of such examples are particles with spin. Here, the wave functions takes value in $\mathbb{C}^l$, i.e the state space is $L^2(\mathbb{R}^n, \mathbb{C}^l)$. More general, one considers a state space $L^2(\mathbb{R}^n, \mathcal{H}_\mathrm{f})$ where $\mathcal{H}_\mathrm{f}$ is a separable Hilbert space denoted as the space of 'fast' or 'fiber' degrees of freedom. In many such systems the Hamiltonian can be expressed as Weyl quantization $\hat{H}^\varepsilon = H(x, -\mathrm{i}\,\varepsilon\,\nabla_x)$ of a symbol $H(q,p)$ on phase space $T^*\mathbb{R}^n$ taking value in the linear self-adjoint operators on $\mathcal{H}_\mathrm{f}$, i.e. $H : T^*\mathbb{R}^n \to \mathcal{L}_\mathrm{sa}(\mathcal{H}_\mathrm{f})$. Here, the small, dimensionless parameter $\varepsilon \ll 1$ controls the separation of the scales. The physical meaning of $\varepsilon$ depends on the concrete example. The asymptotic limit $\varepsilon \to 0$ corresponds to the adiabatic limit where the 'slow' and 'fast' degrees of freedom decouple. At the same time $\varepsilon \to 0$ is the semiclassical limit for the slow degrees of freedom. For a survey of adiabatic problems in physics see the book of Bohm, Mostafazadeh, Koizumi, Niu and Zwanziger [Boh+13].

Also within the context of adiabatic problems semiclassical analysis is very successful and a vast amount of literature exists. The goal of semiclassical analysis is to approximate properties on the scale of the 'slow' or 'semiclassical' degrees of freedom. There are various approaches to derive such approximations. Examples are adiabatic perturbation theory (see e.g. [PST03b; Teu03]), WKB methods (see e.g. [EW96; Car08; WLY13]), Gaussian beams (see e.g. [GRT88; DGR02; JWY08]), frozen Gaussians (see e.g. [DLY16; DLY18]), methods based on coherent states (see e.g. [Hag80; Hag87; Hag89; Hag94; HJ99; HJ01]) or Wigner measures (see e.g [Gér+97; MMP94; Bal+99; BMP01]). What all approaches have in common is that they rely on restricting the state space $\mathcal{H}$ to a subspace associated to a single or a set of eigenvalues $e^{(i)}(q,p)$ of the Hamiltonian's symbol $H(q,p)$ that is gapped away from the rest of the spectrum. Let $e_0(q,p)$ be such an eigenvalue of $H(q,p)$ with projection $P_0(q,p)$ to the respective eigenspace. Using Weyl calculus it is easy to see that up to errors of order $\varepsilon$ the Weyl quantization $\hat{P}_0^{\varepsilon}$ of the eigenprojection $P_0$ commutes with the Hamiltonian operator $\hat{H}^{\varepsilon}$, i.e.

$$\left[\hat{H}^{\varepsilon}, \hat{P}_0^{\varepsilon}\right] = \mathcal{O}(\varepsilon)\,.$$

Hence, the range of $\hat{P}_0^{\varepsilon}$ is invariant under the action of $\hat{H}^{\varepsilon}$ up to errors of order $\varepsilon$. Then, a standard Duhamel argument shows for the evolution operator $\mathrm{e}^{-\mathrm{i}\,\hat{H}^{\varepsilon}\,t}$ on the time-scale of the 'fast' degrees of freedom that

$$\left[\mathrm{e}^{-\mathrm{i}\,\hat{H}^{\varepsilon}\,t}, \hat{P}_0^{\varepsilon}\right] = \mathcal{O}(\varepsilon\,|t|)\,.$$

So, on the 'fast' time-scale the subspace $\hat{P}_0^{\varepsilon}\mathcal{H}$ is invariant under the quantum evolution to errors of order $\varepsilon\,|t|$. However, what we are actually interested in is the dynamics on the time scale of the 'slow' degrees of freedom. Here, the same argument yields only an $\mathcal{O}(1)$ error. Nevertheless, it is known that the operator $\hat{P}_0^{\varepsilon}$ does in fact commute with the unitary quantum evolution $\mathrm{e}^{-\mathrm{i}\,\hat{H}^{\varepsilon}\,t/\varepsilon}$ to errors of order $\varepsilon\,(1+|t|)$, see e.g. [Teu03, Section 2.2]. Then, a standard Duhamel argument shows that within the subspace $\hat{P}_0^{\varepsilon}\mathcal{H}$ the quantum evolution of an observable $\hat{a}^{\varepsilon} := \hat{a}^{\varepsilon} \otimes \mathbf{1}_{\mathcal{H}_{\mathrm{f}}}$, $a : T^*\mathbb{R}^n \to \mathbb{R}$ acting on the slow degrees of freedom can be approximated by classically evolving the symbol $a(q,p)$ using the flow $\Phi_0^t$ of the classical Hamiltonian system $(\mathbb{R}^{2n}, \omega^0, e_0)$, i.e.

$$\left\| \hat{P}_0^{\varepsilon}\left(\hat{a}^{\varepsilon}(t) - \mathrm{op}_{\varepsilon}\left(a(\Phi_0^t)\,\mathbf{1}_{\mathcal{H}_{\mathrm{f}}}\right)\right)\hat{P}_0^{\varepsilon}\right\| = \mathcal{O}(\varepsilon)\,.$$

In addition, for an equilibrium distribution $f : \mathbb{R} \to \mathbb{R}$ and respective steady state $f(\hat{H}^{\varepsilon})$ an application of the Helffer Sjöstrand formula together with the fact that $\hat{P}_0^{\varepsilon}$ commutes with the Hamiltonian $\hat{H}^{\varepsilon}$ to order $\varepsilon$ shows

$$\left|\mathrm{tr}\Big(f(\hat{H}^{\varepsilon})\,\hat{a}^{\varepsilon}\,\hat{P}_0^{\varepsilon}\Big) - \tfrac{1}{(2\pi\varepsilon)^n}\int_{T^*\mathbb{R}^n} f(e_0(z))\,a(z)\,\mathrm{d}z\right| = \mathcal{O}(\varepsilon^{1-n})\,.$$

This means that in case of operator valued symbols, the canonical classical analogues still lead to semiclassical approximations when restricting to the subspace $\hat{P}_0^{\varepsilon}$. But we loose one power of $\varepsilon$ in accuracy. What is unclear at this point is, if and how one can derive higher order semiclassical approximations.

One major challenge in semiclassical analysis is on how one can perturb the subspace $\hat{P}_0^{\varepsilon}\mathcal{H}$ as well as the Hamiltonian system $(\mathbb{R}^{2n}, \omega^0, e_0)$ by a correction of order $\varepsilon$ in order to get higher order semiclassical approximations. In [NS04] Nenciu and Sordoni derived the space-adiabatic projection $\hat{\Pi}^{\varepsilon}$, based on algebraic construction that is due to Hellfer and Sjöstrand [HS90a] and with a different approach and independently Emmrich and Weinstein [EW96]. This projection $\hat{\Pi}^{\varepsilon}$ is related to $\hat{P}_0^{\varepsilon}$ through $\hat{\Pi}^{\varepsilon} = \hat{P}_0^{\varepsilon} + \mathcal{O}(\varepsilon)$ and commutes with the Hamiltonian $\hat{H}^{\varepsilon}$ as well as the unitary evolution operator $\mathrm{e}^{-\mathrm{i}\,\hat{H}^{\varepsilon} t/\varepsilon}$ up to arbitrary order in $\varepsilon$. Hence, the range of $\hat{\Pi}^{\varepsilon}$ is invariant under the action of $\hat{H}^{\varepsilon}$ to any order in $\varepsilon$. We say that the subspace $\hat{\Pi}^{\varepsilon}\,\mathcal{H}$ is almost-invariant. The subspace $\hat{\Pi}^{\varepsilon}\,\mathcal{H}$ is usually referred to as the almost-invariant or space-adiabatic subspace.

So, how do quantum mechanical systems behave when restricting to the almost-invariant subspace $\hat{\Pi}^{\varepsilon}\,\mathcal{H}$? It turns out that restricted to the space-adiabatic subspace the action of the Hamiltonian operator $\hat{H}^{\varepsilon}$ can be approximated to errors of order $\varepsilon^2$ by the Weyl operator $\hat{h}^{\varepsilon}$ with scalar symbol of the form

$$h(q,p) = e_0(q,p) + \varepsilon\, M(q,p)\,. \tag{1.5}$$

The correction $M$, is referred to as 'no-name', 'M' or 'Rammal-Wilkinson' term.

In order to derive higher order semiclassical approximations one has to take into account the geometry of the eigenbundle associated to the eigenvalue $e_0$. Hereto, one considers the Hilbert bundle $E : T^*\mathbb{R}^n \times \mathcal{H}_{\mathrm{f}} \stackrel{P_E}{\to} T^*\mathbb{R}^n$ with $P_E$ the projection onto the first component and equipped with the canonical flat connection $\nabla$ where for $\phi \in \Gamma(E)$ and $X \in \Gamma(T(T^*\mathbb{R}^n))$, $(\nabla_X \phi)(z) = X^j\,\partial_j \phi(z)$. The symbol $H : T^*\mathbb{R}^n \to \mathcal{B}(\mathcal{H}_{\mathrm{f}})$ can be seen as a section in the endomorphism bundle of $E$, i.e. $H \in \Gamma(\mathrm{End}(E))$ acting on sections $\phi \in \Gamma(E)$. Then, one associates to a non-degenerate eigenvalue $e_0 : T^*\mathbb{R}^n \to \mathbb{R}$ of $H$ with eigenprojection $P_0 \in \Gamma(\mathrm{End}(E))$ the eigenbundle $L := \{(z,\phi)\,|\,\phi(z) \in P_0(z)\,\mathcal{H}_{\mathrm{f}}\}$ of $E$. The connection $\nabla$ of $E$ induces a connection on $L$ by projection, i.e. $\nabla_X^{\mathrm{Berry}}\,\phi := P_0 \nabla_X\,\phi$ for $\phi \in \Gamma(L) \subset \Gamma(E)$ and $X \in \Gamma(T(T^*\mathbb{R}^n))$. The resulting connection $\nabla^{\mathrm{Berry}}$ is the famous Berry connection. The Berry connection and its holonomy, the Berry phase, play a significant role in the study of Bloch electrons and vast related fields as investigated in many important physical and mathematical works (e.g. [ST13; PST03b; MMP94; WLY13; CMS04; DL11; Bus87]). The curvature form $R^{\mathrm{Berry}}$ of the Berry connection $\nabla^{\mathrm{Berry}}$, known as Berry curvature, is $\frac{1}{2} R_{ij}^{\mathrm{Berry}}\,\mathrm{d}z^i \wedge \mathrm{d}z^j$ where

$$R_{ij}^{\mathrm{Berry}} = \mathrm{tr}_{\mathcal{H}_{\mathrm{f}}}(P_0\,[\partial_i P_0, \partial_j P_0])$$

see e.g. [ST13, Proposition 6]. In addition, the Berry curvature defines a symplectic form on classical phase space through $\Omega = -\mathrm{i}\,R^{\mathrm{Berry}}$. At the same time the coefficient matrix of the symplectic form $\Omega$ is the imaginary part of the quantum geometric tensor

$$\mathcal{T}_{ij} := 2\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\,\partial_i P_0\,\partial_j P_0)\,.$$

The real part of the quantum geometric tensor defines a metric $g_0$ on phase space known as quantum or Fubini-Study metric. Compared to the Berry curvature the quantum metric is not very well studied but recently gained much interest in the solid state physics community, see e.g. [Pié+16; GYN14; GYN15; Tan+19; Roy14; PG18].

The symplectic form $\Omega$ associated to the Berry curvature $R^{\mathrm{Berry}}$ can be interpreted as geometrical modification to the canonical phase space $(T^*\mathbb{R}^n, \omega^0)$ that results from restricting to the space-adiabatic subspace $\hat{\Pi}^\varepsilon\mathcal{H}$. Together with the classical Hamiltonian $h$ (1.5), the modified symplectic form $\omega^\varepsilon := \omega^0 - \varepsilon\,\mathrm{i}\,R^{\mathrm{Berry}}$ gives rise to an $\varepsilon$-dependent classical Hamiltonian system $(T^*\mathbb{R}^n, \omega^\varepsilon, h)$. Then we have that the quantum evolution of a semiclassical observable $\hat{a}^\varepsilon := \hat{a}^\varepsilon \otimes \mathbf{1}_{\mathcal{H}_\mathrm{f}}$, $a : T^*\mathbb{R}^n \to \mathbb{R}$ satisfies

$$\left\|\hat{\Pi}^\varepsilon \left(\hat{a}^\varepsilon(t) - \mathrm{op}_\varepsilon\left(a(\Phi^t_\varepsilon)\,\mathbf{1}_{\mathcal{H}_\mathrm{f}}\right)\right)\hat{\Pi}^\varepsilon\right\| = \mathcal{O}(\varepsilon^2) \tag{1.6}$$

where $\Phi^t_\varepsilon$ is the flow of the classical Hamiltonian system $(T^*\mathbb{R}^n, \omega^\varepsilon, h)$, see [ST13, Theorem 2]. Moreover, when restricting to the space-adiabatic subspace $\hat{\Pi}^\varepsilon\mathcal{H}$ the expectation value of a thermodynamic equilibrium distribution $f(\hat{H}^\varepsilon)$ with respect to a trace-class semiclassical observable $\hat{a}^\varepsilon$ is approximated by the classical phase space average with respect to the Liouville measure

$$\lambda^\varepsilon := \frac{(-1)^{n(n-1)/2}}{n!}\underbrace{\omega^\varepsilon \wedge \cdots \wedge \omega^\varepsilon}_{n\text{-times}}\,.$$

of the symplectic form $\omega^\varepsilon$, i.e.

$$\left|\mathrm{tr}\Big(f(\hat{H}^\varepsilon)\,\hat{a}^\varepsilon\,\hat{\Pi}^\varepsilon\Big) - \tfrac{1}{(2\pi\varepsilon)^n}\int_{T^*\mathbb{R}^n} f(h)\,a\,\lambda^\varepsilon\right| = \mathcal{O}(\varepsilon^{2-n})\,,$$

see [ST13, Theorem 1]. To conclude, also in the case of Hamiltonians with operator valued symbols the quantum evolution of observables as well as expectation values in thermodynamic equilibrium can be approximated to errors of order $\varepsilon^2$ by a classical Hamiltonian system.

Note, there is a big variety of results on semiclassical approximations of systems where the Hamiltonian's symbol is operator valued. A major drawback of almost all such approaches is that they rely on eigenfunctions $\varphi(q,p)$ of the Hamiltonian $H(q,p)$ to an eigenvalue $e(q,p)$, i.e. a trivialization of the eigenbundle of $H(q,p)$ associated to $e(q,p)$. The main issues with this are: first, $\varphi(q,p)$ in not unique since with $\varphi(q,p)$ also $\mathrm{e}^{\mathrm{i}\,f(q,p)}\,\varphi(q,p)$ for real-valued $f$ is an eigenfunction of $H(q,p)$ to the eigenvalue $e(q,p)$. And second, in some applications the eigenbundle is not trivializable, i.e. such a smooth global choice of $\varphi(q,p)$ does not exist by geometric reasons. Clearly, $\mathbb{R}^{2n}$ is contractible and hence every vector bundle over $\mathbb{R}^{2n}$ is trivializable. Nevertheless, there are applications where the symbols, rather than $\mathbb{R}^{2n}$ are defined of some other manifold. An example hereto are the so called $\tau$-equivariant symbols, see [Teu03, Appendix B]. The concept of $\tau$-equivariant symbols is of big importance in the application to magnetic Bloch electrons. Here, the eigenbundle is not trivializable whenever the Chern number of the respective eigenbundle in non-zero. Hence, the approaches that rely on eigenfunctions are inapplicable to such systems, see Section 1.2 or Chapter 6, respectively.

On the contrary, Emmrich and Weinstein in [EW96] gave a geometric derivation of the transport equation in WKB approximations that is valid even if the eigenbundle is not trivializable. The key difference here is that instead of eigenfunctions they use only the unique projections $P_0$ to the respective eigenspaces. Stiepan and Teufel in [ST13] developed an approach to derive semiclassical approximations of the quantum evolution of semiclassical observables in the Heisenberg picture as well as expectation values of quantum mechanical equilibrium distributions when restricting to the space-adiabatic subspace. Although driving towards semiclassical approximations directly they use tools from space-adiabatic perturbation theory without actually driving towards an effective Hamiltonian in the sense of space-adiabatic perturbation theory. Also in this approach, only the unique projections $P_0$ to the respective eigenspaces $P_0\,\mathcal{H}_\mathrm{f}$ are being used. One major drawback of the results in [ST13] is that they are applicable only when the observable $\hat{a}^\varepsilon$ acts solely on the 'slow' degrees of freedom, i.e. the symbol of $\hat{a}^\varepsilon$ is scalar. This prevents applying the theorems to many interesting physical applications. In [DL17] De Nittis and Lein extended the Egorov theorem (1.6) to observables with operator valued symbols in order to derive ray optics equations in photonic crystals. Another limitation of [ST13] and also [EW96] is that their approaches depend heavily on the fact that, when restricted to the almost-invariant subspace $\hat{\Pi}^\varepsilon\,\mathcal{H}$, the action of the full Hamiltonian $\hat{H}^\varepsilon$ can be approximated to errors of order $\varepsilon^2$ by a Weyl operator with scalar symbol $h$. It was pointed out in [ST13, Chapter 3] that a semiclassical operator approximating the action of the full Hamiltonian $H$ to higher orders is not expected to exist in general. Nonetheless, in this work we prove this expectation to be wrong by showing the existence of a semiclassical operator $\hat{a}^\varepsilon$ for any operator $\hat{A}^\varepsilon$ with operator valued symbol that approximates the action $\hat{A}^\varepsilon$ to arbitrary order in $\varepsilon$ when restricting to the almost-invariant subspace $\hat{\Pi}^\varepsilon\mathcal{H}$.

In recent years higher order semiclassical approximations gained much attention. One of the reasons for this is that many physical phenomena can only be understood when using higher order semiclassical approximations. The derivation of the orbital susceptibility for Bloch bands is one application that is of particular interest in the physics community, as the big variety of recent physics literature in this direction suggests (e.g. [GYN14; GYN15; LZZ15; OF15; Oga16; Rao+15; Pié+16]). Here, first order approximations give no or a wrong answer, namely zero. This topic will be handled in more detail in Section 1.2. Clearly, whether higher order semiclassical approximations for the quantum evolution of observables nor the expectation values in thermodynamic equilibrium can be expressed in terms of a classical Hamiltonian system, see (1.1) and (1.4). Nevertheless, one can still hope for a semiclassical approximation by a modified classical Hamiltonian system and additional quantum corrections. One approach that allows the derivation of semiclassical approximation to arbitrary order in $\varepsilon$ is space-adiabatic perturbation theory. Here, rather than finding a classical Hamiltonian system that approximates quantum mechanical properties, the main goal is to find an effective Hamiltonian $\hat{h}^\varepsilon$ that acts on the 'slow' degrees of freedom and is unitarily equivalent to the full Hamiltonian $\hat{H}^\varepsilon$, see e.g. [PST02; PST03b; Teu03]. Then, the effective Hamiltonian $\hat{h}^\varepsilon$ is admissible to semiclassical approximations. Using space-adiabatic perturbation theory one can derive an Egorov type theorem to arbitrary order in $\varepsilon$, similar to (1.1), for the quantum evolution of observables $\hat{A}^\varepsilon$ with operator valued symbol $A(q,p)$. Hereto, one has to restrict to the almost-invariant subspace $\hat{\Pi}^\varepsilon\mathcal{H}$, i.e. one considers $\hat{\Pi}^\varepsilon \mathrm{e}^{\mathrm{i}\hat{H}^\varepsilon t/\varepsilon} \hat{A}^\varepsilon \mathrm{e}^{-\mathrm{i}\hat{H}^\varepsilon t/\varepsilon} \hat{\Pi}^\varepsilon$ (see e.g.[Teu03, Corollary 3.29.]). As already noted earlier, a major drawback of the approach in [Teu03], as well as almost all other approaches considering Hamiltonians with operator valued symbols, is that they rely on eigenfunctions $\varphi(q,p)$ of the Hamiltonian $H(q,p)$ to an eigenvalue $e(q,p)$. Also, the results to errors of order higher than $\varepsilon^2$ are nowhere explicitly computed and there is no attempt to incorporate parts of the resulting expressions in a modified Hamiltonian system.

To conclude, from a structural applicability perspective there seem to be be two different types of existing results: on the one hand those that provide semiclassical approximation to any order in $\varepsilon$ also when the observable's symbol is operator valued but are inapplicable whenever the eigenbundle is not trivializable. On the other hand those that are applicable in the case of non-trivializable eigenbundles but only lead to approximation to first order. The aim of this work is not less than to give a full solution to this problem.

We will develop a theory to approximate the quantum evolution of semiclassical observables in the Heisenberg picture (Section 5) as well as expectation values of quantum mechanical equilibrium distributions (Section 4) to arbitrary order in $\varepsilon$. Our results are gauge independent, do not rely on trivializability of the eigenbundle and are applicable when the observable's symbol is operator valued. The derivation is particularly transparent and all expressions are given explicitly in terms of the Hamiltonian's symbol $H(q,p)$, the observable's symbol $A(q,p)$, the eigenvalue $e_0(q,p)$, the eigenprojection $P_0(q,p)$ and their derivatives. Moreover, we will show that the restriction to the almost-invariant subspace naturally gives rise to a modified $\varepsilon$-dependent Berry connection, a modified $\varepsilon$-dependent Fubini-Study metric and a closely related modified $\varepsilon$-dependent Hamiltonian system (Section 3). Hereto and in contradiction to the remark in [ST13], we give an explicit construction of effective operators $\hat{a}^\varepsilon$ for Weyl operators $\hat{A}^\varepsilon$ with operator values symbol (Section 3.2). The notion of effective operators within this thesis shall not be confused with the effective operators in the context of space-adiabatic perturbation theory. By an effective operator we mean an operator with scalar symbol $a : \mathbb{R}^{2n} \to \mathbb{C}$ that incorporates the action of the operator $\hat{A}^\varepsilon$ to any order in $\varepsilon$ when restricting to the almost-invariant subspace $\hat{\Pi}^\varepsilon \mathcal{H}$, i.e. a Weyl operator $\hat{a}^\varepsilon$ with scalar symbol satisfying

$$\| \hat{\Pi}^\varepsilon (\hat{A}^\varepsilon - \mathrm{op}_\varepsilon (a \, \mathbf{1}_{\mathcal{H}_\mathrm{f}})) \hat{\Pi}^\varepsilon \| = \mathcal{O}(\varepsilon^\infty) \, .$$

We compute the $\varepsilon^2$ contributions to the semiclassical approximation of equilibrium expectation values and show that, up to quantum corrections discovered by Wigner, all expressions are either incorporated by the modified classical Hamiltonian system or can be expressed in terms of a Fubini-Study metric. To this end, we prove a trace formula for the Liouville measure of general symplectic forms and in particular for semiclassical symplectic forms $\omega^\varepsilon = \omega^0 + \varepsilon \, \Omega$ (Section 2.2). Moreover, we give a scheme on how to extend the approach of [LR10; GL14] leading to an effective numerical method to approximate the time-evolution of quantum mechanical expectation values for the case of Weyl operators with operator valued symbols.

The general results are then applied to a quantum mechanical system with Hamiltonian of Born-Oppenheimer type including an external magnetic field. Here, we prove an Egorov type theorem as well as the semiclassical approximation of equilibrium expectations. Also we will give the explicit expressions for the $\varepsilon$-dependent Hamiltonian system as well as the quantum correction of order $\varepsilon^2$. For an introduction to Born-Oppenheimer type Hamiltonians and a summary of our related results see Section 1.3.

Last but not least we will apply our theory to the system that serves as main motivation for this work. Namely, to a gas of non-interacting fermionic particles in the tight binding approximation on the lattice $\mathbb{Z}^2$ subject to a 'strong' constant magnetic field and an additional electromagnetic field with slowly varying potentials, known as Hofstadter model. Here, we derive an Egorov type theorem to approximate the quantum evolution of observables restricted to adiabatic subspace associated to magnetic Bloch bands. Furthermore, we apply our result on steady states to derive a semiclassical approximation for the free energy per unit area. From the expression for the free energy we can then easily deduce the magnetic susceptibility. Hereto the second order expressions in the semiclassical approximation are crucial. It is worth pointing out that to our knowledge this is the first time a derivation of the orbital susceptibility for magnetic Bloch bands is given. See Section 1.2 for an introduction into Bloch electrons and a summary as well as discussion of our results on the Hofstadter model.

We should note here that from an analytical perspective we make no attempt to achieve greatest generality in this work. Instead we focus mostly on the structural aspects of the problem and avoid distracting technicalities by making stronger assumption than necessary. Note that the algebraic computations and expansions stay the same when relaxing the assumptions. The restrictive assumptions come into play when we turn our results from the level of symbols into statements about operators. As a reference on how to extend our results to more general symbol classes we refer to [Teu03].

## 1.1 Main Results

We will now describe our main results postponing technical details to Section 2 and beyond. We consider a quantum mechanical system described by the Hamiltonian operator $\hat{H}^\varepsilon$ given as Weyl operator acting on $L^2(\mathbb{R}^n, \mathcal{H}_\mathrm{f})$ and with symbol $H : \mathbb{R}^{2n} \to \mathcal{B}_\mathrm{sa}(\mathcal{H}_\mathrm{f})$ taking value in the bounded linear self-adjoint operators on $\mathcal{H}_\mathrm{f}$. Moreover, we assume $e_0 : \mathbb{R}^{2n} \to \mathbb{R}$ to be an isolated, non-degenerate eigenvalue of $H(q,p)$ depending smoothly on $(q,p)$. The projection to the eigenspace associated to $e_0$ is denoted as $P_0$. For the detailed assumptions see Section 2.3.

With the eigenvalue $e_0$ we associate a projection $\hat{\Pi}^\varepsilon$ that commutes with the Hamiltonian $\hat{H}^\varepsilon$ as well as the unitary evolution operator $\mathrm{e}^{-\mathrm{i}\,\hat{H}^\varepsilon t/\varepsilon}$ to arbitrary order in $\varepsilon$. We say that the space $\hat{\Pi}^\varepsilon \mathcal{H}$ is almost-invariant. The derivation of the super-adiabatic projection $\hat{\Pi}^\varepsilon$ is due to Nenciu and Sordoni [NS04] based on the work of Hellfer and Sjöstrand [HS90a]. Our ultimate goal is to derive semiclassical approximations of quantum mechanical equilibrium expectations

$$\mathrm{tr}_{\mathcal{H}}\Big(f(\hat{H}^\varepsilon)\,\hat{A}^\varepsilon\,\hat{\Pi}^\varepsilon\Big)$$

as well as the quantum evolution of observables in the Heisenberg picture

$$\mathrm{e}^{\mathrm{i}\,\hat{H}^\varepsilon t/\varepsilon}\,\hat{A}^\varepsilon\,\mathrm{e}^{-\mathrm{i}\,\hat{H}^\varepsilon t/\varepsilon}$$

within the almost-invariant subspace $\hat{\Pi}^\varepsilon \mathcal{H}$ and this to arbitrary order in $\varepsilon$.

Moreover, we derive a $\varepsilon$-dependent Hamiltonian system $(T^*R^n, \omega^\varepsilon, h)$ that incorporates the semiclassical approximation up to quantum corrections. Hereto, recall that there is a known classical Hamiltonian system $(T^*R^n, \omega^0 - \varepsilon\,\mathrm{i}\,R^{\mathrm{Berry}}, h)$ that approximates the quantum evolution and equilibrium expectations within the almost-invariant subspace $\hat{\Pi}^\varepsilon \mathcal{H}$ to errors of order $\varepsilon^2$, see e.g. [ST13]. Here, the classical Hamiltonian $h$ (1.5) is the scalar symbol of the operator $\hat{h}^\varepsilon$ that approximates the action of the full Hamiltonian $\hat{H}^\varepsilon$ within to the almost-invariant subspace $\hat{\Pi}^\varepsilon \mathcal{H}$ to errors of order $\varepsilon^2$. The Berry curvature $R^{\mathrm{Berry}}$ is the curvature form of the Berry connection $\nabla^{\mathrm{Berry}}$ that results from projecting the Hilbert bundle $E : T^*\mathbb{R}^n \times \mathcal{H}_{\mathrm{f}} \overset{P_E}{\to} T^*\mathbb{R}^n$ using the eigenprojection $P_0(z)$.

We begin the presentation of our main results with the $\varepsilon$-dependent modified Hamiltonian system $(T^*R^n, \omega^\varepsilon, h)$. For the modification of the symplectic form, the basic idea is to modify the eigenprojection $P_0(z)$ where the result is again a pointwise rank-one projection itself. Then, this modified rank-one projection induces a modified Berry connection and so also a modified symplectic form. Hereto, we show that there is an almost-unique rank-one projection $\mathcal{P}^\varepsilon(\varepsilon, z) = P_0(z) + \mathcal{O}(\varepsilon)$ that coincides with the symbol $\pi(\varepsilon, z)$ of the adiabatic projection $\hat{\Pi}^\varepsilon$ up to a $P_0(z)$-diagonal correction of order $\varepsilon$, i.e.

$$\pi(\varepsilon, z) = \mathcal{P}^\varepsilon(\varepsilon, z) + \varepsilon\,P_0(z)\,\tilde{\pi}(\varepsilon, z)\,P_0(z) + \varepsilon\,P_0^\perp(z)\,\tilde{\pi}(\varepsilon, z)\,P_0^\perp(z),$$

see Proposition 3.2. Here, by almost-unique we mean that $\mathcal{P}^\varepsilon(\varepsilon, z)$ is unique up to an error of arbitrary order in $\varepsilon$. The symbols $\mathcal{P}^\varepsilon(\varepsilon, z)$ and $\pi(\varepsilon, z)$ have asymptotic expansions in $\varepsilon$ with coefficients given explicitly in terms of the Hamiltonian symbol $H(z)$, the eigenvalue $e_0(z)$ and the eigenprojection $P_0(z)$.

The explicit algebraic construction of $\mathcal{P}^\varepsilon$ and $\pi(\varepsilon, z)$ are given in Lemma 3.1. For the explicit expressions up to order $\varepsilon^2$, see (3.17) - (3.20).

Analogous to the famous Berry connection $\nabla^{\mathrm{Berry}}$, the family of rank-one projections $\mathcal{P}^\varepsilon(z)$ defines a line-bundle over the classical phase space $T^*\mathbb{R}^n$ that inherits a connection $\nabla^\varepsilon := \mathcal{P}^\varepsilon \nabla$ from the trivial vector bundle $E : T^*\mathbb{R}^n \times \mathcal{H}_\mathrm{f} \overset{P_E}{\to} \mathbb{R}^{2n}$. The resulting connection $\nabla^\varepsilon$ we refer to as the modified Berry connection. The curvature form $R^\varepsilon$ of the modified Berry connection $\nabla^\varepsilon$ is given by $R^\varepsilon = \frac{1}{2} R^\varepsilon_{ij}\, \mathrm{d}z^i \wedge \mathrm{d}z^j$ where

$$R^\varepsilon_{ij} = \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\mathcal{P}^\varepsilon\, [\partial_i \mathcal{P}^\varepsilon, \partial_j \mathcal{P}^\varepsilon])\,,$$

see Proposition 3.9. The modified Berry curvature induces a symplectic form $\omega^\varepsilon$ over the classical phase space $T^*\mathbb{R}^n$ by $\omega^\varepsilon := \omega^0 - \varepsilon\, \mathrm{i}\, R^\varepsilon$, see Proposition 3.10. Then, $\omega^\varepsilon$ defines a $2n$-dimensional symplectic manifold $(T^*R^n, \omega^\varepsilon)$ over the phase space $T^*R^n$. The modified Berry curvature is, up to a factor of $\mathrm{i}$, given as the imaginary part of the modified quantum geometric tensor

$$\mathcal{T}^\varepsilon_{ij} := 2\, \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\mathcal{P}^\varepsilon\, \partial_i \mathcal{P}^\varepsilon\, \partial_j \mathcal{P}^\varepsilon)\,.$$

The real value of the modified quantum geometric tensor defines a Fubini-Study metric $g^\varepsilon$ on phase space $T^*\mathbb{R}^n$. Then, the Fubini-Study metric $g^\varepsilon = g^\varepsilon_{ij}\, \mathrm{d}z^i \otimes \mathrm{d}z^j$ on $T^*\mathbb{R}^n$ is

$$g^\varepsilon_{ij} = \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\mathcal{P}^\varepsilon\, [\partial_i \mathcal{P}^\varepsilon, \partial_j \mathcal{P}^\varepsilon]_+)\,.$$

Here, $[\cdot, \cdot]_+$ denotes the anti-commutator.

To our knowledge, the definition and construction of $\mathcal{P}^\varepsilon$ and thus also of the modified Berry connection $\nabla^\varepsilon$ and the Fubini-Study metric $g^\varepsilon$ is completely new. The projection $\mathcal{P}^\varepsilon(\varepsilon, z)$ naturally emerges from the algebraic construction of the super-adiabatic projection $\hat{\Pi}^\varepsilon$ by introducing an intermediate step, see Lemma 3.1. Therefore, showing the existence and uniqueness of $\mathcal{P}^\varepsilon(\varepsilon, z)$ is quite straight forward provided one is familiar with the construction of the space-adiabatic projection $\hat{\Pi}^\varepsilon$. The main difficulty and advance here clearly lies in the discovery of a natural definition of $\mathcal{P}^\varepsilon(\varepsilon, z)$ such that the associated classical Hamiltonian system incorporates large parts of the higher order semiclassical approximations of thermodynamic equilibrium expectations as well as the quantum evolution of observables. For the special case of Bloch electrons subject to uniform electromagnetic fields Gao, Yang and Niu [GYN14; GYN15] derived a modified Bloch state that is closely related to the first order expansion of $\mathcal{P}^\varepsilon(\varepsilon, z) = P_0(z) + \varepsilon\, P_1(z) + \mathcal{O}(\varepsilon^2)$, for more details see Section 1.2. Compared to the Berry curvature $R^{\mathrm{Berry}}$ the quantum metric $g_{0,ij} = \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\,[\partial_i P_0, \partial_j P_0]_+)$ is not very well studied but recently gained much interest in the solid state physics community, see e.g. [Pié+16; GYN14; GYN15; Tan+19; Roy14; PG18]. To our knowledge, corrections to the quantum metric $g_{0,ij}$ as given by $g^\varepsilon_{ij}$ have nowhere been stated prior to this work.

In order to compare classical phase space averages in thermodynamic equilibrium (1.2) with the semiclassical expansion of thermodynamic equilibrium expectations it is crucial to compute the Lebesgue density $\nu^\varepsilon$ of the symplectic form $\omega^\varepsilon$'s Liouville measure $\lambda^\varepsilon = \nu^\varepsilon\,\mathrm{d}q\,\mathrm{d}p$ (1.3). The Liouville density $\nu^\varepsilon$ is related to the Pfaffian $\mathrm{pf}(\omega^\varepsilon)$ of the symplectic form $\omega^\varepsilon$'s coefficient matrix $\omega^\varepsilon_{ij}$ through

$$\nu^\varepsilon = (-1)^{n(n-1)/2}\,\mathrm{pf}(\omega^\varepsilon)\,. \tag{1.7}$$

Moreover, the symplectic from $\omega^\varepsilon$ resulting from the modified Berry curvature $R^\varepsilon$ takes a particular form, namely $\omega^\varepsilon = \omega^0 + \varepsilon\,\Omega^\varepsilon$. Within this context we prove two trace formulas: One trace formula for the Liouville density $\nu$ of an arbitrary symplectic form $\omega$ (Theorem 2.9) and another trace formula for the $\varepsilon$-expansion of the Liouville density $\nu^\varepsilon$ of on $\varepsilon$-dependent symplectic form $\omega^\varepsilon = \omega^0 + \varepsilon\,\Omega^\varepsilon$ (Proposition 2.7). What is quite remarkable in the proofs of the trace formulas is that while the formula for general symplectic forms $\omega$ follows directly from the $\varepsilon$-expansion of $\nu^\varepsilon$, the reverse direction is rather intricate. Hence, our strategy in Section 2.2 is to first derive the trace formula for $\varepsilon$-expansion of $\nu^\varepsilon$. Then, the general trace formula for the Liouville density $\nu$ is a direct consequence. The proof of Proposition 2.7 is very technical and certainly not straight forward where one of the main issues is to find a suitable framework that helps to keep an overview over the terms and cancellations in the expressions.

*Trace Formula for Liouville Measures (cf. Theorem 2.9)*
Let $\Omega = \frac{1}{2}\sum_{i,j\in\{1,\dots,2n\}} \Omega_{ij}\,\mathrm{d}z^i \wedge \mathrm{d}z^j$ be a symplectic form. Then, the Liouville measure $\lambda$ of $\Omega$ defined by (1.3) can be represented as

$$\lambda = \sum_{\substack{\alpha\in\mathbb{N}_0^n,\\ \sum_{i=1}^n i\,\alpha_i = n}} \left(-\tfrac{1}{2}\right)^{|\alpha|} \prod_{j=1}^n (j^{\alpha_j}\,\alpha_j!)^{-1}\,\mathrm{Tr}_{2n}\Big(\big((\omega^0\,\Omega)^j\big)^{\alpha_j}\Big)\,\mathrm{d}q^1 \wedge \dots \wedge \mathrm{d}p^n\,. \tag{1.8}$$

Recently and using a different route to ours, Krivoruchenko [Kri16] showed that for two skew-symmetric matrices $A, B \in \mathbb{R}^{2n\times 2n}$ it holds that

$$\mathrm{pf}(A)\,\mathrm{pf}(B) = \sum_{\substack{\alpha\in\mathbb{N}_0^n,\\ \sum_{i=1}^n i\,\alpha_i = n}} \left(-\tfrac{1}{2}\right)^{|\alpha|} \prod_{j=1}^{n} (j^{\alpha_j}\,\alpha_j!)^{-1}\,\mathrm{Tr}_{2n}\Big((A\,B)^j\Big)^{\alpha_j}\,.$$

This is a generalization of our trace formula for Liouville densities $\nu$ (Theorem 2.9) as (1.8) follows directly by combining the above result with (1.7) and the well know fact that $\mathrm{pf}(\omega^0) = (-1)^{n(n-1)/2}$.

Nevertheless, for our purposes we require a formula for the $\varepsilon$-expansion of the Liouville measure $\lambda^\varepsilon$ for symplectic forms of the form $\omega^0 + \varepsilon\,\Omega$. To our knowledge, this is the first work where such a formula is stated and proven.

*Trace Formula for semiclassical Liouville Measures (cf. Proposition 2.7)*
For an $\varepsilon$-dependent symplectic form $\omega^\varepsilon := \omega^0 + \varepsilon\,\Omega^\varepsilon$ the respective Liouville measure $\lambda^\varepsilon$ can be represented as

$$\lambda^\varepsilon = \sum_{k=0}^{n} \varepsilon^k\,\lambda_k^\varepsilon = \Big(1 + \sum_{k=1}^{n} \varepsilon^k\,\nu_k^\varepsilon\Big)\,\mathrm{d}q^1\wedge\cdots\wedge\mathrm{d}p^n$$

where

$$\nu_k^\varepsilon = \sum_{\substack{\alpha\in\mathbb{N}_0^k,\\ \sum_{i=1}^k i\,\alpha_i = k}} \left(-\tfrac{1}{2}\right)^{|\alpha|} \prod_{j=1}^{k} (j^{\alpha_j}\,\alpha_j!)^{-1}\,\mathrm{Tr}_{2n}\Big((\omega^0\,\Omega^\varepsilon)^j\Big)^{\alpha_j}$$

for $1 \le k \le n$.

Focusing on the terms up to order $\varepsilon^2$ the density $\nu^\varepsilon$ of the Liouville measure $\lambda^\varepsilon$ is

$$\nu^\varepsilon = 1 - \tfrac{1}{2}\,\varepsilon\,\mathrm{Tr}_{2n}(\omega^0\,\Omega^\varepsilon)) + \tfrac{1}{8}\,\varepsilon^2\,\mathrm{Tr}_{2n}(\omega^0\,\Omega^\varepsilon)^2 - \tfrac{1}{4}\,\varepsilon^2\,\mathrm{Tr}_{2n}(\omega^0\,\Omega^\varepsilon\,\omega^0\,\Omega^\varepsilon) + \mathcal{O}(\varepsilon^3)\,,$$

see Corollary 2.8.

Up to this point all results presented are devoted to the change of the phase space' geometry due to the restriction to the adiabatic subspace $\hat{\Pi}^\varepsilon$. To derive semiclassical approximations for systems with operators having operator valued symbols one crucial step is to 'replace' the full operator by an 'effective' operator that is amendable to semiclassical approximations. Hereto, it was proven in [ST13] that there is an almost-unique semiclassical operator $\hat{h}^\varepsilon$ that approximates the action of the full Hamiltonian $\hat{H}^\varepsilon$ when restricted to the almost-invariant subspace $\hat{\Pi}^\varepsilon\,\mathcal{H}$ to errors of order $\varepsilon^2$.

In this work we will generalize this result in two ways: we show that such an effective operator exists not only for the Hamiltonian operator $\hat{H}^{\varepsilon}$ but for any operator with operator valued symbol and so for approximations to arbitrary order in $\varepsilon$.

*Effective operators (cf. Theorem 3.6)*
Let $B : \mathbb{R}^{2n} \to \mathcal{B}(\mathcal{H}_{\mathrm{f}})$ be a suitable operator valued symbol and define the scalar symbol $b(\varepsilon) : \mathbb{R}^{2n} \to \mathbb{C}$ as re-summation of the asymptotic expansion $\sum_{i=0}^{\infty} \varepsilon^i\, b_i(z)$ with coefficients $b_i(z)$ recursively by

$$b_0 = \mathrm{tr}_{\mathcal{H}_{\mathrm{f}}}\left(B\, P_0\right)$$

and (1.9)

$$b_{j+1} = \mathrm{tr}_{\mathcal{H}_{\mathrm{f}}}\left(\beth_{j+1}\, P_0\right) \quad \text{for} \quad j \geq 0$$

where $\beth_{j+1}$ is the $j+1$-th coefficient of the asymptotic expansion of $\pi \,\#\, (B - b^{(j)} \mathbf{1}_{\mathcal{H}_{\mathrm{f}}}) \,\#\, \pi \asymp \sum_{i=0}^{\infty} \varepsilon^i\, \beth_i$ with $b^{(j)} = \sum_{i=0}^{j} \varepsilon^i\, b_i$. Then,

$$\pi \,\#\, B \,\#\, \pi - \pi \,\#\, b \,\#\, \pi = \mathcal{O}(\varepsilon^{\infty})$$

and

$$\left\| \hat{\Pi}^{\varepsilon}\, \hat{B}^{\varepsilon}\, \hat{\Pi}^{\varepsilon} - \hat{\Pi}^{\varepsilon}\, \hat{b}^{\varepsilon}\, \hat{\Pi}^{\varepsilon} \right\| = \mathcal{O}(\varepsilon^{\infty}).$$

Moreover, for a trace class operator $\hat{B}^{\varepsilon}$ and arbitrary $N \in \mathbb{N}_0$ we have

$$\mathrm{tr}_{\mathcal{H}}\left(\left(\hat{B}^{\varepsilon} - \widehat{b^{(N)}}^{\varepsilon}\right)\hat{\Pi}^{\varepsilon}\right) = \mathcal{O}\left(\varepsilon^{N+1-n}\, \|B\|^{\varepsilon}_{L^1}\right). \tag{1.10}$$

Hence, within the almost-invariant subspace $\hat{\Pi}^{\varepsilon}\mathcal{H}_{\mathrm{f}}$ the action of a Weyl operator $\hat{B}^{\varepsilon}$ can be approximated to arbitrary order by a Weyl operator $\hat{b}^{\varepsilon}$ with scalar symbol $b(\varepsilon, z)$. We call $\hat{b}^{\varepsilon}$ the effective operator of $\hat{B}^{\varepsilon}$ and $b(\varepsilon, z)$ the respective effective symbol. Note, that the effective symbol $b$ is taking values in the reals whenever the symbol of the original operator $\hat{B}^{\varepsilon}$ is taking value in the self-adjoint operators acting on $\mathcal{H}_{\mathrm{f}}$. The coefficients of the asymptotic expansion $b(\varepsilon, z) \asymp \sum_{i=0}^{\infty} \varepsilon^i\, b_i(z)$ are explicitly given in terms of $B(z)$, the Hamiltonian $H(z)$, the eigenvalue $e_0(z)$, the eigenprojection $P_0(z)$ and their derivatives.

The effective symbol $h$ of the Hamiltonian $\hat{H}^{\varepsilon}$ defines a classical Hamiltonian on phase space $T^*\mathbb{R}^n$. Then, $(T^*\mathbb{R}^n, \omega^{\varepsilon}, h)$ defines a classical Hamiltonian system. By the Hamiltonian equations $\omega^{\varepsilon}(X^{\varepsilon}_h, \cdot) = \nabla h$ the Hamiltonian vector field is given by $X_h^{\varepsilon,j} = -(\omega^\varepsilon)^{-1}_{ji}\,\partial_i h$. So, the classical equation of motion are

$$\begin{pmatrix} \dot{q} \\ \dot{p} \end{pmatrix} = -\omega^\varepsilon(q,p)^{-1} \begin{pmatrix} \partial_q h(q,p) \\ \partial_p h(q,p) \end{pmatrix} .$$

For the explicit expression for the classical Hamiltonian $h$ including second order corrections see (3.65).

It is quite remarkable that the action of the 'fast' degrees of freedom can be captured by corrections of the semiclassical operators to arbitrary order in $\varepsilon$ when restricting to the adiabatic subspace. This is one of our key results as it is the basis for all semiclassical approximations in this work. Here, we will focus on the use of effective operators to derive higher order semiclassical approximations using Weyl calculus. Nevertheless, it is expected that by use of the classical Hamiltonian $h$ one can extend the approach of [EW96] leading to an improved WKB approximation.

Despite the fact that the existence of such effective operators prior to this work was not expected or was at least unclear, our derivation of those effective operators is particularly transparent, at least on the level of symbols. The dependency on the $L^1$-norm of the observable in the error estimate of (1.10) is crucial when taking the thermodynamic limit as we will see in Section 6. The proof of this error estimate is very technical and one of the larger parts in the proof of Theorem 3.6.

As already mentioned, one of the main goals of this work is to derive semiclassical approximations of expectation values for thermodynamic equilibrium states. Hereto, one of the crucial and most intricate steps that take the larger part of Chapter 4 is the derivation of the effective operator of the equilibrium state $f(\hat{H}^\varepsilon)$ restricted to the almost-invariant subspace $\hat{\Pi}^\varepsilon\,\mathcal{H}$. Note that prior to this work the existence of a semiclassical operator that approximates the action of the equilibrium state $f(\hat{H}^\varepsilon)$ within the almost-invariant subspace $\hat{\Pi}^\varepsilon\,\mathcal{H}$ to errors of order higher than second order in $\varepsilon$ was unknown, even on a heuristic level.

*Effective stationary states (cf. Proposition 4.3)*
Let $f : \mathbb{R} \to \mathbb{R}$ be a suitable real valued distribution. Then, there exist $\varepsilon$-dependent scalar symbols $f^{\mathrm{sc}}(h)$ and $f^{\mathrm{adi}}(\pi, h)$ such that

$$\left\| \hat{\Pi}^\varepsilon \left( f(\hat{H}^\varepsilon) - \mathrm{op}_\varepsilon\left(f^\varepsilon(h,\pi)\right)\right) \hat{\Pi}^\varepsilon \right\| = \mathcal{O}(\varepsilon^\infty)$$

with

$$f^\varepsilon(h,\pi) = f(h) + \varepsilon^2\, f^{\mathrm{sc}}(h) + \varepsilon^2\, f^{\mathrm{adi}}(\pi, h)\,.$$

For the explicit construction of $f^{\mathrm{sc}}(h)$ and $f^{\mathrm{adi}}(\pi, h)$ see the proof of Proposition 4.3.

The asymptotic expansions of $f^{\mathrm{sc}}(h)$ and $f^{\mathrm{adi}}(\pi, h)$ start with

$$\begin{aligned} f^{\mathrm{sc}}(h) &= -\tfrac{1}{24}\, f'''(e_0)\, \langle\, \omega^0\, \nabla e_0\,,\ \nabla^2 e_0\, \omega^0\, \nabla e_0\,\rangle \\ &\quad + \tfrac{1}{16}\, f''(e_0)\, \mathrm{Tr}_{2n}(\omega^0\, \nabla^2 e_0\, \omega^0\, \nabla^2 e_0) + \mathcal{O}(\varepsilon) \\ &= -\tfrac{1}{24}\, \mathrm{Tr}_{2n}\Big(\omega^0\, \nabla(f''(e_0)\, \nabla^2 e_0\, \omega^0\, \nabla e_0)\Big) \\ &\quad + \tfrac{1}{48}\, f''(e_0)\, \mathrm{Tr}_{2n}\Big((\omega^0\, \nabla^2 e_0)^2\Big) + \mathcal{O}(\varepsilon) \end{aligned}$$

and

$$f^{\mathrm{adi}}(h, \pi) = -\tfrac{1}{4}\, f''(e_0)\, \|\omega^0\, \nabla e_0\|^2_{g_0} + \mathcal{O}(\varepsilon)\,.$$

Here, $g_0$ is the leading order of the modified quantum metric $g^\varepsilon$. The leading order of the quantum correction $f^{\mathrm{sc}}(h)$ coincides with the correction derived by Wigner [Wig32] in the case of a Boltzmann distribution and a semiclassical Hamiltonian, see (1.4). On the contrary, $f^{\mathrm{adi}}(\pi, h)$ results from the adiabatic approximation and thus stems from the fast degrees of freedom.

Up to this point there exists no systematic semiclassical treatment of equilibrium expectations above first order in $\varepsilon$. In particular, for the case non-trivial eigenbands there is no higher order semiclassical approximation known, not for particular application and not even on a heuristic level. We now present one of the main results of this work which gives a semiclassical approximation of quantum mechanical expectation values in thermodynamic equilibrium to arbitrary order in $\varepsilon$.

*Expectation values for stationary states (cf. Theorem 4.4)*
Let $A : \mathbb{R}^{2n} \to \mathcal{B}_{\mathrm{sa}}(\mathcal{H}_{\mathrm{f}})$ be the symbol of a suitable observable $\hat{A}^\varepsilon$. Then, for every $N \in \mathbb{N}_0$ it holds that

$$\begin{aligned} \mathrm{tr}_{\mathcal{H}}\Big(f(\hat{H}^\varepsilon)\, \hat{A}^\varepsilon\, \hat{\Pi}^\varepsilon\Big) =& (2\pi\varepsilon)^{-n} \int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_{\mathrm{f}}}(\pi) \,\#\, f^\varepsilon(h, \pi)\, a^{(N)}\, \mathrm{d}z \\ &- \mathrm{i}\,\varepsilon\, (2\pi\varepsilon)^{-n} \int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_{\mathrm{f}}}(\pi \,\#\, \tfrac{\mathrm{i}}{\varepsilon}\, [\, f^\varepsilon(h, \pi)\,,\, \pi\,]_{\#})\, a^{(N)}\, \mathrm{d}z \\ &+ \mathcal{O}\Big(\varepsilon^{-n+N+1}\, \|A\|^\varepsilon_{L^1}\Big) \end{aligned}$$

Here, $a^{(N)} = \sum_{j=0}^{N} \varepsilon^j\, a_j(z)$ is the expansion to order $N$ of the effective symbol $a : \mathbb{R}^{2n} \to \mathbb{R}$ of $A(z)$ defined by (1.9).

For approximations to errors of order $\varepsilon^3$ the above result can be reformulated to

$$\operatorname{tr}_{\mathcal{H}}\Big(f(\hat{H}^{\varepsilon})\,\hat{A}^{\varepsilon}\,\hat{\Pi}^{\varepsilon}\Big) = (2\pi\varepsilon)^{-n}\Big(\int_{\mathbb{R}^{2n}} f^{\varepsilon}(h,\pi)\,a^{(2)}\,\lambda^{\varepsilon} + \varepsilon^2\int_{\mathbb{R}^{2n}} Q(e_0,g_0)\,a_0\,\mathrm{d}z\Big) + \mathcal{O}\Big(\varepsilon^{3-n}\,\|A\|^{\varepsilon}_{L^1}\Big) \tag{1.11}$$

where $\lambda^{\varepsilon}$ is the Liouville measure (3.74) associated to the Hamiltonian system $(T^*\mathbb{R}^n,\omega^{\varepsilon},h)$. The explicit expressions for the quantum correction $Q(e_0,g_0)$ is

$$Q(e_0,g_0) = \tfrac{1}{2}\operatorname{Tr}_{2n}(\omega^0\,\nabla(f'(e_0)\,g_0\,\omega^0\,\nabla e_0)\,)\,.$$

In Theorem 4.4 we give the first rigorous and systematic derivation of semiclassical approximations of equilibrium expectations to error of orders higher than $\varepsilon^2$. Moreover the results are gauge-invariant and applicable also in case of non-trivializable eigenbundles. As already mentioned, the dependency on the $L^1$-norm of the observable in the error estimate is crucial when taking the thermodynamic limit. The additional quantum corrections to the expectation values of steady states, besides the effective operator of the equilibrium state $f(\hat{H}^{\varepsilon})$, result from the fact that we restrict to the almost-invariant subspace, i.e. we consider $\operatorname{tr}_{\mathcal{H}}\Big(f(\hat{H}^{\varepsilon})\,\hat{A}^{\varepsilon}\,\hat{\Pi}^{\varepsilon}\Big)$ instead of $\operatorname{tr}_{\mathcal{H}}\Big(f(\hat{H}^{\varepsilon})\,\hat{A}^{\varepsilon}\Big)$. It is worth pointing out that other than the band energy $e_0$ and the distribution function $f$, the second order quantum corrections depend only on the quantum metric $g_0$. This corroborates the general importance of quantum metric. The modified $\varepsilon$-dependent classical Hamiltonian system $(T^*\mathbb{R}^n,\omega^{\varepsilon},h)$ incorporates big parts of the semiclassical approximation of equilibrium expectations to error of order $\varepsilon^3$ (1.11). Although we expect this to be true to arbitrary order, we will not prove it in this work.

Next, we discuss the semiclassical approximation of the quantum evolution of observables in the Heisenberg picture also known as Egorov type theorem. There are already existent works on Egorov type theorems to arbitrary order. One limitation that all such results have in common is their reliance on the trivializability of the eigenbundle. Also, in most derivations of Egorov type theorems big effort has to be taken in order to make the results gauge invariant. In this work we derive an Egorov type theorem that is based upon eigenprojections rather than eigenfunctions and is therefore gauge invariant by definition and applicable also in case of non-trivial eigenbundles. The applicability to non-trivializable eigenbundles is of particular importance in many applications as magnetic Bloch bands (see Section 1.2) or locally isolated eigenbands in the time-dependent Born-Oppenheimer approximation (see Section 1.3). In addition, we show that at least in the approximation to errors of order $\varepsilon^3$ the modified classical Hamiltonian system incorporates the quantum evolution of observables, up to quantum corrections. Note, with the derivation of effective operators in the sense of Theorem 3.6 in hand, the derivation of an Egorov type theorem is comparatively straight forward. Here, we mainly follow the strategy of [ST13, Theorem 2].

*Egorov type theorem (cf. Theorem 5.2)*
Let $A : \mathbb{R}^{2n} \to \mathcal{B}_{\mathrm{sa}}(\mathcal{H}_{\mathrm{f}})$ be the symbol of a suitable observable $\hat{A}^{\varepsilon}$ with quantum mechanical time-evolution

$$\hat{A}^{\varepsilon}(t) := \mathrm{e}^{\mathrm{i}\hat{H}^{\varepsilon}t/\varepsilon}\hat{A}^{\varepsilon}\mathrm{e}^{-\mathrm{i}\hat{H}^{\varepsilon}t/\varepsilon}\,.$$

In addition, let $\Phi_{\varepsilon}^{t}$ be the classical flow associated to the Hamiltonian system $(T^*\mathbb{R}^n, \omega^{\varepsilon}, h)$ and $a(\Phi_{\varepsilon}^{t})$ the classical evolution of the effective symbol of $\hat{A}^{\varepsilon}$. Then, there exists an $\varepsilon$-dependent semiclassical symbol $\mathfrak{A}(t) : \mathbb{R}^{2n} \to \mathbb{R}$ such that

$$\left\|\hat{\Pi}^{\varepsilon}\left(\hat{A}^{\varepsilon}(t) - \mathrm{op}_{\varepsilon}\left(a(\Phi_{\varepsilon}^{t}) + \varepsilon^2\,\mathfrak{A}(t)\right)\right)\hat{\Pi}^{\varepsilon}\right\| \leq \mathcal{O}\Big(\varepsilon^{N+1}\sum_{j=0}^{N+3}|t|^j\Big)$$

for every $N \in \mathbb{N}$.

The semiclassical symbol $\mathfrak{A}(t) : \mathbb{R}^{2n} \to \mathbb{R}$ has an asymptotic expansion $\mathfrak{A}(t) \asymp \sum_{j=0}^{\infty}\varepsilon^{2j}\,\mathfrak{A}_{2j}^{N}(t)$ with $\mathfrak{A}_{2j}^{N}(t) : \mathbb{R}^{2n} \to \mathbb{R}$ inductively given by

$$\mathfrak{A}_{0}^{N}(t) := \int_0^t \mathfrak{A}_{h,\varepsilon}^{c,N}(a(\Phi_{\varepsilon}^{\tau})) \circ \Phi_{\varepsilon}^{t-\tau}\,\mathrm{d}\tau$$

and

$$\mathfrak{A}_{2j}^{N}(t) := \int_0^t \mathfrak{A}_{h,\varepsilon}^{c,N}(\mathfrak{A}_{2(j-1)}^{N}(\tau)) \circ \Phi_{\varepsilon}^{t-\tau}\,\mathrm{d}\tau \quad \text{for } j \geq 1\,.$$

For the construction of the $\varepsilon$-dependent symbol $\mathfrak{A}_{h,\varepsilon}^{c,N}(a)(z) : \mathbb{R}^{2n} \to \mathbb{R}$ see Proposition 5.1, in particular (5.14). Regarding the explicit expressions to errors of order $\varepsilon^3$ we have

$$\begin{aligned}\mathfrak{A}_{0}^{2}(t) = {} & 2\,\mathrm{i}\int_0^t \{e_0\,, a_0(\Phi_{\varepsilon}^{\tau})\}_3 \circ \Phi_{\varepsilon}^{t-\tau}\,\mathrm{d}\tau \\ & - \tfrac{1}{2}\int_0^t \mathrm{tr}_{\mathcal{H}_{\mathrm{f}}}(\{\{e_0\,, P_0\}\ , \{a_0(\Phi_{\varepsilon}^{\tau})\,, P_0\}\}) \circ \Phi_{\varepsilon}^{t-\tau}\,\mathrm{d}\tau + \mathcal{O}(\varepsilon)\,.\end{aligned}$$

As a consequence, for the quantum evolution of the expectation value of a non-stationary state $\rho(t) = \mathrm{e}^{-\mathrm{i}\hat{H}^{\varepsilon} t/\varepsilon}\, \rho_0\, \mathrm{e}^{\mathrm{i}\hat{H}^{\varepsilon} t/\varepsilon}$ with initial state $\rho_0 = \hat{\Pi}^{\varepsilon}\rho_0\,\hat{\Pi}^{\varepsilon}$ it holds that

$$\begin{aligned}\mathrm{tr}_{\mathcal{H}}(\rho(t)\,\hat{A}^{\varepsilon}) &= \mathrm{tr}_{\mathcal{H}}(\rho_0\,\hat{\Pi}^{\varepsilon}\,\hat{A}^{\varepsilon}(t)\,\hat{\Pi}^{\varepsilon}) \\ &= \mathrm{tr}_{\mathcal{H}}\Big(\rho_0\,\mathrm{op}_{\varepsilon}\Big(a(\Phi^t_{\varepsilon}) + \varepsilon^2\,\mathfrak{A}(t)\Big)\Big) + \mathcal{O}(\varepsilon^{\infty})\,.\end{aligned}$$

The way we stated the Egorov theorem it seems like the modified $\varepsilon$-dependent classical Hamiltonian system $(T^*\mathbb{R}^n, \omega^{\varepsilon}, h)$ incorporates big parts of the semiclassical approximation of the quantum evolution of observables to arbitrary order. Although we expect this statement to be true, in this work we will prove it only for the semiclassical approximation to errors of order $\varepsilon^3$. At this point it may as well be that the higher order corrections to the classical Hamiltonian system lead to additional correction terms.

Last but not least, in Section 5.2 we will introduce a scheme to derive numerical approximation schemes for the time evolution of quantum mechanical expectation values $\mathrm{tr}_{\mathcal{H}}(\hat{\rho}^{\psi_t}\,\hat{A}^{\varepsilon})$ with initial wave function $\psi_0 \in \hat{\Pi}^{\varepsilon}\mathcal{H}$ and this to arbitrary order in $\varepsilon$. Hereto, we reformulates the corrections $\mathfrak{A}^N_j(t)$ for fixed $N \in \mathbb{N}_0$ leading to

$$\mathfrak{A}^N_j(t,z) = \sum_{j=0}^{N} \varepsilon^j \sum_{k=0}^{l_j} \Gamma_{j,k}(t, z, D^{m_{j,k}} a \circ \Phi^t_{\varepsilon}(z))$$

where

$$\Gamma_{j,k}(t,z) : \mathbb{R}^{\overbrace{2d \times \cdots \times 2d}^{m_{j,k} \text{ times}}} \to \mathbb{R}$$

are explicitly defined linear mappings from the space of $m_{j,k}$-tensors to the real numbers that are independent of the effective observable $a$. Then we derive a first order system of initial value problems for the components of $\Gamma^{j,k}(t,z)$ such that the vectorization of this system can be written as

$$\frac{\partial}{\partial t}\vec{\Gamma}(t,z) = N(t,z)\,\vec{\Gamma}(t,z) + b(t,z)$$

where the components of the Matrix $N(t,z)$ and the vector $b(t,z)$ are given explicitly in terms of the classical Hamiltonian $h$, the symbol of the adiabatic projection $\pi$ as well as their derivatives, evaluated along the classical flow $\Phi^t_{\varepsilon}$. Then, the Wigner type phase space method developed in [GL14] can directly be applied leading to a very effective algorithm to approximate the evolution of quantum mechanical expectation values. In Section 7.4, we validate the accuracy and efficiency of the resulting algorithm by applying it to a simple quantum system of Born-Oppenheimer type with matrix valued potential

$$V(x) = \begin{pmatrix} \tanh(x) & \delta \\ \delta & -\tanh(x) \end{pmatrix}, \qquad \delta > 0\,.$$

Due to the success of semiclassical approximation for Hamiltonians with operator valued symbols there is a huge amount of literature on this topic. We give a short overview over the contributions that we believe are most important where we will focus mostly on higher order semiclassical approximations. For a short survey over the literature related to semiclassical approximation to error of order $\varepsilon^2$, see [ST13, Section 6].

The first appearance of the first order corrections to the symplectic form $\omega^0$ and the energy $e_0$ is in [LF91] where they use Weyl calculus to diagonalize operators with matrix valued symbols. Here, the change of coordinates due to the symplectic form is used as technical tool rather than as the coordinates for the 'slow' degrees of freedom. Independently, Chang and Niu [CN96] formally derive the first order corrections to the classical equations of motion to approximate the evolution of wave packets for the case of Bloch electrons. The first rigorous proof of the Egorov theorem to errors of order $\varepsilon^2$ in the case of Bloch electrons without strong magnetic field is given in [PST03b] and was slightly generalized in [DL11]. In [ST13] the proof of Egorov's theorem is then extended to the case of a non-trivializable eigenbundle. In addition, a semiclassical approximation of thermodynamic equilibrium distribution is proven in [ST13]. The results in [ST13] are very similar to Theorem 5.2 and Theorem 4.4 but limited to errors of order $\varepsilon^2$ and to observables with scalar symbol. The first order semiclassical model has been studied intensely an led to big advances in the theory of solid state physics, see [XCN10] for a review.

As already mentioned, for the case of a trivializable eigenbundle one can use space-adiabatic perturbation theory to derive an Egorov type theorem in the sense of Theorem 5.2, see e.g. [Teu03]. For the special case of particles with spin an Egorov theorem to arbitrary order in $\varepsilon$ was proven in [BG04]. Related to the theory of Bloch electrons, Blount pioneered the work of systematically extending semiclassical theory up to second order by using phase space quantum mechanics [Blo62b]. Recently and completely independent to this work, Gao, Yang and Niu [GYN14; GYN15] have constructed a second order semiclassical theory for Bloch electrons under uniform electromagnetic fields. Here, they introduced a positional shift $a'$ for the case of Bloch bands with trivializable geometry. This positional shift acts as correction to the

Berry phase and induces a Berry connection that is very similar to the next to leading order part of the modified Berry connection $\nabla^\varepsilon$. In addition, a second order correction to the wave-packet energy is given in this work. The approach can not be applied in the case where the Bloch bundle is non-trivializable as in the case of magnetic Bloch bundles with non-zero Chern number (see e.g. [DN80a; DN80b]). Moreover, [GYN14; GYN15] is based on formal computations which includes making the correct guesses for certain needed objects. Thus, the approach does hardly reflect the structure of the problem and none of the statements is rigorously proven. We will give a more detailed comparison of our results with [GYN14; GYN15] in Section 1.2.

The existence of semiclassical operators that approximate the action of operators with operator valued symbols restricted to the adiabatic subspace to errors of order $\varepsilon^2$ is well known and has previously been used e.g. in [EW96; ST13; DL17]. To higher orders the existence of such effective operators has previously been neither claimed nor proven.

## 1.2 Magnetic Bloch Bands

The understanding of Electrons within a two dimensional crystal subject to electromagnetic fields is one of the central problems of solid state physics. Such Bloch electrons are described by the underlying Schrödinger equation

$$\mathrm{i}\,\partial_t \psi(x,t) = \hat{H}^{\varepsilon}_{B_0}\psi(x,t)$$

with Hamiltonian

$$\hat{H} = \tfrac{1}{2}\Big( -\mathrm{i}\nabla_x + \tfrac{1}{2}\mathbf{B}_0\, x - A(\varepsilon x)\Big)^2 + V_\Gamma(x) + \Phi(\varepsilon x)\,.$$

The potential $V_\Gamma : \mathbb{R}^2 \to \mathbb{R}$, generated by the nuclei of the crystal, is periodic with respect to the regular lattice $\Gamma$ with basis $\gamma_1, \gamma_2 \in \mathbb{R}^2$, i.e. $\Gamma = \{a\,\gamma_1 + b\,\gamma_2 : a, b \in \mathbb{Z}\}$. The strong constant magnetic field perpendicular to the plane is represented by $\mathbf{B}_0 = \left(\begin{smallmatrix} 0 & B_0 \\ -B_0 & 0 \end{smallmatrix}\right)$ with $B_0 \in \mathbb{R}$. The potentials $A(\varepsilon x)$ and $\Phi(\varepsilon x)$ are slowly varying on the scale of the lattice $\Gamma$ which is expressed through the dimensionless semiclassical parameter $0 < \varepsilon \ll 1$.

The dynamics of Bloch electrons and properties in thermodynamic equilibrium are considered of big importance, as the big variety of past and recent works in theoretical physics (e.g. [Blo62b; Zak68; Hof76; Tho+82; Ber84; SN99; GA03; Blo05; XCN10; GYN15; LZZ15; OF15; Oga16; Rao+15;

Pié+16]) and mathematical literature (e.g. [DN80a; DN80b; Nov81; Bus87; Bel88; GRT88; RB90; HST01; PST03a; DGR04; Pan07; ST13]) in this direction suggests. Also the spectral properties of Hamiltonians with slowly varying external potentials are studied intensely as can be seen by the large number of mathematical articles (e.g. [HS89b; HS89a; HS90b; HKS90; GMS91; AJ09; HK15]). Due to the enormous amount of literature in this direction we can mention only a small part here. For a review of the mathematical and physical literature until 1991 we refer to [Nen91]. A well known approach in understanding Bloch Hamiltonians is the Peierls substitution and the derivation of effective Hamiltonians as done in (e.g. [Pei33; Blo62a; Nen89; Nen91; FT16; DL11; DP10]). While in the limiting cases $B_0 = 0$ and $B_0 \to \infty$ the construction of unitarily equivalent effective Hamiltonians is well understood (see e.g. [PST03a; DP10; DL11]), for the case $B_0 \neq 0$ the validity and the meaning of Peierls substitution was absolutely unclear (see e.g. [Zak86; Zak91]) until recently. The main obstruction in the case of magnetic Bloch bands ($B_0 \neq 0$) is the fact that the associated Bloch bands are non-trivializable. A first derivation of a unitary equivalent effective Hamiltonian for the case of magnetic Bloch bands was given in [FT16].

Although many problems have already been solved, there are many properties of electrons in crystals that can not be described at all or at least not in a satisfying manner. One of this properties is the magnetic susceptibility which, as many other phenomena, can be explained by using a second-order semiclassical theory for Bloch electrons. Recently, Gao, Yang and Niu [GYN14; GYN15] have constructed such a theory under uniform electromagnetic fields, including a derivation for the first-order correction to the Berry curvature. As already noted, this approach can not be applied in the case where the Bloch bundle is non-trivializable as in the case of magnetic Bloch bundles with non-zero Chern number (see e.g. [DN80a; DN80b]). As already mentioned, [GYN14; GYN15] is based on formal computations, does hardly reflect the structure of the problem and none of the statements is rigorously proven. In [LZZ15] a second-order semiclassical theory for the dynamics of Bloch electrons without external magnetic field is derived rigorously using WKB-type solutions to the underlying Schrödinger equation. Their results can be used to describe the dynamics of certain wave packets up to second order but the resulting equations depend on the shape of the wave packet and the choice of phase in the Bloch waves. In addition, the approach can not be used when an external magnetic field is present and therefore is inapplicable to compute properties like the magnetic susceptibility. Moreover a trivialization of the Bloch bundle is used in this approach as well, making it inapplicable to the case of magnetic Bloch bands. Also, there are several recent works on the derivation of the magnetic susceptibility using Green's functions, see e.g. [OF15; Oga16; Rao+15; Pié+16]. To conclude, despite the huge interest in higher order semiclassical approximations and especially the magnetic susceptibility of Bloch electrons there is no existing result for the case of magnetic Bloch bands with non-trivial geometry, not even on a heuristic level. This is the main motivation for this work.

In the following we will explain how our theory can be applied to Bloch electrons in order to derive a higher order semiclassical theory that is rigorously proven and applicable also when the Bloch band are non-trivializable.

Clearly, the Hamiltonian $\hat{H}$ can not be expressed as Weyl quantization of an operator valued symbol. We will briefly show how the problem can be reformulated allowing the use of Weyl calculus. Hereto, we transform the Hamiltonian $\hat{H}$ unitarily using the magnetic Bloch-Floquet transform. Note, that we will not go much into detail here. For a detailed introduction to the magnetic Bloch-Floquet transform, see e.g [FT16].

We assume the flux per unit cell of the strong magnetic field $\mathbf{B}_0$ to be a rational multiple of $2\pi$, i.e. $B_0\,(\gamma_1 \times \gamma_2) = 2\pi\,\frac{p}{q}, p \in \mathbb{Z}, q \in \mathbb{N}$ where $\gamma_1, \gamma_2 \in \mathbb{R}^2$ is the basis of the lattice $\Gamma$. Further, we consider the sublattice $\Gamma_q \subset \Gamma$ with basis $\gamma_1^q = q\,\gamma_1$ and $\gamma_2^q = \gamma_2$. The Brillouin zone $M^*$ is the centered fundamental cell of $\Gamma_q^*$, the reciprocal lattice to $\Gamma_q$.

The unperturbed Hamiltonian

$$\hat{H}_{B_0} = \tfrac{1}{2}\Big(-\mathrm{i}\nabla_x + \tfrac{1}{2}\mathbf{B}_0\,x\Big)^2 + V_\Gamma(x)$$

fibers in magnetic Bloch-Floquet representation as

$$\mathcal{U}_{BF}\,\hat{H}_{B_0}\,\mathcal{U}_{BF}^{-1} = \int_{M^*}^{\oplus} H_{\mathrm{per}}(k)$$

where

$$H_{\mathrm{per}}(k) = \tfrac{1}{2}\Big(-\mathrm{i}\nabla_y + \tfrac{1}{2}\mathbf{B}_0\,y + k\Big)^2 + V_\Gamma(y)\,.$$

Then, $H_{\mathrm{per}}(k)$ is bounded from below and has a compact resolvent. Thus, the fibered Hamiltonian $H_{\mathrm{per}}(k)$ has a discrete spectrum with eigenvalues $e^{(m)}(k)$ of finite multiplicity that accumulate at infinity. The eigenbundle associated to an eigenvalue $e^{(m)}(k)$ is known as Bloch bundle. While in the non-magnetic case ($B_0 = 0$) the Bloch bundle is always trivial, a magnetic

Bloch bundle is trivializable only when its Chern number is zero. In addition, $H_{\mathrm{per}}(k)$ is called to be $\tau$-equivariant in the sense that for every $\gamma^* \in \Gamma_q^*$

$$H_{\mathrm{per}}(k-\gamma^*) = \tau(\gamma^*)\, H_{\mathrm{per}}(k-\gamma^*)\, \tau(\gamma^*)^{-1}$$

where the operator $\tau(\gamma^*)$ acts on a function $f \in L^2(\mathbb{R}^2)$ as

$$(\tau(\gamma^*)f)(y) := \mathrm{e}^{\mathrm{i}\,\langle \gamma^*\,,\, y\rangle} f(y)\,.$$

The magnetic Bloch-Floquet transform $\mathcal{U}_{BF}$ maps the full Hamiltonian $\hat{H}$ to

$$\hat{H}^{\varepsilon} = \mathcal{U}_{BF}\, \hat{H}\, \mathcal{U}_{BF}^{-1} = \tfrac{1}{2}\Big( -\mathrm{i}\nabla_y + \tfrac{1}{2}\mathbf{B}_0\, y + k - A(\mathrm{i}\,\varepsilon\,\nabla_k^{\tau})\Big)^2 + V_\Gamma(y) + \Phi(\mathrm{i}\,\varepsilon\,\nabla_k^{\tau})$$

where $\nabla_k^{\tau}$ denotes the derivative with $\tau$-equivariant boundary conditions. Then, $\hat{H}^{\varepsilon}$ can be represented as the $\tau$-quantization of the $\tau$-equivariant operator valued symbol

$$\begin{aligned} H(r,k) &= \mathcal{U}_{BF}\, \hat{H}\, \mathcal{U}_{BF}^{-1} = \tfrac{1}{2}\Big( -\mathrm{i}\nabla_y + \tfrac{1}{2}\mathbf{B}_0\, y + k - A(r)\Big)^2 + V_\Gamma(y) + \Phi(r) \\ &= H_{\mathrm{per}}(k - A(r)) + \Phi(r)\,. \end{aligned}$$

For details on the $\tau$-quantization we refer to [Teu03, Appendix B].

So, we transformed the original problem to a system driven by a Hamiltonian that can be expressed as quantization of an operator valued symbol. Usually the non-trivializability of the Bloch bundle is considered as the main obstruction to overcome in the magnetic Bloch case. As noted several times, this is no issue in our case. Still, there are some obstructions that prevent us from applying our theory to this general case.

- While $\hat{H}^{\varepsilon}$ is the $\tau$-quantization of $H(r,k)$, our approach is based upon Weyl symbols defined on $\mathbb{R}^{2n}$: since all our results hold for $\tau$-equivariant symbols with the same proofs we can neglect this issue, see [Teu03].
- While $H(r,k)$ is in general unbounded, we assume the symbols to take value in the bounded operators on a Hilbert space $\mathcal{H}_{\mathrm{f}}$: clearly, it is not a straight forward task to extend our results to unbounded operators. Nevertheless, adiabatic-perturbation theory was applied to Bloch operators and since most of our results base on the techniques of space-adiabatic perturbation theory we do not expect serious issues when extending our results to Bloch operators as done in [Teu03].
- The restriction that the eigenvalues must be non-degenerate is a limitation of our approach and at this point we do not see much way around this.

Nonetheless, in Section 6 we will apply our results to a simplified model. Namely, a gas of non-interacting fermionic particles in the tight binding approximation on the lattice $\mathbb{Z}^2$ subject to a constant magnetic field and an additional electromagnetic field with slowly varying potentials, known as Hofstadter model. Here, the single particle Hamiltonian is

$$H^{A^\varepsilon} = \sum_{|\alpha|=1} T_\alpha^{A^\varepsilon} + \phi^\varepsilon$$

acting as bounded self-adjoint operator on $\ell^2(\mathbb{Z}^2)$. The magnetic translations $T_\alpha^{A^\varepsilon}$ are defined by

$$(T_\alpha^{A^\varepsilon}\psi)_\beta = \mathrm{e}^{-\mathrm{i}\langle\alpha\,,\,A^\varepsilon(\beta)\rangle}\psi_{\beta-\alpha} \quad \text{for} \quad \psi \in \ell^2(\mathbb{Z}^2) \quad \text{and} \quad \alpha,\beta \in \mathbb{Z}^2\,.$$

The magnetic vector potential $A^\varepsilon : \mathbb{R}^2 \to \mathbb{R}^2$ is given by

$$A^\varepsilon(r) = -\tfrac{1}{2}\mathbf{B}_0\, r + A(\varepsilon\, r) \qquad \text{where} \qquad A(r) = A_b(r) - \tfrac{1}{2}\mathbf{b}\, r$$

with $\mathbf{B}_0 = \left(\begin{smallmatrix} 0 & B_0 \\ -B_0 & 0 \end{smallmatrix}\right)$, $B_0 = 2\pi\frac{p}{q}$, $p \in \mathbb{Z}$, $q \in \mathbb{N}$, $\mathbf{b} = \left(\begin{smallmatrix} 0 & b \\ -b & 0 \end{smallmatrix}\right)$, $b \in \mathbb{R}$ and $A_b : \mathbb{R}^2 \to \mathbb{R}^2$ smooth and bounded together with all its derivatives. The electric potential $\phi^\varepsilon$ is a multiplication operator defined by

$$(\phi^\varepsilon\psi)_\beta = \phi(\varepsilon\beta)\psi_\beta \quad \text{for} \quad \psi \in \ell^2(\mathbb{Z}^2), \beta \in \mathbb{Z}^2 \quad \text{where} \quad \phi(r) = \phi_b(r) + \mathcal{E}\cdot r$$

with $\mathcal{E} \in \mathbb{R}^2$ and $\phi_b : \mathbb{R}^2 \to \mathbb{R}$ smooth and bounded with all its derivatives. Then, an application of the respective magnetic Bloch-Floquet transform (6.2) to $H^{A^\varepsilon}$ yields

$$\hat{H}^\varepsilon = \mathcal{U}_{BF}^{B_0} H^{A^\varepsilon} \mathcal{U}_{BF}^{B_0 *} = H_0(k - A(\mathrm{i}\varepsilon\nabla_k^\tau)) + \phi(\mathrm{i}\varepsilon\nabla_k^\tau)$$

where $H_0(k)$ acts on $L^2(M_q, \mathbb{C}^q)$ as matrix valued multiplication operator, see (6.3).

In the following we will explain our main results in the context of Hofstadter electrons. Note that in this application we focus on second order semiclassical approximations. Clearly, our approach allows an extension of the results to semiclassical approximations of arbitrary order in $\varepsilon$.

We begin with the modified classical Hamiltonian system. So, let $e^{(m)}$, $1 \le m \le q$ be an isolated eigenvalue of $H_0(k)$ with $P_0^{(m)}(k)$ the associated spectral projection. Then, $\tilde{e}^{(m)}(r,k) := e^{(m)}(k - A(r)) + \phi(r)$ is an isolated eigenvalue of $H(r,k)$ with spectral projection $\tilde{P}_0^{(m)}(r,k) = P_0^{(m)}(k - A(r))$. After a change of coordinates to kinetic momentum $\kappa = k - A(r)$, the $\varepsilon$-

dependent classical Hamiltonian system associated to $e^{(m)}$ is $(\omega^{(m)}_{\mathrm{KM}}(r,\kappa), h^{(m)})$. Here, the classical Hamiltonian $h^{(m)}$ is given explicitly by (6.7) and the coefficient matrix of the symplectic form $\omega^{(m)}_{\mathrm{KM}}(r,\kappa)$ is of the form

$$\omega^{(m)}_{\mathrm{KM}}(r,\kappa) = \begin{pmatrix} -\mathbf{B}(r) & \mathbf{1}_2 \\ -\mathbf{1}_2 & \varepsilon\,\mathbf{\Omega}^{(m)}(r,\kappa) \end{pmatrix} + \varepsilon^2 \begin{pmatrix} 0 & \mathbf{L}^{(m)}(r,\kappa) \\ -(\mathbf{L}^{(m)})^T(r,\kappa) & 0 \end{pmatrix}$$

where $\mathbf{B}(r) = B(r)\,\mathrm{J}_2 = B(r)\,\left(\begin{smallmatrix} 0 & 1 \\ -1 & 0 \end{smallmatrix}\right)$, $B(r) = \nabla \times A(r)$; $\mathbf{L}^{(m)}(r,\kappa)$ is given by (6.9) and $\mathbf{\Omega}^{(m)}(r,\kappa) = \Omega^{(m)}(r,\kappa)\,\mathrm{J}_2$ with

$$\begin{aligned}\Omega^{(m)}(r,\kappa) = {} & 2\,\mathfrak{Im}\,\mathrm{tr}_{\mathbb{C}^q}\Big(\partial_1 P^{(m)}_0\,\partial_2 P^{(m)}_0\,P^{(m)}_0\Big)(\kappa) \\ & + \varepsilon\,\partial_\kappa \times \left(B(r)\,S^{(m)}(\kappa) + W^{(m)}(\kappa)\,\nabla\phi(r)\right)\end{aligned}$$

the modified Berry curvature for the $m$-th band (see Equation 6.6).

The associated Hamiltonian equations are (6.15)

$$\begin{pmatrix} \dot r \\ \dot\kappa \end{pmatrix} = \frac{1}{\nu^{(m)}}\left[\begin{pmatrix} -\varepsilon\,\mathbf{\Omega}^{(m)} & \mathbf{1}_2 \\ -\mathbf{1}_2 & \mathbf{B} \end{pmatrix} + \varepsilon^2 \begin{pmatrix} 0 & -\mathrm{J}_2\,(\mathbf{L}^{(m)})^T\,\mathrm{J}_2 \\ \mathrm{J}_2\,\mathbf{L}^{(m)}\,\mathrm{J}_2 & 0 \end{pmatrix}\right]\begin{pmatrix} \partial_r h^{(m)} \\ \partial_\kappa h^{(m)} \end{pmatrix}.$$

where

$$\nu^{(m)}(r,\kappa) = \ 1 + \varepsilon\,B(r)\,\Omega^{(m)}(\kappa) + \varepsilon^2\,\mathrm{Tr}_2\Big(\mathbf{L}^{(m)}(r,\kappa)\Big)$$

is, up to errors of order $\varepsilon^3$, the density of the Liouville measure $\lambda^{(m)}_\varepsilon$ of the symplectic form $\omega^{(m)}_{\mathrm{KM}}(r,\kappa)$, i.e.

$$\lambda^{(m)}_\varepsilon = \Big(\nu^{(m)}(r,\kappa) + \mathcal{O}(\varepsilon^3)\Big)\,\mathrm{d}r_1 \wedge \cdots \wedge \mathrm{d}\kappa_n\,.$$

This is the first time that a Hamiltonian system for the second order semi-classical approximations of magnetic Bloch electrons is given. Also within the context of Bloch electrons without strong Magnetic field, to our knowledge there is no result known of such generality. The only comparable results the are those in [GYN14; GYN15] and [LZZ15]. Where in [GYN14; GYN15] uniform electromagnetic fields are considered, in [LZZ15] no magnetic field is considered at all. If we restrict our results to a trivializable Bloch bundle and uniform electromagnetic field then the correction to the Berry phase

$$B(r)\,S^{(m)}(\kappa) + W^{(m)}(\kappa)\,\nabla\phi(r)$$

coincides exactly with the positional shift in [GYN14]. Since in case of a uniform electromagnetic field the expression $\mathbf{L}^{(m)}(r,\kappa)$ vanishes, our symplectic and thus also the Liouville measure coincides with the one in [GYN14]. In

[GYN15], an additional correction to the positional shift 'magically' occurs. Due to the simple and natural structure of our approach, in contrast to most other approaches, an assignment to the effective energy and the Berry curvature arise naturally. Hence, we think that rather than introducing this additional correction to the positional shift this correction should have been incorporated in the effective energy. Nevertheless, we have to admit that we did not do a detailed comparison of our effective Hamiltonian with the wave-packet energy in [GYN14; GYN15]. If we assume a vanishing magnetic and constant electric field then our results coincide with the ones in [LZZ15].

Before we get to our results on steady states we briefly discuss our results on the second-order approximation of the quantum evolution of magnetic Bloch electrons. Hereto, let $\hat{R}$ be a self-adjoint operator acting on $\ell^2(\mathbb{Z}^2)$ such that $\hat{O}^\varepsilon = \mathcal{U}^{B_0} \hat{R}\, \mathcal{U}^{B_0 *}$ is a Weyl operator with $\tau$-equivariant symbol. Moreover, let $\tilde{o}^{(m)}$ be the effective symbol of $O$ associated to the Bloch band $e^{(m)}$ and $o^{(m)}(r,\kappa)$ the second order effective symbol in kinetic momentum representation $o^{(m)}(r,\kappa) := \sum_{i=0}^{2} \varepsilon^i\, \tilde{o}_i^{(m)}(r, \kappa + A(r))$.

*Egorov Theorem for Hofstadter Electrons (cf. Proposition 6.4)*
Let $A_b(r) = 0$, $B_0 = 2\pi \frac{p}{q}$, $p \in \mathbb{Z}$, $q \in \mathbb{N}$ and $m \in \{1, \ldots, q\}$ for $q$ odd or $m \in \{1, \ldots, q\} \setminus \{q/2, q/2+1\}$ for $q$ even. Then,

$$\begin{aligned}
&\hat{\Pi}^{\varepsilon(m)} \mathcal{U}^{B_0}\, \mathrm{e}^{\mathrm{i}\, H^{A^\varepsilon} t/\varepsilon}\, \hat{R}\, \mathrm{e}^{-\mathrm{i}\, H^{A^\varepsilon} t/\varepsilon}\, U^{B_0 *}\, \hat{\Pi}^{\varepsilon(m)} \\
&\quad = \hat{\Pi}^{\varepsilon(m)} \operatorname{op}_\varepsilon \Big( \big( o^{(m)}(\Phi_t^{(m)}) + \varepsilon^2\, \mathfrak{A}^{(m)}(t) \big)(r, k + \tfrac{1}{2}\, \mathbf{b}\, r) \Big)\, \hat{\Pi}^{\varepsilon(m)} \\
&\qquad + \mathcal{O}\Big( \varepsilon^{N+1}\, \|O\|^\varepsilon_{0,r} \sum_{j=0}^{5} |t|^j \Big)
\end{aligned}$$

where the Hamiltonian flow $\Phi_t^{(m)}$ is the flow of the Hamiltonian system $(h^{(m)}, \omega_{\mathrm{KM}}^{(m)})$ and the quantum correction $\mathfrak{A}^{(m)}(t)$ is given by (6.26).

In particular, for $\psi_t = \mathrm{e}^{-\mathrm{i}\, H^{A^\varepsilon} t/\varepsilon}\, \psi_0$ where the initial state $\psi_0 \in \ell^2(\mathbb{Z}^2)$ satisfies $\mathcal{U}^{B_0}\, \psi_0 = \widetilde{\psi}_0 \in \hat{\Pi}^{\varepsilon(m)} L^2(M_q, \mathbb{C}^q)$ we have

$$\begin{aligned}
&\big\langle \psi_t\,,\, \hat{R}\, \psi_t \big\rangle_{\ell^2(\mathbb{Z}^2)} \\
&= \Big\langle \widetilde{\psi}_0\,,\, \operatorname{op}_\varepsilon \Big( \big( o^{(m)}(\Phi_t^{(m)}) + \varepsilon^2\, \mathfrak{A}^{(m)}(t) \big)(r, k + \tfrac{1}{2}\, \mathbf{b}\, r) \Big)\, \widetilde{\psi}_0 \Big\rangle_{L^2(M_q, \mathbb{C}^q)} + \mathcal{O}(\varepsilon^3)\,.
\end{aligned}$$

To our knowledge this is the first time that a complete second-order semiclassical approximation of the quantum evolution of Bloch electrons is given. Note, the assumption that the magnetic field is constant is only a technicality that simplifies the computations and leads to a more readable result. As already stated, Gao et al. [GYN14] gave a derivation of the modified

Hamiltonian system but the additional quantum corrections are nowhere mentioned in this work. This probably is due to the fact that they consider only semiclassical wave-packets. Clearly, by applying space-adiabatic perturbation theory [PST03a; Teu03] one can derive a second-order semiclassical approximation for the quantum evolution of Bloch electrons but as already mentioned space-adiabatic perturbation theory is applicable only when the Chern number vanishes. Also, space-adiabatic perturbation theory makes no statement about the associated modified classical Hamiltonian system.

Finally, we get to the results that are one of the main motivations of this work. Namely, the semiclassical approximation of equilibrium expectations for magnetic Bloch bands including an application of that result leading to a second-order approximation of the free energy and an exact formula for the magnetic susceptibility. Hereto, we assume $\hat{R}$, $\hat{O}^{\varepsilon}$, $\tilde{o}^{(m)}$ and $o^{(m)}$ as above.

*Equilibrium Expectations for Hofstadter Electrons (cf. Proposition 6.1)*
Let $f : \mathbb{R} \to \mathbb{R}$ be a suitable real valued distribution and $B_0 = 2\pi\frac{p}{q}$, $p \in \mathbb{Z}$, $q$ odd. Then,

$$\begin{aligned}\operatorname{tr}_{\ell^2(\mathbb{Z}^2)}(\hat{R}\, f(H^{A^\varepsilon})) = & \frac{1}{(2\,\pi\,\varepsilon)^2} \sum_{m=1}^{q} \Big( \int_{\mathbb{R}^2\times M_q} o^{(m)}\, f^\varepsilon(h^{(m)}, \pi^{(m)})\, \lambda^{\varepsilon,(m)} \\ & + \int_{\mathbb{R}^2\times M_q} o^{(m)}\, Q(h_0^{(m)}, g_0^{(m)})\, \mathrm{d}r\, \mathrm{d}\kappa \Big) \\ & + \mathcal{O}(\varepsilon\, \|O\|_{L^1})\end{aligned}$$

where $M_q := [0, 2\,\pi/q) \times [0, 2\,\pi)$ is the reduced Brillouin zone. The effective equilibrium state $f^\varepsilon(h^{(m)}, \pi^{(m)})$ is given by (B.67) and the quantum correction $Q(h_0^{(m)}, g_0^{(m)})$ by (B.65).

To our knowledge there is no comparable result to the above in the literature, not for the case of trivializable Bloch bundles and not even on a heuristic level. Note, that the dependency of the error estimate on the $L^1$-norm of the observable is crucial when taking a thermodynamic limit as we will see in our next result, the free energy per unit volume.

For a gas of non-interacting Hofstadter electrons at temperature $T = \beta^{-1}$ and chemical potential $\mu$ the free energy per unit volume is defined by

$$p(B^\varepsilon, \beta, \mu) := \frac{1}{\beta} \lim_{j\to\infty} \frac{\varepsilon^2}{|\Lambda_j|} \operatorname{tr}_{\ell^2(\mathbb{Z}^2)} \left( \chi_j(\varepsilon x)\, \ln\left(1 + \mathrm{e}^{-\beta(H^{A^\varepsilon} - \mu)}\right)\right) .$$

Here, $\chi_j : \mathbb{R}^2 \to [0, 1]$ is a sequence of smooth cutoff functions supported in $\Lambda_j := [-j, j]^2$ such that $\chi_j(z) = 1$ for all $z \in \Lambda_{j-1}$ where with an abuse of notation we define $|\Lambda_j| = \|\chi_j\|_{L^1}$.

*Free Energy (cf. Proposition 6.2)*
Let $q$ odd, $B_0 = 2\pi\frac{p}{q}$ and $A_b(r) = \phi(r) = 0$. Then, for $\varepsilon > 0$ small enough, $\beta > 0$ and $\mu \in \mathbb{R}$ it holds that

$$p(B^\varepsilon, \beta, \mu) = -\tfrac{q}{(2\pi)^2} \sum_{m=1}^{q} \Big( \int_{\mathbb{T}_q} F_{\beta,\mu}(h^{(m)}(\kappa))\, \nu^{(m)}(\kappa)\, \mathrm{d}\kappa \\ - \varepsilon^2 \int_{\mathbb{T}_q} Q_{\mathrm{pr}}^{(m)}(\kappa)\, \mathrm{d}\kappa \Big) + \mathcal{O}(\varepsilon^3)$$

where $\mathbb{T}_q$ is the torus $[0, \frac{2\pi}{q})^2$, $F_{\beta,\mu}(x) = -\beta^{-1} \ln\left(1 + e^{-\beta(x-\mu)}\right)$ is the anti-derivative of the Fermi-Dirac distribution $f_{\beta,\mu}(x) = (1 + \mathrm{e}^{\beta(x-\mu)})^{-1}$ and

$$Q_{\mathrm{pr}}^{(m)} = b^2\, f'_{\beta,\mu}(e^{(m)}) \left( \tfrac{1}{24} \det\left(\nabla^2 e^{(m)}\right) + \tfrac{1}{4} \|\nabla e^{(m)\perp}\|^2_{g_0^{(m)}} \right).$$

The first expression in the quantum correction $Q_{\mathrm{pr}}^{(m)}$ is well established and known as Landau-Peierls magnetic energy, see e.g. [Blo62b]. It results from the semiclassical approximation (1.4) for a purely semiclassical system. On the contrary, the second term of $Q_{\mathrm{pr}}^{(m)}$ stems from the adiabatic approximation and to our knowledge is completely new, at least in this generality. There are several recent works on the approximation of the free energy or grand canonical potential to second order in the magnetic fields, e.g. [BCS12; Sav12; GYN15; GS11; OF15; Oga16; Rao+15; Pié+16]. While [BCS12; Sav12] use magnetic perturbation theory, [GYN15] is based upon semiclassical wave packets and [GS11; OF15; Oga16; Rao+15; Pié+16] use Green's functions to approximate the free energy. None of those works are applicable to magnetic Bloch bands. Hence, their results are valid only for weak constant magnetic fields while our results can be applied for arbitrary constant magnetic fields by expressing the magnetic field as field with rational flux plus a small perturbation. In addition, [OF15; Oga16] is limited to time-reversal case, i.e. a centrosymmetric potential where the Berry curvature $\Omega^0$ vanishes. In [GS11; Rao+15; Pié+16] a formula for the approximation of the grand potential to second order in terms of Greens functions for two-dimensional tight-binding models is given. For a two-band model, the explicit expression in terms of Bloch functions is then given in [Pié+16]. The results in case of a two-band model are surely very similar to our results. Nevertheless, we will not give a exact comparison here. Hence, it is not clear at this point whether the results coincide exactly. In [GYN15] the grand potential to second order in the magnetic field for a three dimensional model is determined. In contrast to the previously discussed works, here the Landau-Peierls energy is only introduced artificially and is no direct result of the approach. Thus, we are quite confident that the second term of the quantum correction $Q_{\mathrm{pr}}^{(m)}$ is missing in this work but also here we will not give a more detailed comparison. The results in [BCS12; Sav12] are not very explicit and thus are very difficult to compare with our results.

The free energy gives rise to many interesting physical quantities. An example hereto is the orbital magnetization defined by $\mathrm{M}(B_0,\beta,\mu)=\partial_{B^\varepsilon}p(B^\varepsilon,\beta,\mu)$. By the fact that

$$\partial^j_{B^\varepsilon}p\,(B_0,\beta,\mu)=b^{-j}\,\partial^j_\varepsilon p\,(B^\varepsilon,\beta,\mu)\Big|_{\varepsilon=0}$$

we get

$$\mathrm{M}(B_0,\beta,\mu)=-\,\tfrac{q}{(2\pi)^2}\sum_{m=1}^{q}\Big(\int_{\mathbb{T}_q}F_{\beta,\mu}(e^{(m)}(\kappa))\,\mathcal{M}^{(m)}(\kappa) \\ +\,f_{\beta,\mu}(e^{(m)}(\kappa))\,\Omega_0^{(m)}(\kappa)\,\mathrm{d}\kappa$$

which reproduces the result in [ST13]. Clearly, only a first order theory is needed to determine the orbital magnetization. On the contrary, for the orbital susceptibility

$$\mathcal{S}(B_0,\beta,\mu)=\partial^2_{B^\varepsilon}p(B^\varepsilon,\beta,\mu)=b^{-2}\,\partial^2_\varepsilon p\,(B^\varepsilon,\beta,\mu)\Big|_{\varepsilon=0}$$

the first order theory gives a wrong answer, namely zero. Here, only a higher order theory gives the correct answer being one of the main motivations for this work as well as [Blo62b; GYN14; GYN15; GS11; OF15; Oga16; Rao+15; Pié+16]. We get the following result.

*Susceptibility (cf. Corollary 6.3)*
Let $q$ odd, $B_0=2\pi\frac{p}{q}$ and $A_b(r)=\phi(r)=0$. Then for $0<\beta<\infty$ and $\mu\in\mathbb{R}$ the magnetic susceptibility is

$$\begin{aligned}\mathcal{S}&(B_0,\beta,\mu)\\ &=-\frac{q}{(2\pi)^2}\sum_{m=1}^{q}\int_{\mathbb{T}_q}f_{\beta,\mu}(e^{(m)}(\kappa))\Big(2\,S^{(m)}\times\nabla e^{(m)}+3\,\mathcal{M}^{(m)}\,\Omega_0\\ &\qquad+\langle\,\nabla^\perp e^{(m)}\,,\,W^{(m)}\,\nabla^\perp e^{(m)}\,\rangle-2\,\mathrm{tr}_{\mathbb{C}^q}\Big(\mathcal{M}_{op}^{(m)}\,(H_0-e^{(m)})^{-1}\,\mathcal{M}_{op}^{*(m)}\,P_0^{(m)}\Big)\\ &\qquad+\mathrm{i}\,\mathrm{tr}_{\mathbb{C}^q}\Big(\nabla\mathcal{M}_{op}^{(m)}\times\nabla P_0^{(m)}\,P_0^{(m)}\Big)\\ &\qquad+\tfrac14\,\mathrm{tr}_{\mathbb{C}^q}\Big(\mathrm{Tr}_2(\nabla^{2\,\perp}P_0^{(m)}\,\nabla^{2\,\perp}(H_0-e^{(m)})\,)\,P_0^{(m)}\Big)\Big)(\kappa)\\ &\quad+f'_{\beta,\mu}(e^{(m)}(\kappa))\,\Big((\mathcal{M}^{(m)})^2-\tfrac{1}{12}\,\det\Big(\nabla^2e^{(m)}\Big)-\tfrac12\,\|\nabla e^{(m)\,\perp}\|^2_{g_0^{(m)}}\Big)(\kappa)\,\mathrm{d}\kappa\,.\end{aligned}$$

It's worth noting that the result above is not an approximation but an exact formula for the orbital susceptibility and clearly this is the first time a formula for the orbital susceptibility is given for magnetic Bloch bands.

## 1.3 Born-Oppenheimer Type Hamiltonians

The effective description of molecules is of big importance in chemistry as well as theoretical physics. The molecular Hamiltonian for $l$ nuclei and $m$ electrons is

$$\hat{H}_{mol} = -\tfrac{\hbar^2}{2\,m_n}\Delta_x + \hat{H}_e(x)$$

acting on the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^{3l}) \otimes L^2(\mathbb{R}^{3m})$ where

$$\hat{H}_e(x) = -\tfrac{\hbar^2}{2\,m_e}\Delta_y + V_e(y) + V_n(x) + V_{en}(x, y)\,.$$

Here, $V_e$ is the electronic and $V_n$ the nucleonic repulsion and $V_{en}$ the attraction between nuclei and electrons. The potentials $V_n$ and $V_e$ may include external electro-static fields. For notational simplicity we ignore spin and assume all nuclei have the same mass $m_n$.

Even though the linear time-dependent Schrödinger equation

$$\mathrm{i}\,\hbar\,\tfrac{\partial}{\partial\tau}\psi(\tau) = \hat{H}_{mol}\,\psi(\tau), \qquad \phi(\tau_0) = \psi_0 \in L^2(\mathbb{R}^{3\,(l+m)}) \tag{1.12}$$

is a linear partial differential equation, its direct numerical treatment is notoriously difficult for two reasons:

- The dimension $3(l+m)$ of configuration space is large. Even a simple molecule as $CO_2$ contains, 3 nuclei and 22 electrons resulting in a $3\,(l+m) = 75$ dimensional configuration space.
- Long Microscopic times $\tau$ have to be considered to observe finite motion of the nuclei.

Already in 1927, Born and Oppenheimer [BO27] realized that the large disparity between the mass of the light electrons and heavy nuclei can be exploited to explain general features of molecular spectra. Here, the physical intuition is the following. Due to their lower mass the electrons move much faster than the nuclei. Hence, the electrons can adjust their state quickly to the movement of the slow nuclei. So, if the electrons start in the $N$-th bound state, they stay in the $N$-th bound state although the nuclei are moving. This results in the bound state of the new nuclei position. Born and Oppenheimer realized that the small ratio $m_e/m_n$ can be used as expansion parameter for the energy levels of the molecular Hamiltonian (1.13) leading to the time-independent Born-Oppenheimer approximation.

In addition, London [Lon28] realized that the nuclei position dependent bound states and electronic energies act as effective potential for the movement of the nuclei. Moreover, due to their large mass the nuclei can be treated semiclassically. This approach is known as time-dependent Born-Oppenheimer approximation and is the most important tool for studying the quantum dynamics of molecules.

The number of works on Born-Oppenheimer type approximations is immense and we can only mention a small fraction here. In what follows, we will give a short overview on what from out perspective are the most relevant works. For a review of existing literature see [HJ07].

The first rigorous proof of the time-independent Born-Oppenheimer approximation is due to Combes, Duclos and Seiler [CS79; CDS81]. Hagedorn [Hag87] showed the expansion to arbitrary order in $\varepsilon = \sqrt{m_e/m_n}$ assuming smooth potentials which was generalized to general molecules in [Kle+92].

The time-dependent Born-Oppenheimer approximation was first proven by Hagedorn for smooth potentials in [Hag80] and extended to approximations of arbitrary order in [Hag86]. A generalization to Coulomb potentials then followed in [Hag88]. In [ST01; PST07] space-adiabatic perturbation theory was applied to proof the time-dependent Born-Oppenheimer approximation for an isolated subsets of the spectrum of $H_e(x)$. One of the main advantages of this approach compared to many others is the separation of the adiabatic and semiclassical approximation. This separation is also related to some numerical approaches in chemical physics where in contrast to the semiclassical treatment of the nuclei, the idea is to handle the nuclei quantum mechanically using the electronic energy band $E(x)$ as effective potential. Due to the fewer approximations this approach is expected to yield better results.

Also within the context of Born-Oppenheimer type approximations most approaches rely on eigenfunctions with the drawback that the results are often gauge dependent. In addition, the eigenvalue bands of $\hat{H}_e(x)$ are in general only isolated locally in the nucleonic configuration space $\mathbb{R}^{3l}$ as they may cross or merge into the continuous spectrum. In such cases, one has to restrict to solutions of the Schrödinger equation that are initially and stay supported in the region $\Lambda \subset \mathbb{R}^{3l}$ where the considered energy band $e_v(x)$ satisfies the gap condition. Then, the respective eigenprojection $P_0 : \Gamma \to \mathcal{B}(\mathcal{H}_\mathrm{f})$ defines a vector bundle that is non-trivial in general. The reason for this is that in contrast to $\mathbb{R}^{3l}$ the region $\Gamma$ may not be contractible.

To our knowledge our approach is the first that is applicable also in such a regime. Nevertheless, here we will restrict to the case where the eigenvalue is isolated globally, i.e. $\Lambda = \mathbb{R}^{3l}$.

Our goal within the application to Born-Oppenheimer type Hamiltonians is to derive the respective modified classical Hamiltonian system (Section 7.1) and show an Egorov type theorem (Section 7.3) as well as the second order semiclassical approximation of equilibrium expectations (Section 7.2). In Section 7.4 we apply the numerical scheme developed in Section 5.2 to a simple example of Born-Oppenheimer type in order to validate the accuracy and efficiency of the respective numerical algorithm.

We consider the molecular Hamiltonian for $l$ nuclei and $m$ electrons subject to an external magnetic field $\mathbf{B}$ in atomic units $(m_e = \hbar = 1)$, i.e.

$$\hat{H}^{\varepsilon}_{mol} = \tfrac{m_e}{2\,m_n}(-\mathrm{i}\,\nabla_x + A(x))^2 + \hat{H}^{\varepsilon}_e(x) \tag{1.13}$$

where

$$\hat{H}_e(x) = \tfrac{1}{2}(-\mathrm{i}\,\nabla_y - A(y))^2 + V_e(y) + V_n(x) + V_{en}(x,y)\,.$$

The magnetic vector potential $A : \mathbb{R}^n \to \mathbb{R}^n$ is assumed to be smooth and bounded. By an abuse of notation $A : \mathbb{R}^{3l} \to \mathbb{R}^{3l}$ or $A : \mathbb{R}^{3m} \to \mathbb{R}^{3m}$ is the extension of the vector potential obtained by repeating the vector potential $A : \mathbb{R}^3 \to \mathbb{R}^3$ of the external magnetic field $\mathbf{B} = \nabla \times A$, $l$ or $m$ times, respectively. The electrons are treated as point-like. Hence the electronic repulsion is

$$V_e(y) = \sum_{i=0}^{m-1} \sum_{j=i+1}^{k} \frac{1}{y_i - y_j}\,.$$

For physical and technical reasons, the nuclei are modeled to have an extended, rigid charge distribution $\rho \in \mathbb{C}_0^\infty(\mathbb{R}^3)$, $\rho \geq 0$, $\|\rho\|_{L^1} = 1$. Hence the nucleonic repulsion is

$$V_n(x) = \sum_{i=0}^{l-1} \sum_{j=i+1}^{l} \int_{\mathbb{R}^6} \frac{\rho(\xi - x_i)\,\rho(\xi' - x_j)}{|\xi - \xi'|}\,\mathrm{d}\xi\,\mathrm{d}\xi'$$

and the attractive potential between electrons and nuclei satisfies

$$V_{en}(x,y) = -\sum_{i=0}^{l} \sum_{j=1}^{m} \int_{\mathbb{R}^3} \frac{\rho(\xi - x_i)}{|\xi - y_j|}\,\mathrm{d}\xi\,.$$

Assuming nuclei and electrons having a kinetic energy of comparable magnitude, one finds for the speeds that $|v_n| \approx \varepsilon\,|v_e|$ where $\varepsilon$ is the small dimensionless parameter

$$\varepsilon = \sqrt{\tfrac{m_e}{m_n}}\,.$$

Hence, the dynamics of the nuclei must be followed over microscopic times of order $\varepsilon^{-1}$ to observe motion over finite distances. Rescaling the time to $\varepsilon\,\tau = t$ the Schrödinger equation (1.12) becomes

$$\mathrm{i}\,\varepsilon\,\tfrac{\partial}{\partial t}\psi(t) = \hat{H}^{\varepsilon}_{mol}\,\psi(t), \qquad \phi(t_0) = \psi_0 \in L^2(\mathbb{R}^{3\,(l+m)})$$

and $\hat{H}^{\varepsilon}_{mol}$ is the Weyl quantization of the symbol

$$H_{mol}(q,p) = \tfrac{1}{2}(p - \varepsilon\,A(q))^2 + \hat{H}_e(q)\,.$$

The main goal here is to apply our approach in order to derive an $\varepsilon$-dependent classical Hamiltonian system $(h, \omega^{\varepsilon})$ that, up to quantum corrections, approximates the quantum evolution of observables and equilibrium expectations to errors of third order in $\varepsilon$. Clearly, $H_{mol}(q,p)$ does not fulfill our assumptions (see Section 2.3) preventing us to apply our results directly. This is so for several reasons.

- While $H_{mol}(q,p)$ takes value in the unbounded operators on $\mathcal{H}_{\mathrm{f}} = L^2(\mathbb{R}^{3m})$, we assume the symbols to take value in the bounded operators: clearly, it is not a straight forward task to extend our results to unbounded operators. Nevertheless, this is only a technical issue and the domain questions arising have to be dealt case by case, see [Teu03]. We will thus assume $H_e$ to take values in the bounded operators on $\mathcal{H}_{\mathrm{f}}$ from here.
- Similar to the application to magnetic Bloch bands, the restriction that the eigenvalues must be non-degenerate is a limitation of our approach and at this point we do not see much way around this. Also our approach does not allow to handle subsets of energy bands which is clearly a limitation compared to adiabatic-perturbation theory.
- While $H_{mol}(q,p)$ is growing quadratically in $p$, we assume the Hamiltonian to be bounded with respect to $q$ and $p$: Even if we relax our assumptions on the Hamiltonian to Hörmander symbol classes, our approach would still be inapplicable since Hörmander symbol classes impose an increasing gap condition to the energy bands. In particular we would require the energy gap to increase quadratically in the momenta $p$ which is not fulfilled by the molecular energy bands in

general. This causes a qualitative change in the sense that the adiabatic decoupling is no longer uniform. Hence, a momentum cut-off needs to be introduced.

In Section 7 we consider the Hamiltonian operator $\hat{H}^\varepsilon$ acting on $\mathcal{H} = L^2(\mathbb{R}^n) \otimes \mathcal{H}_\mathrm{f}$ for $\mathcal{H}_\mathrm{f}$ some separable Hilbert space and given as Weyl-operator with symbol

$$H(q,p) = \tfrac{1}{2}\,|p - \varepsilon\,A(q)|^2\,\mathbf{1}_{\mathcal{H}_f} + V(q), \qquad \text{for} \quad (q,p) = z \in \mathbb{R}^{2n} \tag{1.14}$$

The magnetic vector potential $A : \mathbb{R}^n \to \mathbb{R}^n$ is assumed to be smooth and bounded. The operator valued potential $V(q)$ is assumed to be bounded together with all it's derivatives and to take value in the continuous linear self-adjoint operators on $\mathcal{H}_\mathrm{f}$. In addition, we assume $V(x)$ to have a non-degenerate isolated eigenvalue $e_v(x)$ with eigenprojection $P_0(q)$. Then,

$$e(q,p) = \tfrac{1}{2}\,|p - \varepsilon\,A(q)|^2 + e_v(q)$$

is an isolated non-degenerate eigenvalue of $H(q,p)$ with eigenprojection $P_0(q)$.

Clearly, due the quadratic growth of $H(q,p)$ our results are still not directly applicable. Nevertheless, we can at least formally determine the modified Hamiltonian system associated to $H(q,p)$, see Section 7.1. The associated classical Hamiltonian is

$$h(q,p) = \ \tfrac{1}{2}\,|p - \varepsilon\,A(q)|^2 + e_v(q) + \tfrac{1}{2}\,\varepsilon^2\,\|p - \varepsilon\,A(q)\|^2_{W(q)} + \mathcal{O}(\varepsilon^3)$$

with

$$W_{ij}(q) := \mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big(\big[\,\partial_i P_0\,|\,(V - e_v)^{-1}\,|\,\partial_j P_0\,\big]_+\Big)(q)$$

where $(V - e_v)^{-1}$ is the reduced resolvent on $P_0^\perp\,\mathcal{H}_\mathrm{f}$. Note, the second order correction to the classical Hamiltonian can be represented as

$$\begin{aligned} \tfrac{1}{2}\,\|\kappa\|^2_{W(q)} &= \tfrac{1}{2}\,\kappa_i\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}([\,\partial_i P_0\,|\,(V - e_v)^{-1}\,|\,\partial_j P_0\,]_+)(q)\,\kappa_j \\ &= \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\langle\kappa\,,\,\nabla P_0(q)\rangle\,(V(q) - e_v(q))^{-1}\,\langle\nabla P_0(q)\,,\,\kappa\rangle) \end{aligned}$$

and thus coincides with the $\mathcal{M}$ term in [PST07]. Nonetheless, the classical Hamiltonian $h$ does not include the Born-Huang potential and therefore does not coincide with the symbol of the effective Hamiltonian that results from adiabatic perturbation theory, cf. [PST07]. It turns out that the Born-Huang potential is closely related to the quantum metric $g_0$, see Remark 7.1. As we will see later in our result on equilibrium expectations as well as the evolution of observables, one can include the Born-Huang potential into the classical Hamiltonian which actually results in a simplification of the quantum corrections. Nevertheless, at this point we state the classical Hamiltonian system the way it results from our general approach.

The coefficient matrix of the modified symplectic form is

$$\omega^\varepsilon(q,p) = \ \omega^0 + \varepsilon\,\mathbf{\Omega}(q,p) + \mathcal{O}(\varepsilon^3)\,.$$

with modified Berry curvature

$$\mathbf{\Omega}(q,p) = \begin{pmatrix} \Omega(q,p) & \varepsilon\,W(q) \\ -\varepsilon\,W(q) & 0 \end{pmatrix}$$

where

$$\begin{aligned}\Omega^{ij}(q,p) = &- \mathrm{i}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}([\,\partial_i P_0\,,\partial_j P_0\,]\,P_0)(q) \\ &- \varepsilon\,(\partial_i W_{jl}(q) - \partial_j W_{il}(q))\,(p-\varepsilon\,A(q))_l\,.\end{aligned}$$

The associated Fubini-Studi metric $\mathbf{g}^\varepsilon$ is

$$\mathbf{g}^\varepsilon(q,p) = \mathbf{g}_0(q) + \mathcal{O}(\varepsilon) = \begin{pmatrix} g_0(q) & 0 \\ 0 & 0 \end{pmatrix} + \mathcal{O}(\varepsilon)$$

where

$$g_0^{ij}(q) = \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\,[\partial_i P_0(q), \partial_j P_0(q)]_+)\,.$$

The Liouville measure of the symplectic form $\omega^\varepsilon$ satisfies

$$\lambda^\varepsilon = \nu^\varepsilon(q,p)\,\mathrm{d}q_1\wedge\cdots\wedge\mathrm{d}p_n = \Big(1+\varepsilon^2\,\mathrm{Tr}_n(W)(q) + \mathcal{O}(\varepsilon^3)\Big)\,\mathrm{d}q_1\wedge\cdots\wedge\mathrm{d}p_n\,.$$

Then, the Hamiltonian equations of motion are

$$\dot q \ = p - \varepsilon\,A(q) + \mathcal{O}(\varepsilon^3)$$

and (1.15)

$$\begin{aligned}\dot p_i = &-\partial_i e_v(q) + \varepsilon\,\langle \partial_i A(q)\,,\,p-\varepsilon\,A(q)\rangle \\ &- \varepsilon\,\Omega^{ij}(q,p)\,(p-\varepsilon\,A(q))_j \\ &- \tfrac{1}{2}\,\varepsilon^2\,\langle p-\varepsilon\,A(q)\,,\,\partial_i W(q)\,(p-\varepsilon\,A(q))\rangle \\ &+ \varepsilon^2\,W_{ij}(q)\,\partial_j e_v(q) + \mathcal{O}(\varepsilon^3)\,.\end{aligned}$$

To our knowledge, the modified Berry connection and thus also the symplectic form and the quantum metric for Born-Oppenheimer type Hamiltonians have nowhere been stated before, not even on a heuristic level.

As addressed already, we need to cut off large momenta to make our approach applicable. Hereto, we replace $|\,p - \varepsilon\, A(q)\,|^2$ by a smooth function that flattens at large momenta. Then, the symbol $H(q,p)$ (1.14) changes to

$$H_\lambda := \tfrac{1}{2}\,\chi_\lambda\Big(|\,p - \varepsilon\, A(q)\,|^2\Big) + V(q)$$

where $\chi_\lambda : \mathbb{R} \to \mathbb{R}$ is a smooth and monotonically non-decreasing function satisfying that $\chi_\lambda(x) = x$ for $x \leq \lambda$ and $\chi_\lambda(x)$ is constant for $x \geq \lambda + 1$. Clearly, $H_\lambda$ satisfies Assumptions 2.10 and 2.11 with eigenvalue $e_\lambda(q,p) = \frac{1}{2}\,\chi_\lambda\Big(|\,p - \varepsilon\, A(q)\,|^2\Big) + e_v(q)$ and eigenprojection $P_0(q)$. Thus, we are now able to apply the theory developed in Chapter 2 - 5 where we aim to express as much as possible in terms of quantities that stem from the original Hamiltonian $\hat{H}^\varepsilon$.

We start with our results on equilibrium expectations. So, let $f$ a suitable equilibrium distribution. Think of a Boltzmann $\mathrm{e}^{-\beta\, x}$ or Fermi-Dirac $(1 + \mathrm{e}^{\beta(x-\mu)})^{-1}$ distribution, as example.

*Equilibrium Expectations for Born-Oppenheimer Type Hamiltonians (cf. Proposition 7.3)*
The equilibrium expectation with respect to a suitable observable $\hat{R}^\varepsilon$ with symbol $R : \mathbb{R}^{2n} \to \mathcal{B}_{\mathrm{sa}}(\mathcal{H}_{\mathrm{f}})$ satisfies

$$\begin{aligned}
&\mathrm{tr}_{\mathcal{H}}\left(f(\hat{H}_\lambda^\varepsilon)\,\hat{R}^\varepsilon\,\hat{\Pi}_\lambda^\varepsilon\right)\\
&\qquad= (2\pi\varepsilon)^{-n}\int_{\Lambda_\lambda}\Big(f(h(q,p)) + \varepsilon^2\,Q_{\mathrm{BO}}(q,p)\Big)\,r(q,p)\,\nu^\varepsilon(q)\,\mathrm{d}q\,\mathrm{d}p\\
&\qquad\quad + (2\pi\varepsilon)^{-n}\Big(\int_{\mathbb{R}^{2n}\setminus\Lambda_\lambda} f^\varepsilon(h_\lambda,\pi_\lambda)\,r_\lambda(q,p)\,\nu_\lambda^\varepsilon(q,p)\,\mathrm{d}q\,\mathrm{d}p\\
&\qquad\qquad + \varepsilon^2\int_{\mathbb{R}^{2n}\setminus\Lambda_\lambda} Q(h_{\lambda,0},\mathbf{g}_0)(q,p)\,r_\lambda(q,p)\,\mathrm{d}q\,\mathrm{d}p\Big)\\
&\qquad\quad + \mathcal{O}\Big(\varepsilon^{3-n}\Big)
\end{aligned} \tag{1.16}$$

with quantum correction to the equilibrium state

$$\begin{aligned}
Q_{\mathrm{BO}}(q,p) = {}& \tfrac{1}{2}\,f'(e(q,p))\,\mathrm{Tr}_n(g_0(q)) + \tfrac{1}{4}\,f''(e(q,p))\,\|p - \varepsilon\, A(q)\|^2_{g_0(q)}\\
&- \tfrac{1}{8}\,f''(e(q,p))\,\Delta e_v(q)\\
&- \tfrac{1}{24}\,f'''(e(q,p))\,\Big(\|p - \varepsilon\, A(q)\|^2_{\nabla^2 e_v(q)} + |\nabla e_v(q)|^2\Big)\,.
\end{aligned}$$

In the first summand of the r.h.s. of (1.16) we restrict the integration over phase space to $\Lambda_\lambda := \{(q,p) \in \mathbb{R}^{2n} : |p - \varepsilon\, A(q)|^2 \leq \lambda\}$. The scalar symbol $r(q,p)$ is the effective symbol of $R(q,p)$ associated to $H(q,p) = \frac{1}{2}\,|p - \varepsilon\, A(q)|^2 + V(q)$ and eigenvalue $e(q,p) = \frac{1}{2}\,|p - \varepsilon\, A(q)|^2 + e_v(q)$.

The effective equilibrium distribution $f^\varepsilon(h_\lambda, \pi_\lambda)$ as well as the quantum correction $Q(h_{\lambda,0}, \mathrm{g}_0)$ are the expressions that follow directly from applying Theorem 4.4 to the l.h.s of (1.16). The classical Hamiltonian system $(\mathbb{R}^{2n}, \omega^\varepsilon_\lambda, h_\lambda)$ is determined in Section 7.1.

Besides the computational effort to compute the explicit expressions for the classical Hamiltonian system $(h, \omega^\varepsilon)$ and the quantum correction as well as their analogues including the momentum cutoff, the above result follows directly from Theorem 4.4.

Note, a simple Taylor expansion shows that the first summand of the quantum correction $Q_{\mathrm{BO}}(q,p)$ can be incorporated in the classical Hamiltonian system by including the Born-Huang potential into the classical Hamiltonian, i.e. $\tilde{h}(q,p) = h(q,p) + \frac{1}{2}\,\mathrm{Tr}_n(g_0(q))$.

We expect that for rapidly decreasing $f$ one can let $\lambda$ tend to infinity with the result that

$$
\begin{aligned}
&\lim_{\lambda\to\infty} \mathrm{tr}_{\mathcal{H}} \Big( f(\hat{H}^\varepsilon_\lambda)\, \hat{R}^\varepsilon\, \hat{\Pi}^\varepsilon_\lambda \Big) \\
&\qquad = (2\pi\varepsilon)^{-n} \int_{\Lambda_\lambda} \Big( f(h(q,p)) + \varepsilon^2\, Q_{\mathrm{BO}}(q,p) \Big)\, r(q,p)\, \nu^\varepsilon(q)\, \mathrm{d}q\, \mathrm{d}p \\
&\qquad\quad + \mathcal{O}\Big(\varepsilon^{3-n}\Big)\,.
\end{aligned}
$$

Nevertheless, this is not proven in this work. For a rough argumentation on why we expect the above to be true, see Remark 7.4.

Next, we present our result on the semiclassical approximation of the quantum evolution of an observable $\hat{R}^\varepsilon$ within the Heisenberg picture of quantum mechanics. Clearly, one can directly apply Theorem 5.2 the time-evolved observable $\hat{R}^\varepsilon(t,\lambda) := \mathrm{e}^{\mathrm{i}\,\hat{H}^\varepsilon_\lambda\, t/\varepsilon}\, \hat{R}^\varepsilon\, \mathrm{e}^{-\mathrm{i}\,\hat{H}^\varepsilon_\lambda}$. As already mentioned we aim the express as much as possible in terms of the classical Hamiltonian system $(h, \omega^\varepsilon)$ associated to the original Hamiltonian symbol $H(q,p)$. This leads to some technical difficulties one has to take care of. First of all, we limit the energy to a range where the original Hamiltonian symbol $H(q,p)$ coincides with $H_\lambda(q,p)$. Hereto, we cut off large energies by introducing the operator $\zeta_\mu(\hat{H}^\varepsilon_\lambda)$ where $\zeta_\mu : \mathbb{R} \to \mathbb{R}$, $\mu > 0$ is a smooth cutoff function satisfying $\zeta_\mu(x) = 1$ for $x \le \mu$ and $\zeta_\mu(x) = 0$ for $x \ge \mu+1$. Moreover, we have to be quite careful regarding the flow $\Phi^t_\varepsilon$ of the Hamiltonian equations of motion (1.15) as it may not be defined for arbitrary $(q,p) \in \mathbb{R}^{2n}, t > 0$. This leads to the following proposition as well as its proof to be quite technical.

*Egorov theorem for Born-Oppenheimer type Hamiltonians (cf. Proposition 7.5)* There exist $\lambda_\mu > \tilde\lambda_\mu > 0$ and a $T_{\mu,\lambda_\mu} > 0$ such that for $\hat\Pi^\varepsilon_{\lambda_\mu}$ the super-adiabatic projection associated to $H_{\lambda_\mu}$ with eigenvalue $e_{\lambda_\mu}$ and $0 \le t < T_{\mu,\lambda_\mu}$ we have

$$\begin{aligned}\Big\| \hat\Pi^\varepsilon_{\lambda_\mu} \Big( \mathrm{e}^{\mathrm{i}\,\hat H^\varepsilon_{\lambda_\mu} t/\varepsilon}\, \hat R^\varepsilon\, \mathrm{e}^{-\mathrm{i}\,\hat H^\varepsilon_{\lambda_\mu} t/\varepsilon} - \mathrm{op}_\varepsilon \Big( \Big( r(\Phi^t_\varepsilon) + \varepsilon^2\, \mathfrak{A}(t) \Big)\, \xi_{\tilde\lambda_\mu,\lambda_\mu} \Big) \Big)\, \hat\Pi^\varepsilon_{\lambda_\mu}\, \zeta_\mu(\hat H^\varepsilon_{\lambda_\mu}) \Big\| \\ = \mathcal{O}(\varepsilon^3)\,.\end{aligned}$$

Here, $\xi_{\tilde\lambda_\mu,\lambda_\mu}$ is a smooth cutoff function with $\xi_{\tilde\lambda_\mu,\lambda_\mu}(q,p) = 1$ for $(q,p) \in \Lambda_{\tilde\lambda_\mu}$ and $\xi_{\tilde\lambda_\mu,\lambda_\mu}(q,p) = 0$ for $(q,p) \in \mathbb{R} \setminus \Lambda_{(\tilde\lambda_\mu+\lambda_\mu)/2}$ where $\Lambda_\lambda := \{(q,p) \in \mathbb{R}^{2n} : |p - \varepsilon\, A(q)|^2 \le \lambda\}$. The scalar symbol $r(q,p)$ is the effective symbol of $R(q,p)$ associated to $H(q,p) = \frac{1}{2}\, |p - \varepsilon\, A(q)|^2 + V(q)$ and eigenvalue $e(q,p) = \frac{1}{2}\, |p - \varepsilon\, A(q)|^2 + e_v(q)$. The quantum correction $\mathfrak{A}(t)$ is given by

$$\mathfrak{A}(t) = \int_0^t \mathfrak{A}^c_h(r_0(\Phi^\tau_\varepsilon)) \circ \Phi^{t-\tau}_\varepsilon\, \mathrm{d}\tau$$

with

$$\begin{aligned}\mathfrak{A}^c_h(r_0)(q,p) = &- \tfrac{1}{2}\, \mathrm{Tr}_n\Big( \partial^2_{pq} r_0(q,p)\, g_0(q) \Big) - \tfrac{1}{4}\, \langle \partial_p r_0(q,p)\,,\, \nabla\, \mathrm{Tr}_n(g_0(q)) \rangle \\ &+ \tfrac{1}{4}\, \partial^2_{p_j p_l} r_0(q,p)\, (p - \varepsilon\, A(q))_i\, \partial_i g^{jl}_0(q) \\ &+ \tfrac{1}{24}\, \partial^3_{p_i p_j p_l} r_0(q,p)\, \partial^3_{ijl} e_v(q,p) + \mathcal{O}(\varepsilon)\,.\end{aligned}$$

Note here, the reason for introducing $\xi_{\tilde\lambda_\mu,\lambda_\mu}$ is that the Weyl quantization of $r(\Phi^t_\varepsilon) + \varepsilon^2\, \mathfrak{A}(t))$ may not make sense for all $t \in [0, T_{\mu,\lambda_\mu})$ as the Hamiltonian flow $\Phi^t_\varepsilon$ may not exist for arbitrary $(q,p) \in \mathbb{R}^{2n}$ and $t \in [0, T_{\mu,\lambda_\mu})$. Including the cut-off, the expression $(r(\Phi^t_\varepsilon) + \varepsilon^2\, \mathfrak{A}(t))\, \xi_{\tilde\lambda_\mu,\lambda_\mu}$ is smooth and bounded with all its derivatives for any $t \in [0, T_{\mu,\lambda_\mu})$.

Also here, the inclusion of the Born-Huang potential into the classical Hamiltonian, i.e. $\tilde h(q,p) = h(q,p) + \frac{1}{2}\, \mathrm{Tr}_n(g_0(q))$ leads to a simplification of the quantum correction $\mathfrak{A}^c_h(r_0)(q,p)$. Note that apart from the Born-Huang potential also the sign of the expression $\frac{1}{2}\, \varepsilon^2\, \|p - \varepsilon\, A(q)\|^2_{W(q)}$ differs in our classical Hamiltonian when compared to the symbol the effective Hamiltonian the results for space-adiabatic perturbation theory, c.f. [PST07]. One can alter the coefficient matrix of the symplectic form $\omega^\varepsilon$ to obtain a second order Egorov theorem using the effective Hamiltonian form [PST07] but this results in an $\tilde\omega^\varepsilon$ that is not skew-symmetric and therefore does not define a symplectic form, see Remark 7.6.

# 2 Weyl Calculus, Liouville Measures and Assumptions

This chapter consists of three mainly independent sections. In Section 2.1 we give a general overview over Weyl calculus and state known results that are used throughout this thesis. In contrast, the results of Section 2.2 are very general and to our knowledge mostly new. There, we will drive the Lebesgue density of the Liouville measure of an arbitrary symplectic form $\Omega$ on $\mathbb{R}^{2n}$. In addition, we will derive the Lebesgue density of the Liouville measure for the special case of a semiclassical symplectic form $\omega^\varepsilon = \omega^0 + \varepsilon\,\Omega$. Besides the general importance of these trace formulae we will use them in the analysis of the structure of expectation values for stationary states. In the third and last section of this chapter we state the assumptions on the Hilbert space $\mathcal{H}$, the Hamiltonian $\hat{H}^\varepsilon$ and the eigenvalue $e_0(z)$ on which we will restrict to throughout this thesis.

## 2.1 Weyl Calculus, Notation and Other Useful Identities

Let $X$ be a Banach space and $k \in \mathbb{R}$. We define

$$S^k(X) := \left\{ f \in C^\infty(\mathbb{R}^{2n}, X) : \sup_{z\in\mathbb{R}^{2n}} \left\| \langle z\rangle^k \, \partial_z^\alpha f(z) \right\|_X < \infty \text{ for all } \alpha \in \mathbb{N}_0^{2n} \right\}$$

where $\langle z\rangle := (1 + |z|^2)^{1/2}$. The family of seminorms

$$\|f\|_{k,r,X} := \max_{\substack{\alpha\in\mathbb{N}_0^{2n}\\ |\alpha|\le r}} \sup_{z\in\mathbb{R}^{2n}} \left\| \langle z\rangle^k \, \partial_z^\alpha f(z) \right\|_X$$

turns $S^k(X)$ into a Fréchet space. For $B \in S^k(X)$ with $k > 2n$ it holds that

$$\begin{aligned}\|\partial_z^\alpha B\|_{L^1(\mathbb{R}^{2n},X)} &= \int_{\mathbb{R}^{2n}} \|\partial_z^\alpha B(z)\|_X \,\mathrm{d}z = \int_{\mathbb{R}^{2n}} \langle z\rangle^{-k} \|\langle z\rangle^k\, \partial_z^\alpha B(z)\|_X \,\mathrm{d}z \\ &\le \|B\|_{k,|\alpha|,X} \int_{\mathbb{R}^{2n}} \langle z\rangle^{-k} \,\mathrm{d}z < \infty\end{aligned}$$

for all $\alpha \in \mathbb{N}_0^{2n}$. Thus, $B$ is Bochner-integrable together with all its derivatives.

The space of maps $B : [0, \varepsilon_0) \to S^k(X)$ with

$$\|B\|^\varepsilon_{k,r,X} := \sup_{\varepsilon\in[0,\varepsilon_0)} \|B(\varepsilon)\|_{k,r,X} < \infty$$

for all $r \in \mathbb{N}_0$ is denoted by $S^k(\varepsilon, X)$. Similar to above, for $B \in S^k(\varepsilon, X)$ with $k > 2n$ we have

$$\begin{aligned}\|\partial_z^\alpha B\|^\varepsilon_{L^1(\mathbb{R}^{2n},X)} &:= \sup_{\varepsilon\in[0,\varepsilon_0)} \|\partial_z^\alpha B(\varepsilon)\|_{L^1(\mathbb{R}^{2n},X)} = \sup_{\varepsilon\in[0,\varepsilon_0)} \int_{\mathbb{R}^{2n}} \|\partial_z^\alpha B(\varepsilon, z)\|_X \,\mathrm{d}z \\ &\le \|B\|^\varepsilon_{k,|\alpha|,X} \int_{\mathbb{R}^{2n}} \langle z\rangle^{-k} \,\mathrm{d}z < \infty\end{aligned}$$

for all $\alpha \in \mathbb{N}_0^{2n}$. Hence, also here $B$ is Bochner-integrable together with all its derivatives. We call the elements of $S^k(X)$ and $S^k(\varepsilon, X)$ symbols. To increase readability, we will omit the $\varepsilon$ and $z$ dependence of symbols in $S^k(\varepsilon, X)$ in many computations and statements throughout this thesis, e.g. we write $\partial_i B$ for $\frac{\partial}{\partial z_i} B(\varepsilon, z)$.

If for $B \in S^k(\varepsilon, X)$ there exist $B_j \in S^k(\varepsilon, X)$, $j \in \mathbb{N}_0$ such that

$$\sup_{\varepsilon\in[0,\varepsilon_0)} \left\| \varepsilon^{-(N+1)} \left( B(\varepsilon) - \sum_{j=0}^{N} \varepsilon^j B_j(\varepsilon) \right) \right\|_{k,r,X} < \infty$$

for all $r \in \mathbb{N}_0$ and $N \in \mathbb{N}_0$, then we say that $B$ has an asymptotic expansion $\sum_{j=0}^m \varepsilon^j B_j(\varepsilon)$ and write $B \asymp \sum_{j=0}^\infty \varepsilon^j B_j(\varepsilon)$ in $S^k(\varepsilon, X)$. We denote $B^{(m)}(\varepsilon) := \sum_{j=0}^m \varepsilon^j B_j(\varepsilon)$. If $B \in S^k(\varepsilon, X)$ has an asymptotic expansion with $B_j(\varepsilon) = 0$ for all $0 \le j \le N$ and all $\varepsilon \in [0, \varepsilon_0)$ we write

$$B = \mathcal{O}(\varepsilon^{N+1}) \quad \text{in } S^k(\varepsilon, X)$$

and if $B_j(\varepsilon) = 0$ for all $j \ge 0$ and all $\varepsilon \in [0, \varepsilon_0)$ we write

$$B = \mathcal{O}(\varepsilon^\infty) \quad \text{in } S^k(\varepsilon, X)\,.$$

Note that for $B_j \in S^k(\varepsilon, X)$, $j \in \mathbb{N}_0$ the series $\sum_{j=0}^{\infty} \varepsilon^j B_j(\varepsilon)$ does not converge in general. However, one can always find a symbol $B \in S^k(\varepsilon, X)$ such that $B \asymp \sum_{j=0}^{\infty} \varepsilon^j B_j(\varepsilon)$.

**Lemma 2.1** *Let $(B_j(\varepsilon))_{j\geq 0}$ be a sequence in $S^k(\varepsilon, X)$ . In addition, let $\chi : \mathbb{R} \to \mathbb{R}$ be a smooth cutoff function supported in $\overline{\mathrm{B}_2(0)}$ with $\chi(x) = 1$ on $\mathrm{B}_1(0)$. Then there exists a sequence $(\lambda_j)_{j\geq 0}$ in $\mathbb{R}$, $\lambda_j \overset{j\to\infty}{\to} \infty$ such that*

$$B(\varepsilon) := \sum_{j=0}^{\infty} \varepsilon^j \chi(\varepsilon \lambda_j) B_j(\varepsilon) \in S^k(\varepsilon, X)$$

*and*

$$B \asymp \sum_{j=0}^{\infty} \varepsilon^j B_j(\varepsilon) \qquad \textit{in } S^k(\varepsilon, X) .$$

This Lemma was proven several times for the case where the $B_j \in S^k(X)$ are $\varepsilon$ independent see e.g. [Zwo12, Theorem 4.15] or [Fol89, Proposition 2.26]. Yet, for $B_j \in S^k(\varepsilon, X)$ the same proves hold with just minor adjustments.

Now let $\mathcal{H}_\mathrm{f}$ be a separable Hilbert space. We denote the Banach space of continuous linear operators by $\mathcal{B}(\mathcal{H}_\mathrm{f})$ and use the following abbreviations

$$\|B(\varepsilon)\|_{k,r} := \|B(\varepsilon)\|_{k,r,\mathcal{B}(\mathcal{H}_\mathrm{f})} , \qquad \|B\|^\varepsilon_{k,r} := \|B\|^\varepsilon_{k,r,\mathcal{B}(\mathcal{H}_\mathrm{f})} ,$$
$$\|B(\varepsilon)\|_{L^1} := \|B(\varepsilon)\|_{L^1(\mathbb{R}^{2n},\mathcal{B}(\mathcal{H}_\mathrm{f}))} \quad \text{and} \quad \|B\|^\varepsilon_{L^1} := \|B\|^\varepsilon_{L^1(\mathbb{R}^{2n},\mathcal{B}(\mathcal{H}_\mathrm{f}))} .$$

For a symbol $B \in S^k(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f}))$, $k \geq 0$ we define its Weyl quantization $\hat{B}^\varepsilon = \mathrm{op}_\varepsilon(B)$ by the action on a Schwartz function $\psi \in \mathscr{S}(\mathcal{H}_\mathrm{f}) = \bigcap_{k=0}^{\infty} S^k(\mathcal{H}_\mathrm{f})$

$$\left(\hat{B}^\varepsilon \psi\right)(x) = \frac{1}{(2\pi\varepsilon)^n} \int_{\mathbb{R}^{2n}} B\left(\varepsilon, \tfrac{1}{2}(x+q), p\right) \mathrm{e}^{\mathrm{i}p\cdot(x-q)/\varepsilon} \psi(q) \,\mathrm{d}q \,\mathrm{d}p . \tag{2.1}$$

By the Calderon-Vaillancourt theorem there exists a constant $C_n$ independent of $B$ and $\varepsilon$ such that

$$\|\hat{B}^\varepsilon\|_{\mathcal{B}(\mathcal{H})} \leq C_n \|B(\varepsilon)\|_{0,2n+1} \tag{2.2}$$

for all $\varepsilon \in [0, \varepsilon_0)$ (see e.g. [Fol89, Theorem 2.73] or [Mar02, Theorem 2.8.1]). Therefore, $\hat{B}^\varepsilon$ can be extended to a continuous linear operator on $L^2(\mathbb{R}^n, \mathcal{H}_\mathrm{f})$. By (2.1) one can easily see that the adjoint of a Weyl quantized operator $\hat{B}^\varepsilon$ agrees with the quantization of the pointwise adjoint symbol $B^*$. As a consequence, the Weyl quantization of a symbol $B$ taking values in $\mathcal{B}_{\mathrm{sa}}(\mathcal{H}_\mathrm{f})$, the self-adjoint bounded linear operators on $\mathcal{H}_\mathrm{f}$, is self-adjoint.

By $\mathscr{S}(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f})) = \bigcap_{k=0}^{\infty} S^k(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f}))$ we denote the Schwartz functions from $\mathbb{R}^{2n}$ to $\mathcal{B}(\mathcal{H}_\mathrm{f})$ uniformly bounded with respect to $\varepsilon$ and define $\sigma(\mathfrak{D}_z, \mathfrak{D}_y) = \langle \omega^0 \, \mathfrak{D}_z \, , \, \mathfrak{D}_y \rangle$ where $\mathfrak{D}_z := \frac{1}{\mathrm{i}} \nabla_z$ and $\omega^0$ is the canonical symplectic form with coefficient matrix

$$\omega^0 = \begin{pmatrix} 0 & \mathbf{1}_{\mathbb{R}^n} \\ -\mathbf{1}_{\mathbb{R}^n} & 0 \end{pmatrix} .$$

For $R, B \in \mathscr{S}(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f}))$ we have

$$\hat{R}^\varepsilon \, \hat{B}^\varepsilon = \mathrm{op}_\varepsilon \left( \mathrm{e}^{\mathrm{i} \frac{\varepsilon}{2} \sigma(\mathfrak{D}_z, \mathfrak{D}_y)} R(z) \, B(y) \Big|_{y=z} \right) =: \mathrm{op}_\varepsilon \left( R \# B \right)$$

where $\mathrm{e}^{\mathrm{i} \frac{\varepsilon}{2} \sigma(\mathfrak{D}_z, \mathfrak{D}_y)}$ is defined as a Fourier multiplier (see e.g. [Zwo12, Theorem 4.11]). The bilinear map $\#$, called Moyal product, extends uniquely to

$$\# : S^{k_1}(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f})) \times S^{k_2}(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f})) \to S^{k_1+k_2}(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f}))$$

and is continuous with respect to the Fréchet topologies uniformly in $\varepsilon$, i.e. there exists an $\tilde{r} \in \mathbb{N}_0$ and a constant $C_r < \infty$ for any $r \in \mathbb{N}_0$, $k_1, k_2 \geq 0$ such that

$$\|(R\#B)(\varepsilon)\|_{k_1+k_2,r} \leq C_r \|R(\varepsilon)\|_{k_1,\tilde{r}} \|B(\varepsilon)\|_{k_2,\tilde{r}} \quad \text{for all } \varepsilon \in [0, \varepsilon_0), \tag{2.3}$$

see e.g. in the proof of [Zwo12, Theorem 4.17] or [Fol89, Proposition 2.41]. Let $R, B, A \in \mathscr{S}(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f}))$ then

$$\begin{aligned} ((R \# B) \# A)(z) &= \mathrm{e}^{\mathrm{i} \frac{\varepsilon}{2} \sigma(\mathfrak{D}_y, \mathfrak{D}_z)} \Big( \mathrm{e}^{\mathrm{i} \frac{\varepsilon}{2} \sigma(\mathfrak{D}_x, \mathfrak{D}_y)} R(x) \, B(y) \Big|_{y=x} \Big) \, A(z) \Big|_{z=y} \\ &= \mathrm{e}^{\mathrm{i} \frac{\varepsilon}{2} \sigma(\mathfrak{D}_x + \mathfrak{D}_y, \mathfrak{D}_z)} \mathrm{e}^{\mathrm{i} \frac{\varepsilon}{2} \sigma(\mathfrak{D}_x, \mathfrak{D}_y)} R(x) \, B(y) \, A(z) \Big|_{z=y=x} \\ &= \mathrm{e}^{\mathrm{i} \frac{\varepsilon}{2} \sigma(\mathfrak{D}_x, \mathfrak{D}_z)} \mathrm{e}^{\mathrm{i} \frac{\varepsilon}{2} \sigma(\mathfrak{D}_y, \mathfrak{D}_z)} \mathrm{e}^{\mathrm{i} \frac{\varepsilon}{2} \sigma(\mathfrak{D}_x, \mathfrak{D}_y)} R(x) \, B(y) \, A(z) \Big|_{z=y=x} . \end{aligned}$$

It is easy to verify that the same is true for $(R \# (B \# A))(z)$, showing the associativity of the Moyal product $\#$.

For $R \in S^{k_1}(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f}))$ and $B \in S^{k_2}(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f}))$ the Moyal product $R\#B \in S^{k_1+k_2}(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f}))$ has an explicit asymptotic expansion

$$R\#B \asymp \sum_{j=0}^{\infty} \varepsilon^j \, \{R(\varepsilon) \, , B(\varepsilon)\}_j$$

where (2.4)

$$\{R(\varepsilon) \, , B(\varepsilon)\}_j := \left(\tfrac{\mathrm{i}}{2}\right)^j \tfrac{1}{j!} \, \sigma(\mathfrak{D}_z, \mathfrak{D}_y)^j R(\varepsilon, z) \, B(\varepsilon, y) \Big|_{y=z} .$$

The map $\{\cdot\,,\cdot\}_j$ is a generalization of the Poisson bracket $\{\cdot\,,\cdot\}$ which is defined by

$$\{R(\varepsilon)\,,B(\varepsilon)\} := \sum_{i=1}^{n} \Big(\partial_{p_i} R(\varepsilon)\,\partial_{q_i} B(\varepsilon) - \partial_{q_i} R(\varepsilon)\,\partial_{p_i} B(\varepsilon)\Big)\,.$$

The generalized Poisson bracket can be reformulated as

$$\{R(\varepsilon)\,,B(\varepsilon)\}_j = \tfrac{1}{(2\mathrm{i})^j\,j!} \sum_{\alpha,\beta\in\{1,\ldots,2n\}^j} \omega^0_{\alpha_1\beta_1}\cdots\omega^0_{\alpha_j\beta_j}\,\nabla^j_\beta R(\varepsilon,z)\,\nabla^j_\alpha B(\varepsilon,z) \tag{2.5}$$

and thus for $j=1$ agrees with the Poisson bracket $\{\cdot\,,\cdot\}$ up to a factor of $2\mathrm{i}$. The remainder maps of the Moyal expansion $R_N : S^{k_1}(\varepsilon,\mathcal{B}(\mathcal{H}_\mathrm{f})) \times S^{k_2}(\varepsilon,\mathcal{B}(\mathcal{H}_\mathrm{f})) \to S^{k_1+k_2}(\varepsilon,\mathcal{B}(\mathcal{H}_\mathrm{f}))$

$$R_N(R,B) := \varepsilon^{-(N+1)}\Big(R\#B - \sum_{j=0}^{N} \varepsilon^j\,\{R(\varepsilon)\,,B(\varepsilon)\}_j\Big)$$

are continuous with respect to the Fréchet topologies, i.e. for any $N,r\in\mathbb{N}_0$ there exists an $\tilde r\in\mathbb{N}_0$ and a constant $C_r<\infty$ such that

$$\|R_N(R,B)(\varepsilon)\|_{k_1+k_2,r} \le C_r\,\|R(\varepsilon)\|_{k_1,\tilde r}\,\|B(\varepsilon)\|_{k_2,\tilde r} \quad \text{for all } \varepsilon\in[0,\varepsilon_0)\,. \tag{2.6}$$

By (2.5) it is easy to see that

$$\begin{aligned}&\{R(\varepsilon)\,,B(\varepsilon)\}_j + \{B(\varepsilon)\,,R(\varepsilon)\}_j \\ &\quad= \tfrac{1}{(2\mathrm{i})^j\,j!} \sum_{\alpha,\beta\in\{1,\ldots,2n\}^j} \omega^0_{\alpha_1\beta_1}\cdots\omega^0_{\alpha_j\beta_j} \begin{cases}[\,\nabla^j_\beta R(\varepsilon,z),\nabla^j_\alpha B(\varepsilon,z)\,], & j \text{ odd}\\ [\,\nabla^j_\beta R(\varepsilon,z),\nabla^j_\alpha B(\varepsilon,z)\,]_+, & j \text{ even}\end{cases}\end{aligned}$$

and (2.7)

$$\begin{aligned}&\{R(\varepsilon)\,,B(\varepsilon)\}_j - \{B(\varepsilon)\,,R(\varepsilon)\}_j \\ &\quad= \tfrac{1}{(2\mathrm{i})^j\,j!} \sum_{\alpha,\beta\in\{1,\ldots,2n\}^j} \omega^0_{\alpha_1\beta_1}\cdots\omega^0_{\alpha_j\beta_j} \begin{cases}[\,\nabla^j_\beta R(\varepsilon,z),\nabla^j_\alpha B(\varepsilon,z)\,]_+, & j \text{ odd}\\ [\,\nabla^j_\beta R(\varepsilon,z),\nabla^j_\alpha B(\varepsilon,z)\,], & j \text{ even}\end{cases}\end{aligned}$$

where $[\cdot,\cdot]$ denotes the commutator and $[\cdot,\cdot]_+$ the anti-commutator. If $R\in S^{k_1}(\varepsilon,\mathcal{B}(\mathcal{H}_\mathrm{f}))$ and $B\in S^{k_2}(\varepsilon,\mathcal{B}(\mathcal{H}_\mathrm{f}))$ commute as for example when $B$ is given by $B(\varepsilon,z)=b(\varepsilon,z)\,\mathbf{1}_{\mathcal{H}_\mathrm{f}}$ where $b\in S^{k_2}(\varepsilon,\mathbb{C})$ is a scalar symbol then

$$\begin{aligned}R\,\#\,B - B\,\#\,R &\asymp 2\,\varepsilon\,\{R,B\}_1 + 2\,\varepsilon^3\,\{R,B\}_3 + \mathcal{O}(\varepsilon^5)\\ &= -\mathrm{i}\,\varepsilon\,\{R,B\} + 2\,\varepsilon^3\,\{R,B\}_3 + \mathcal{O}(\varepsilon^5)\,.\end{aligned}$$

We also want to work with triple Moyal products i.e., $A\#B\#R$ for $A \in S^{k_1}(\varepsilon,\mathcal{B}(\mathcal{H}_\mathrm{f}))$, $B \in S^{k_2}(\varepsilon,\mathcal{B}(\mathcal{H}_\mathrm{f}))$ and $R \in S^{k_3}(\varepsilon,\mathcal{B}(\mathcal{H}_\mathrm{f}))$ with this in mind we denote

$$\{A\,|R\,|\,B\}_j := \tfrac{1}{(2\mathrm{i})^j\, j!} \sum_{\alpha,\beta\in\{1,\dots,2n\}^j} \omega^0_{\alpha_1\beta_1}\cdots\omega^0_{\alpha_j\beta_j}\,\nabla^j_\beta A(\varepsilon,z)\,R(\varepsilon,z)\,\nabla^j_\alpha B(\varepsilon,z)$$

and

$$[\,A\,|R\,|\,B\,] := A\,R\,B - B\,R\,A\,.$$

Then a simple computation shows

$$\begin{aligned} A\#R\#B = A\,R\,B + \varepsilon\,A\,\{R\,,B\}_1 + \varepsilon\,\{A\,|R\,|\,B\}_1 + \varepsilon\,\{A\,,R\}_1\,B \\ + \varepsilon^2\,\{\{A\,,R\}_1\,\,,B\}_1 + \varepsilon^2\,\{A\,R\,,B\}_2 + \mathcal{O}(\varepsilon^3)\,. \end{aligned} \tag{2.8}$$

We call $B \in S^k(\varepsilon,\mathcal{B}(\mathcal{H}_\mathrm{f}))$ a classical symbol if $B$ has an asymptotic expansion with coefficients $B_j$ that do not depend on $\varepsilon$, i.e. $B(\varepsilon) \asymp \sum_{j=0}^\infty \varepsilon^j B_j$, $B_j \in S^k(\mathcal{B}(\mathcal{H}_\mathrm{f}))$ for all $j \in \mathbb{N}_0$. If $R$ and $B$ are classical symbols then also the Moyal product $R\#B$ is a classical symbol an asymptotic expansion given by

$$(R\#B)(\varepsilon) \asymp \sum_{j=0}^\infty \varepsilon^j\,(R\#B)_j = \sum_{j=0}^\infty \varepsilon^j \sum_{\substack{\alpha\in\mathbb{N}_0^3,\\ |\alpha|=j}} \{R_{\alpha_1}\,,B_{\alpha_2}\}_{\alpha_3}\,. \tag{2.9}$$

Moreover, the remainder satisfies that for any $N, r \in \mathbb{N}_0$ there exist $\tilde r \geq r$ and $C_r < \infty$ such that

$$\begin{aligned} &\varepsilon^{-(N+1)}\Big\|(R\,\#\,B)(\varepsilon) - \sum_{j=0}^N \varepsilon^j\,(R\,\#\,B)_j\Big\|_{k_1+k_2,r} \\ &= \Big\|\sum_{0\leq\alpha_1,\alpha_2\leq N} \varepsilon^{|\alpha|}\Big((R_{\alpha_1}\,\#\,B_{\alpha_2})(\varepsilon) - \sum_{j=0}^{N-|\alpha|}\varepsilon^j(R_{\alpha_1}\,\#\,B_{\alpha_2})_j\Big) \\ &\quad + \Big((R-R^{(N)})\,\#\,(B-B^{(N)})\Big)(\varepsilon)\Big\|_{0,r} \\ &\leq C_r\Big(\sum_{i=0}^N \|R_i\|_{k_1,\tilde r}\,\sum_{i=0}^N \|B_i\|_{k_2,\tilde r} \\ &\quad + \varepsilon^{-(N+1)}\|(R-R^{(N)})(\varepsilon)\|_{k_1,\tilde r}\,\|(B-B^{(N)})(\varepsilon)\|_{k_2,\tilde r}\Big) \end{aligned} \tag{2.10}$$

for all $\varepsilon \in [0,\varepsilon_0)$.

We also want to take traces of Weyl operators. By $\mathcal{J}(\mathcal{H}_\mathrm{f}) \subset \mathcal{B}(\mathcal{H}_\mathrm{f})$ we denote the Banach space of trace-class operators on $\mathcal{H}_\mathrm{f}$ with trace norm $\|B\|_1 := \mathrm{tr}_{\mathcal{H}_\mathrm{f}}|B|$ and for $B \in S^k(\varepsilon,\mathcal{J}(\mathcal{H}_\mathrm{f}))$ abbreviate

$$\|B(\varepsilon)\|_{k,r,1} := \|B(\varepsilon)\|_{k,r,\mathcal{J}(\mathcal{H}_\mathrm{f})} \qquad \text{and} \qquad \|B\|^\varepsilon_{k,r,1} := \|B\|^\varepsilon_{k,r,\mathcal{J}(\mathcal{H}_\mathrm{f})}\,.$$

The Moyal product restricts to maps

$$\# : S^{k_1}(\varepsilon, \mathcal{J}(\mathcal{H}_{\mathrm{f}})) \times S^{k_2}(\varepsilon, \mathcal{B}(\mathcal{H}_{\mathrm{f}})) \to S^{k_1+k_2}(\varepsilon, \mathcal{J}(\mathcal{H}_{\mathrm{f}}))$$

and (2.11)

$$\# : S^{k_1}(\varepsilon, \mathcal{B}(\mathcal{H}_{\mathrm{f}})) \times S^{k_2}(\varepsilon, \mathcal{J}(\mathcal{H}_{\mathrm{f}})) \to S^{k_1+k_2}(\varepsilon, \mathcal{J}(\mathcal{H}_{\mathrm{f}})).$$

Continuity of Moyal product and asymptotic expansion holds as well with respect to the trace norm $\|\cdot\|_1$ on $\mathcal{J}(\mathcal{H}_{\mathrm{f}})$. One crucial observation is that a Weyl operator $\hat{B}^{\varepsilon}$ with symbol $B \in S^k(\varepsilon, \mathcal{J}(\mathcal{H}_{\mathrm{f}}))$, $k > 2n$ is trace class and its trace can be computed by a phase space integral

$$\mathrm{tr}_{L^2(\mathbb{R}^n,\mathcal{H}_{\mathrm{f}})}\left(\hat{B}^{\varepsilon}\right) = (2\pi\varepsilon)^{-n} \int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_{\mathrm{f}}}(B(\varepsilon, z))\,\mathrm{d}z\,. \tag{2.12}$$

Moreover, for two Weyl operators $\hat{B}^{\varepsilon}$, $\hat{R}^{\varepsilon}$ with symbols $B \in S^{k_1}(\varepsilon, \mathcal{B}(\mathcal{H}_{\mathrm{f}}))$ and $R \in S^{k_2}(\varepsilon, \mathcal{B}(\mathcal{H}_{\mathrm{f}}))$,$k_1, k_2 \geq 0$ satisfying that $\|\mathrm{tr}_{\mathcal{H}_{\mathrm{f}}}(B\,R)\|_{L^1(\mathbb{R}^{2n})} < \infty$ the composition $\hat{B}^{\varepsilon}\,\hat{R}^{\varepsilon}$ is trace class with

$$\mathrm{tr}_{L^2(\mathbb{R}^n,\mathcal{H}_{\mathrm{f}})}\left(\hat{B}^{\varepsilon}\,\hat{R}^{\varepsilon}\right) = (2\pi\varepsilon)^{-n} \int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_{\mathrm{f}}}(B(\varepsilon, z)\,R(\varepsilon, z))\,\mathrm{d}z \tag{2.13}$$

see e.g. [ST13, Section 2.2]. In particular, if $B \in S^k(\varepsilon, \mathcal{B}(\mathcal{H}_{\mathrm{f}}))$, $k > 2n$ and $R \in S^0(\varepsilon, \mathcal{J}(\mathcal{H}_{\mathrm{f}}))$ then $\hat{B}^{\varepsilon}\,\hat{R}^{\varepsilon}$ is trace class since

$$\begin{aligned}\int_{\mathbb{R}^{2n}} |\mathrm{tr}_{\mathcal{H}_{\mathrm{f}}}(B(\varepsilon, z)\,R(\varepsilon, z))|\,\mathrm{d}z &\leq \int_{\mathbb{R}^{2n}} \|B(\varepsilon, z)\|\,|\mathrm{tr}_{\mathcal{H}_{\mathrm{f}}}(R(\varepsilon, z))|\,\mathrm{d}z \\ &\leq \|B\|^{\varepsilon}_{L^1}\,\|R\|^{\varepsilon}_{0,0,1} < \infty\end{aligned} \tag{2.14}$$

holds for all $\varepsilon \in [0, \varepsilon_0)$. In the case of scalar symbols $B \in S^k(\varepsilon, \mathbb{C})$, $k > 2n$ and $R \in S^0(\varepsilon, \mathbb{C})$ we have

$$\mathrm{tr}_{L^2(\mathbb{R}^n)}\left(\hat{B}^{\varepsilon}\,\hat{R}^{\varepsilon}\right) = (2\pi\varepsilon)^{-n} \int_{\mathbb{R}^{2n}} B(\varepsilon, z)\,R(\varepsilon, z)\,\mathrm{d}z$$

see e.g. [Ron84].

For later reference we will also state some identities for symbols that take value in the orthogonal rank-one projections on $\mathcal{H}_{\mathrm{f}}$. So, let the symbol $\mathrm{P} \in S^0(\varepsilon, \mathcal{J}(\mathcal{H}_{\mathrm{f}}))$ take value in the rank-one projections on $\mathcal{H}_{\mathrm{f}}$. Then, there exists an orthonormal basis $\{\psi_i(\varepsilon, z)\}_{i\in\mathbb{N}_0}$ of $\mathcal{H}_{\mathrm{f}}$ for every $z \in \mathbb{R}^{2n}$, $\varepsilon \in [0, \varepsilon_0)$

such that $P(\varepsilon, z) = |\psi_0(\varepsilon, z)\rangle\langle\psi_0(\varepsilon, z)|$. Hence, for every $A \in S^k(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f}))$ and every $z \in \mathbb{R}^{2n}$, $\varepsilon \in [0, \varepsilon_0)$ it holds that

$$\begin{aligned} \mathrm{P}(\varepsilon, z)\, \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(A\,\mathrm{P})(\varepsilon, z) &= \Big(|\psi_0\rangle\langle\psi_0| \sum_{j=0}^{\infty} \langle\psi_i|\, A\, |\psi_0\rangle\langle\psi_0|\, |\psi_i\rangle\Big)(\varepsilon, z) \\ &= \Big(|\psi_0\rangle\langle\psi_0|\langle\psi_0|\, A\, |\psi_0\rangle\Big)(\varepsilon, z) \\ &= \Big(|\psi_0\rangle\langle\psi_0|\, A\, |\psi_0\rangle\langle\psi_0|\Big)(\varepsilon, z) \\ &= \mathrm{P}(\varepsilon, z)\, A(\varepsilon, z)\, \mathrm{P}(\varepsilon, z) \end{aligned} \tag{2.15}$$

The following statements about first and second order derivatives of symbols taking value in the rank-one projections will be used many times throughout this thesis. For any $i \in \{1, \dots, 2n\}$ we have

$$\partial_i \mathrm{P}(\varepsilon, z) = \partial_i(\mathrm{P}(\varepsilon, z)\, \mathrm{P}(\varepsilon, z)) = \mathrm{P}(\varepsilon, z)\, \partial_i \mathrm{P}(\varepsilon, z) + \partial_i \mathrm{P}(\varepsilon, z)\, \mathrm{P}(\varepsilon, z)\,.$$

Consequently, $\mathrm{P}(\varepsilon, z)\, \partial_i \mathrm{P}(\varepsilon, z)\, \mathrm{P}(\varepsilon, z) = \mathrm{P}^\perp(\varepsilon, z)\, \partial_i \mathrm{P}(\varepsilon, z)\, \mathrm{P}^\perp(\varepsilon, z) = 0$ where $\mathrm{P}^\perp(\varepsilon, z) := \mathbf{1}_{\mathcal{H}_\mathrm{f}} - \mathrm{P}(\varepsilon, z)$ is the orthogonal complement of $\mathrm{P}$. Therefore, first order derivatives of $\mathrm{P}$ are off-diagonal with rank less or equal to two. Moreover, a simple computation shows

$$\begin{aligned} \partial^2_{ij} \mathrm{P}(\varepsilon, z) =& \mathrm{P}(z)\, \partial^2_{ij} \mathrm{P}(\varepsilon, z)\, \mathrm{P}^\perp(\varepsilon, z) + \mathrm{P}^\perp(\varepsilon, z)\, \partial^2_{ij} \mathrm{P}(\varepsilon, z)\, \mathrm{P}(\varepsilon, z) \\ &- \mathrm{P}(\varepsilon, z)\, \left[\, \partial_i \mathrm{P}(\varepsilon, z)\, , \partial_j \mathrm{P}(\varepsilon, z)\,\right]_+\, \mathrm{P}(\varepsilon, z) \\ &+ \mathrm{P}^\perp(\varepsilon, z)\, \left[\, \partial_i \mathrm{P}(\varepsilon, z)\, , \partial_j \mathrm{P}(\varepsilon, z)\,\right]_+\, \mathrm{P}^\perp(\varepsilon, z) \end{aligned} \tag{2.16}$$

for every $i, j \in \{1, \dots, 2n\}$.

## 2.2 Density of Liouville Measures

We consider a symplectic form $\Omega = \sum_{i<j} \Omega_{ij}\, \mathrm{d}z_i \wedge \mathrm{d}z_j$ with skew-symmetric coefficient matrix $\Omega \in \mathbb{R}^{2n \times 2n}$. The symplectic form $\Omega$ defines a symplectic manifold $(\mathbb{R}^{2n}, \Omega)$ over $\mathbb{R}^{2n}$. The natural volume form $\lambda$ on the symplectic manifold $(\mathbb{R}^{2n}, \Omega)$, also known as Liouville measure is given by

$$\lambda := \frac{(-1)^{n(n-1)/2}}{n!}\, \Omega^{\wedge n} = \frac{(-1)^{n(n-1)/2}}{n!}\, \underbrace{\Omega \wedge \dots \wedge \Omega}_{n\text{-times}}\,.$$

The Liouville measure is of big importance in classical mechanics. By Liouville's theorem the Liouville measure $\lambda$ is invariant under the classical Hamiltonian flow $\Phi^t$ associated to a classical Hamiltonian system $(\mathbb{R}^{2n}, \Omega, h)$

with Hamiltonian $h : \mathbb{R}^{2n} \to \mathbb{R}$. Moreover, for a system of identical non-interacting particles in phase space $(\mathbb{R}^{2n}, \Omega)$ with one-particle Hamiltonian $h$ in a thermodynamic equilibrium state with density $\rho(h)$, the expectation value with respect an the observable $a : \mathbb{R}^{2n} \to \mathbb{R}$ is

$$\langle a \rangle_{\rho(h)} = \int_{\mathbb{R}^{2n}} a\, \rho(h)\, \lambda\,.$$

The Liouville measure $\lambda$ can be represented by using the so called Pfaffian $\mathrm{pf}(\Omega)$ which is defined by the equation

$$\tfrac{1}{n!}\, \Omega^{\wedge n} = \mathrm{pf}(\Omega)\, \mathrm{d}q_1 \wedge \cdots \mathrm{d}q_n \wedge \mathrm{d}p_1 \wedge \cdots \wedge \mathrm{d}p_n\,.$$

Clearly, we get

$$\lambda = (-1)^{n(n-1)/2}\, \mathrm{pf}(\Omega)\, \mathrm{d}q_1 \wedge \cdots \mathrm{d}q_n \wedge \mathrm{d}p_1 \wedge \cdots \wedge \mathrm{d}p_n\,.$$

In this section we will derive a trace formula for the density of a general Liouville measure with respect to the Lebesgue measure $\mathrm{d}q \wedge \mathrm{d}p = \mathrm{d}q^1 \wedge \cdots \wedge \mathrm{d}q^n \wedge \mathrm{d}p^1 \wedge \cdots \wedge \mathrm{d}p^n$, i.e. we derive the density $\nu : \mathbb{R}^{2n} \to \mathbb{R}$ satisfying

$$\lambda = \nu\, \mathrm{d}q \wedge \mathrm{d}p\,. \tag{2.17}$$

By $\nu = (-1)^{n(n-1)/2}\, \mathrm{pf}(\Omega)$, the trace formula for the Liouville density $\nu$ directly yields a trace formula for the Pfaffian $\mathrm{pf}(\Omega)$ for skew-symmetric matrices $\Omega$. The resulting density $\nu$ is of surprisingly simple form. Namely, a sum where each summand is given as product of terms of the form

$$\mathrm{Tr}_{2n}\Big((\omega^0\, \Omega)^l\Big)\,.$$

Here, $\omega^0 = \left(\begin{smallmatrix} 0 & \mathbf{1}_n \\ -\mathbf{1}_n & 0 \end{smallmatrix}\right)$ is the coefficient matrix of the canonical symplectic form.

Moreover, we will derive the Lebesgue density of the Liouville measure associated to the symplectic form $\omega^\varepsilon = \omega^0 + \varepsilon\, \Omega$ where $\varepsilon \in \mathbb{R}$, $\omega^0$ is the canonical symplectic form and $\Omega$ is an arbitrary symplectic form on $\mathbb{R}^{2n}$. What is remarkable is that it is straight forward to deduce the density of the Liouville measure for the general case from the case where we use the special form $\omega^\varepsilon$ as symplectic form. This is due to the fact that

$$\begin{aligned}\lambda^\varepsilon :=& \frac{(-1)^{n(n-1)/2}}{n!} \underbrace{\omega^\varepsilon \wedge \cdots \wedge \omega^\varepsilon}_{n\text{-times}} \\ =& \frac{(-1)^{n(n-1)/2}}{n!} \underbrace{(\omega^0 + \varepsilon\,\Omega) \wedge \cdots \wedge (\omega^0 + \varepsilon\,\Omega)}_{n\text{-times}} \\ =& \sum_{k=0}^{n} \varepsilon^k \lambda_k^\varepsilon\end{aligned}$$

with

$$\lambda_k^\varepsilon := \frac{(-1)^{n(n-1)/2}}{n!} \sum_{1\le l_1<\ldots<l_k\le n} \omega^0 \wedge \cdots \wedge \underset{\substack{|\\ l_1 th}}{\Omega} \wedge \cdots \wedge \underset{\substack{|\\ l_k th}}{\Omega} \wedge \cdots \wedge \omega^0 \,. \tag{2.18}$$

for $0 \le k \le n$. Then,

$$\lambda_n^\varepsilon := \frac{(-1)^{n(n-1)/2}}{n!} \underbrace{\Omega \wedge \cdots \wedge \Omega}_{n\text{-times}} \,. \tag{2.19}$$

Therefore our strategy is to derive the density of the Liouville measure for the special case $\omega^\varepsilon = \omega^0 + \varepsilon\,\Omega$ and then deduce the density for a general symplectic form $\Omega$ directly from this result.

Before we begin with the derivation of the trace formulae we give a brief motivation for the first two lemmata of this section. By the fact that $a \wedge b = b \wedge a$ for any two 2-forms $a, b$

$$\begin{aligned}&\sum_{1\le l_1<\ldots<l_k\le n} \omega^0 \wedge \cdots \wedge \underset{\substack{|\\ l_1 th}}{\Omega} \wedge \cdots \wedge \underset{\substack{|\\ l_k th}}{\Omega} \wedge \cdots \wedge \omega^0 \\ &= \binom{n}{k} \underbrace{\Omega \wedge \cdots \wedge \Omega}_{k\text{-times}} \wedge \underbrace{\omega^0 \wedge \cdots \wedge \omega^0}_{n-k\text{-times}} \,.\end{aligned} \tag{2.20}$$

By definition of $\omega^\varepsilon$

$$\omega^\varepsilon = \sum_{1\le i<j\le 2n} (\omega_{ij}^0 + \varepsilon\,\Omega_{ij})\,\mathrm{d}z^i \wedge \mathrm{d}z^j = \tfrac{1}{2} \sum_{i,j=1}^{2n} (\omega_{ij}^0 + \varepsilon\,\Omega_{ij})\,\mathrm{d}z^i \wedge \mathrm{d}z^j \,.$$

Hence,

$$\underbrace{\Omega \wedge \cdots \wedge \Omega}_{k\text{-times}} \wedge \underbrace{\omega^0 \wedge \cdots \wedge \omega^0}_{n-k\text{-times}}$$
$$= \left(\frac{1}{2}\right)^n \sum_{\substack{\alpha,\beta \in \{1,\ldots,2n\}^k \\ \gamma,\eta \in \{1,\ldots,2n\}^{n-k}}} \Omega_{\alpha_1\beta_1} \cdots \Omega_{\alpha_k\beta_k} \, \omega^0_{\gamma_1\eta_1} \cdots \omega^0_{\gamma_{n-k}\eta_{n-k}}$$
$$\mathrm{d}z^{\alpha_1} \wedge \mathrm{d}z^{\beta_1} \wedge \cdots \wedge \mathrm{d}z^{\alpha_n} \wedge \mathrm{d}z^{\beta_n} \wedge \mathrm{d}z^{\gamma_1} \wedge \mathrm{d}z^{\eta_1} \wedge \cdots \wedge \mathrm{d}z^{\gamma_{n-k}} \wedge \mathrm{d}z^{\eta_{n-k}} \,. \tag{2.21}$$

Combining (2.18)- (2.21)

$$\lambda_k^\varepsilon = \frac{(-1)^{n(n-1)/2}}{k!\,(n-k)!} \left(\frac{1}{2}\right)^n \sum_{\substack{\alpha,\beta \in \{1,\ldots,2n\}^k \\ \gamma,\eta \in \{1,\ldots,2n\}^{n-k}}} \Omega_{\alpha_1\beta_1} \cdots \Omega_{\alpha_k\beta_k} \, \omega^0_{\gamma_1\eta_1} \cdots \omega^0_{\gamma_{n-k}\eta_{n-k}}$$
$$\mathrm{d}z^{\alpha_1} \wedge \mathrm{d}z^{\beta_1} \wedge \cdots \wedge \mathrm{d}z^{\alpha_n} \wedge \mathrm{d}z^{\beta_n} \wedge \mathrm{d}z^{\gamma_1} \wedge \mathrm{d}z^{\eta_1} \wedge \cdots \wedge \mathrm{d}z^{\gamma_{n-k}} \wedge \mathrm{d}z^{\eta_{n-k}} \,. \tag{2.22}$$

Sorting the $\mathrm{d}z^{\alpha_i}$s, $\mathrm{d}z^{\beta_i}$s, $\mathrm{d}z^{\gamma_i}$s and $\mathrm{d}z^{\eta_i}$s in the above equation using the anti-commutativity of the wedge product (which only leads to variations of the sign in the summands) we get a function satisfying (2.17). But this sorting has to be done for each $\alpha, \beta, \gamma, \eta$ separately. So, at this point it is not clear how to do this sorting in a structured way that leads to a closed form for the density $\nu$. By definition of the symplectic form $\omega^0$

$$\omega^0_{ij} \neq 0 \Longleftrightarrow j = \lfloor i+n \rceil_{2n} \tag{2.23}$$

where the modulo function $\lfloor \cdot \rceil_l : \mathbb{Z} \to \{1, \ldots, l\}$, $l \in \mathbb{N}_0$ is given as follows: For $i \in \mathbb{Z}$ with unique decomposition $i = j + k\,l$, $j \in \{1, \ldots, l\}$ and $k \in \mathbb{Z}$ we define

$$\lfloor i \rceil_l := j \,. \tag{2.24}$$

It follows directly from (2.23) that

$$\sum_{j \in \{1,\ldots,2n\}} \omega^0_{ij} \, \mathrm{d}z^i \wedge \mathrm{d}z^j = \omega^0_{i\lfloor i+n \rceil_{2n}} \, \mathrm{d}z^i \wedge \mathrm{d}z^{\lfloor i+n \rceil_{2n}} \,.$$

From the above and the anti-commutativity of the wedge product we conclude that for non-vanishing terms in (2.22) the multi-indices $\alpha, \beta$ and $\gamma, \nu$ must stem from disjoint index sets. We obtain

$$\lambda_k^\varepsilon = \frac{(-1)^{n(n-1)/2}}{k!\,(n-k)!}\left(\frac{1}{2}\right)^k \sum_{\substack{I\subset\{1,\dots,n\},\\ |I|=k}} \left(\sum_{\alpha,\beta\in L^k} \Omega_{\alpha_1\beta_1}\cdots\Omega_{\alpha_k\beta_k}\,\mathrm{d}z^{\alpha_1}\wedge\mathrm{d}z^{\beta_1}\wedge\cdots\wedge\mathrm{d}z^{\alpha_k}\wedge\mathrm{d}z^{\beta_k}\right) \bigwedge\left(\sum_{\gamma,\nu\in L_c^{n-k}} \omega^0_{\gamma_1\nu_1}\cdots\omega^0_{\gamma_{n-k}\nu_{n-k}}\,\mathrm{d}z^{\gamma_1}\wedge\mathrm{d}z^{\nu_1}\wedge\cdots\wedge\mathrm{d}z^{\gamma_{n-k}}\wedge\mathrm{d}z^{\nu_{n-k}}\right)$$

where here and in the following we write $L := I\cup(I+n)$ and $L_c := I^c\cup(I^c+n)$ with $I^c = \{1,\dots,n\}\setminus I$ for every $I\subset\{1,\dots,n\}$, $|I| = k$ and $M+n := \{i+n|\, i\in M\}$ for every set $M\subset\{1,\dots,n\}$. Note here that by the simple structure of $\omega^0$ the second factor in the formula above is fairly simple to compute. So, the main issue is the first part that includes the symplectic form $\Omega$. We will do the sorting of the $\mathrm{d}z^{\alpha_i}$s and $\mathrm{d}z^{\beta_i}$s in

$$\sum_{\alpha,\beta\in L^k} \Omega_{\alpha_1\beta_1}\cdots\Omega_{\alpha_k\beta_k}\,\mathrm{d}z^{\alpha_1}\wedge\mathrm{d}z^{\beta_1}\wedge\cdots\wedge\mathrm{d}z^{\alpha_k}\wedge\mathrm{d}z^{\beta_k}$$

inductively where we prove the most important part of the induction step in a separate lemma.

To simplify the proofs we introduce to following map that will be of big importance throughout this section. For $k\in\mathbb{N}$, $m_1,\dots,m_{k-1}\in\{1,\dots,2n\}$ we define the linear map

$$\Lambda^k_{m_1,\dots,m_{k-1}} : \overbrace{\mathbb{R}^{2n\times 2n}\times\cdots\times\mathbb{R}^{2n\times 2n}}^{k\text{-times}} \mapsto \mathbb{R}^{2n\times 2n}$$

recursively by

$$\begin{aligned} \Lambda^1_{i,j}(B^1) &:= B^1_{i\,j}\,, \\ \Lambda^2_{m_1;i,j}(B^1,B^2) &:= B^2_{i\,m_1}\,\omega^0_{m_1\,\lfloor m_1+n\rfloor_{2n}}\,B^1_{\lfloor m_1+n\rfloor_{2n}\,j} \\ &\quad + B^1_{i\,\lfloor m_1+n\rfloor_{2n}}\,\omega^0_{\lfloor m_1+n\rfloor_{2n}\,m_1}\,B^2_{m_1\,j} \end{aligned} \tag{2.25}$$

and

$$\Lambda^k_{m_1,\dots,m_{k-1};i,j}(B^1,\dots,B^k)$$
$$:= \sum_{l=1}^{k-1} \Lambda^{k-1}_{m_1,\dots,m_{k-2};i,j}(B^1,\dots,\Lambda^2_{m_{k-1}}(B^l,B^k),\dots,B^{k-1}) \qquad \text{for } k>2\,. \tag{2.26}$$

Note here that $\Lambda^k_{m_1,\dots,m_{k-1};i,j}(B^1,\dots,B^k)$ defines an skew-symmetric matrix for every $k\in\mathbb{N}$, $m_1,\dots,m_k\in\{1,\dots,2n\}$ and arbitrary skew-symmetric matrices $B^1,\dots,B^k\in\mathbb{R}^{2n\times 2n}$, for a proof see Lemma A.1.

**Lemma 2.2** *Let $k\in\mathbb{N}$, $I\subset\{1,\dots,n\}$, $|I|=k$, $L=I\cup(I+n)$ and $B^j\in\mathbb{R}^{2n\times 2n}$ for $j=1,\dots,k$ be skew-symmetric matrices. Then,*

$$\begin{aligned}
&\sum_{\alpha,\beta\in L^k} B^1_{\alpha_1\,\beta_1}\cdots B^k_{\alpha_k\,\beta_k}\,\mathrm{d}z^{\alpha_1}\wedge\mathrm{d}z^{\beta_1}\wedge\cdots\wedge\mathrm{d}z^{\alpha_k}\wedge\mathrm{d}z^{\beta_k}\\
&\quad=\sum_{m\in L}\quad\sum_{\alpha,\beta\in L^{k-1}_{\lfloor m\rfloor_n}}\\
&\qquad\Big(-B^1_{\alpha_1\,\beta_1}\cdots B^{k-1}_{\alpha_{k-1}\,\beta_{k-1}}\operatorname{Tr}_{\{m\}}(\omega^0\,\Lambda^1(B^k))\\
&\qquad\quad+\sum_{l=1}^{k-1}B^1_{\alpha_1\,\beta_1}\cdots B^{l-1}_{\alpha_{l-1}\,\beta_{l-1}}\,\Lambda^2_{m;\alpha_l,\beta_l}(B^l,B^k)\\
&\qquad\quad B^{l+1}_{\alpha_{l+1}\beta_{l+1}}\cdots B^{k-1}_{\alpha_{k-1}\,\beta_{k-1}}\Big)\\
&\qquad\mathrm{d}z^{\alpha_1}\wedge\mathrm{d}z^{\beta_1}\wedge\cdots\wedge\mathrm{d}z^{\alpha_{k-1}}\wedge\mathrm{d}z^{\beta_{k-1}}\wedge\mathrm{d}q^{\lfloor m\rfloor_n}\wedge\mathrm{d}p^{\lfloor m\rfloor_n}
\end{aligned} \tag{2.27}$$

*where $\Lambda^1$ and $\Lambda^2$ are defined by (2.25) and*

$$L_{\lfloor m\rfloor_n} := (I\setminus\{\lfloor m\rfloor_n\})\cup((I\setminus\{\lfloor m\rfloor_n\})+n)\,.$$

*with $\lfloor m\rfloor_n$ given by (2.24). The partial trace $\operatorname{Tr}_M(R)$ of a matrix $R\in\mathbb{R}^{2n\times 2n}$ with respect to a set $M\subset\{1,\dots,2n\}$ is given by*

$$\operatorname{Tr}_M(R) := \sum_{m\in M} R_{m\,m}\,.$$

Proof  Let $k\in\mathbb{N}$, $I\subset\{1,\dots,n\}$, $|I|=k$, $L=I\cup(I+n)$ and $B^j\in\mathbb{R}^{2n\times 2n}$ for $j=1,\dots,k$ be skew-symmetric matrices. The anti-commutativity of the wedge product implies for $\alpha,\beta\in L^k$ that

$$\mathrm{d}z^{\alpha_1}\wedge\mathrm{d}z^{\beta_1}\wedge\cdots\wedge\mathrm{d}z^{\alpha_k}\wedge\mathrm{d}z^{\beta_k}\neq 0 \iff \bigcup_{i=1}^{k}\{\alpha_i,\beta_i\}=L\,.$$

Hence, by separating the sum over $\beta_k$ from the rest the sum

$$\sum_{\alpha,\beta\in L^k} B^1_{\alpha_1\,\beta_1}\ \cdots\ B^k_{\alpha_k\,\beta_k}\,\mathrm{d}z^{\alpha_1}\wedge\mathrm{d}z^{\beta_1}\wedge\cdots\wedge\mathrm{d}z^{\alpha_k}\wedge\mathrm{d}z^{\beta_k}$$

splits into six parts. We get

$$\sum_{\alpha,\beta\in L^k} B^1_{\alpha_1\,\beta_1}\ \cdots\ B^k_{\alpha_k\,\beta_k}\,\mathrm{d}z^{\alpha_1}\wedge\mathrm{d}z^{\beta_1}\wedge\cdots\wedge\mathrm{d}z^{\alpha_k}\wedge\mathrm{d}z^{\beta_k}$$
$$=(I)+(II)+(III)+(IV)+(V)+(VI)$$

where

$$(I)=\sum_{m\in I+n}\ \sum_{\alpha,\beta\in L^{k-1}_{\lfloor m\rfloor n}} B^1_{\alpha_1\,\beta_1}\ \cdots\ B^{k-1}_{\alpha_{k-1}\,\beta_{k-1}}\ B^k_{(m-n)\,m}$$
$$\mathrm{d}z^{\alpha_1}\wedge\mathrm{d}z^{\beta_1}\wedge\cdots\wedge\mathrm{d}z^{\alpha_{k-1}}\wedge\mathrm{d}z^{\beta_{k-1}}\wedge\mathrm{d}z^{m-n}\wedge\mathrm{d}z^{m}\,,$$

$$(II)=\sum_{m\in I}\ \sum_{\alpha,\beta\in L^{k-1}_{\lfloor m\rfloor n}} B^1_{\alpha_1\,\beta_1}\ \cdots\ B^{k-1}_{\alpha_{k-1}\,\beta_{k-1}}\ B^k_{(m+n)\,m}$$
$$\mathrm{d}z^{\alpha_1}\wedge\mathrm{d}z^{\beta_1}\wedge\cdots\wedge\mathrm{d}z^{\alpha_{k-1}}\wedge\mathrm{d}z^{\beta_{k-1}}\wedge\mathrm{d}z^{m+n}\wedge\mathrm{d}z^{m}\,,$$

$$(III)=\sum_{m\in I+n}\ \sum_{l=1}^{k-1}\ \sum_{\alpha,\beta\in L^{k-1}_{\lfloor m\rfloor n}} B^1_{\alpha_1\,\beta_1}\ \cdots\ B^l_{(m-n)\,\beta_l}\ \cdots\ B^k_{\alpha_l\,m}$$
$$\mathrm{d}z^{\alpha_1}\wedge\mathrm{d}z^{\beta_1}\wedge\cdots\wedge\mathrm{d}z^{m-n}\wedge\mathrm{d}z^{\beta_l}\wedge\cdots\wedge\mathrm{d}z^{\beta_{k-1}}\wedge\mathrm{d}z^{\alpha_l}\wedge\mathrm{d}z^{m}\,,$$

$$(IV)=\sum_{m\in I}\ \sum_{l=1}^{k-1}\ \sum_{\alpha,\beta\in L^{k-1}_{\lfloor m\rfloor n}} B^1_{\alpha_1\,\beta_1}\ \cdots\ B^l_{(m+n)\,\beta_l}\ \cdots\ B^k_{\alpha_l\,m}$$
$$\mathrm{d}z^{\alpha_1}\wedge\mathrm{d}z^{\beta_1}\wedge\cdots\wedge\mathrm{d}z^{m+n}\wedge\mathrm{d}z^{\beta_l}\wedge\cdots\wedge\mathrm{d}z^{\beta_{k-1}}\wedge\mathrm{d}z^{\alpha_l}\wedge\mathrm{d}z^{m}\,,$$

$$(V)=\sum_{m\in I+n}\ \sum_{l=1}^{k-1}\ \sum_{\alpha,\beta\in L^{k-1}_{\lfloor m\rfloor n}} B^1_{\alpha_1\,\beta_1}\ \cdots\ B^l_{\alpha_l\,(m-n)}\ \cdots\ B^k_{\beta_l\,m}$$
$$\mathrm{d}z^{\alpha_1}\wedge\mathrm{d}z^{\beta_1}\wedge\cdots\wedge\mathrm{d}z^{\alpha_l}\wedge\mathrm{d}z^{m-n}\wedge\cdots\wedge\mathrm{d}z^{\beta_l}\wedge\mathrm{d}z^{m}\,,$$

and

$$(VI) = \sum_{m\in I} \sum_{l=1}^{k-1} \sum_{\alpha,\beta \in L^{k-1}_{\lfloor m \rfloor_n}} B^1_{\alpha_1\,\beta_1} \,\cdots\, B^l_{\alpha_l\,(m+n)} \cdots B^k_{\beta_l\, m} \\ \mathrm{d}z^{\alpha_1} \wedge \mathrm{d}z^{\beta_1} \wedge \cdots \wedge \mathrm{d}z^{\alpha_l} \wedge \mathrm{d}z^{m+n} \wedge \cdots \wedge \mathrm{d}z^{\beta_l} \wedge \mathrm{d}z^m \,.$$

Next we analyze each of the six parts. For $(I)$ assume $m > n$ and $\alpha, \beta \in L^{k-1}_{\lfloor m \rfloor_n}$ then,

$$\begin{aligned} & B^1_{\alpha_1\,\beta_1} \,\cdots\, B^{k-1}_{\alpha_{k-1}\,\beta_{k-1}} B^k_{(m-n)\,m} \\ & \quad \mathrm{d}z^{\alpha_1} \wedge \mathrm{d}z^{\beta_1} \wedge \cdots \wedge \mathrm{d}z^{\alpha_{k-1}} \wedge \mathrm{d}z^{\beta_{k-1}} \wedge \mathrm{d}z^{m-n} \wedge \mathrm{d}z^m \\ & \qquad = B^1_{\alpha_1\,\beta_1} \,\cdots\, B^{k-1}_{\alpha_{k-1}\,\beta_{k-1}} B^k_{(m-n)\,m} \\ & \qquad \quad \mathrm{d}z^{\alpha_1} \wedge \mathrm{d}z^{\beta_1} \wedge \cdots \wedge \mathrm{d}z^{\alpha_{k-1}} \wedge \mathrm{d}z^{\beta_{k-1}} \wedge \mathrm{d}q^{m-n} \wedge \mathrm{d}p^{m-n} \\ & \qquad = -B^1_{\alpha_1\,\beta_1} \,\cdots\, B^{k-1}_{\alpha_{k-1}\,\beta_{k-1}} \omega^0_{m\,\lfloor m+n \rfloor_{2n}} B^k_{\lfloor m+n \rfloor_{2n}\,m} \\ & \qquad \quad \mathrm{d}z^{\alpha_1} \wedge \mathrm{d}z^{\beta_1} \wedge \cdots \wedge \mathrm{d}z^{\alpha_{k-1}} \wedge \mathrm{d}z^{\beta_{k-1}} \wedge \mathrm{d}q^{\lfloor m \rfloor_n} \wedge \mathrm{d}p^{\lfloor m \rfloor_n} \\ & \qquad = -B^1_{\alpha_1\,\beta_1} \,\cdots\, B^{k-1}_{\alpha_{k-1}\,\beta_{k-1}} \mathrm{Tr}_{\{m\}}(\omega^0\, B^k) \\ & \qquad \quad \mathrm{d}z^{\alpha_1} \wedge \mathrm{d}z^{\beta_1} \wedge \cdots \wedge \mathrm{d}z^{\alpha_{k-1}} \wedge \mathrm{d}z^{\beta_{k-1}} \wedge \mathrm{d}q^{\lfloor m \rfloor_n} \wedge \mathrm{d}p^{\lfloor m \rfloor_n} \end{aligned} \tag{2.28}$$

where in the second equality we used that

$$\omega^0_{ij} = \begin{cases} 1 & \text{for } i \le n,\ j = i+n \\ -1 & \text{for } i > n,\ j = i+n \\ 0 & \text{otherwise} \end{cases} . \tag{2.29}$$

Regarding $(II)$ let $m \le n$ and $\alpha, \beta \in L^{k-1}_{\lfloor m \rfloor_n}$ then,

$$\begin{aligned} & B^1_{\alpha_1\,\beta_1} \,\cdots\, B^{k-1}_{\alpha_{k-1}\,\beta_{k-1}} B^k_{(m+n)\,m} \\ & \quad \mathrm{d}z^{\alpha_1} \wedge \mathrm{d}z^{\beta_1} \wedge \cdots \wedge \mathrm{d}z^{\alpha_{k-1}} \wedge \mathrm{d}z^{\beta_{k-1}} \wedge \mathrm{d}z^{m+n} \wedge \mathrm{d}z^m \\ & \qquad = B^1_{\alpha_1\,\beta_1} \,\cdots\, B^{k-1}_{\alpha_{k-1}\,\beta_{k-1}} B^k_{(m+n)\,m} \\ & \qquad \quad \mathrm{d}z^{\alpha_1} \wedge \mathrm{d}z^{\beta_1} \wedge \cdots \wedge \mathrm{d}z^{\alpha_{k-1}} \wedge \mathrm{d}z^{\beta_{k-1}} \wedge \mathrm{d}p^{m} \wedge \mathrm{d}q^{m} \\ & \qquad = -B^1_{\alpha_1\,\beta_1} \,\cdots\, B^{k-1}_{\alpha_{k-1}\,\beta_{k-1}} B^k_{(m+n)\,m} \\ & \qquad \quad \mathrm{d}z^{\alpha_1} \wedge \mathrm{d}z^{\beta_1} \wedge \cdots \wedge \mathrm{d}z^{\alpha_{k-1}} \wedge \mathrm{d}z^{\beta_{k-1}} \wedge \mathrm{d}q^{\lfloor m \rfloor_n} \wedge \mathrm{d}p^{\lfloor m \rfloor_n} \\ & \qquad = -B^1_{\alpha_1\,\beta_1} \,\cdots\, B^{k-1}_{\alpha_{k-1}\,\beta_{k-1}} \omega^0_{m\,(m+n)} B^k_{(m+n),m} \\ & \qquad \quad \mathrm{d}z^{\alpha_1} \wedge \mathrm{d}z^{\beta_1} \wedge \cdots \wedge \mathrm{d}z^{\alpha_{k-1}} \wedge \mathrm{d}z^{\beta_{k-1}} \wedge \mathrm{d}q^{\lfloor m \rfloor_n} \wedge \mathrm{d}p^{\lfloor m \rfloor_n} \\ & \qquad = -B^1_{\alpha_1\,\beta_1} \,\cdots\, B^{k-1}_{\alpha_{k-1}\,\beta_{k-1}} \mathrm{Tr}_{\{m\}}(\omega^0\, B^k) \\ & \qquad \quad \mathrm{d}z^{\alpha_1} \wedge \mathrm{d}z^{\beta_1} \wedge \cdots \wedge \mathrm{d}z^{\alpha_{k-1}} \wedge \mathrm{d}z^{\beta_{k-1}} \wedge \mathrm{d}q^{\lfloor m \rfloor_n} \wedge \mathrm{d}p^{\lfloor m \rfloor_n} \end{aligned} \tag{2.30}$$

where in the second equality we used the anti-commutativity of the wedge product. By (2.28) and (2.30) we obtain

$$
\begin{aligned}
(I) + (II) = -\sum_{m \in L} \sum_{\alpha,\beta \in L^{k-1}_{\lfloor m \rfloor_n}} & B^1_{\alpha_1\,\beta_1} \cdots B^{k-1}_{\alpha_{k-1}\,\beta_{k-1}} \operatorname{Tr}_{\{m\}}(\omega^0\, B^k) \\
& \mathrm{d}z^{\alpha_1} \wedge \mathrm{d}z^{\beta_1} \wedge \cdots \wedge \mathrm{d}z^{\alpha_{k-1}} \wedge \mathrm{d}z^{\beta_{k-1}} \wedge \mathrm{d}q^{\lfloor m \rfloor_n} \wedge \mathrm{d}p^{\lfloor m \rfloor_n}
\end{aligned}
\tag{2.31}
$$

For (III), let $m \in I + n$, $l \in \{1, \ldots, k-1\}$ and $\alpha, \beta \in L^{k-1}_{\lfloor m \rfloor_n}$. Then,

$$
\begin{aligned}
& B^1_{\alpha_1\,\beta_1} \cdots B^l_{(m-n)\,\beta_l} \cdots B^k_{\alpha_l\,m} \\
& \qquad \mathrm{d}z^{\alpha_1} \wedge \mathrm{d}z^{\beta_1} \wedge \cdots \wedge \mathrm{d}z^{m-n} \wedge \mathrm{d}z^{\beta_l} \wedge \cdots \wedge \mathrm{d}z^{\alpha_l} \wedge \mathrm{d}z^{m} \\
& \qquad = B^1_{\alpha_1\,\beta_1} \cdots B^l_{(m-n)\,\beta_l} \cdots B^k_{\alpha_l\,m} \\
& \qquad\quad \mathrm{d}z^{\alpha_1} \wedge \mathrm{d}z^{\beta_1} \wedge \cdots \wedge \mathrm{d}q^{\lfloor m \rfloor_n} \wedge \mathrm{d}z^{\beta_l} \wedge \cdots \wedge \mathrm{d}z^{\alpha_l} \wedge \mathrm{d}p^{\lfloor m \rfloor_n}\,.
\end{aligned}
\tag{2.32}
$$

By the anti-commutativity of the wedge product it holds that

$$
\begin{aligned}
& \mathrm{d}z^1 \wedge \mathrm{d}z^2 \wedge \cdots \wedge \mathrm{d}z^i \wedge \cdots \wedge \mathrm{d}z^j \wedge \cdots \wedge \mathrm{d}z^k \\
& \qquad = -\,\mathrm{d}z^1 \wedge \mathrm{d}z^2 \wedge \cdots \wedge \mathrm{d}z^j \wedge \cdots \wedge \mathrm{d}z^i \wedge \cdots \wedge \mathrm{d}z^k
\end{aligned}
$$

for any $1 \leq i < j \leq k$. This implies

$$
\begin{aligned}
& B^1_{\alpha_1\,\beta_1} \cdots B^l_{(m-n)\,\beta_l} \cdots B^k_{\alpha_l\,m} \\
& \qquad \mathrm{d}z^{\alpha_1} \wedge \mathrm{d}z^{\beta_1} \wedge \cdots \wedge \mathrm{d}q^{\lfloor m \rfloor_n} \wedge \mathrm{d}z^{\beta_l} \wedge \cdots \wedge \mathrm{d}z^{\alpha_l} \wedge \mathrm{d}p^{\lfloor m \rfloor_n} \\
& \qquad = -B^1_{\alpha_1\,\beta_1} \cdots B^{l-1}_{\alpha_{l-1}\,\beta_{l-1}} B^k_{\alpha_l\,m} B^l_{(m-n)\,\beta_l} B^{l+1}_{\alpha_{l+1}\,\beta_{l+1}} \cdots B^{k-1}_{\alpha_{k-1}\,\beta_{k-1}} \\
& \qquad\quad z^{\alpha_1} \wedge \mathrm{d}z^{\beta_1} \wedge \cdots \wedge \mathrm{d}z^{\alpha_l} \wedge \mathrm{d}z^{\beta_l} \wedge \cdots \wedge \mathrm{d}z^{\beta_{k-1}} \wedge \mathrm{d}q^{\lfloor m \rfloor_n} \wedge \mathrm{d}p^{\lfloor m \rfloor_n}\,.
\end{aligned}
\tag{2.33}
$$

By definition of $\omega^0$ (2.29)

$$
\begin{aligned}
& -B^1_{\alpha_1\,\beta_1} \cdots B^{l-1}_{\alpha_{l-1}\,\beta_{l-1}} B^k_{\alpha_l\,m} B^l_{(m-n)\,\beta_l} B^{l+1}_{\alpha_{l+1}\,\beta_{l+1}} \cdots B^{k-1}_{\alpha_{k-1}\,\beta_{k-1}} \\
& \quad z^{\alpha_1} \wedge \mathrm{d}z^{\beta_1} \wedge \cdots \wedge \mathrm{d}z^{\alpha_l} \wedge \mathrm{d}z^{\beta_l} \wedge \cdots \wedge \mathrm{d}z^{\beta_{k-1}} \wedge \mathrm{d}q^{\lfloor m \rfloor_n} \wedge \mathrm{d}p^{\lfloor m \rfloor_n} \\
& \quad = B^1_{\alpha_1\,\beta_1} \cdots B^{l-1}_{\alpha_{l-1}\,\beta_{l-1}} B^k_{\alpha_l\,m}\, \omega^0_{m\,(m-n)}\, B^l_{(m-n)\,\beta_l} B^{l+1}_{\alpha_{l+1}\,\beta_{l+1}} \cdots B^{k-1}_{\alpha_{k-1}\,\beta_{k-1}} \\
& \qquad z^{\alpha_1} \wedge \mathrm{d}z^{\beta_1} \wedge \cdots \wedge \mathrm{d}z^{\alpha_l} \wedge \mathrm{d}z^{\beta_l} \wedge \cdots \wedge \mathrm{d}z^{\beta_{k-1}} \wedge \mathrm{d}q^{\lfloor m \rfloor_n} \wedge \mathrm{d}p^{\lfloor m \rfloor_n} \\
& \quad = B^1_{\alpha_1\,\beta_1} \cdots B^{l-1}_{\alpha_{l-1}\,\beta_{l-1}} B^k_{\alpha_l\,m}\, \omega^0_{m\,\lfloor m+n \rfloor_{2n}}\, B^l_{\lfloor m+n \rfloor_{2n}\,\beta_l} B^{l+1}_{\alpha_{l+1}\,\beta_{l+1}} \cdots B^{k-1}_{\alpha_{k-1}\,\beta_{k-1}} \\
& \qquad z^{\alpha_1} \wedge \mathrm{d}z^{\beta_1} \wedge \cdots \wedge \mathrm{d}z^{\alpha_l} \wedge \mathrm{d}z^{\beta_l} \wedge \cdots \wedge \mathrm{d}z^{\beta_{k-1}} \wedge \mathrm{d}q^{\lfloor m \rfloor_n} \wedge \mathrm{d}p^{\lfloor m \rfloor_n}\,.
\end{aligned}
\tag{2.34}
$$

Combining (2.32)- (2.34) yields

$$(III) = \sum_{m\in I+n} \sum_{l=1}^{k-1} \sum_{\alpha,\beta\in L^{k-1}_{\lfloor m\rfloor_n}} B^1_{\alpha_1\,\beta_1}\cdots B^{l-1}_{\alpha_{l-1}\,\beta_{l-1}}\, B^k_{\alpha_l\,m}\,\omega^0_{m\,\lfloor m+n\rfloor_{2n}}\, B^l_{\lfloor m+n\rfloor_{2n}\,\beta_l}\, B^{l+1}_{\alpha_{l+1}\,\beta_{l+1}}\cdots B^{k-1}_{\alpha_{k-1}\,\beta_{k-1}} z^{\alpha_1}\wedge \mathrm{d}z^{\beta_1}\wedge\cdots\wedge \mathrm{d}z^{\alpha_l}\wedge \mathrm{d}z^{\beta_l}\wedge\cdots\wedge \mathrm{d}z^{\beta_{k-1}}\wedge \mathrm{d}q^{\lfloor m\rfloor_n}\wedge \mathrm{d}p^{\lfloor m\rfloor_n}\,. \tag{2.35}$$

With similar arguments as for (2.35) we get

$$(IV) = \sum_{m\in I} \sum_{l=1}^{k-1} \sum_{\alpha,\beta\in L^{k-1}_{\lfloor m\rfloor_n}} B^1_{\alpha_1\,\beta_1}\cdots B^{l-1}_{\alpha_{l-1}\,\beta_{l-1}}\, B^k_{\alpha_l\,m}\,\omega^0_{m\,\lfloor m+n\rfloor_{2n}}\, B^l_{\lfloor m+n\rfloor_{2n}\,\beta_l}\, B^{l+1}_{\alpha_{l+1}\,\beta_{l+1}}\cdots B^{k-1}_{\alpha_{k-1}\,\beta_{k-1}} z^{\alpha_1}\wedge \mathrm{d}z^{\beta_1}\wedge\cdots\wedge \mathrm{d}z^{\alpha_l}\wedge \mathrm{d}z^{\beta_l}\wedge\cdots\wedge \mathrm{d}q^{\lfloor m\rfloor_n}\wedge \mathrm{d}p^{\lfloor m\rfloor_n}\,. \tag{2.36}$$

Then, adding (2.35) and (2.36)

$$(III)+(IV) = \sum_{m\in L} \sum_{l=1}^{k-1} \sum_{\alpha,\beta\in L^{k-1}_{\lfloor m\rfloor_n}} B^1_{\alpha_1\,\beta_1}\cdots B^{l-1}_{\alpha_{l-1}\,\beta_{l-1}}\, B^k_{\alpha_l\,m}\,\omega^0_{m\,\lfloor m+n\rfloor_{2n}}\, B^l_{\lfloor m+n\rfloor_{2n}\,\beta_l}\, B^{l+1}_{\alpha_{l+1}\,\beta_{l+1}}\cdots B^{k-1}_{\alpha_{k-1}\,\beta_{k-1}} z^{\alpha_1}\wedge \mathrm{d}z^{\beta_1}\wedge\cdots\wedge \mathrm{d}z^{\alpha_l}\wedge \mathrm{d}z^{\beta_l}\wedge\cdots\wedge \mathrm{d}q^{\lfloor m\rfloor_n}\wedge \mathrm{d}p^{\lfloor m\rfloor_n}\,. \tag{2.37}$$

For $(V)$, assume $m\in I+n$, $l\in\{1,\ldots,k-1\}$ and $\alpha,\beta\in L^{k-1}_{\lfloor m\rfloor_n}$. Then, similar to (2.33) we get

$$\begin{aligned} &B^1_{\alpha_1\,\beta_1}\cdots B^l_{\alpha_l\,(m-n)}\cdots B^k_{\beta_l\,m}\, \mathrm{d}z^{\alpha_1}\wedge \mathrm{d}z^{\beta_1}\wedge\cdots\wedge \mathrm{d}z^{\alpha_l}\wedge \mathrm{d}z^{m-n}\wedge\cdots\wedge \mathrm{d}z^{\beta_l}\wedge \mathrm{d}z^m \\ &= -B^1_{\alpha_1\,\beta_1}\cdots B^{l-1}_{\alpha_{l-1}\,\beta_{l-1}}\, B^l_{\alpha_l\,(m-n)}\, B^k_{\beta_l\,m}\, B^{l+1}_{\alpha_{l+1}\,\beta_{l+1}}\cdots B^{k-1}_{\alpha_{k-1}\,\beta_{k-1}}\, \mathrm{d}z^{\alpha_1}\wedge \mathrm{d}z^{\beta_1}\wedge\cdots\wedge \mathrm{d}z^{\alpha_l}\wedge \mathrm{d}z^{\beta_l}\wedge\cdots\wedge \mathrm{d}q^{\lfloor m\rfloor_n}\wedge \mathrm{d}p^{\lfloor m\rfloor_n}\,. \end{aligned} \tag{2.38}$$

By the skew-symmetry of $B^k$ and the definition of $\omega^0$ (2.29) we obtain

$$\begin{aligned}
&- B^1_{\alpha_1\,\beta_1} \cdots B^{l-1}_{\alpha_{l-1}\,\beta_{l-1}} \, B^l_{\alpha_l\,(m-n)} \, B^k_{\beta_l\,m} \, B^{l+1}_{\alpha_{l+1}\,\beta_{l+1}} \cdots B^{k-1}_{\alpha_{k-1}\,\beta_{k-1}} \\
&\quad \mathrm{d}z^{\alpha_1} \wedge \mathrm{d}z^{\beta_1} \wedge \cdots \wedge \mathrm{d}z^{\alpha_l} \wedge \mathrm{d}z^{\beta_l} \wedge \cdots \wedge \mathrm{d}q^{\lfloor m \rfloor_n} \wedge \mathrm{d}p^{\lfloor m \rfloor_n} \\
&\quad = B^1_{\alpha_1\,\beta_1} \cdots B^{l-1}_{\alpha_{l-1}\,\beta_{l-1}} \, B^l_{\alpha_l\,\lfloor m+n \rfloor_{2n}} \, \omega^0_{\lfloor m+n \rfloor_{2n}\,m} \, B^k_{m\,\beta_l} \, B^{l+1}_{\alpha_{l+1}\,\beta_{l+1}} \cdots B^{k-1}_{\alpha_{k-1}\,\beta_{k-1}} \\
&\quad\quad \mathrm{d}z^{\alpha_1} \wedge \mathrm{d}z^{\beta_1} \wedge \cdots \wedge \mathrm{d}z^{\alpha_l} \wedge \mathrm{d}z^{\beta_l} \wedge \cdots \wedge \mathrm{d}q^{\lfloor m \rfloor_n} \wedge \mathrm{d}p^{\lfloor m \rfloor_n} \,.
\end{aligned} \tag{2.39}$$

Combining (2.38) and (2.39) we get

$$\begin{aligned}
(V) = &\sum_{m \in I+n} \sum_{l=1}^{k-1} \sum_{\alpha,\beta \in L^{k-1}_{\lfloor m \rfloor_n}} \\
&B^1_{\alpha_1\,\beta_1} \cdots B^{l-1}_{\alpha_{l-1}\,\beta_{l-1}} \, B^l_{\alpha_l\,\lfloor m+n \rfloor_{2n}} \, \omega^0_{\lfloor m+n \rfloor_{2n}\,m} \, B^k_{m\,\beta_l} \, B^{l+1}_{\alpha_{l+1}\,\beta_{l+1}} \cdots B^{k-1}_{\alpha_{k-1}\,\beta_{k-1}} \\
&\mathrm{d}z^{\alpha_1} \wedge \mathrm{d}z^{\beta_1} \wedge \cdots \wedge \mathrm{d}z^{\alpha_l} \wedge \mathrm{d}z^{\beta_l} \wedge \cdots \wedge \mathrm{d}q^{\lfloor m \rfloor_n} \wedge \mathrm{d}p^{\lfloor m \rfloor_n} \,.
\end{aligned} \tag{2.40}$$

Similar to (2.40) we get for $(VI)$ that

$$\begin{aligned}
(VI) = &\sum_{m \in I} \sum_{l=1}^{k-1} \sum_{\alpha,\beta \in L^{k-1}_{\lfloor m \rfloor_n}} \\
&B^1_{\alpha_1\,\beta_1} \cdots B^{l-1}_{\alpha_{l-1}\,\beta_{l-1}} \, B^l_{\alpha_l\,\lfloor m+n \rfloor_{2n}} \, \omega^0_{\lfloor m+n \rfloor_{2n}\,m} \, B^k_{m\,\beta_l} \, B^{l+1}_{\alpha_{l+1}\,\beta_{l+1}} \cdots B^{k-1}_{\alpha_{k-1}\,\beta_{k-1}} \\
&\mathrm{d}z^{\alpha_1} \wedge \mathrm{d}z^{\beta_1} \wedge \cdots \wedge \mathrm{d}z^{\alpha_l} \wedge \mathrm{d}z^{\beta_l} \wedge \cdots \wedge \mathrm{d}q^{\lfloor m \rfloor_n} \wedge \mathrm{d}p^{\lfloor m \rfloor_n} \,.
\end{aligned} \tag{2.41}$$

Adding (2.31), (2.37), (2.40) and (2.41) and applying the definitions of $\Lambda^1$ and $\Lambda^2$ shows (2.27), finishing the proof. □

**Lemma 2.3** *Let $k \in \mathbb{N}$, $B^j \in \mathbb{R}^{2n \times 2n}$ for $j = 1, \ldots, k$ be skew-symmetric matrices and $I \subset \{1, \ldots, n\}$, $|I| = k$, $L = I \cup (I+n)$ then*

$$\begin{aligned}
&\sum_{\alpha,\beta \in L^k} B^1_{\alpha_1\,\beta_1} \cdots B^k_{\alpha_k\,\beta_k} \, \mathrm{d}z^{\alpha_1} \wedge \mathrm{d}z^{\beta_1} \wedge \cdots \wedge \mathrm{d}z^{\alpha_k} \wedge \mathrm{d}z^{\beta_k} \\
&\quad = \sum_{p \in P(k)} (-1)^{|p|} \sum_{\substack{m \in L^k \\ \lfloor m_i \rfloor_n \neq \lfloor m_j \rfloor_n, \\ 1 \leq i < j \leq k}} \\
&\quad\quad \prod_{j \in \{1,\ldots,|p|\}} \mathrm{Tr}_{\{m_{(p_j)_{|p_j|}}\}} \Big( \omega^0 \, \Lambda^{|p_j|}_{m_{(p_j)_1},\ldots,m_{(p_j)_{(|p_j|-1)}}} \big( B^{(p_j)_1}, \ldots, B^{(p_j)_{|p_j|}} \big) \Big) \\
&\quad\quad \mathrm{d}q^{\lfloor m_1 \rfloor_n} \wedge \mathrm{d}p^{\lfloor m_1 \rfloor_n} \wedge \cdots \wedge \mathrm{d}q^{\lfloor m_k \rfloor_n} \wedge \mathrm{d}p^{\lfloor m_k \rfloor_n}
\end{aligned} \tag{2.42}$$

*where $P(k)$ denotes the set of all partitions of $\{1,\ldots,k\}$ and for $p \in P(k)$ we write $\{p_1,\ldots,p_{|p|}\} = p$ with $p_i = ((p_i)_1,\ldots,(p_i)_{|p_i|})$ for every $1 \le i \le |p|$ and $(p_i)_1 < (p_i)_2 < \ldots < (p_i)_{|p_i|}$. The linear maps $\Lambda^l_{m_1,\ldots,m_l}$ are defined by (2.26).*

REMARK 2.4 At this point we did not proof any symmetry in the arguments $m_j$ and $B_j$ of $\Lambda$. Hence, sorting the $(p_i)_j$s is important to make the above formula well-defined. In what follows we will always imply such a sorting in the arguments of $\Lambda$ as long as not noted differently. Later in this section we will see that

$$\begin{aligned}&\mathrm{Tr}_{\{m_{j_l}\}}\Big(\omega^0\,\Lambda^l_{m_{j_1},\ldots,m_{j_{l-1}}}(B^{j_1},\ldots,B^{j_l})\Big)\\&\quad+\mathrm{Tr}_{\{\lfloor m_{j_l}+n\rfloor_{2n}\}}\Big(\omega^0\,\Lambda^l_{m_{j_1},\ldots,m_{j_{l-1}}}(B^{j_1},\ldots,B^{j_l})\Big)\end{aligned}$$

is actually independent of the ordering of the $j_i$s making the above formula well-defined also without implying this sorting.

PROOF The proof is by induction on $k$. Let $k = 1$ and let $I_1 \in \{1,\ldots n\}$, $B^1 \in \mathbb{R}^{2n\times 2n}$ skew-symmetric be arbitrary. Then, $I = \{I_1\}$, $L = \{I_1, I_1+n\}$ which implies

$$\sum_{\alpha,\beta\in L} B^1_{\alpha_1\,\beta_1}\,\mathrm{d}z^{\alpha_1}\wedge\mathrm{d}z^{\beta_1} = B^1_{I_1\,(I_1+n)}\,\mathrm{d}q^{I_1}\wedge\mathrm{d}p^{I_1} + B^1_{I_1\,(I_1+n)}\,\mathrm{d}p^{I_1}\wedge\mathrm{d}q^{I_1}\,.$$

By definition of $\omega^0$ and the anti-commutativity of the wedge product we get

$$\begin{aligned}&B^1_{I_1\,(I_1+n)}\,\mathrm{d}q^{I_1}\wedge\mathrm{d}p^{I_1} + B^1_{(I_1+n)\,I_1}\,\mathrm{d}p^{I_1}\wedge\mathrm{d}q^{I_1}\\&\qquad= B^1_{I_1\,(I_1+n)}\,\mathrm{d}q^{I_1}\wedge\mathrm{d}p^{I_1} - B^1_{(I_1+n)\,I_1}\,\mathrm{d}q^{I_1}\wedge\mathrm{d}p^{I_1}\\&\qquad= -\omega^0_{(I_1+n)\,I_1}\,B^1_{I_1\,(I_1+n)}\,\mathrm{d}q^{I_1}\wedge\mathrm{d}p^{I_1} - \omega^0_{I_1\,(I_1+n)}\,B^1_{(I_1+n)\,I_1}\,\mathrm{d}q^{I_1}\wedge\mathrm{d}p^{I_1}\\&\qquad= -\sum_{m_1\in L}\mathrm{Tr}_{\{m_1\}}(\omega^0\,\Lambda^1(B^1))\,.\end{aligned}$$

Now, assume (2.42) holds for fixed $k$ and every $B^j \in \mathbb{R}^{2n\times 2n}$, $j = 1,\ldots,k$ skew-symmetric and every $I \subset \{1,\ldots,n\}$, $|I| = k$; we prove it for $k+1$. Fix

$B^j \in \mathbb{R}^{2n\times 2n}$, $j = 1,\dots,k+1$ skew-symmetric and $I \subset \{1,\dots,n\}$, $|I| = k+1$. By Lemma 2.3 we have

$$\begin{aligned}
&\sum_{\alpha,\beta\in L^{k+1}} B^1_{\alpha_1\,\beta_1}\ \cdots\ B^{k+1}_{\alpha_{k+1}\,\beta_{k+1}}\,\mathrm{d}z^{\alpha_1}\wedge\mathrm{d}z^{\beta_1}\wedge\cdots\wedge\mathrm{d}z^{\alpha_{k+1}}\wedge\mathrm{d}z^{\beta_{k+1}}\\
&\quad= -\sum_{m_{k+1}\in L}\ \sum_{\alpha,\beta\in L^k_{\lfloor m_{k+1}\rfloor_n}} B^1_{\alpha_1\,\beta_1}\cdots B^k_{\alpha_k\,\beta_k}\,\mathrm{Tr}_{\{m_{k+1}\}}\Big(\omega^0\,\Lambda^1(B^{k+1})\Big)\\
&\qquad \mathrm{d}z^{\alpha_1}\wedge\mathrm{d}z^{\beta_1}\wedge\cdots\wedge\mathrm{d}z^{\alpha_k}\wedge\mathrm{d}z^{\beta_k}\wedge\mathrm{d}q^{\lfloor m_{k+1}\rfloor_n}\wedge\mathrm{d}p^{\lfloor m_{k+1}\rfloor_n}\\
&\qquad+\sum_{m_{k+1}\in L}\ \sum_{\alpha,\beta\in L^k_{\lfloor m_{k+1}\rfloor_n}}\\
&\qquad\quad\sum_{l=1}^{k} B^1_{\alpha_1\,\beta_1}\cdots\breve{B^l}_{\alpha_l\,\beta_l}\cdots B^k_{\alpha_k\,\beta_k}\,\Lambda^2_{m_{k+1};\alpha_l,\beta_l}(B^l,B^{k+1})\\
&\qquad \mathrm{d}z^{\alpha_1}\wedge\mathrm{d}z^{\beta_1}\wedge\cdots\wedge\mathrm{d}z^{\alpha_k}\wedge\mathrm{d}z^{\beta_k}\wedge\mathrm{d}q^{\lfloor m_{k+1}\rfloor_n}\wedge\mathrm{d}p^{\lfloor m_{k+1}\rfloor_n}\\
&\quad=: (I)+(II)
\end{aligned}\tag{2.43}$$

where we make use of the notation where

$$B^1_{\alpha_1\,\beta_1}\cdots\breve{B^l}_{\alpha_l\,\beta_l}\cdots B^k_{\alpha_k\,\beta_k} = B^1_{\alpha_1\,\beta_1}\cdots {B^{l-1}}_{\alpha_{l-1}\,\beta_{l-1}}\,{B^{l+1}}_{\alpha_{l+1}\,\beta_{l+1}}\cdots B^k_{\alpha_k\,\beta_k}\,.$$

Applying the induction assumption to $(I)$ yields

$$\begin{aligned}
&\sum_{m_{k+1}\in L}\ \sum_{\alpha,\beta\in L^k_{\lfloor m_{k+1}\rfloor_n}} -B^1_{\alpha_1\,\beta_1}\cdots B^k_{\alpha_k\,\beta_k}\,\mathrm{Tr}_{\{m_{k+1}\}}\Big(\omega^0\,\Lambda^1(B^{k+1})\Big)\\
&\quad \mathrm{d}z^{\alpha_1}\wedge\mathrm{d}z^{\beta_1}\wedge\cdots\wedge\mathrm{d}z^{\alpha_k}\wedge\mathrm{d}z^{\beta_k}\wedge\mathrm{d}q^{\lfloor m_{k+1}\rfloor_n}\wedge\mathrm{d}p^{\lfloor m_{k+1}\rfloor_n}\\
&\quad=\sum_{m_{k+1}\in L}\sum_{p\in P(k)}(-1)^{|p|+1}\sum_{\substack{m\in L^k_{\lfloor m_{k+1}\rfloor_n}\\ \lfloor m_i\rfloor_n\neq\lfloor m_j\rfloor_n,\\ 1\le i<j\le k}}\mathrm{Tr}_{\{m_{k+1}\}}\Big(\omega^0\,\Lambda^1(B^{k+1})\Big)\\
&\qquad\quad\prod_{j\in\{1,\dots,|p|\}}\mathrm{Tr}_{\{m_{(p_j)_{|p_j|}}\}}\Big(\omega^0\,\Lambda^{|p_j|}_{m_{(p_j)_1},\dots,m_{(p_j)_{(|p_j|-1)}}}(B^{(p_j)_1},\dots,B^{(p_j)_{|p_j|}})\Big)\\
&\qquad\quad\mathrm{d}q^{\lfloor m_1\rfloor_n}\wedge\mathrm{d}p^{\lfloor m_1\rfloor_n}\wedge\cdots\wedge\mathrm{d}q^{\lfloor m_{k+1}\rfloor_n}\wedge\mathrm{d}p^{\lfloor m_{k+1}\rfloor_n}\,.
\end{aligned}\tag{2.44}$$

By Lemma A.1 $\Lambda^2_{m_{k+1};i,j}(B^l, B^{k+1})$ is a skew-symmetric matrix for any $m_{k+1} \in L$, $1 \leq l \leq k$. Hence, replacing $B_l$ by $\Lambda^2_{m_{k+1};\alpha_l,\beta_l}(B^l, B^{k+1})$ in the induction assumption and applying it to $(II)$ for every $l \in \{1, \ldots, k\}$. We obtain

$$(II) = \sum_{m_{k+1}\in L} \sum_{p=\{p_1,\ldots,p_{|p|}\}\in P(k)} (-1)^{|p|} \sum_{r=1}^{|p|} \sum_{l\in p_r} \sum_{\substack{m\in L^k_{\lfloor m_{k+1}\rfloor_n} \\ \lfloor m_i\rfloor_n \neq \lfloor m_j\rfloor_n, \\ 1\leq i<j\leq k}} \mathrm{Tr}_{\{m_{(p_r)_{|p_r|}}\}}\Big( \omega^0\, \Lambda^{|p_r|}_{m_{(p_r)_1},\ldots,m_{(p_r)_{(|p_r|-1)}}}(B^{(p_r)_1}, \ldots, \Lambda^2_{m_{k+1};\alpha_l,\beta_l}(B^l, B^{k+1}), \ldots, B^{(p_r)_{|p_r|}})\Big) \prod_{j\in\{1,\ldots,|p|\}\setminus\{r\}} \mathrm{Tr}_{\{m_{(p_j)_{|p_j|}}\}}\Big(\omega^0\, \Lambda^{|p_j|}_{m_{(p_j)_1},\ldots,m_{(p_j)_{(|p_j|-1)}}}(B^{(p_j)_1}, \ldots, B^{(p_j)_{|p_j|}})\Big) \mathrm{d}q^{\lfloor m_1\rfloor_n} \wedge \mathrm{d}p^{\lfloor m_1\rfloor_n} \wedge \cdots \wedge \mathrm{d}q^{\lfloor m_k\rfloor_n} \wedge \mathrm{d}p^{\lfloor m_k\rfloor_n} \tag{2.45}$$

where in addition we used the fact that $\bigcup_{r=1}^{|p|} p_r = \{1, \ldots, k\}$ for any partition $p$ of $\{1, \ldots, k\}$. By definition of $\Lambda^k$ we have

$$\sum_{l\in p_r} \mathrm{Tr}_{\{m_{(p_r)_{|p_r|}}\}}\Big( \omega^0\, \Lambda^{|p_r|}_{m_{(p_r)_1},\ldots,m_{(p_r)_{(|p_r|-1)}}}(B^{(p_r)_1}, \ldots, \Lambda^2_{m_{k+1};\alpha_l,\beta_l}(B^l, B^{k+1}), \ldots, B^{(p_r)_{|p_r|}})\Big) = \mathrm{Tr}_{\{m_{(p_r)_{|p_r|}}\}}\Big(\omega^0\, \Lambda^{|p_r|+1}_{m_{(p_r)_1},\ldots,m_{(p_r)_{(|p_r|-1)}},m_{k+1}}(B^{(p_r)_1}, \ldots, B^{(p_r)_{|p_r|}}, B^{k+1})\Big) \tag{2.46}$$

for any $p_r \in p$ where $p \in P(k)$. Combining (2.45) and (2.46) we obtain

$$(II) = \sum_{p=\{p_1,\ldots,p_{|p|}\}\in P(k)} (-1)^{|p|} \sum_{r=1}^{|p|} \sum_{m_{k+1}\in L} \sum_{\substack{m\in L^k_{\lfloor m_{k+1}\rfloor_n} \\ \lfloor m_i\rfloor_n \neq \lfloor m_j\rfloor_n, \\ 1\leq i<j\leq k}} \mathrm{Tr}_{\{m_{(p_r)_{|p_r|}}\}}\Big(\omega^0\, \Lambda^{|p_r|+1}_{m_{(p_r)_1},\ldots,m_{(p_r)_{(|p_r|-1)}},m_{k+1}}(B^{(p_r)_1}, \ldots, B^{(p_r)_{|p_r|}}, B^{k+1})\Big) \prod_{j\in\{1,\ldots,|p|\}\setminus\{r\}} \mathrm{Tr}_{\{m_{(p_j)_{|p_j|}}\}}\Big(\omega^0\, \Lambda^{|p_j|}_{m_{(p_j)_1},\ldots,m_{(p_j)_{(|p_j|-1)}}}(B^{(p_j)_1}, \ldots, B^{(p_j)_{|p_j|}})\Big) \mathrm{d}q^{\lfloor m_1\rfloor_n} \wedge \mathrm{d}p^{\lfloor m_1\rfloor_n} \wedge \cdots \wedge \mathrm{d}q^{\lfloor m_k\rfloor_n} \wedge \mathrm{d}p^{\lfloor m_k\rfloor_n}\,. \tag{2.47}$$

Finally, combining (2.44), (2.43) and (2.47) yields

$$\sum_{\alpha,\beta\in L^{k+1}} B^1_{\alpha_1\,\beta_1} \cdots B^k_{\alpha_{k+}\,\beta_{k+1}}\,\mathrm{d}z^{\alpha_1}\wedge \mathrm{d}z^{\beta_1}\wedge\cdots\wedge \mathrm{d}z^{\alpha_{k+}}\wedge \mathrm{d}z^{\beta_{k+1}}$$
$$= \sum_{p\in P(k+1)} (-1)^{|p|} \sum_{\substack{m\in L^{k+1}\\ \lfloor m_i\rfloor_n\neq\lfloor m_j\rfloor_n,\\ 1\le i<j\le k+1}} \prod_{j\in\{1,\ldots,|p|\}} \mathrm{Tr}_{\{m_{(p_j)_{|p_j|}}\}}\Big(\omega^0\,\Lambda^{|p_j|}_{m_{(p_j)_1},\ldots,m_{(p_j)_{(|p_j|-1)}}}(B^{(p_j)_1},\ldots,B^{(p_j)_{|p_j|}})\Big)$$
$$\mathrm{d}q^{\lfloor m_1\rfloor_n}\wedge \mathrm{d}p^{\lfloor m_1\rfloor_n}\wedge\cdots\wedge \mathrm{d}q^{\lfloor m_{k+1}\rfloor_n}\wedge \mathrm{d}p^{\lfloor m_{k+1}\rfloor_n}$$

which finishes the proof. □

To get an overview over what is left to derive the Lebesgue density $\nu^\varepsilon$ of the Liouville measure $\lambda^\varepsilon$ of $\omega^\varepsilon$ we give an outline of the procedure where we restrict to $\lambda^\varepsilon_n$. Replacing the $B^i$s in (2.42) and choosing $k = n$ we get

$$\sum_{\alpha,\beta\in\{1,\ldots,2n\}^n} \Omega_{\alpha_1\,\beta_1} \cdots \Omega_{\alpha_n\,\beta_n}\,\mathrm{d}z^{\alpha_1}\wedge \mathrm{d}z^{\beta_1}\wedge\ldots\wedge \mathrm{d}z^{\alpha_n}\wedge \mathrm{d}z^{\beta_n}$$
$$= \sum_{\substack{m\in\{1,\ldots,2n\}^n\\ \lfloor m_i\rfloor_n\neq\lfloor m_j\rfloor_n,\\ 1\le i<j\le n}} \sum_{p\in P(n)} (-1)^{|p|} \prod_{j\in\{1,\ldots,|p|\}} \mathrm{Tr}_{\{m_{(p_j)_{|p_j|}}\}}\Big(\omega^0\,\Lambda^{|p_j|}_{m_{(p_j)_1},\ldots,m_{(p_j)_{(|p_j|-1)}}}(\Omega)\Big)$$
$$\mathrm{d}q^{\lfloor m_1\rfloor_n}\wedge \mathrm{d}p^{\lfloor m_1\rfloor_n}\wedge\ldots\wedge \mathrm{d}q^{\lfloor m_n\rfloor_n}\wedge \mathrm{d}p^{\lfloor m_n\rfloor_n}$$

where by an abuse of notation we write

$$\Lambda^j_{m_1,\ldots,m_{j-1}}(\overbrace{B,\ldots,B}^{j\text{-times}}) =: \Lambda^j_{m_1,\ldots,m_{j-1}}(B)\,.$$

By the fact that wedge products of two-forms commute we have

$$\mathrm{d}q^{\lfloor m_1\rfloor_n}\wedge \mathrm{d}p^{\lfloor m_1\rfloor_n}\wedge\ldots\wedge \mathrm{d}q^{\lfloor m_n\rfloor_n}\wedge \mathrm{d}p^{\lfloor m_n\rfloor_n} = \mathrm{d}q^1\wedge \mathrm{d}p^1\wedge\ldots\wedge \mathrm{d}q^n\wedge \mathrm{d}p^n$$

for any $m_1, \ldots, m_n \in \{1, \ldots, 2n\}$. Moreover, by the anti-commutativity of the wedge product

$$
\begin{aligned}
&\mathrm{d}q^1 \wedge \mathrm{d}p^1 \wedge \cdots \wedge \mathrm{d}q^{n-2} \wedge \mathrm{d}p^{n-2} \wedge \mathrm{d}q^{n-1} \wedge \mathrm{d}p^{n-1} \wedge \mathrm{d}q^n \wedge \mathrm{d}p^n \\
&= (-1)\, \mathrm{d}q^1 \wedge \mathrm{d}p^1 \wedge \cdots \wedge \mathrm{d}q^{n-2} \wedge \mathrm{d}p^{n-2} \wedge \mathrm{d}q^{n-1} \wedge \mathrm{d}q^n \wedge \mathrm{d}p^{n-1} \wedge \mathrm{d}p^n \\
&= (-1)\,(-1)^2\, \mathrm{d}q^1 \wedge \mathrm{d}p^1 \wedge \cdots \wedge \mathrm{d}q^{n-2} \wedge \mathrm{d}q^{n-1} \wedge \mathrm{d}q^n \wedge \mathrm{d}p^{n-2} \wedge \mathrm{d}p^{n-1} \wedge \mathrm{d}p^n \\
&\vdots \\
&= (-1)^{(\sum_{i=1}^{n-1} i)}\, \mathrm{d}q^1 \wedge \cdots \wedge \mathrm{d}q^n \wedge \mathrm{d}p^1 \wedge \cdots \wedge \mathrm{d}p^n \\
&= (-1)^{(n(n-1)/2)}\, \mathrm{d}q^1 \wedge \cdots \wedge \mathrm{d}q^n \wedge \mathrm{d}p^1 \wedge \cdots \wedge \mathrm{d}p^n \,.
\end{aligned}
\tag{2.48}
$$

Combining the above equations yields

$$
\begin{aligned}
&\sum_{\alpha,\beta \in \{1,\ldots,2n\}^n} \Omega_{\alpha_1\,\beta_1} \cdots \Omega_{\alpha_n\,\beta_n}\, \mathrm{d}z^{\alpha_1} \wedge \mathrm{d}z^{\beta_1} \wedge \ldots \wedge \mathrm{d}z^{\alpha_n} \wedge \mathrm{d}z^{\beta_n} \\
&\quad = (-1)^{n(n-1)/2} \sum_{p \in P(n)} (-1)^{|p|} \\
&\quad \sum_{\substack{m \in \{1,\ldots,2n\}^n \\ \lfloor m_i \rfloor_n \neq \lfloor m_j \rfloor_n, \\ 1 \le i < j \le n}} \prod_{j \in \{1,\ldots,|p|\}} \mathrm{Tr}_{\{m_{(p_j)_{|p_j|}}\}}\Big(\omega^0\, \Lambda^{|p_j|}_{m_{(p_j)_1},\ldots,m_{(p_j)_{(|p_j|-1)}}}(\Omega)\Big) \\
&\quad \mathrm{d}q^1 \wedge \cdots \wedge \mathrm{d}q^n \wedge \mathrm{d}p^1 \wedge \mathrm{d}p^n \,.
\end{aligned}
$$

Now, assume

$$
0 = \sum_{p \in P(n)} (-1)^{|p|} \prod_{j \in \{1,\ldots,|p|\}} \mathrm{Tr}_{\{m_{(p_j)_{|p_j|}}\}}\Big(\omega^0\, \Lambda^{|p_j|}_{m_{(p_j)_1},\ldots,m_{(p_j)_{(|p_j|-1)}}}(\Omega)\Big) \tag{2.49}
$$

whenever $m_i = m_j$ for some $i \neq j$. Then,

$$
\begin{aligned}
&\sum_{\alpha,\beta \in \{1,\ldots,2n\}^n} \Omega_{\alpha_1\,\beta_1} \cdots \Omega_{\alpha_n\,\beta_n}\, \mathrm{d}z^{\alpha_1} \wedge \mathrm{d}z^{\beta_1} \wedge \ldots \wedge \mathrm{d}z^{\alpha_n} \wedge \mathrm{d}z^{\beta_n} \\
&\quad = (-1)^{n(n-1)/2} \sum_{p \in P(n)} (-1)^{|p|} \prod_{j \in \{1,\ldots,|p|\}} \mathrm{Tr}_{2n}\Big(\omega^0\, \Lambda^{|p_j|}(\Omega)\Big) \\
&\quad \mathrm{d}q^1 \wedge \cdots \wedge \mathrm{d}q^n \wedge \mathrm{d}p^1 \wedge \mathrm{d}p^n \,.
\end{aligned}
$$

where we denote

$$
\Lambda^i(\Omega) := \sum_{m \in \{1,\ldots,2n\}^{j-1}} \Lambda^j_{m_1,\ldots,m_{j-1}}(\Omega)\,.
$$

From the definition of $\Lambda^i$ it's easy to see that $\Lambda^i(\Omega) = C\,(\Omega\,\omega^0)^{i-1}\,\Omega$ for some natural number $C$. Comparing the above result with $\lambda_n^\varepsilon$ (2.21) we conclude that the above is exactly of the form what we are looking for. So, the main points left are the prove of (2.49) and derive the exact formula for $\mathrm{Tr}_{2n}\Big(\omega^0\,\Lambda^{|p_j|}(\Omega)\Big)$.

To show (2.49) we have to go quite deep into the structure of $\Lambda^j_{m_1,\dots,m_{j-1})}(\Omega)$. In general, the terms

$$\sum_{p\in P(k)}(-1)^{|p|}\prod_{j\in\{1,\dots,|p|\}}\mathrm{Tr}_{\{m_{(p_j)_{|p_j|}}\}}\Big(\omega^0\,\Lambda^{|p_j|}_{m_{(p_j)_1},\dots,m_{(p_j)_{(|p_j|-1)}}}(\Omega)\Big)$$

are very complex. To keep a better overview over the structure we introduce a new short notation. From the definition of $\Lambda^j_{m_1,\dots,m_{j-1})}(\Omega)$ (2.26) it is easy to see that each summand in the explicit formula of $\Lambda^k_{m_1,\dots,m_{j-1})}(\Omega)$ is of the form

$$\begin{gathered}\Omega_{i\,m_{l_1}}\,\omega^0_{m_{l_1}\,\lfloor m_{l_1}+n\rfloor_{2n}}\,\Omega_{\lfloor m_{l_1}+n\rfloor_{2n}\,\lfloor m_{l_2}+n\rfloor_{2n}}\\ \cdots\,\Omega_{m_{l_{k-2}}\,\lfloor m_{l_{k-1}}+n\rfloor_{2n}}\,\omega^0_{\lfloor m_{l_{k-1}}+n\rfloor_{2n}\,m_{l_{k-1}}}\,\Omega_{m_{l_{k-1}}\,j}\,.\end{gathered}$$

From this one can see that the only differences between the summands are the ordering of the indices $m_j$ as well as whether the first index of $\omega^0$ associated to $m_j$ is $m_j$ or $\lfloor m_j+n\rfloor_{2n}$. So we can uniquely identify any term of this form just by using those two properties. In what follows we will use the following notation. For $m_1,\dots,m_k,i,j\in\{1,\dots,2n\}$ and $1\le l\le k$ we write

$$\begin{aligned} l^{\downarrow}_{ji} &:= \Omega_{j\,m_l}\,\omega^0_{m_l\,\lfloor m_l+n\rfloor_{2n}}\,\Omega_{\lfloor m_l+n\rfloor_{2n}\,i}\\ l^{\uparrow}_{ji} &:= \Omega_{j\,\lfloor m_l+n\rfloor_{2n}}\,\omega^0_{\lfloor m_l+n\rfloor_{2n}\,m_l}\,\Omega_{m_l\,i}\,. \end{aligned}\tag{2.50}$$

We call the number (as $l$ in the above) the index and the arrow ($\uparrow$ or $\downarrow$) the direction of such a symbol. In addition, we define a product or contraction of two such symbols by merging the $\Omega$s that meet. As an example we have

$$\begin{aligned}(2^{\downarrow}\,3^{\uparrow})_{ji} &= (\Omega_{j\,m_2}\,\omega^0_{m_2\,\lfloor m_2+n\rfloor_{2n}}\,\Omega_{\lfloor m_2+n\rfloor_{2n}\,i}\rightleftharpoons\Omega_{j\,\lfloor m_3+n\rfloor_{2n}}\,\omega^0_{\lfloor m_3+n\rfloor_{2n}\,m_3}\,\Omega_{m_3\,i})_{ji}\\ &=\Omega_{j\,m_2}\,\omega^0_{m_2\,\lfloor m_2+n\rfloor_{2n}}\,\boldsymbol{\Omega}_{\lfloor \mathbf{m_2+n}\rfloor_{\mathbf{2n}}\,\lfloor\mathbf{m_3+n}\rfloor_{\mathbf{2n}}}\,\omega^0_{\lfloor m_3+n\rfloor_{2n}\,m_3}\,\Omega_{m_3\,i}\,.\end{aligned}$$

Furthermore, we introduce a 'partial trace' for these symbols where we insert an additional $\omega^0$. For a matrix $B\in\mathbb{R}^{2n\times 2n}$ we write

$$\mathrm{Tr}_{1^{\downarrow}}(B):=\omega^{\mathbf{0}}_{\mathbf{m_1}\,\lfloor\mathbf{m_1+n}\rfloor_{\mathbf{2n}}}\,B_{\lfloor m_1+n\rfloor_{2n}\,m_1}$$

and

$$\mathrm{Tr}_{1^{\uparrow}}(B):=\omega^{\mathbf{0}}_{\lfloor\mathbf{m_1+n}\rfloor_{\mathbf{2n}}\,\mathbf{m_1}}\,B_{m_1\,\lfloor m_1+n\rfloor_{2n}}\,.$$

Here, we again use $\downarrow$ if $m_1$ occurs at the first index of $\omega^0$ and $\uparrow$ when the first index of $\omega^0$ is $\lfloor m_1+n\rfloor_{2n}$. Then, as an example we have

$$\begin{aligned}\mathrm{Tr}_{1^\downarrow}(2^\downarrow 3^\uparrow) := \omega^{\mathbf{0}}_{\mathbf{m_1}\,\lfloor \mathbf{m_1}+\mathbf{n}\rfloor_{\mathbf{2n}}}\,\Omega_{\lfloor \mathbf{m_1}+\mathbf{n}\rfloor_{\mathbf{2n}}\,m_2}\,\omega^0_{m_2\,\lfloor m_2+n\rfloor_{2n}}\\ \Omega_{\lfloor m_2+n\rfloor_{2n}\,\lfloor m_3+n\rfloor_{2n}}\,\omega^0_{\lfloor m_3+n\rfloor_{2n}\,m_3}\,\Omega_{m_3\,\mathbf{m_1}}\,.\end{aligned}$$

To simplify the computations following we also introduce a special case. We write

$$\mathrm{Tr}_{1^\uparrow}() := \mathrm{Tr}_{1^\uparrow}(\Omega) = \omega^0_{\lfloor m_1+n\rfloor_{2n}\,m_1}\,\Omega_{m_1\,\lfloor m_1+n\rfloor_{2n}}\,.$$

Moreover we introduce the inversion operator $\overline{(\cdot)}$ for the directions $\downarrow$ and $\uparrow$, i.e. for $\alpha\in\{\uparrow,\downarrow\}$

$$\overline{\alpha} = \begin{cases}\uparrow, & \text{for } \alpha=\downarrow\\ \downarrow, & \text{for } \alpha=\uparrow\end{cases}\,. \tag{2.51}$$

For a collection of properties regarding this notation, (see Lemma A.2). Furthermore, for a set $R=\{R_1,\dots,R_k\}$ we denote the set of all permutations of $R$ by $\mathrm{Sym}(R)$. For $\sigma\in\mathrm{Sym}(R)$ we write $\sigma_i=\sigma(R_i)$ for $1\le i\le k$.

In the next step we express $\Lambda^k_{m_1,\dots,m_{k-1}}(\Omega)$ in the short notation introduced above. We start with $\Lambda^2_{m_1}(\Omega)$. Now, let $m\in\{1,\dots,2n\}^n$ then

$$\begin{aligned}\Lambda^2_{m_1;i,j}(\Omega) &= \Omega_{i\,m_1}\,\omega^0_{m_1\,\lfloor m_1+n\rfloor_{2n}}\,\Omega_{\lfloor m_1+n\rfloor_{2n}\,j}\\ &\quad+\Omega_{i\,\lfloor m_1+n\rfloor_{2n}}\,\omega^0_{\lfloor m_1+n\rfloor_{2n}\,m_1}\,\Omega_{m_1\,j}\\ &= 1^\downarrow+1^\uparrow\,.\end{aligned} \tag{2.52}$$

For $\Lambda^3_{m_1,m_2;i,j}(\Omega)$, let's have a closer look at the definition

$$\Lambda^3_{m_1,m_2;i,j}(\Omega) :=\ \Lambda^{k-1}_{m_1,\dots,m_{k-2};i,j}(\Omega,\Lambda^2_{m_2}(\Omega))+\Lambda^{k-1}_{m_1,\dots,m_{k-2};i,j}(\Lambda^2_{m_2}(\Omega),\Omega)\,.$$

This means that in (2.52) every $\Omega$ will be replaced by $\Lambda^2_{m_2}(\Omega)$. Replacing the first $\Omega$ in $1^\downarrow$ will add a $(2^\downarrow+2^\uparrow)$ in front of the $1^\downarrow$. Replacing the second $\Omega$ in $1^\downarrow$ will add a $(2^\downarrow+2^\uparrow)$ after the $1^\downarrow$. The equivalent holds for the $1^\uparrow$ summand of $\Lambda^2_{m_1;i,j}(\Omega)$. Hence,

$$\begin{aligned}\Lambda^3_{m_1,m_2}(\Omega) &= 2^\downarrow 1^\downarrow+2^\uparrow 1^\downarrow+1^\downarrow 2^\downarrow+1^\downarrow 2^\uparrow+2^\downarrow 1^\uparrow+2^\uparrow 1^\uparrow+1^\uparrow 2^\downarrow+1^\uparrow 2^\uparrow\\ &= \sum_{\alpha\in\{\uparrow,\downarrow\}^2}\ \sum_{\sigma\in\mathrm{Sym}(\{1,2\})}\sigma_1^{\alpha_1}\,\sigma_2^{\alpha_2}\,.\end{aligned}$$

Inductively, we get

$$\Lambda^k_{m_1,\ldots,m_{k-1}}(\Omega) = \sum_{\alpha\in\{\uparrow,\downarrow\}^{k-1}} \sum_{\sigma\in\mathrm{Sym}(\{1,\ldots,k-1\})} \sigma_1^{\alpha_1}\cdots\sigma_{k-1}^{\alpha_{k-1}} \quad \text{for } k\geq 2\,. \tag{2.53}$$

Note here that the above shows that $\Lambda^k_{m_1,\ldots,m_{k-1}}(\Omega)$ is independent of the ordering of the $m_j$s. Now, consider $\Lambda^k_{m_1,\ldots,m_{l-1},\lfloor m_l+n\rfloor_{2n},m_{l+1},\ldots,m_{k-1}}(\Omega)$ for $l\in\{1,\ldots,k-1\}$. Clearly, replacing $m_l$ by $\lfloor m_l+n\rfloor_{2n}$ in (2.53) every $l^\uparrow$ will turn to $l^\downarrow$ and vice versa. Since all possibilities to distribute the indices and directions are already included in $\Lambda^k_{m_1,\ldots,m_{k-1}}(\Omega)$ we conclude

$$\Lambda^k_{m_1,\ldots,m_{l-1},\lfloor m_l+n\rfloor_{2n},m_{l+1},\ldots,m_{k-1}}(\Omega) = \Lambda^k_{m_1,\ldots,m_{k-1}}(\Omega) \tag{2.54}$$

for every $1\leq l\leq k-1$. Also, one can easily see that

$$\begin{aligned}
&\mathrm{Tr}_{\{m_k\}}(\omega^0\,\Lambda^k_{m_1,\ldots,m_{k-1}}(\Omega))\\
&\quad= \omega^0_{m_k\,\lfloor m_k+n\rfloor_{2n}}\,\Lambda^k_{m_1,\ldots,m_{k-1};\lfloor m_k+n\rfloor_{2n},m_k}(\Omega)\\
&\quad= \sum_{\alpha\in\{\uparrow,\downarrow\}^{k-1}} \sum_{\sigma\in\mathrm{Sym}(\{1,\ldots,k-1\})} \mathrm{Tr}_{k^\downarrow}(\sigma_1^{\alpha_1}\cdots\sigma_{k-1}^{\alpha_{k-1}})
\end{aligned}$$

as well as (2.55)

$$\begin{aligned}
&\mathrm{Tr}_{\{\lfloor m_k+n\rfloor_{2n}\}}(\omega^0\,\Lambda^k_{m_1,\ldots,m_{k-1}}(\Omega))\\
&\quad= \sum_{\alpha\in\{\uparrow,\downarrow\}^{k-1}} \sum_{\sigma\in\mathrm{Sym}(\{1,\ldots,k-1\})} \mathrm{Tr}_{k^\uparrow}(\sigma_1^{\alpha_1}\cdots\sigma_{k-1}^{\alpha_{k-1}})\,.
\end{aligned}$$

Combining (2.55) and (A.3) we have

$$\begin{aligned}
&\mathrm{Tr}_{\{m_k\}}(\omega^0\,\Lambda^k_{m_1,\ldots,m_{k-1}}(\Omega)) + \mathrm{Tr}_{\{\lfloor m_k+n\rfloor_{2n}\}}(\omega^0\,\Lambda^k_{m_1,\ldots,m_{k-1}}(\Omega))\\
&\quad= \sum_{\alpha\in\{\uparrow,\downarrow\}^{k}} \sum_{\sigma\in\mathrm{Sym}(\{1,\ldots,k-1\})} \mathrm{Tr}_{k^{\sigma_k}}(\sigma_1^{\alpha_1}\cdots\sigma_{k-1}^{\alpha_{k-1}})\\
&\quad= \sum_{\alpha\in\{\uparrow,\downarrow\}^{k}} \sum_{\sigma\in\mathrm{Sym}(\{1,\ldots,k\}\setminus\{j\})} \mathrm{Tr}_{j^{\sigma_k}}(\sigma_1^{\alpha_1}\cdots\sigma_{k-1}^{\alpha_{k-1}})\,.
\end{aligned} \tag{2.56}$$

for any $1\leq j\leq k$.

Now, we are set to derive the explicit formula for

$$\sum_{p\in P(n)}(-1)^{|p|} \sum_{\substack{m\in\{1,\ldots,2n\}^n\\ \lfloor m_i\rfloor_n\neq\lfloor m_j\rfloor_n,\\ 1\leq i<j\leq n}} \prod_{j\in\{1,\ldots,|p|\}} \mathrm{Tr}_{\{m_{(p_j)_{|p_j|}}\}}\Big(\omega^0\,\Lambda^{|p_j|}_{m_{(p_j)_1},\ldots,m_{(p_j)_{(|p_j|-1)}}}(\Omega)\Big)\,.$$

As we can see by the following lemma.

**Lemma 2.5** *Let $k \in \mathbb{N}$. Then,*

$$\sum_{p \in P(k)} (-1)^{|p|} \sum_{\substack{m \in \{1,\dots,2n\}^k \\ \lfloor m_i \rfloor_n \neq \lfloor m_l \rfloor_n, \\ 1 \leq i < l \leq k}} \prod_{j \in \{1,\dots,|p|\}} \mathrm{Tr}_{\{m_{(p_j)_{|p_j|}}\}} \Big( \omega^0 \, \Lambda^{|p_j|}_{m_{(p_j)_1},\dots,m_{(p_j)_{(|p_j|-1)}}} (\Omega) \Big)$$
$$= k! \sum_{\substack{\alpha \in \mathbb{N}_0^k, \\ \sum_{i=1}^k i \, \alpha_i = k}} (-1)^{|\alpha|} \, 2^{k-|\alpha|} \prod_{j=1}^{k} (j^{\alpha_j} \, \alpha_j!)^{-1} \, \mathrm{Tr}_{2n} \Big( (\omega^0 \, \Omega)^j \Big)^{\alpha_j} . \tag{2.57}$$

PROOF We start with the following observation. By (2.55)

$$\sum_{p \in P(k)} (-1)^{|p|} \sum_{\substack{m \in \{1,\dots,2n\}^k \\ \lfloor m_i \rfloor_n \neq \lfloor m_l \rfloor_n, \\ 1 \leq i < l \leq k}} \prod_{j \in \{1,\dots,|p|\}} \mathrm{Tr}_{\{m_{(p_j)_{|p_j|}}\}} \Big( \omega^0 \, \Lambda^{|p_j|}_{m_{(p_j)_1},\dots,m_{(p_j)_{(|p_j|-1)}}} (\Omega) \Big)$$
$$= \sum_{p \in P(k)} (-1)^{|p|} \sum_{\substack{m \in \{1,\dots,2n\}^k \\ \lfloor m_i \rfloor_n \neq \lfloor m_j \rfloor_n, \\ 1 \leq i < j \leq k}} \prod_{j \in \{1,\dots,|p|\}}$$
$$\Bigg( \sum_{\alpha \in \{\uparrow,\downarrow\}^{|p_j|-1}} \sum_{\sigma \in \mathrm{Sym}(\{(p_j)_1,\dots,(p_j)_{(|p_j|-1)}\})} \mathrm{Tr}_{(p_j)^{\downarrow}_{|p_j|}} \big( \sigma_1^{\alpha_1} \cdots \sigma_{|p_j|-1}^{\alpha_{|p_j|-1}} \big) \Bigg) \tag{2.58}$$

Combining (2.54) and (2.56) yields

$$\sum_{p \in P(k)} (-1)^{|p|} \sum_{\substack{m \in \{1,\dots,2n\}^k \\ \lfloor m_i \rfloor_n \neq \lfloor m_l \rfloor_n, \\ 1 \leq i < l \leq k}} \prod_{j \in \{1,\dots,|p|\}}$$
$$\Bigg( \sum_{\alpha \in \{\uparrow,\downarrow\}^{|p_j|-1}} \sum_{\sigma \in \mathrm{Sym}(\{(p_j)_1,\dots,(p_j)_{(|p_j|-1)}\})} \mathrm{Tr}_{(p_j)^{\downarrow}_{|p_j|}} \big( \sigma_1^{\alpha_1} \cdots \sigma_{|p_j|-1}^{\alpha_{|p_j|-1}} \big) \Bigg)$$
$$= \sum_{p \in P(k)} (-1)^{|p|} \sum_{\substack{m \in \{1,\dots,n\}^k \\ m_i \neq m_l, \\ 1 \leq i < l \leq k}} \prod_{j \in \{1,\dots,|p|\}}$$
$$\Bigg( \sum_{\alpha \in \{\uparrow,\downarrow\}^{|p_j|}} \sum_{\sigma \in \mathrm{Sym}(\{(p_j)_1,\dots,(p_j)_{(|p_j|-1)}\})} 2^{|p_j|-1} \, \mathrm{Tr}_{(p_j)^{\alpha_{|p_j|}}_{|p_j|}} \big( \sigma_1^{\alpha_1} \cdots \sigma_{|p_j|-1}^{\alpha_{|p_j|-1}} \big) \Bigg)$$
$$= \sum_{p \in P(k)} (-1)^{|p|} \, 2^{k-|p|} \sum_{\substack{m \in \{1,\dots,n\}^k \\ m_i \neq m_l, \\ 1 \leq i < l \leq k}} \prod_{j \in \{1,\dots,|p|\}}$$
$$\Bigg( \sum_{\alpha \in \{\uparrow,\downarrow\}^{|p_j|}} \sum_{\sigma \in \mathrm{Sym}(\{(p_j)_1,\dots,(p_j)_{(|p_j|-1)}\})} \mathrm{Tr}_{(p_j)^{\alpha_{|p_j|}}_{|p_j|}} \big( \sigma_1^{\alpha_1} \cdots \sigma_{|p_j|-1}^{\alpha_{|p_j|-1}} \big) \Bigg) .$$

Now, choose an arbitrary $m \in \{1, \dots, n\}^k$ with $m_i = m_l$ for some $i \neq l$ and a $p \in P(k)$. We define as $M_1$ the set of all partitions of $\{1, \dots, k\}$ that include a set $\xi$ with $i, l \in \xi$, i.e.

$$M_1 := \{p \in P(k) | \exists \xi \in p : i, l \in \xi\} .$$

In addition, for $\tilde{p} \in M_1$ with $\xi \in \tilde{p}$ and $i, l \in \xi$ we define the set of all partitions of $\{1, \dots, k\}$ that result from splitting $\xi$ into two sets $\xi_1$ and $\xi_2$ where one of the two sets includes $i$ and the other one $l$, i.e.

$$M^{\tilde{p}} := \{p \in P(k) | \exists \xi_1, \xi_2 \in p : i \in \xi_1, l \in \xi_2, \xi_1 \cup \xi_2 = \xi\} .$$

Clearly, the union of the sets $M^{\tilde{p}}$ over all $\tilde{p}$ in $M_1$ results in the set of all partitions of $\{1, \dots, k\}$ satisfying that there are two distinct $\xi_1, \xi_2 \in p$ with $i \in \xi_1$ and $l \in \xi_2$. Also, for an arbitrary $p \in P(k)$ there are two possibilities. Either there is a $\xi \in p$ with $i, l \in \xi$ or there are $\xi_1, \xi_2 \in p$ with $i \in \xi_1$ and $j \in \xi_2$. It is therefore obvious that

$$\bigcup_{\tilde{p} \in M_1} \left( M^{\tilde{p}} \cup \{\tilde{p}\} \right) = P(k) .$$

This fact together with Lemma A.7 shows that for every $m \in \{1, \dots, n\}^k$ with $m_i = m_l$ for some $i \neq l$

$$\begin{aligned}
&\sum_{p \in P(k)} (-1)^{|p|} \, 2^{k-|p|} \prod_{j \in \{1,\dots,|p|\}} \\
&\quad \Bigg( \sum_{\alpha \in \{\uparrow,\downarrow\}^{|p_j|}} \sum_{\sigma \in \mathrm{Sym}(\{(p_j)_1,\dots,(p_j)_{(|p_j|-1)}\})} \mathrm{Tr}_{(p_j)_{|p_j|}^{\alpha_{|p_j|}}} \big( \sigma_1^{\alpha_1} \cdots \sigma_{|p_j|-1}^{\alpha_{|p_j|-1}} \big) \Bigg) \\
&\quad = \sum_{\tilde{p} \in M_1} \Bigg( (-1)^{|\tilde{p}|} \, 2^{k-|\tilde{p}|} \prod_{j \in \{1,\dots,|\tilde{p}|\}} \\
&\qquad \Bigg( \sum_{\alpha \in \{\uparrow,\downarrow\}^{|\tilde{p}_j|}} \sum_{\sigma \in \mathrm{Sym}(\{(\tilde{p}_j)_1,\dots,(\tilde{p}_j)_{(|\tilde{p}_j|-1)}\})} \mathrm{Tr}_{(\tilde{p}_j)_{|\tilde{p}_j|}^{\alpha_{|\tilde{p}_j|}}} \big( \sigma_1^{\alpha_1} \cdots \sigma_{|\tilde{p}_j|-1}^{\alpha_{|\tilde{p}_j|-1}} \big) \Bigg) \\
&\qquad + \sum_{p \in M^{\tilde{p}}} (-1)^{|p|} \, 2^{k-|p|} \prod_{j \in \{1,\dots,|p|\}} \\
&\qquad \Bigg( \sum_{\alpha \in \{\uparrow,\downarrow\}^{|p_j|}} \sum_{\sigma \in \mathrm{Sym}(\{(p_j)_1,\dots,(p_j)_{(|p_j|-1)}\})} \mathrm{Tr}_{(p_j)_{|p_j|}^{\alpha_{|p_j|}}} \big( \sigma_1^{\alpha_1} \cdots \sigma_{|p_j|-1}^{\alpha_{|p_j|-1}} \big) \Bigg) \Bigg) \\
&\quad = 0 .
\end{aligned}$$

It follows that

$$
\begin{aligned}
&\sum_{\substack{m\in\{1,\dots,n\}^k\\ m_i\neq m_l,\\ 1\leq i<l\leq k}} \sum_{p\in P(k)} (-1)^{|p|}\, 2^{k-|p|} \prod_{j\in\{1,\dots,|p|\}} \\
&\quad\Bigg(\sum_{\alpha\in\{\uparrow,\downarrow\}^{|p_j|}} \sum_{\sigma\in\mathrm{Sym}(\{(p_j)_1,\dots,(p_j)_{(|p_j|-1)}\})} \mathrm{Tr}_{{(p_j)}_{|p_j|}}^{\alpha_{|p_j|}}\big(\sigma_1^{\alpha_1}\cdots\sigma_{|p_j|-1}^{\alpha_{|p_j|-1}}\big)\Bigg) \\
&\quad= \sum_{m\in\{1,\dots,n\}^k} \sum_{p\in P(k)} (-1)^{|p|}\, 2^{k-|p|} \prod_{j\in\{1,\dots,|p|\}} \\
&\qquad\Bigg(\sum_{\alpha\in\{\uparrow,\downarrow\}^{|p_j|}} \sum_{\sigma\in\mathrm{Sym}(\{(p_j)_1,\dots,(p_j)_{(|p_j|-1)}\})} \mathrm{Tr}_{{(p_j)}_{|p_j|}}^{\alpha_{|p_j|}}\big(\sigma_1^{\alpha_1}\cdots\sigma_{|p_j|-1}^{\alpha_{|p_j|-1}}\big)\Bigg)
\end{aligned} \tag{2.59}
$$

Since the $m_j$s in the above formula are independent of each other we can split up the sum over $m\in\{1,\dots,n\}^k$ depending on each partition $p$ in a way that the resulting sums are interchangeable with the product. This yields

$$
\begin{aligned}
&\sum_{p\in P(k)} (-1)^{|p|}\, 2^{k-|p|} \sum_{m\in\{1,\dots,n\}^k} \prod_{j\in\{1,\dots,|p|\}} \\
&\quad\Bigg(\sum_{\alpha\in\{\uparrow,\downarrow\}^{|p_j|}} \sum_{\sigma\in\mathrm{Sym}(\{(p_j)_1,\dots,(p_j)_{(|p_j|-1)}\})} \mathrm{Tr}_{{(p_j)}_{|p_j|}}^{\alpha_{|p_j|}}\big(\sigma_1^{\alpha_1}\cdots\sigma_{|p_j|-1}^{\alpha_{|p_j|-1}}\big)\Bigg) \\
&\quad= \sum_{p\in P(k)} (-1)^{|p|}\, 2^{k-|p|} \prod_{j\in\{1,\dots,|p|\}} \Bigg(\sum_{\sigma\in\mathrm{Sym}(\{(p_j)_1,\dots,(p_j)_{(|p_j|-1)}\})} \\
&\qquad\sum_{\alpha\in\{\uparrow,\downarrow\}^{|p_j|}} \sum_{\{m_{(p_j)_1},\dots,m_{(p_j)_{|p_j|}}\}\in\{1,\dots,n\}^{|p_j|}} \mathrm{Tr}_{{(p_j)}_{|p_j|}}^{\alpha_{|p_j|}}\big(\sigma_1^{\alpha_1}\cdots\sigma_{|p_j|-1}^{\alpha_{|p_j|-1}}\big)\Bigg)
\end{aligned} \tag{2.60}
$$

As is easy to see, for every fixed $p\in P(k)$, $j\in\{1,\dots,|p|\}$ and $\sigma\in\mathrm{Sym}(\{(p_j)_1,\dots,(p_j)_{(|p_j|-1)}\})$ we have

$$
\begin{aligned}
&\sum_{\alpha\in\{\uparrow,\downarrow\}^{|p_j|}} \sum_{\{m_{(p_j)_1},\dots,m_{(p_j)_{|p_j|}}\}\in\{1,\dots,n\}^{|p_j|}} \mathrm{Tr}_{{(p_j)}_{|p_j|}}^{\alpha_{|p_j|}}\big(\sigma_1^{\alpha_1}\cdots\sigma_{|p_j|-1}^{\alpha_{|p_j|-1}}\big) \\
&\qquad= \mathrm{Tr}_{2n}\Big((\omega^0\,\Omega)^{|p_j|}\Big)\,.
\end{aligned} \tag{2.61}
$$

Combining (2.60), (2.61) and the fact that $|\mathrm{Sym}(\{(p_j)_1, \ldots, (p_j)_{(|p_j|-1)}\})| = (|p_j| - 1)!$ we obtain

$$\sum_{m\in\{1,\ldots,n\}^k} \sum_{p\in P(k)} (-1)^{|p|}\, 2^{k-|p|} \prod_{j\in\{1,\ldots,|p|\}} \Bigg( \sum_{\alpha\in\{\uparrow,\downarrow\}^{|p_j|}} \sum_{\sigma\in \mathrm{Sym}(\{(p_j)_1,\ldots,(p_j)_{(|p_j|-1)}\})} \mathrm{Tr}_{(p_j)_{|p_j|}^{\alpha_{|p_j|}}} (\sigma_1^{\alpha_1} \cdots \sigma_{|p_j|-1}^{\alpha_{|p_j|-1}}) \Bigg) \tag{2.62}$$
$$= \sum_{p\in P(k)} (-1)^{|p|}\, 2^{k-|p|} \prod_{j\in\{1,\ldots,|p|\}} (|p_j| - 1)!\; \mathrm{Tr}_{2n}\Big( (\omega^0\, \Omega)^{|p_j|} \Big)\,.$$

Then, by (2.58)- (2.59) and (2.62) we get

$$\sum_{\substack{m\in\{1,\ldots,2n\}^k\\ \lfloor m_i\rfloor_n \neq \lfloor m_l\rfloor_n,\\ 1\le i<l\le k}} \sum_{p\in P(k)} (-1)^{|p|} \prod_{j\in\{1,\ldots,|p|\}} \mathrm{Tr}_{\{m_{(p_j)_{|p_j|}}\}} \Big( \omega^0\, \Lambda^{|p_j|}_{m_{(p_j)_1},\ldots,m_{(p_j)_{(|p_j|-1)}}} (\Omega) \Big)$$
$$= \sum_{p\in P(k)} (-1)^{|p|}\, 2^{k-|p|} \prod_{j\in\{1,\ldots,|p|\}} (|p_j| - 1)!\; \mathrm{Tr}_{2n}\Big( (\omega^0\, \Omega)^{|p_j|} \Big)\,. \tag{2.63}$$

Now, note that the summands in the above result only depend on the cardinalities of the partition $p \in P(k)$. As an example consider $k = 3$ and the partitions $\{\{1\}, \{2, 3\}\}$ and $\{\{3\}, \{1, 2\}\}$ then

$$(-1)^{|p|}\, 2^{k-|p|} \prod_{j\in\{1,\ldots,|p|\}} (|p_j| - 1)!\; \mathrm{Tr}_{2n}\Big( (\omega^0\, \Omega)^{|p_j|} \Big)$$
$$= (-1)^2\, 2^{3-2} 0!\; \mathrm{Tr}_{2n}\Big( (\omega^0\, \Omega) \Big)\; 1!\; \mathrm{Tr}_{2n}\Big( (\omega^0\, \Omega)^2 \Big)$$

for either of the partitions. Thus, we simplify our result to a sum over all partitions with distinct cardinalities. To that end we first compute the number of partitions with given cardinalities $r_1, \ldots, r_s$. Note, that the number of possibilities to distribute the numbers $\{1, \ldots .k\}$ into $s$ sets with cardinalities $r_1, \ldots, r_s$ is given by the multinomial coefficient $\binom{k}{r_1, r_2, \ldots, r_s}$. In the set of partitions with cardinalities $r_1, \ldots, r_s$ we do not differentiate between permutations of equal sets. Thus we divide the multinomial coefficient by the number of permutations of sets with identical cardinality, i.e. we divide by the product $\prod_{j=1}^k | \bigcup_{i\in\{1,\ldots,s\},\, r_i = j} \{r_i\}|\,!$. Also note that the set of all partitions with distinct cardinalities can be expressed by $\{\beta \in \mathbb{N}_0^k | \sum_{i=1}^k i\, \beta_i = k\}$.

Here, $\beta_i$ encodes the number of sets with cardinality $i$. Then, the number of partitions with cardinalities given by $\alpha \in \{\beta \in \mathbb{N}_0^k | \sum_{i=1}^k i\,\beta_i = k\}$ is

$$\binom{k}{\underbrace{1,\ldots,1}_{\alpha_1\text{-times}},\ldots,\underbrace{k,\ldots,k}_{\alpha_k\text{-times}}} \prod_{i=1}^k \frac{1}{\alpha_i!} = \frac{k!}{\prod_{j=1}^k (j!)^{\alpha_j}} \prod_{i=1}^k \frac{1}{\alpha_i!} = \frac{k!}{\prod_{i=1}^k (i!)^{\alpha_i}\,\alpha_i!}\,.$$

Therefore,

$$\begin{aligned}
&\sum_{p\in P(k)} (-1)^{|p|}\, 2^{k-|p|} \prod_{j\in\{1,\ldots,|p|\}} (|p_j|-1)!\, \mathrm{Tr}_{2n}\Big((\omega^0\,\Omega)^{|p_j|}\Big) \\
&\quad = \sum_{\substack{\alpha\in\mathbb{N}_0^k,\\ \sum_{i=1}^k i\,\alpha_i = k}} (-1)^{|\alpha|}\, 2^{n-|\alpha|} \frac{k!}{\prod_{i=1}^k (i!)^{\alpha_i}\,\alpha_i!} \prod_{j=1}^k \Big((j-1)!\,\mathrm{Tr}_{2n}\Big((\omega^0\,\Omega)^j\Big)\Big)^{\alpha_j} \\
&\quad = k! \sum_{\substack{\alpha\in\mathbb{N}_0^k,\\ \sum_{i=1}^k i\,\alpha_i = k}} (-1)^{|\alpha|}\, 2^{k-|\alpha|} \prod_{j=1}^k (j^{\alpha_j}\,\alpha_j!)^{-1}\, \mathrm{Tr}_{2n}\Big((\omega^0\,\Omega)^j\Big)^{\alpha_j}
\end{aligned}$$

To finish the proof we combine the above result with (2.63). □

REMARK 2.6 The equation (2.57) can be expressed in a slightly different way using integer partitions. For an integer partition $\xi$ of $k \in \mathbb{N}$ we write $\xi \vdash k$. We will make use of two distinct ways of expressing an integer partition $\xi \vdash k$. Namely,

$$\xi = \xi_1 \geq \xi_2 \geq \cdots \xi_s \geq 0 \quad \text{and} \quad \xi = 1^{\alpha_1}\, 2^{\alpha_2} \cdots k^{\alpha_k}, \alpha \in \mathbb{N}_0^k\,.$$

Clearly, we have $|\alpha| = \sum_{i=1}^k \alpha_i = s$ and $\sum_{i=1}^k i\,\alpha_i = k$. It follows that $\alpha \in \{\beta \in \mathbb{N}_0^k | \sum_{i=1}^k i\,\beta_i = k\}$ whenever $\xi$ is an integer partition of $k$ and vice versa we can associate any $\alpha \in \{\beta \in \mathbb{N}_0^k | \sum_{i=1}^k i\,\beta_i = k\}$ with an integer partition $\xi \vdash k$.

Hence, we can represent (2.57) as

$$\begin{aligned}
&\sum_{\substack{m\in\{1,\ldots,2n\}^k\\ \lfloor m_i\rfloor_n \neq \lfloor m_l\rfloor_n,\\ 1\leq i<l\leq k}} \sum_{p\in P(k)} (-1)^{|p|} \prod_{j\in\{1,\ldots,|p|\}} \mathrm{Tr}_{\{m_{(p_j)_{|p_j|}}\}}\Big(\omega^0\,\Lambda^{|p_j|}_{m_{(p_j)_1},\ldots,m_{(p_j)_{(|p_j|-1)}}}(\Omega)\Big) \\
&\quad = k! \sum_{\xi\vdash k} (-1)^{|\alpha|}\, 2^{k-|\alpha|} \prod_{j=1}^k (j^{\alpha_j}\,\alpha_j!)^{-1}\, \mathrm{Tr}_{2n}\Big((\omega^0\,\Omega)^j\Big)^{\alpha_j}\,.
\end{aligned}$$

**Proposition 2.7** *Let $\varepsilon \in \mathbb{R}$, $\Omega = \sum_{1\leq i<j\leq 2n} \Omega_{ij}\, \mathrm{d}z^i \wedge \mathrm{d}z^j$ be a symplectic form on $\mathbb{R}^{2n}$ and let $\omega^0$ be the canonical symplectic form on $\mathbb{R}^{2n}$. Then, the Liouville measure $\lambda^\varepsilon$ of $\omega^\varepsilon := \omega^0 + \varepsilon\, \Omega$ defined by*

$$\lambda^\varepsilon := \tfrac{(-1)^{n(n-1)/2}}{n!} \underbrace{\omega^\varepsilon \wedge \cdots \wedge \omega^\varepsilon}_{n\text{-times}} \tag{2.64}$$

*satisfies*

$$\lambda^\varepsilon = \sum_{k=0}^{n} \varepsilon^k \lambda_k^\varepsilon = \Big(1 + \sum_{k=1}^{n} \varepsilon^k \nu_k^\varepsilon\Big)\, \mathrm{d}q^1 \wedge \cdots \wedge \mathrm{d}p^n$$

*where*

$$\nu_k^\varepsilon = \sum_{\substack{\alpha\in\mathbb{N}_0^k,\\ \sum_{i=1}^k i\,\alpha_i = k}} \Big(-\tfrac{1}{2}\Big)^{|\alpha|} \prod_{j=1}^{k} (j^{\alpha_j}\, \alpha_j!)^{-1}\, \mathrm{Tr}_{2n}\Big((\omega^0\,\Omega)^j\Big)^{\alpha_j}$$

*for $1 \leq k \leq n$.*

PROOF Substituting the definition of $\omega^\varepsilon$ into (2.64) we get

$$\lambda^\varepsilon = \sum_{k=0}^{n} \varepsilon^k \lambda_k^\varepsilon$$

with

$$\lambda_k^\varepsilon := \frac{(-1)^{n(n-1)/2}}{n!} \sum_{1\leq l_1<\ldots<l_k\leq n} \omega^0 \wedge \cdots \wedge \underset{l_1 th}{\Omega} \wedge \cdots \wedge \underset{l_k th}{\Omega} \wedge \cdots \wedge \omega^0\,. \tag{2.65}$$

By the fact that $a \wedge b = b \wedge a$ for any two 2-forms $a, b$

$$\begin{aligned}&\sum_{1\leq l_1<\ldots<l_k\leq n} \omega^0 \wedge \cdots \wedge \underset{l_1 th}{\Omega} \wedge \cdots \wedge \underset{l_k th}{\Omega} \wedge \cdots \wedge \omega^0 \\ &= \binom{n}{k} \underbrace{\Omega \wedge \cdots \wedge \Omega}_{k\text{-times}} \wedge \underbrace{\omega^0 \wedge \cdots \wedge \omega^0}_{n-k\text{-times}}\,.\end{aligned} \tag{2.66}$$

By definition of $\omega^\varepsilon$

$$\omega^\varepsilon = \sum_{1\leq i<j\leq 2n} (\omega_{ij}^0 + \varepsilon\,\Omega_{ij})\, \mathrm{d}z^i \wedge \mathrm{d}z^j = \tfrac{1}{2} \sum_{i,j=1}^{2n} (\omega_{ij}^0 + \varepsilon\,\Omega_{ij})\, \mathrm{d}z^i \wedge \mathrm{d}z^j\,.$$

Hence,

$$\underbrace{\Omega \wedge \cdots \wedge \Omega}_{k\text{-times}} \wedge \underbrace{\omega^0 \wedge \cdots \wedge \omega^0}_{n-k\text{-times}}$$
$$= \left(\frac{1}{2}\right)^n \sum_{\substack{\alpha,\beta \in \{1,\dots,2n\}^k \\ \gamma,\nu \in \{1,\dots,2n\}^{n-k}}} \Omega_{\alpha_1\beta_1} \cdots \Omega_{\alpha_k\beta_k} \, \omega^0_{\gamma_1\nu_1} \cdots \omega^0_{\gamma_{n-k}\nu_{n-k}}$$
$$\mathrm{d}z^{\alpha_1} \wedge \mathrm{d}z^{\beta_1} \wedge \cdots \wedge \mathrm{d}z^{\alpha_n} \wedge \mathrm{d}z^{\beta_n} \wedge \mathrm{d}z^{\gamma_1} \wedge \mathrm{d}z^{\nu_1} \wedge \cdots \wedge \mathrm{d}z^{\gamma_{n-k}} \wedge \mathrm{d}z^{\nu_{n-k}} \,. \tag{2.67}$$

Combining (2.65)- (2.67)

$$\lambda^\varepsilon_k = \frac{(-1)^{n(n-1)/2}}{k!\,(n-k)!} \left(\frac{1}{2}\right)^n \sum_{\substack{\alpha,\beta \in \{1,\dots,2n\}^k \\ \gamma,\nu \in \{1,\dots,2n\}^{n-k}}} \Omega_{\alpha_1\beta_1} \cdots \Omega_{\alpha_k\beta_k} \, \omega^0_{\gamma_1\nu_1} \cdots \omega^0_{\gamma_{n-k}\nu_{n-k}}$$
$$\mathrm{d}z^{\alpha_1} \wedge \mathrm{d}z^{\beta_1} \wedge \cdots \wedge \mathrm{d}z^{\alpha_n} \wedge \mathrm{d}z^{\beta_n} \wedge \mathrm{d}z^{\gamma_1} \wedge \mathrm{d}z^{\nu_1} \wedge \cdots \wedge \mathrm{d}z^{\gamma_{n-k}} \wedge \mathrm{d}z^{\nu_{n-k}} \,. \tag{2.68}$$

By (2.23) we have for any $I \subset \{1,\dots,n\}, |I| = k$ with complement $I^c := \{1,\dots,n\} \setminus I$ that

$$\sum_{\gamma,\nu \in (\{1,\dots,2n\}\setminus I)^{n-k}} \omega^0_{\gamma_1\nu_1} \cdots \omega^0_{\gamma_{n-k}\nu_{n-k}} \mathrm{d}z^{\gamma_1} \wedge \mathrm{d}z^{\nu_1} \wedge \cdots \wedge \mathrm{d}z^{\gamma_{n-k}} \wedge \mathrm{d}z^{\nu_{n-k}}$$
$$= \sum_{\gamma,\nu \in (I^c \cup (I^c+n))^{n-k}} \omega^0_{\gamma_1\nu_1} \cdots \omega^0_{\gamma_{n-k}\nu_{n-k}} \mathrm{d}z^{\gamma_1} \wedge \mathrm{d}z^{\nu_1} \wedge \cdots \wedge \mathrm{d}z^{\gamma_{n-k}} \wedge \mathrm{d}z^{\nu_{n-k}} \,. \tag{2.69}$$

Furthermore,

$$\omega^0_{ij} = \begin{cases} 1 & \text{for } i \le n,\ j = i+n \\ -1 & \text{for } i > n,\ j = i+n \\ 0 & \text{otherwise} \end{cases} .$$

Therefore,

$$\sum_{i,j=1}^{2n} \omega^0_{ij} \, \mathrm{d}z^i \wedge \mathrm{d}z^j = \sum_{i=1}^n \mathrm{d}q^i \wedge \mathrm{d}p^i - \sum_{i=1}^n \mathrm{d}p^i \wedge \mathrm{d}q^i = 2\sum_{i=1}^n \mathrm{d}q^i \wedge \mathrm{d}p^i \,.$$

Clearly, the above statement generalizes to

$$\sum_{\gamma,\nu\in(I^c\cup(I^c+n))^{n-k}} \omega^0_{\gamma_1\nu_1} \cdots \omega^0_{\gamma_{n-k}\nu_{n-k}} \mathrm{d}z^{\gamma_1}\wedge \mathrm{d}z^{\nu_1}\wedge\cdots\wedge \mathrm{d}z^{\gamma_{n-k}}\wedge \mathrm{d}z^{\nu_{n-k}} \\ = 2^{n-k}\sum_{\gamma\in(I^c)^{n-k}} \mathrm{d}q^{\gamma_1}\wedge \mathrm{d}p^{\gamma_1}\wedge\cdots\wedge \mathrm{d}q^{\gamma_{n-k}}\wedge \mathrm{d}p^{\gamma_{n-k}} \tag{2.70}$$

where $I\subset\{1,\dots,n\}, |I|=k$ with complement $I^c:=\{1,\dots,n\}\setminus I$. By the skew-symmetry of the wedge product we can conclude that the summands in the above result are zero whenever $\gamma\in(I^c)^{n-k}$ satisfies that $\gamma_i=\gamma_j$ for some $1\le i<j\le n-k$. Hence,

$$\sum_{\gamma\in(I^c)^{n-k}} \mathrm{d}q^{\gamma_1}\wedge \mathrm{d}p^{\gamma_1}\wedge\cdots\wedge \mathrm{d}q^{\gamma_{n-k}}\wedge \mathrm{d}p^{\gamma_{n-k}} \\ = \sum_{\substack{\gamma\in(I^c)^{n-k},\\ \gamma_i\neq\gamma_j,\\ 1\le i<j\le n-k}} \mathrm{d}q^{\gamma_1}\wedge \mathrm{d}p^{\gamma_1}\wedge\cdots\wedge \mathrm{d}q^{\gamma_{n-k}}\wedge \mathrm{d}p^{\gamma_{n-k}}\,. \tag{2.71}$$

We are now at the point where it's rather straight forward to deduce $\lambda_0^\varepsilon$. Combining (2.68) - (2.71) we get

$$\lambda_0^\varepsilon = \frac{(-1)^{n(n-1)/2}}{(n)!}\sum_{\substack{\gamma\in\{1,\dots,n\}^n,\\ \gamma_i\neq\gamma_j,\\ 1\le i<j\le n}} \mathrm{d}q^{\gamma_1}\wedge \mathrm{d}p^{\gamma_1}\wedge\cdots\wedge \mathrm{d}q^{\gamma_n}\wedge \mathrm{d}p^{\gamma_n}\,. \tag{2.72}$$

By the fact that wedge products of two-forms commute we have that

$$\mathrm{d}q^{\gamma_1}\wedge \mathrm{d}p^{\gamma_1}\wedge\cdots\wedge \mathrm{d}q^{\gamma_n}\wedge \mathrm{d}p^{\gamma_n} = \mathrm{d}q^1\wedge \mathrm{d}p^1\wedge\cdots\wedge \mathrm{d}q^n\wedge \mathrm{d}p^n \tag{2.73}$$

for any $\gamma\in\{1,\dots,n\}^n$ satisfying $\gamma_i\neq\gamma_j$ for every $1\le i<j\le n-k$. In addition by (2.48)

$$\mathrm{d}q^1\wedge \mathrm{d}p^1\wedge\cdots\wedge \mathrm{d}q^{n-2}\wedge \mathrm{d}p^{n-2}\wedge \mathrm{d}q^{n-1}\wedge \mathrm{d}p^{n-1}\wedge \mathrm{d}q^n\wedge \mathrm{d}p^n \\ = (-1)^{(n(n-1)/2)}\,\mathrm{d}q^1\wedge\cdots\wedge \mathrm{d}q^n\wedge \mathrm{d}p^1\wedge\cdots\wedge \mathrm{d}p^n\,. \tag{2.74}$$

Note here that the cardinality of the set of all multiindices in $(I^c)^{n-k}$ with distinct indices is given by the number of all permutations of the set $\{1,\ldots,n-k\}$ which is $(n-k)!$. Thus,

$$\sum_{\substack{\gamma\in(I^c)^{n-k},\\ \gamma_i\neq\gamma_j,\\ 1\leq i<j\leq n-k}} 1 = |\{\gamma\in(I^c)^{n-k}|\gamma_i\neq\gamma_j \quad \forall\, 1\leq i<j\leq n-k\}| = (n-k)! \tag{2.75}$$

and in particular

$$|\{\{1,\ldots,n\}^n|\gamma_i\neq\gamma_j \quad \forall\, 1\leq i<j\leq n\}| = n!\,. \tag{2.76}$$

By combining (2.72) - (2.74) and (2.76) we obtain

$$\lambda_0^\varepsilon = \mathrm{d}q^1\wedge\cdots\wedge\mathrm{d}q^n\wedge\mathrm{d}p^1\wedge\cdots\wedge\mathrm{d}p^n\,.$$

From now on let $k\geq 1$. By the anti-commutativity of the wedge product we have for $\alpha,\beta\in\{1,\ldots,2n\}^k$ and $\gamma,\nu\in\{1,\ldots,2n\}^{n-k}$ that

$$\mathrm{d}z^{\alpha_1}\wedge\mathrm{d}z^{\beta_1}\wedge\cdots\wedge\mathrm{d}z^{\alpha_n}\wedge\mathrm{d}z^{\beta_n}\wedge\mathrm{d}z^{\gamma_1}\wedge\mathrm{d}z^{\nu_1}\wedge\cdots\wedge\mathrm{d}z^{\gamma_{n-k}}\wedge\mathrm{d}z^{\nu_{n-k}} = 0$$

whenever two of the indices are identical. Hence, we have for $I\subset\{1,\ldots,2n\}$, $|I|=2k$, $\alpha,\beta\in I^k$ and $\gamma,\nu\in\{1,\ldots,2n\}^{n-k}$ that

$$\begin{aligned}\mathrm{d}z^{\wedge\alpha}\wedge\mathrm{d}z^{\wedge\beta}\wedge\mathrm{d}z^{\wedge\gamma}\wedge\mathrm{d}z^{\wedge\nu}\neq 0 \Longleftrightarrow & \bigcup_{i\in\{1,\ldots,k\}}\{\alpha_i,\beta_i\} = I \qquad \text{and}\\ & \bigcup_{i\in\{1,\ldots,n-k\}}\{\gamma_i,\nu_i\} = \{1,\ldots,2n\}\backslash I\,.\end{aligned} \tag{2.77}$$

Combining (2.69)- (2.71) and (2.77) we conclude that for non-vanishing terms in (2.68) the multi-indices $\alpha,\beta$ and $\gamma,\nu$ must stem from disjoint index sets. We obtain

$$\begin{aligned}\lambda_k^\varepsilon =& \frac{(-1)^{n(n-1)/2}}{k!\,(n-k)!}\left(\frac{1}{2}\right)^k \sum_{\substack{I\subset\{1,\ldots,n\},\\ |I|=k}} \sum_{\alpha,\beta\in L^k} \sum_{\substack{\gamma\in(I^c)^{n-k},\\ \gamma_i\neq\gamma_j,\\ 1\leq i<j\leq n-k}} \Omega_{\alpha_1\beta_1}\cdots\Omega_{\alpha_k\beta_k}\\ & \mathrm{d}z^{\alpha_1}\wedge\mathrm{d}z^{\beta_1}\wedge\cdots\wedge\mathrm{d}z^{\alpha_k}\wedge\mathrm{d}z^{\beta_k}\wedge\mathrm{d}q^{\gamma_1}\wedge\mathrm{d}p^{\gamma_1}\wedge\cdots\wedge\mathrm{d}q^{\gamma_{n-k}}\wedge\mathrm{d}p^{\gamma_{n-k}}\,.\end{aligned} \tag{2.78}$$

where $L := I \cup (I+n)$. By Lemma 2.3 with $B^j = \Omega$, $j = 1, \ldots, k$ we have

$$\begin{aligned}
&\sum_{\alpha,\beta \in L^k} \Omega_{\alpha_1\beta_1} \cdots \Omega_{\alpha_k\beta_k} \, \mathrm{d}z^{\alpha_1} \wedge \mathrm{d}z^{\beta_1} \wedge \cdots \wedge \mathrm{d}z^{\alpha_k} \wedge \mathrm{d}z^{\beta_k} \\
&\qquad = \sum_{p \in P(k)} (-1)^{|p|} \sum_{\substack{m \in L^k \\ \lfloor m_i \rfloor_n \neq \lfloor m_j \rfloor_n, \\ 1 \le i < j \le k}} \\
&\qquad\qquad \prod_{j \in \{1,\ldots,|p|\}} \mathrm{Tr}_{\{m_{(p_j)_{|p_j|}}\}} \Big( \omega^0 \, \Lambda^{|p_j|}_{m_{(p_j)_1},\ldots,m_{(p_j)_{(|p_j|-1)}}} (\Omega) \Big) \\
&\qquad\quad \mathrm{d}q^{\lfloor m_1 \rfloor_n} \wedge \mathrm{d}p^{\lfloor m_1 \rfloor_n} \wedge \cdots \wedge \mathrm{d}q^{\lfloor m_k \rfloor_n} \wedge \mathrm{d}p^{\lfloor m_k \rfloor_n} .
\end{aligned} \tag{2.79}$$

Analogous to (2.73) and (2.74) it follows for every $m \in L^k$, $\lfloor m_i \rfloor_n \neq \lfloor m_j \rfloor_n$, $1 \le i < j \le k$ and every $\gamma \in (I^c)^{n-k}$ that

$$\begin{aligned}
&\mathrm{d}q^{\lfloor m_1 \rfloor_n} \wedge \mathrm{d}p^{\lfloor m_1 \rfloor_n} \wedge \cdots \wedge \mathrm{d}q^{\lfloor m_k \rfloor_n} \wedge \mathrm{d}p^{\lfloor m_k \rfloor_n} \\
&\qquad \wedge \mathrm{d}q^{\gamma_1} \wedge \mathrm{d}p^{\gamma_1} \wedge \cdots \wedge \mathrm{d}q^{\gamma_{n-k}} \wedge \mathrm{d}p^{\gamma_{n-k}} \\
&\qquad = (-1)^{n(n-1)/2} \, \mathrm{d}q^1 \wedge \cdots \wedge \mathrm{d}q^n \wedge \mathrm{d}p^1 \wedge \cdots \wedge \mathrm{d}p^n .
\end{aligned} \tag{2.80}$$

Combining (2.75) and (2.78) - (2.80) yields

$$\begin{aligned}
\lambda_k^\varepsilon = &\frac{1}{k!} \left(\frac{1}{2}\right)^k \sum_{p \in P(k)} (-1)^{|p|} \sum_{\substack{I \subset \{1,\ldots,n\}, \\ |I| = k}} \sum_{\substack{m \in L^k \\ \lfloor m_i \rfloor_n \neq \lfloor m_j \rfloor_n, \\ 1 \le i < j \le k}} \\
&\qquad \prod_{j \in \{1,\ldots,|p|\}} \mathrm{Tr}_{\{m_{(p_j)_{|p_j|}}\}} \Big( \omega^0 \, \Lambda^{|p_j|}_{m_{(p_j)_1},\ldots,m_{(p_j)_{(|p_j|-1)}}} (\Omega) \Big) \\
&\quad \mathrm{d}q^1 \wedge \cdots \wedge \mathrm{d}q^n \wedge \mathrm{d}p^1 \wedge \cdots \wedge \mathrm{d}p^n .
\end{aligned} \tag{2.81}$$

As is easy to see, it holds that

$$\begin{aligned}
&\{m \in \{1, \ldots, 2n\}^k | \lfloor m_i \rfloor_n \neq \lfloor m_j \rfloor_n \quad \forall\, 1 \le i < j \le k\} \\
&\qquad = \bigcup_{\substack{I \subset \{1,\ldots,n\}, \\ |I| = k}} \{m \in L_I^k | \lfloor m_i \rfloor_n \neq \lfloor m_j \rfloor_n \quad \forall\, 1 \le i < j \le k\} .
\end{aligned}$$

where additionally for $I_1, I_2 \subset \{1, \ldots, n\}$, $|I_1| = |I_2| = k$, $I_1 \neq I_2$ we have

$$\begin{aligned}
\emptyset = &\{m \in L_{I_1}^k | \lfloor m_i \rfloor_n \neq \lfloor m_j \rfloor_n \quad \forall\, 1 \le i < j \le k\} \\
&\cap \{m \in L_{I_2}^k | \lfloor m_i \rfloor_n \neq \lfloor m_j \rfloor_n \quad \forall\, 1 \le i < j \le k\} .
\end{aligned}$$

Therefore, we represent (2.81) as

$$\lambda_k^\varepsilon = \frac{1}{k!}\left(\frac{1}{2}\right)^k \sum_{p\in P(k)} (-1)^{|p|} \sum_{\substack{m\in\{1,\dots,2n\}^k\\ \lfloor m_i\rfloor_n \neq \lfloor m_j\rfloor_n,\\ 1\le i<j\le k}} \prod_{j\in\{1,\dots,|p|\}} \mathrm{Tr}_{\{m_{(p_j)_{|p_j|}}\}}\Big(\omega^0\, \Lambda^{|p_j|}_{m_{(p_j)_1},\dots,m_{(p_j)_{(|p_j|-1)}}}(\Omega)\Big) \mathrm{d}q^1\wedge\dots\wedge \mathrm{d}q^n \wedge \mathrm{d}p^1\wedge\dots\wedge\mathrm{d}p^n\,.$$

Applying Lemma 2.5 to the above result shows

$$\begin{aligned}\lambda_k^\varepsilon &= \frac{1}{k!\,2^k}\,k! \sum_{\substack{\alpha\in\mathbb{N}_0^k,\\ \sum_{i=1}^k i\,\alpha_i = k}} (-1)^{|\alpha|}\,2^{k-|\alpha|} \prod_{j=1}^k (j^{\alpha_j}\,\alpha_j!)^{-1}\,\mathrm{Tr}_{2n}\Big((\omega^0\,\Omega)^j\Big)^{\alpha_j} \\ &\quad \mathrm{d}q^1\wedge\dots\wedge \mathrm{d}q^n \wedge \mathrm{d}p^1\wedge\dots\wedge\mathrm{d}p^n \\ &= \sum_{\substack{\alpha\in\mathbb{N}_0^k,\\ \sum_{i=1}^k i\,\alpha_i = k}} \Big(-\tfrac{1}{2}\Big)^{|\alpha|} \prod_{j=1}^k (j^{\alpha_j}\,\alpha_j!)^{-1}\,\mathrm{Tr}_{2n}\Big((\omega^0\,\Omega)^j\Big)^{\alpha_j} \\ &\quad \mathrm{d}q^1\wedge\dots\wedge \mathrm{d}q^n \wedge \mathrm{d}p^1\wedge\dots\wedge\mathrm{d}p^n\end{aligned}$$

which finishes proof. □

**Corollary 2.8** *Let $\varepsilon > 0$ small enough, $\Omega$ a symplectic form on $\mathbb{R}^{2n}$ with the coefficients $\Omega_{ij}\in S^0(\varepsilon,\mathbb{R})$ and let $\omega^0$ be the canonical symplectic form on $\mathbb{R}^{2n}$. Then, the Liouville measure $\lambda^\varepsilon$ of $\omega^\varepsilon := \omega^0 + \varepsilon\,\Omega$ is given by*

$$\lambda^\varepsilon = \nu^\varepsilon\,\mathrm{d}q^1\wedge\mathrm{d}q^2\wedge\dots\wedge\mathrm{d}p^n$$

*with*

$$\nu^\varepsilon = 1 - \tfrac{1}{2}\,\varepsilon\,\mathrm{Tr}_{2n}(\omega^0\,\Omega)) + \tfrac{1}{8}\,\varepsilon^2\,\mathrm{Tr}_{2n}(\omega^0\,\Omega)^2 - \tfrac{1}{4}\,\varepsilon^2\,\mathrm{Tr}_{2n}(\omega^0\,\Omega\,\omega^0\,\Omega) + \mathcal{O}(\varepsilon^3)\,.$$

PROOF By Proposition 2.7, $\nu^\varepsilon = 1 + \sum_{k=1}^n \varepsilon^k\,\nu_k^\varepsilon$ with

$$\nu_k^\varepsilon = \sum_{\substack{\alpha\in\mathbb{N}_0^k,\\ \sum_{i=1}^k i\,\alpha_i = k}} \Big(-\tfrac{1}{2}\Big)^{|\alpha|} \prod_{j=1}^k (j^{\alpha_j}\,\alpha_j!)^{-1}\,\mathrm{Tr}_{2n}\Big((\omega^0\,\Omega)^j\Big)^{\alpha_j}$$

for $1\le k\le n$. Then,

$$\nu_1^\varepsilon = -\tfrac{1}{2}\,\mathrm{Tr}_{2n}\Big((\omega^0\,\Omega)\Big)\,.$$

and

$$
\begin{aligned}
\nu_2^\varepsilon = & \left(-\tfrac{1}{2}\right)^2 \, (1^2\, 2!)^{-1} \, \mathrm{Tr}_{2n}\Big((\omega^0\, \Omega)\Big)^2 \\
& + \left(-\tfrac{1}{2}\right) \, (2^1\, 1!)^{-1} \, \mathrm{Tr}_{2n}\Big((\omega^0\, \Omega)^2\Big) \\
= & \tfrac{1}{8} \, \mathrm{Tr}_{2n}\Big((\omega^0\, \Omega)\Big)^2 \\
& - \tfrac{1}{4} \, \mathrm{Tr}_{2n}\Big((\omega^0\, \Omega)^2\Big) \, .
\end{aligned}
$$

Since, $\Omega_{ij} \in S^0(\varepsilon, \mathbb{R})$ this finishes the proof. □

**Theorem 2.9** *Let $\Omega = \frac{1}{2} \sum_{i,j \in \{1,\dots,2n\}} \Omega_{ij} \, \mathrm{d}z^i \wedge \mathrm{d}z^j$ a symplectic form. Then, the Liouville measure of $\Omega$ is given by*

$$
\lambda = \sum_{\substack{\alpha \in \mathbb{N}_0^n, \\ \sum_{i=1}^n i\, \alpha_i = n}} \left(-\tfrac{1}{2}\right)^{|\alpha|} \prod_{j=1}^{n} (j^{\alpha_j} \, \alpha_j!)^{-1} \, \mathrm{Tr}_{2n}\Big((\omega^0\, \Omega)^j\Big)^{\alpha_j} \, \mathrm{d}q^1 \wedge \cdots \wedge \mathrm{d}p^n \, .
$$

PROOF Let $\Omega = \frac{1}{2} \sum_{i,j \in \{1,\dots,2n\}} \Omega_{ij} \, \mathrm{d}z^i \wedge \mathrm{d}z^j$ a symplectic form and define $\tilde{\omega} = \omega^0 + \Omega$ with Liouville measure $\tilde{\lambda}$. By $(2.19)$ we have that $\lambda = \tilde{\lambda}_n$. Then, the assertion follows by applying Proposition 2.7 with $\omega^\varepsilon = \tilde{\omega}$ and $\varepsilon = 1$. □

## 2.3 Assumptions

We consider a composite system with state space

$$
\mathcal{H} = L^2(\mathbb{R}^n) \otimes \mathcal{H}_\mathrm{f} \cong L^2(\mathbb{R}^n, \mathcal{H}_\mathrm{f}) \, .
$$

Here $L^2(\mathbb{R}^n)$ is the state space of the 'slow degrees of freedom' and the separable Hilbert space $\mathcal{H}_\mathrm{f}$ is the state space of 'fast or fiber degrees of freedom'.

**Assumption 2.10** *We consider a Hamiltonian $\hat{H}^\varepsilon$ on $\mathcal{H}$ given as the Weyl quantization of a symbol*

$$
H(z) = H_0(z) + \varepsilon H^1(z) + \xi \cdot z
$$

*with $H_0 \in S^0(\mathcal{B}_{sa}(\mathcal{H}_\mathrm{f}))$, $H^1$ a classical symbol in $S^0(\varepsilon, \mathcal{B}_{sa}(\mathcal{H}_\mathrm{f}))$ and $\xi \in \mathbb{R}^{2n}$.*

Then $\hat{H}_0^\varepsilon$ and $\hat{H^1}^\varepsilon$ are bounded operators on $\mathcal{H}$. Thus, $\hat{H}^\varepsilon$ is self-adjoint on $D(\hat{H}^\varepsilon) \subset \mathcal{H}$ with $D(\hat{H}^\varepsilon)$ being the maximal domain of the operator $\xi_q \cdot x - \mathrm{i}\, \varepsilon\, \xi_p \cdot \nabla_x$ where $\xi = \binom{\xi_q}{\xi_p}$.

**Assumption 2.11** (Gap Condition) *We assume that the principal symbol $H_0(z)$ of the Hamiltonian $H(z)$ has a non-degenerate eigenvalue $e_0(z)$ such that $e_0 : \mathbb{R}^{2n} \to \mathbb{R}$ is continuous and satisfies the uniform gap condition*

$$\operatorname{dist}(e_0(z), \sigma(H_0(z)) \backslash \{e_0(z)\}) \geq g > 0 \tag{2.82}$$

*for every $z \in \mathbb{R}^{2n}$. We denote the eigenprojection of $H_0(z)$ associated to the eigenvalue $e_0(z)$ by $P_0(z)$, i.e.*

$$H_0(z)\, P_0(z) = e_0(z)\, P_0(z).$$

The gap condition implies that for any $z_0 \in \mathbb{R}^{2n}$ there exists a neighborhood $U_{z_0} \subset \mathbb{R}^{2n}$ of $z_0$ such that the positively oriented complex circle $\gamma(z_0) = \{|z - e_0(z_0)| = \frac{g}{2}\}$ satisfies

$$\operatorname{dist}\Big(\gamma(z_0), \sigma(H_0(z))\}\Big) \geq \frac{g}{4} \qquad \text{for all } z \in U_{z_0}\,.$$

Therefore the eigenprojection

$$P_0(z) = \frac{\mathrm{i}}{2\pi} \oint_{\gamma(z_0)} (H_0(z) - \xi)^{-1}\, \mathrm{d}\xi \qquad \text{for all } z \in U_{z_0}$$

is smooth and bounded with all its derivatives on $U_{z_0}$. As is easy to see, it follows that $P_0 \in S^0(\mathcal{B}(\mathcal{H}_\mathrm{f}))$. Moreover, since $H_0 \in S^0(\mathcal{B}_{sa}(\mathcal{H}_\mathrm{f}))$ and $H_0(z)\, P_0(z) = e_0(z)\, P_0(z)$ we conclude $e_0 \in S^0(\mathbb{R})$.

# 3 Space-Adiabatic Perturbation Theory

The main goal of this chapter is to derive a effective theory for systems with operator-valued symbol within the almost-invariant subspace $\hat{\Pi}^{\varepsilon}\mathcal{H}$. The derivation of the space-adiabatic projection $\hat{\Pi}^{\varepsilon}$ is well known and was done several times in the past (see e.g. [Teu03], [NS04] or [EW96]). Nevertheless, we derive $\hat{\Pi}^{\varepsilon}$ in Section 3.1 where we slightly vary the derivation. This variation leads to a pointwise projection $\mathcal{P}^{\varepsilon}$ that is used Section 3.3 to define the modified Berry connection $\nabla^{\varepsilon}$. In Section 3.2 we construct scalar effective operators that approximate the action of operator-valued symbols $B \in S^k(\varepsilon, \mathcal{B}(\mathcal{H}_{\mathrm{f}}))$, $k \geq 0$ up to any order in $\varepsilon$. As already mentioned, in the third section of this chapter we define the modified Berry connection from which we deduce a symplectic form $\omega^{\varepsilon}$. This symplectic form together with the effective operator $h$ of the Hamiltonian $H$ defines a $\varepsilon$-dependent Hamiltonian system $(T^*\mathbb{R}^n\omega^{\varepsilon}, h)$. Later, in Chapter 4 and 5 we show that this $\varepsilon$-dependent Hamiltonian system incorporates most expressions of the semiclassical approximation of expectation values for stationary state as well as the time propagation of observables with operator-valued symbols in the Heisenberg picture of quantum mechanics.

## 3.1 The Almost-Invariant Subspace

In this section we will show that there is a projection $\hat{\Pi}^{\varepsilon}$ associated to an isolated eigenvalue $e_0(z)$ of $H_0(z)$ such that the subspace $\hat{\Pi}^{\varepsilon}\mathcal{H}$ is almost-invariant under the action of $\hat{H}^{\varepsilon}$. In addition, we prove the existence of a pointwise rank-one projection $\mathcal{P}^{\varepsilon}(z)$ taking values in the self-adjoint trace-class operators $\mathcal{J}_{\mathrm{sa}}(\mathcal{H}_{\mathrm{f}})$ that is closely related to the adiabatic projection $\hat{\Pi}^{\varepsilon}$. In Section 3.3 we will use $\mathcal{P}^{\varepsilon}$ to define a modified Berry connection leading us to a symplectic form on the classical phase space. The existence of the almost-invariant subspace $\hat{\Pi}^{\varepsilon}\mathcal{H}$ was proven several times in the literature. We will follow the strategy of the proof of [Teu03, Theorem 3.2] which is due to Nenciu and Sordoni [NS04] and based on the work of Helffer and

Sjöstrand [HS90a]. The basic idea is to recursively construct a classical symbol $\pi \in S^0(\varepsilon, \mathcal{B}_{\mathrm{sa}}(\mathcal{H}_{\mathrm{f}}))$ satisfying

$$\begin{aligned} &\text{(i)} \quad \pi \# \pi = \pi + \mathcal{O}(\varepsilon^\infty) \\ &\text{(ii)} \quad H \,\#\, (\pi) - \pi \,\#\, H = \mathcal{O}(\varepsilon^\infty)\,. \end{aligned}$$

In addition, it is known that $\pi$ indeed takes value in the trace-class operators, i.e. $\pi \in S^0(\varepsilon, \mathcal{J}_{\mathrm{sa}}(\mathcal{H}_{\mathrm{f}}))$, see [ST13, Proposition 1]. The main idea in the construction of $\mathcal{P}^\varepsilon$ is to decompose $\pi$ into a almost pointwise projection $P$ and a remainder $\tilde{\pi}$. This is achieved by extending the recursion of $\pi$ by two additional steps. Then $\hat{\pi}^\varepsilon$ and $P(z)$ are almost projections as operators acting on $\mathcal{H}$ and $\mathcal{H}_{\mathrm{f}}$, respectively. Finally, one defines $\hat{\Pi}^\varepsilon$ and $\mathcal{P}^\varepsilon(z)$ as spectral projections of $\hat{\pi}^\varepsilon$ and $P(z)$ to their spectrum near one.

**Lemma 3.1** *Let Assumption 2.10 and 2.11 hold and fix $N \in \mathbb{N}_0$. Then there exist unique $P_j, \tilde{\pi}_i \in S^0(\mathcal{J}_{\mathrm{sa}}(\mathcal{H}_{\mathrm{f}}))$, $i, j \in \mathbb{N}_0$, $j \leq N$, $i \leq N-1$ such that $P^{(N)} = \sum_{j=0}^{N} \varepsilon^j P_j$, $\tilde{\pi}^{(N-1)} = \sum_{j=0}^{N-1} \varepsilon^j \tilde{\pi}_j$ and $\pi^{(N)} = P^{(N)} + \varepsilon\, \tilde{\pi}^{(N-1)}$ satisfy*

$$\begin{aligned} &\textit{(i)} \quad P^{(N)} P^{(N)} - P^{(N)} = \mathcal{O}(\varepsilon^{N+1}) \\ &\textit{(ii)} \quad P_0^\perp\, \tilde{\pi}^{(N-1)}\, P_0 = P_0\, \tilde{\pi}^{(N-1)}\, P_0^\perp = 0 \\ &\textit{(iii)} \quad \pi^{(N)} \,\#\, \pi^{(N)} - \pi^{(N)} = \mathcal{O}(\varepsilon^{N+1}) \\ &\textit{(iv)} \quad H \,\#\, \pi^{(N)} - \pi^{(N)} \,\#\, H = \mathcal{O}(\varepsilon^{N+1}) \end{aligned} \tag{3.1}$$

*where $P_0$ is the eigenprojection of $H_0$ corresponding to $e_0$.*

PROOF We start our proof with the following observation. Recall that $P_0$ is the eigenprojection of $H_0$ to the eigenvalue $e_0$. Then, making use of the asymptotic expansion of the Moyal product it hold that $P_0 \,\#\, P_0 = P_0\, P_0 + \mathcal{O}(\varepsilon) = P_0 + \mathcal{O}(\varepsilon)$ as well as $[\, H \,, P_0\,]_\# = [\, H_0 \,, P_0\,] + \mathcal{O}(\varepsilon) = \mathcal{O}(\varepsilon)$. In addition, since $e_0$ is non-degenerate by assumption, $P_0$ takes value in the self-adjoint rank-one projections on $\mathcal{H}_{\mathrm{f}}$ and thus $P_0 \in S^0(\mathcal{J}(\mathcal{H}_{\mathrm{f}}))$.

Now, assume there are $P_j \in S^0(\mathcal{J}_{\mathrm{sa}}(\mathcal{H}_{\mathrm{f}}))$ for $0 \leq j \leq N$ and $\tilde{\pi}_j \in S^0(\mathcal{J}_{\mathrm{sa}}(\mathcal{H}_{\mathrm{f}}))$ for $0 \leq j \leq N-1$ such that (i)-(iv) holds. We prove it for $N+1$. By induction assumption

$$P^{(N)}\, P^{(N)} - P^{(N)} = \mathcal{O}(\varepsilon^{N+1})\,.$$

Then, defining $\tilde{G}_{N+1}$by

$$\tilde{G}_{N+1} := (P^{(N)}\, P^{(N)})_{N+1}, \tag{3.2}$$

$P_{N+1}$ must satisfy

$$0 = (P^{(N+1)}\, P^{(N+1)} - P^{(N+1)})_{N+1} = P_0\, P_{N+1} + P_{N+1}\, P_0 - P_{N+1} + \tilde{G}_{N+1}\,.$$

This uniquely determines the diagonal part of $P_{N+1}$ to be

$$P^D_{N+1} = -P_0\, \tilde{G}_{N+1}\, P_0 + P_0^\perp\, \tilde{G}_{N+1}\, P_0^\perp\,. \tag{3.3}$$

In addition, we have

$$\begin{aligned} P_0\, \tilde{G}_{N+1}\, (\mathbf{1}_{\mathcal{H}_\mathrm{f}} - P_0) =& \Big(P_0\, \varepsilon^{-(N+1)}(P^{(N)}\, P^{(N)} - P^{(N)})\, (\mathbf{1}_{\mathcal{H}_\mathrm{f}} - P_0)\Big)_0 \\ =& \Big(\varepsilon^{-(N+1)}\, P^{(N)}\, (P^{(N)}\, P^{(N)} - P^{(N)})\, (\mathbf{1}_{\mathcal{H}_\mathrm{f}} - P^{(N)})\Big)_0 \\ =& \Big(\, \varepsilon^{-(N+1)}(P^{(N)}\, P^{(N)} - P^{(N)})\, (P^{(N)} - P^{(N)}\, P^{(N)})\Big)_0 \\ =& 0\,. \end{aligned} \tag{3.4}$$

Similarly, $(\mathbf{1}_{\mathcal{H}_\mathrm{f}} - P_0)\, \tilde{G}_{N+1}\, P_0 = 0$ showing that $\tilde{G}_{N+1}$ is diagonal with respect to $P_0$. As a consequence,

$$(P^{(N)} + \varepsilon^{N+1}\, P^D_{N+1})\, (P^{(N)} + \varepsilon^{N+1}\, P^D_{N+1}) - (P^{(N)} + \varepsilon^{N+1}\, P^D_{N+1}) = \mathcal{O}(\varepsilon^{N+2})\,.$$

We define $u^{(N)} := P^{(N)} + \varepsilon^{N+1}\, P^D_{N+1} + \varepsilon\tilde{\pi}^{(N-1)}$. Then, (iii) yields

$$u^{(N)} \,\#\, u^{(N)} - u^{(N)} = \mathcal{O}(\varepsilon^{N+1})\,.$$

Therefore,

$$w^{(N)} := u^{(N)} + \varepsilon^{N+1}\, \tilde{\pi}_N$$

has to satisfy

$$0 = (w^{(N)} \,\#\, w^{(N)} - w^{(N)})_{N+1} = P_0\, \tilde{\pi}_N + \tilde{\pi}_N\, P_0 - \tilde{\pi}_N + G_{N+1}$$

where

$$G_{N+1} := (u^{(N)} \,\#\, u^{(N)})_{N+1}\,.$$

This uniquely determines $\tilde{\pi}_N$ to be

$$\tilde{\pi}_N = -P_0\, G_{N+1}\, P_0 + P_0^\perp\, G_{N+1}\, P_0^\perp\,. \tag{3.5}$$

The proof of $G_{N+1}$ being diagonal with respect to $P_0$ is very similar to (3.4). Consequently, $\tilde{\pi}_N$ is diagonal with respect to $P_0$ and $w^{(N)}$ satisfies (iii) up to order $\mathcal{O}(\varepsilon^{N+2})$.

Finally, using induction assumption (iv) we have

$$[\,H\,,w^{(N)}\,]_{\#} = \mathcal{O}(\varepsilon^{N+2})$$

and define

$$([\,H\,,w^{(N)}\,]_{\#})_{N+1} = F_{N+1}\,.$$

The diagonal part of $P^{D}_{N+1}$ and $\tilde{\pi}_{N+1}$ being fixed already, $P^{OD}_{N+1}$ has to fulfill the equation $[H_0, P^{OD}_{N+1}] = -F_{N+1}$, i.e.

$$H_0\,P_0\,P^{OD}_{N+1}\,P_0^{\perp} - P_0\,P^{OD}_{N+1}\,P_0^{\perp}\,H_0 = -P_0\,P^{OD}_{N+1}\,P_0^{\perp}\,(H_0 - e_0) = -P_0\,F_{N+1}\,P_0^{\perp}$$

and

$$H_0\,P_0^{\perp}\,P^{OD}_{N+1}\,P_0 - P_0^{\perp}\,P^{OD}_{N+1}\,P_0\,H_0 = (H_0 - e_0)\,P_0^{\perp}\,P^{OD}_{N+1}\,P_0 = -P_0^{\perp}\,F_{N+1}\,P_0\,.$$

This uniquely determines the off diagonal part of $P_{N+1}$ to be

$$P^{OD}_{N+1} = P_0\,F_{n+1}\,(H_0 - e_0)^{-1}\,P_0^{\perp} - P_0^{\perp}\,(H_0 - e_0)^{-1}\,F_{n+1}\,P_0\,. \tag{3.6}$$

where $(H_0 - e_0)^{-1} = P_0^{\perp}\,(H_0 - e_0)^{-1}\,P_0^{\perp}$ is the reduced resolvent on $P_0^{\perp}\mathcal{H}_{\mathrm{f}}$. Since $w^{(N)}\#w^{(N)} - w^{(N)} = \mathcal{O}(\varepsilon^{N+2})$ and $w_0 = P_0$ we have

$$\begin{aligned} P_0\,F_{N+1}\,P_0 &= \Big(\varepsilon^{N+1}\,(P_0\,H\,\#\,w^{(N)}\,P_0 - P_0\,H\,\#\,w^{(N)}\,P_0)\Big)_0 \\ &= \Big(\varepsilon^{N+1}\,(w^{(N)}\,\#\,H\,\#\,w^{(N)}\,\#\,w^{(N)} - w^{(N)}\,\#\,H\,\#\,w^{(N)}\,\#\,w^{(N)})\Big)_0 \\ &= 0 \end{aligned}$$

and similarly $(\mathbf{1}_{\mathcal{H}_{\mathrm{f}}} - P_0)\,F_{N+1}\,(\mathbf{1}_{\mathcal{H}_{\mathrm{f}}} - P_0) = 0$. So, $F_{N+1}$ is off diagonal with respect to $P_0$. Therefore,

$$\Big[\,H\,,P^{(N+1)} + \varepsilon\tilde{\pi}^{(N)}\Big] = \mathcal{O}(\varepsilon^{N+2})\,.$$

To sum up, we have that $P^{(N+1)} + \varepsilon\,\tilde{\pi}^{(N)}$ satisfies (i)-(iv). What is left is to proof that $P_{N+1}$ and $\tilde{\pi}_N$ take value in the self-adjoint linear operators and are bounded with all their derivatives with respect to the trace norm. Clearly, $G_{N+1}$ takes value in the trace-class operators by definition. In addition, by (2.11) we conclude $G_{N+1} \in S^0(\mathcal{J}(\mathcal{H}_{\mathrm{f}}))$ and $F_{N+1} \in S^0(\mathcal{J}(\mathcal{H}_{\mathrm{f}}))$ which directly implies $P_{N+1} \in S^0(\mathcal{J}(\mathcal{H}_{\mathrm{f}}))$ and $\tilde{\pi}_N \in S^0(\mathcal{J}(\mathcal{H}_{\mathrm{f}}))$. Regarding the self-adjointness note that $\tilde{G}_{N+1}$ is obviously self-adjoint for all $z \in \mathbb{R}^{2n}$ by the symmetry of its definition and since all $P_j$ for $0 \leq j \leq N$ are self-adjoint by assumption. Therefore, the diagonal part of $P_{N+1}$ is self-adjoint. By the expansion of the Moyal product for classical symbols (2.9) together with (2.7) it is easy to see that $G_{N+1}$ takes value in the self-adjoint operators and thus also $\tilde{\pi}_N$. Similarly, by (2.7) the self-adjointness of $F_{N+1}$ and thus also $P^{OD}_{N+1}$ follows which finishes the proof. □

**Proposition 3.2** (Super-adiabatic projection) *Let Assumption 2.10 and 2.11 hold and let $\varepsilon > 0$ small enough. Then there exist a pointwise rank-one projection $\mathcal{P}^\varepsilon \in S^0(\varepsilon, \mathcal{J}_{\mathrm{sa}}(\mathcal{H}_{\mathrm{f}}))$ and an orthogonal projection $\hat{\Pi}^\varepsilon \in \mathcal{B}_{\mathrm{sa}}(\mathcal{H})$ satisfying*

$$\|[\hat{H}^\varepsilon, \hat{\Pi}^\varepsilon]\| = \mathcal{O}(\varepsilon^\infty), \tag{3.7}$$

$$\|\hat{\Pi}^\varepsilon - \hat{\pi}^\varepsilon\| = \mathcal{O}(\varepsilon^\infty), \tag{3.8}$$

*where*

$$\hat{\pi}^\varepsilon = \mathrm{op}_\varepsilon\left(P + \varepsilon\,\tilde{\pi}\right), \qquad \tilde{\pi} = P_0\,\tilde{\pi}\,P_0 + P_0^\perp\,\tilde{\pi}\,P_0^\perp$$

*and*

$$\mathcal{P}^\varepsilon = P + \mathcal{O}(\varepsilon^\infty) \qquad \textit{in } S^0(\varepsilon, \mathcal{J}(\mathcal{H}_{\mathrm{f}}))\,. \tag{3.9}$$

*$P$ and $\tilde{\pi}$ are classical symbols in $S^0(\varepsilon, \mathcal{J}_{\mathrm{sa}}(\mathcal{H}_{\mathrm{f}}))$. The symbol $P(\varepsilon, z)$ and thus also $\mathcal{P}^\varepsilon(\varepsilon, z)$ and $\hat{\Pi}^\varepsilon$ are related to the eigenvalue $e_0(z)$ through its associated eigenprojection $P_0(z)$ which is the principal symbol of $P(\varepsilon, z)$.*

PROOF For the derivation of the super-adiabatic projection $\hat{\Pi}^\varepsilon$ we follow the idea of [NS04]. Also the derivation of the pointwise projection $\mathcal{P}^\varepsilon(\varepsilon, z)$ is based on this approach. By Lemma 3.1 there exist $P_j, \tilde{\pi}_j \in S^0(\mathcal{J}_{\mathrm{sa}}(\mathcal{H}_{\mathrm{f}}))$, $j \in \mathbb{N}_0$ such that (3.1) is satisfied for any $N \in \mathbb{N}_0$. A resummation (Lemma 2.1) of $(P_j)_{j\in\mathbb{N}_0}$ and $(\tilde{\pi}_j)_{j\in\mathbb{N}_0}$ results in symbols $P, \tilde{\pi} \in S^0(\varepsilon, \mathcal{J}(\mathcal{H}_{\mathrm{f}}))$ with asymptotic expansions $P \asymp \sum_{j=0}^\infty \varepsilon^j\,P_j$ and $\tilde{\pi} \asymp \sum_{j=0}^\infty \varepsilon^j\,\tilde{\pi}_j$ where $\tilde{\pi}$ is diagonal with respect to $P_0$.

Then, $\pi = P + \varepsilon\,\tilde{\pi}$ is an almost Moyal projection, i.e. $\pi \,\#\, \pi - \pi = \mathcal{O}(\varepsilon^\infty)$. Hence, $\hat{\pi}^\varepsilon$ satisfies $\|\hat{\pi}^\varepsilon\,\hat{\pi}^\varepsilon - \hat{\pi}^\varepsilon\| = \mathcal{O}(\varepsilon^\infty)$. We define $\hat{\Pi}^\varepsilon$ as the spectral projection of $\hat{\pi}^\varepsilon$ for its spectrum near one, i.e. $\hat{\Pi}^\varepsilon = \chi_{[\frac{1}{2},\frac{3}{2}]}(\hat{\pi}^\varepsilon)$. Then, $\hat{\Pi}^\varepsilon$ satisfies (3.7) and (3.8), for details see e.g. [NS04] or [Teu03, Section 3.2].

By definition $P(\varepsilon, z)$ takes value in the almost pointwise projections on $\mathcal{H}_{\mathrm{f}}$, i.e. there is a constant $C_{r,N} > 0$ for every $r \in \mathbb{N}_0$ and $N \in \mathbb{N}_0$ such that

$$\|P^2 - P\|^\varepsilon_{0,r} \leq C_{r,N}\,\varepsilon^N\,.$$

In particular, it holds for every $N \in \mathbb{N}_0$ that

$$\|P^2(\varepsilon, z) - P(\varepsilon, z)\|_{\mathcal{B}(\mathcal{H}_\mathrm{f})} \leq C_{0,N}\, \varepsilon^N \qquad \text{for any } \varepsilon \in [0, \varepsilon_0) \text{ and } z \in \mathbb{R}^{2n}\,.$$

It follows from the spectral mapping theorem for self-adjoint operators that there is a constant $C_N > 0$ for every $N \in \mathbb{N}_0$ such that

$$\sigma(P(\varepsilon, z)) \subset [-C_N\, \varepsilon^N, C_N\, \varepsilon^N] \cup [1 - C_N\, \varepsilon^N, 1 + C_N\, \varepsilon^N] =: \sigma_0^\varepsilon \cup \sigma_1^\varepsilon\,.$$

Therefore, we can define

$$\mathcal{P}^\varepsilon(\varepsilon, z) = \frac{\mathrm{i}}{2\,\pi} \int_{|\zeta - 1| < 1/2} (P(\varepsilon, z) - \zeta)^{-1}\, \mathrm{d}\zeta\,.$$

for $z \in \mathbb{R}^{2n}$ and $\varepsilon$ small enough. Then, it is easy to see that $\mathcal{P}^\varepsilon(\varepsilon, z)$ depends smoothly on $z$, is bounded with all it derivatives and takes value in the pointwise projections on $\mathcal{H}_\mathrm{f}$. In addition, defining $E(\varepsilon, z, \cdot)$ as the projection valued measure of $P(\varepsilon, z)$ we have

$$P(\varepsilon, z) = \int_{\sigma_0^\varepsilon \cup \sigma_1^\varepsilon} \lambda\, E(\varepsilon, z, \mathrm{d}\lambda) = \int_{\sigma_1^\varepsilon} \lambda\, E(\varepsilon, z, \mathrm{d}\lambda) + \mathcal{O}(\varepsilon^N) = \mathcal{P}^\varepsilon(\varepsilon, z) + \mathcal{O}(\varepsilon^N)$$

for every $N \in \mathbb{N}_0$. Moreover, since $\mathcal{P}^\varepsilon(\varepsilon, z)$ depends smoothly on $\varepsilon$ and $\mathcal{P}^\varepsilon(0, z) = P_0(z)$ we conclude that $\mathcal{P}^\varepsilon$ actually takes value in the pointwise rank-one projections on $\mathcal{H}_\mathrm{f}$, finishing the proof.

□

**Corollary 3.3** *Let $A \in S^k(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f}))$ for $k > 2n$. Then $\hat{A}^\varepsilon\, \hat{\Pi}^\varepsilon$ and $\hat{A}^\varepsilon\, \hat{\pi}^\varepsilon$ are trace class with*

$$\mathrm{tr}_\mathcal{H}(\hat{A}^\varepsilon\, \hat{\pi}^\varepsilon) = \mathcal{O}(\varepsilon^{-n}\, \|A\|_{L^1})$$

*and*

$$\mathrm{tr}_\mathcal{H}(\hat{A}^\varepsilon\, \hat{\Pi}^\varepsilon) = \mathrm{tr}_\mathcal{H}(\hat{A}^\varepsilon\, \hat{\pi}^\varepsilon)(1 + \mathcal{O}(\varepsilon^\infty))\,. \tag{3.10}$$

**Corollary 3.4** *The diagonal Hamiltonian $\hat{\Pi}^\varepsilon \hat{H}^\varepsilon \hat{\Pi}^\varepsilon + \hat{\Pi}^{\varepsilon\perp} \hat{H}^\varepsilon \hat{\Pi}^{\varepsilon\perp}$ is self-adjoint on $D(\hat{H}^\varepsilon)$ and the projection $\hat{\Pi}^\varepsilon$ almost commutes with the unitary time evolution operator, i.e.*

$$\left\| \left[ \mathrm{e}^{-\mathrm{i}\, \hat{H}^\varepsilon t/\varepsilon}, \hat{\Pi}^\varepsilon \right] \right\| = \mathcal{O}(\varepsilon^\infty\, |t|)$$

*and*

$$\left\| \mathrm{e}^{-\mathrm{i}\, \hat{H}^\varepsilon t/\varepsilon} - \mathrm{e}^{-\mathrm{i}\, (\hat{\Pi}^\varepsilon \hat{H}^\varepsilon \hat{\Pi}^\varepsilon + \hat{\Pi}^{\varepsilon\perp} \hat{H}^\varepsilon \hat{\Pi}^{\varepsilon\perp})\, t/\varepsilon} \right\| = \mathcal{O}(\varepsilon^\infty\, |t|).$$

See [ST13][Corollary 1] for a proof of Corollary 3.3 and Corollary 3.4.

In order to explicitly compute the contributions form super-adiabatic subspaces up to the second order in $\varepsilon$ we need to know the explicit formulas for $\tilde{\pi}$, $P$ and $\pi$ up to the order $\varepsilon^2$. We follow the construction of Lemma 3.1 starting with $P_0$, the eigenprojection of $H_0$ corresponding to $e_0$. Since $P_0\,P_0 - P_0 = 0$ we have $P_1^D = 0$.

Next, we want to compute $\tilde{\pi}_0$. By (3.2)

$$G_1 = \{P_0\,,P_0\}_1 = -\tfrac{\mathrm{i}}{2}\,\omega^0_{ij}\,\partial_j P_0\,\partial_i P_0 = -\tfrac{\mathrm{i}}{4}\,\omega^0_{ij}\,\left[\,\partial_j P_0\,,\partial_i P_0\,\right]\,.$$

Thus (3.3) yields

$$\tilde{\pi}_0 = -\tfrac{1}{4}\,P_0\,\mathrm{Tr}_{2n}(\omega^0\,\Omega_0^{op})\,P_0 + \tfrac{1}{4}\,P_0^\perp\,\mathrm{Tr}_{2n}(\omega^0\,\Omega_0^{op})\,P_0^\perp$$

where

$$\Omega^{op}_{0,ij} := -\mathrm{i}\,\left[\,\partial_i P_0\,,\partial_j P_0\,\right]\,.$$

Regarding $P_1^{OD}$, we define $w^{(1)} := P_0 + \varepsilon\,\tilde{\pi}_0$. Then

$$\begin{aligned}([H,w^{(1)}]_\#)_1 =& H_0\,\tilde{\pi}_0 - \tilde{\pi}_0\,H_0 + H_0^1\,P_0 - P_0\,H_0^1\\ &+ \{H_0 + \xi\cdot z\,,P_0\}_1 - \{P_0\,,H_0 + \xi\cdot z\}_1 =: F_1\end{aligned}$$

where we used that $\xi\cdot z$ and $\tilde{\pi}$ commute. Then, combining (B.2) and (B.3) with (3.6) leads to

$$\begin{aligned}P_1^{OD} =& \tfrac{\mathrm{i}}{2}\,P_0\langle\,\omega^0\,\nabla P_0\,,\,\nabla(H_0+e_0) + 2\,\xi\,\rangle(H_0-e_0)^{-1} - P_0\,H_0^1\,(H_0-e_0)^{-1}\\ &- \tfrac{\mathrm{i}}{2}\,(H_0-e_0)^{-1}\langle\,\nabla(H_0+e_0)+2\,\xi\,,\,\omega^0\,\nabla P_0\,\rangle P_0 - (H_0-e_0)^{-1}\,H_0^1\,P_0\,.\end{aligned} \tag{3.11}$$

We can reformulate $P_1 = P_1^{OD}$ by defining

$$M^{op}_{ij} := -\tfrac{\mathrm{i}}{2}\,\partial_i P_0\,\partial_j(H_0 - e_0)\,.$$

such that

$$\{P_0\,,H_0 - e_0\}_1 = \mathrm{Tr}_{2n}(\omega^0\,M^{op})$$

and

$$\{H_0 - e_0\,,P_0\}_1 = \mathrm{Tr}_{2n}((\omega^0\,M^{op})^*)$$

resulting in

$$
\begin{aligned}
P_1 = &- P_0 \,(\, \mathrm{Tr}_{2n}(\omega^0\, M^{op}) + H_0^1 \,)(H_0 - e_0)^{-1} \\
&+ \mathrm{i}\, P_0 \,\langle\, \omega^0\, \nabla P_0 \,,\, \nabla e_0 + \xi \,\rangle\, (H_0 - e_0)^{-1} \\
&- (H_0 - e_0)^{-1}\, (\, \mathrm{Tr}_{2n}((\omega^0\, M^{op})^*) + H_0^1 \,)\, P_0 \\
&- \mathrm{i}\, (H_0 - e_0)^{-1}\, \langle\, \nabla e_0 + \xi \,,\, \omega^0\, \nabla P_0 \,\rangle\, P_0
\end{aligned}
\tag{3.12}
$$

where $\mathrm{Tr}_{2n}(\cdot)$ is the trace on $\mathbb{C}^{2n}$.

Having $P_1$, we define

$$
\mathcal{T}_{ij}^{op} = \mathcal{T}_{0,ij}^{op} + \varepsilon\, \mathcal{T}_{1,ij}^{op} := \partial_i P_0\, \partial_j P_0 + \varepsilon\, \partial_i P_1\, \partial_j P_0 + \varepsilon\, \partial_i P_0\, \partial_j P_1 \,, \tag{3.13}
$$

$$
\begin{aligned}
\Omega_{ij}^{op} &= \Omega_{0,ij}^{op} + \varepsilon\, \Omega_{1,ij}^{op} := \tfrac{1}{\mathrm{i}}(\mathcal{T}_{ij}^{op} - (\mathcal{T}_{ij}^{op})^*) \\
&= - \mathrm{i}\, [\, \partial_i P_0 \,,\, \partial_j P_0 \,] - \varepsilon\, \mathrm{i}\, [\, \partial_i P_1 \,,\, \partial_j P_0 \,] - \varepsilon\, \mathrm{i}\, [\, \partial_i P_0 \,,\, \partial_j P_1 \,] \,,
\end{aligned}
\tag{3.14}
$$

and

$$
\begin{aligned}
g_{ij}^{op} &= g_{0,ij}^{op} + \varepsilon\, g_{1,ij}^{op} := \mathcal{T}_{0,ij}^{op} + (\mathcal{T}_{0,ij}^{op})^* \\
&= [\, \partial_i P_0 \,,\, \partial_j P_0 \,]_+ + \varepsilon\, [\, \partial_i P_1 \,,\, \partial_j P_0 \,]_+ + \varepsilon\, [\, \partial_i P_0 \,,\, \partial_j P_1 \,]_+
\end{aligned}
$$

for $1 \le i, j \le 2n$. Then

$$
\mathcal{T}_{ij}^{op} := \tfrac{1}{2} g_{ij}^{op} + \tfrac{\mathrm{i}}{2} \Omega_{ij}^{op} \,.
$$

We proceed by computing $P_2^D$ and observe that

$$
((P_0 + \varepsilon\, P_1)(P_0 + \varepsilon\, P_1))_2 = P_1\, P_1 \,.
$$

Thus, by (3.3)

$$
P_2^D = - P_0\, P_1\, P_1\, P_0 + P_0^\perp\, P_1\, P_1\, P_0^\perp \,.
$$

Regarding $\tilde{\pi}_1$ we define $u^{(1)} := P_0 + \varepsilon\, P_1 + \varepsilon\, \tilde{\pi}_0 + \varepsilon^2 P_2^D$. Then

$$
\begin{aligned}
(u^{(1)} \# u^{(1)})_2 = &\tilde{\pi}_0\, P_1 + P_1\, \tilde{\pi}_0 + \tilde{\pi}_0\, \tilde{\pi}_0 \\
&- \tfrac{\mathrm{i}}{2}\, \omega_{ij}^0\, \partial_j P_0\, \partial_i P_1 - \tfrac{\mathrm{i}}{2}\, \omega_{ij}^0\, \partial_j P_1\, \partial_i P_0 \\
&- \tfrac{\mathrm{i}}{2}\, \omega_{ij}^0\, \partial_j P_0\, \partial_i \tilde{\pi}_0 - \tfrac{\mathrm{i}}{2}\, \omega_{ij}^0\, \partial_j \tilde{\pi}_0\, \partial_i P_0 \\
&- \tfrac{1}{8}\, \omega_{ij}^0\, \omega_{lm}^0\, \partial_{jm}^2 P_0\;\, \partial_{il}^2 P_0 \\
&=: G_2
\end{aligned}
$$

where we used that $P_0\, P_2^D + P_2^D\, P_0 + P_1\, P_1 - P_2^D = 0$ by definition of $P_2^D$. By (3.5)

$$\tilde{\pi}_1 = -P_0\, G_2\, P_0 + P_0^\perp\, G_2\, P_0^\perp$$

Applying (B.4) yields

$$\begin{aligned} P_0\, \tilde{\pi}_1\, P_0 = & -\tfrac{1}{4}\, P_0\, \mathrm{Tr}_{2n}(\omega^0\, \Omega_1^{op})\, P_0 \\ & + \tfrac{1}{16}\, P_0\, \mathrm{Tr}_{2n}(\omega^0\, \Omega_0^{op})\, \mathrm{Tr}_{2n}(\omega^0\, \Omega_0^{op})\, P_0 \\ & - \tfrac{1}{8}\; P_0\, \mathrm{Tr}_{2n}(\omega^0\, \Omega_0^{op}\, \omega^0\, \Omega_0^{op})\, P_0 \\ & - \tfrac{1}{8}\, P_0\, \mathrm{Tr}_{2n}(\omega^0\, \nabla^2 P_0\, P_0^\perp\, \omega^0\, \nabla^2 P_0)\, P_0\,. \end{aligned} \tag{3.15}$$

A similar computation using (B.5) leads to

$$\begin{aligned} P_0^\perp\, \tilde{\pi}_1\, P_0^\perp = & \tfrac{1}{4}\, P_0^\perp\, \mathrm{Tr}_{2n}(\omega^0\, \Omega_1^{op})\, P_0^\perp \\ & - \tfrac{1}{16}\, P_0^\perp\, \mathrm{Tr}_{2n}(\omega^0\, \Omega_0^{op})\, \mathrm{Tr}_{2n}(\omega^0\, \Omega_0^{op})\, P_0^\perp \\ & + \tfrac{1}{8}\, P_0^\perp\, \mathrm{Tr}_{2n}(\omega^0\, \Omega_0^{op}\, \omega^0\, \Omega_0^{op})\, P_0^\perp \\ & + \tfrac{1}{8}\, P_0^\perp\, \mathrm{Tr}_{2n}(\omega^0\, \nabla^2 P_0\, P_0\, \omega^0\, \nabla^2 P_0)\, P_0^\perp\,. \end{aligned} \tag{3.16}$$

To summarize, the Moyal projection $\pi$ is given by

$$\pi = P + \varepsilon\, \tilde{\pi} \tag{3.17}$$

where the expansion of $P$ starts with

$$P = P_0 + \varepsilon\, P_1 - \varepsilon^2\, P_0\, P_1\, P_1\, P_0 + \varepsilon^2\, P_0^\perp\, P_1\, P_1\, P_0^\perp + \varepsilon^2\, P_2^{OD} + \mathcal{O}(\varepsilon^3)$$

where

$$\begin{aligned} P_1 = & -P_0\, (\, \mathrm{Tr}_{2n}(\omega^0\, M^{op}) + H_0^1\, )(H_0 - e_0)^{-1} \\ & + \mathrm{i}\, P_0 \langle\, \omega^0\, \nabla P_0\, ,\, \nabla e_0 + \xi\, \rangle\, (H_0 - e_0)^{-1} \\ & - (H_0 - e_0)^{-1}\, (\, \mathrm{Tr}_{2n}((\omega^0\, M^{op})^*) + H_0^1\, )\, P_0 \\ & - \mathrm{i}\, (H_0 - e_0)^{-1} \langle\, \nabla e_0 + \xi\, ,\, \omega^0\, \nabla P_0\, \rangle P_0\,. \end{aligned} \tag{3.18}$$

Note here that we did not compute $P_2^{OD}$ since it will not be needed for later computations. The expansion of $\tilde{\pi}$ is given by

$$\tilde{\pi} = \tilde{\pi}_0 + \varepsilon\, P_0\, \tilde{\pi}_1\, P_0 + \varepsilon\, P_0^\perp\, \tilde{\pi}_1\, P_0^\perp + \mathcal{O}(\varepsilon^2) \tag{3.19}$$

where

$$\tilde{\pi}_0 = -\tfrac{1}{4}\, P_0\, \mathrm{Tr}_{2n}(\omega^0\, \Omega_0^{op})\, P_0 + \tfrac{1}{4}\, P_0^\perp\, \mathrm{Tr}_{2n}(\omega^0\, \Omega_0^{op})\, P_0^\perp\,,$$

$$\begin{aligned} P_0\, \tilde{\pi}_1\, P_0 = &- \tfrac{1}{4}\, P_0\, \mathrm{Tr}_{2n}(\omega^0\, \Omega_1^{op})\, P_0 \\ &+ \tfrac{1}{16}\, P_0\, \mathrm{Tr}_{2n}(\omega^0\, \Omega_0^{op})\, \mathrm{Tr}_{2n}(\omega^0\, \Omega_0^{op})\, P_0 \\ &- \tfrac{1}{8}\, P_0\, \mathrm{Tr}_{2n}(\omega^0\, \Omega_0^{op}\, \omega^0\, \Omega_0^{op})\, P_0 \\ &- \tfrac{1}{8}\, P_0\, \mathrm{Tr}_{2n}(\omega^0\, \nabla^2 P_0\, P_0^\perp\, \omega^0\, \nabla^2 P_0)\, P_0 \end{aligned}$$

and

$$\begin{aligned} P_0^\perp\, \tilde{\pi}_1\, P_0^\perp = &\tfrac{1}{4}\, P_0^\perp\, \mathrm{Tr}_{2n}(\omega^0\, \Omega_1^{op})\, P_0^\perp \\ &- \tfrac{1}{16}\, P_0^\perp\, \mathrm{Tr}_{2n}(\omega^0\, \Omega_0^{op})\, \mathrm{Tr}_{2n}(\omega^0\, \Omega_0^{op})\, P_0^\perp \\ &+ \tfrac{1}{8}\, P_0^\perp\, \mathrm{Tr}_{2n}(\omega^0\, \Omega_0^{op}\, \omega^0\, \Omega_0^{op})\, P_0^\perp \\ &+ \tfrac{1}{8}\, P_0^\perp\, \mathrm{Tr}_{2n}(\omega^0\, \nabla^2 P_0\, P_0\, \omega^0\, \nabla^2 P_0)\, P_0^\perp. \end{aligned} \tag{3.20}$$

In addition, by (B.6)

$$\begin{aligned} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0^\perp\, \tilde{\pi}_1\, P_0^\perp) = &- \tfrac{1}{4}\, \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\, \mathrm{Tr}_{2n}(\omega^0\, \Omega_1^{op})) \\ &- \tfrac{1}{8}\, \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\, \mathrm{Tr}_{2n}(\omega^0\, \Omega_0^{op}\, \omega^0\, \Omega_0^{op})) \\ &+ \tfrac{1}{16}\, \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\, \mathrm{Tr}_{2n}(\omega^0\, \Omega_0^{op})\, \mathrm{Tr}_{2n}(\omega^0\, \Omega_0^{op})) \\ &+ \tfrac{1}{8}\, \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\, \mathrm{Tr}_{2n}(\omega^0\, \nabla^2 P_0\, P_0^\perp\, \omega^0\, \nabla^2 P_0))\,. \end{aligned}$$

## 3.2 Effective Operators

The goal of this section is the following: to an arbitrary Weyl operator $\hat{B}^\varepsilon$ with $B \in S^k(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f}))$ we want to associate a Weyl operator $\hat{b}^\varepsilon$ with scalar symbol $b \in S^k(\varepsilon, \mathbb{C})$ that approximates the action of $\hat{B}^\varepsilon$ restricted to the adiabatic subspace $\hat{\Pi}^\varepsilon \mathcal{H}$ to arbitrary order in $\varepsilon$, i.e.

$$\|\hat{\Pi}^\varepsilon\, \hat{B}^\varepsilon\, \hat{\Pi}^\varepsilon - \hat{\Pi}^\varepsilon\, \hat{b}^\varepsilon\, \hat{\Pi}^\varepsilon\| = \mathcal{O}(\varepsilon^\infty)\,.$$

We will refer to $b$ as the effective Symbol of $B$ or $\hat{B}^\varepsilon$, respectively. The Weyl quantization $\hat{b}^\varepsilon$ of $b$ will be called the effective Operator of $\hat{B}^\varepsilon$. Before we begin with the actual construction of the effective operator we introduce the basic idea. For now, assume that $B$ is a classical symbol in $S^k(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f}))$.

In addition assume that for some $N \in \mathbb{N}_0$ there is a classical symbol $R \in S^k(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f}))$ such that

$$\pi \# (B - R) \# \pi = \mathcal{O}(\varepsilon^N). \tag{3.21}$$

Then, $\pi \# (B-R) \# \pi$ is a classical symbol which has an asymptotic expansion that starts with the order $N$ term, i.e.

$$\pi \# (B - R) \# \pi \asymp \sum_{i=N}^{\infty} \varepsilon^i \, (\pi \# (B - R) \# \pi)_i \,.$$

Since $\pi$ is a Moyal projection we have

$$\pi \# (B - R) \# \pi = \pi \# \pi \# (B - R) \# \pi \# \pi \,.$$

Thus, we can express the leading order coefficient of the asymptotic expansion of $\pi \# (B - R) \# \pi$ as

$$\begin{aligned}(\pi \# (B - R) \# \pi)_N &= (\pi \# \pi \# (B - R) \# \pi \# \pi)_N \\ &= P_0 \, (\pi \# (B - R) \# \pi)_N \, P_0\end{aligned}$$

where in the last equality we used the assumption (3.21). Since $P_0$ is a rank-one projection we can express the last term in the above equation as a scalar multiple of the projection $P_0$. More precisely, applying (2.15) yields

$$P_0 \, (\pi \# (B - R) \# \pi)_N \, P_0 = \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0 \, (\pi \# (B - R) \# \pi)_N) \, P_0$$

In addition, since

$$\begin{aligned}&\pi \# \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0 \, (\pi \# (B - R) \# \pi)_N) \# \pi \\ &\qquad = \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0 \, (\pi \# (B - R) \# \pi)_N) \, P_0 + \mathcal{O}(\varepsilon)\end{aligned}$$

we obtain

$$\pi \# (B - R) \# \pi - \varepsilon^N \, \pi \# \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0 \, (\pi \# (B - R) \# \pi)_N) \# \pi = \mathcal{O}(\varepsilon^{N+1}) \,. \tag{3.22}$$

Now we want to use (3.22) to construct the effective operator $b$. Obviously, for $N = 0$ and $R = 0$ the assumption (3.21) is satisfied for any classical symbol $B$ in $S^k(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f}))$. Therefore, defining

$$b_0 := \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0 \, (\pi \# B \# \pi)_0) = \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0 \, B_0)$$

we have

$$\pi \# (B - b_0 \mathbf{1}_{\mathcal{H}_\mathrm{f}}) \# \pi = \pi \# B \# \pi - \pi \# b_0 \# \pi = \mathcal{O}(\varepsilon) \,.$$

But now $\pi \# (B - b_0 \mathbf{1}_{\mathcal{H}_\mathrm{f}}) \# \pi$ satisfies assumption (3.21) for $N = 1$ and $R = b_0 \mathbf{1}_{\mathcal{H}_\mathrm{f}}$. It follows by (3.22) that

$$\pi \# (B - b^{(1)} \mathbf{1}_{\mathcal{H}_\mathrm{f}}) \# \pi = \pi \# (B - b_0 \mathbf{1}_{\mathcal{H}_\mathrm{f}}) \# \pi - \varepsilon \, \pi \# b_1 \# \pi = \mathcal{O}(\varepsilon^2) \,.$$

where

$$b_1 := \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0 \, (\pi \# (B - b_0 \mathbf{1}_{\mathcal{H}_\mathrm{f}}) \# \pi)_1) \,.$$

Clearly, we can apply the above procedure inductively and so, for any $N \in \mathbb{N}_0$ construct $b^{(N)}$ satisfying

$$\pi \# (B - b^{(N)} \mathbf{1}_{\mathcal{H}_\mathrm{f}}) \# \pi = \mathcal{O}(\varepsilon^{N+1}) \,. \tag{3.23}$$

The recursion for $b^{(N)}$ is given by

$$b_0 = \mathrm{tr}_{\mathcal{H}_\mathrm{f}} \, (B_0 \, P_0)$$

and (3.24)

$$b_j = \mathrm{tr}_{\mathcal{H}_\mathrm{f}} \left( (\pi \# (B - b^{(j-1)} \mathbf{1}_{\mathcal{H}_\mathrm{f}}) \# \pi)_j \, P_0 \right) \quad \text{for} \quad j \geq 1 \,.$$

The symbol of the effective operator $b$ is then obtained by a resummation according to Lemma 2.1. So we can say that in the space of symbols we already know that the effective symbol $b$ approximates the action of a classical symbol $B$ restricted by the Moyal projection $\pi$. Moreover, applying the Calderon-Vaillancourt theorem (2.2) the result about symbols (3.23) can be turned into a statement about operators, i.e.

$$\| \hat{\Pi}^\varepsilon \, \hat{B}^\varepsilon \, \hat{\Pi}^\varepsilon - \hat{\Pi}^\varepsilon \, \hat{b}^\varepsilon \, \hat{\Pi}^\varepsilon \| = \mathcal{O}(\varepsilon^\infty) \,. \tag{3.25}$$

At this point it seems that we reached our goal to derive effective operators already. However, our actual goal is to proof (3.25) for arbitrary $B \in S^k(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f}))$. So, also for symbols $B$ that are no classical symbols. The main issue here is the following: the asymptotic expansion of the Moyal product of two classical symbols is unique if one restricts to coefficients that do not depend on $\varepsilon$. If one of the symbols is not classical there is no such unique asymptotic expansion. This makes it quite difficult to control the remainder of an asymptotic expansion especially when one only has the information about the $\varepsilon$ order of a term, e.g. $\pi \# (B - R) \# \pi = \mathcal{O}(\varepsilon)$. Therefore, to prove

(3.25) we will have to keep track of the explicit form of the remainder in the induction step. On the other hand we can already derive the recursion of the effective symbol $b$ of an arbitrary $B \in S^k(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f}))$ from (3.24).

For a symbol $B \in S^k(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f}))$, $k \geq 0$ we define

$$b_0(\varepsilon) = \mathrm{tr}_{\mathcal{H}_\mathrm{f}}\left(B(\varepsilon)\, P_0\right)$$

and (3.26)

$$b_{j+1}(\varepsilon) = \mathrm{tr}_{\mathcal{H}_\mathrm{f}}\left(\daleth_{j+1}(\varepsilon)\, P_0\right) \quad \text{for} \quad j \geq 0$$

where $\daleth_{j+1}$ is the $j+1$-th coefficient of the asymptotic expansion of $\pi \,\#\, (B - b^{(j)} \mathbf{1}_{\mathcal{H}_\mathrm{f}}) \,\#\, \pi \asymp \sum_{j=0}^{\infty} \varepsilon^j \, \daleth_j(\varepsilon)$ given by

$$\daleth_{j+1}(\varepsilon) = \sum_{\substack{\alpha \in \mathbb{N}_0^4, \\ |\alpha| = j+1}} \left\{ \left\{ \pi_{\alpha_1}, B(\varepsilon) \right\}_{\alpha_2}, \pi_{\alpha_3} \right\}_{\alpha_4} - \sum_{i=0}^{j} \sum_{\substack{\alpha \in \mathbb{N}_0^4, \\ |\alpha| = j+1-i}} \left\{ \left\{ \pi_{\alpha_1}, b_i(\varepsilon) \right\}_{\alpha_2}, \pi_{\alpha_3} \right\}_{\alpha_4} .$$

Since $P_0$ is a symbol in $S^0(\mathcal{J}_\mathrm{sa}(\mathcal{H}_\mathrm{f}))$ and $B \in S^k(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f}))$, clearly $b_0$ is a symbol in $S^k(\varepsilon, \mathbb{C})$. Assuming $b_i \in S^k(\varepsilon, \mathbb{C})$ for a $j \geq 0$ and any $j \geq i \geq 0$ we have $b_{j+1} \in S^k(\varepsilon, \mathbb{C})$ since all $\pi_l \in S^0(\mathcal{J}_\mathrm{sa}(\mathcal{H}_\mathrm{f}))$ take value in the trace class operators for every $l \geq 0$. By induction $b_j$ is a symbol in $S^k(\varepsilon, \mathbb{C})$ for any $j \geq 0$. A similar argument shows that there exist $\tilde{r} \in N_0$ and $C_{r,j} < \infty$ for any $r, j \in \mathbb{N}_0$ such that

$$\|b_j(\varepsilon)\|_{k,r} \leq C_{r,j} \, \|B(\varepsilon)\|_{k,\tilde{r}} \,. \tag{3.27}$$

Then a resummation according to Lemma 2.1 defines a symbol $b \in S^k(\varepsilon, \mathbb{C})$ where $b(\varepsilon) \asymp \sum_{j=0}^{\infty} \varepsilon^j \, b_j(\varepsilon)$.

Assume $B \in S^k(\varepsilon, \mathcal{B}_\mathrm{sa}(\mathcal{H}_\mathrm{f}))$ to take value in the self-adjoint operators on $\mathcal{H}_\mathrm{f}$. Then, $b_0$ takes value in $\mathbb{R}$. Considering the associativity of the Moyal product, the definition of $\daleth_1(\varepsilon)$ is symmetric. Moreover, all symbols included in $\daleth_1(\varepsilon)$ take value in the self-adjoint operators. Therefore, $\daleth_1(\varepsilon)$ takes value in the self-adjoint operators on $\mathcal{H}_\mathrm{f}$ and thus $b_1$ takes value in $\mathbb{R}$. Inductively it is easy to show that every $b_j$ and thus also $b$ take value in $\mathbb{R}$, i.e. $b \in S^k(\varepsilon, \mathbb{R})$.

The main goal for the rest of this section is to proof that $\hat{b}^\varepsilon$ approximates the action $\hat{B}^\varepsilon$ restricted to the almost-invariant subspace $\hat{\Pi}^\varepsilon \mathcal{H}$. We start by proving that the effective symbol $b$ given by (3.26) cancels the terms in the asymptotic expansion of $\pi \,\#\, B \,\#\, \pi$ order by order. This is done in the following proposition.

**Proposition 3.5** *Let $B$ be a symbol in $S^k(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f}))$, $k \geq 0$ with effective symbol $b \in S^k(\varepsilon, \mathbb{C})$ given as resummation of (3.26). Then, for every $N \in \mathbb{N}_0$ it holds that $\pi \# (B - b^{(N)} \mathbf{1}_{\mathcal{H}_\mathrm{f}}) \# \pi$ has the asymptotic expansion*

$$\begin{aligned}\pi \# (B - b^{(N)} \mathbf{1}_{\mathcal{H}_\mathrm{f}}) \# \pi \asymp \sum_{i=N+1}^{\infty} \varepsilon^i \Bigg( &\sum_{\substack{\alpha \in \mathbb{N}_0^4, \\ |\alpha| = i}} \Big\{ \{ \pi_{\alpha_1}, B(\varepsilon) \}_{\alpha_2}, \pi_{\alpha_3} \Big\}_{\alpha_4} \\ &- \sum_{j=0}^{N} \sum_{\substack{\alpha \in \mathbb{N}_0^4, \\ |\alpha| = i-j}} \Big\{ \{ \pi_{\alpha_1}, b_j(\varepsilon) \}_{\alpha_2}, \pi_{\alpha_3} \Big\}_{\alpha_4} \Bigg)\end{aligned} \tag{3.28}$$

*In particular,*

$$\sum_{\substack{\alpha \in \mathbb{N}_0^4, \\ |\alpha| = i}} \Big\{ \{ \pi_{\alpha_1}, B(\varepsilon) \}_{\alpha_2}, \pi_{\alpha_3} \Big\}_{\alpha_4} - \sum_{j=0}^{i} \sum_{\substack{\alpha \in \mathbb{N}_0^4, \\ |\alpha| = i-j}} \Big\{ \{ \pi_{\alpha_1}, b_j(\varepsilon) \}_{\alpha_2}, \pi_{\alpha_3} \Big\}_{\alpha_4} = 0 \tag{3.29}$$

*for every $0 \leq i \leq N$.*

PROOF Let $B \in S^k(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f}))$, $k \geq 0$ with effective symbol $b \in S^k(\varepsilon, \mathbb{C})$. We prove (3.28) and (3.29) by induction over $N \in \mathbb{N}_0$. For the induction basis ($N = 0$) we start with the following observation. We have

$$\begin{aligned}\sum_{\substack{\alpha \in \mathbb{N}_0^4, \\ |\alpha| = 0}} \Big\{ \{ \pi_{\alpha_1}, B(\varepsilon) - b_0(\varepsilon) \mathbf{1}_{\mathcal{H}_\mathrm{f}} \}_{\alpha_2}, \pi_{\alpha_3} \Big\}_{\alpha_4} &= P_0 \left( B(\varepsilon) - \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(B(\varepsilon)\, P_0)\, \mathbf{1}_{\mathcal{H}_\mathrm{f}} \right) P_0 \\ &= P_0\, B(\varepsilon)\, P_0 - P_0\, B(\varepsilon)\, P_0 = 0\end{aligned}$$

where for the second equation we applied (2.15) using the fact that $P_0$ is a rank-one projection. By the asymptotic expansion of the Moyal product (2.4) for symbols in $S^k(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f}))$ we have

$$\begin{aligned}&\pi \# (B - b_0 \mathbf{1}_{\mathcal{H}_\mathrm{f}}) \# \pi \\ &\quad \asymp P_0 \left( B(\varepsilon) - \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(B(\varepsilon)\, P_0) \mathbf{1}_{\mathcal{H}_\mathrm{f}} \right) P_0 \\ &\qquad + \sum_{i=1}^{\infty} \varepsilon^i \sum_{\alpha \in \mathbb{N}_0^4, |\alpha| = i} \Big\{ \{ \pi_{\alpha_1}, B(\varepsilon) - b_0(\varepsilon) \mathbf{1}_{\mathcal{H}_\mathrm{f}} \}_{\alpha_2}, \pi_{\alpha_3} \Big\}_{\alpha_4} \\ &\quad = \sum_{i=1}^{\infty} \varepsilon^i \sum_{\alpha \in \mathbb{N}_0^4, |\alpha| = i} \Big\{ \{ \pi_{\alpha_1}, B(\varepsilon) - b_0(\varepsilon) \mathbf{1}_{\mathcal{H}_\mathrm{f}} \}_{\alpha_2}, \pi_{\alpha_3} \Big\}_{\alpha_4}\end{aligned}$$

which proves (3.28) for $N = 0$.

Now let (3.28) and (3.29) hold for $N \in \mathbb{N}_0$ we will prove it for $N+1$. First, we define $\mathcal{B}_{j,\alpha} \in S^k(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f}))$ for $j \in \mathbb{N}_0$, $j \leq N$ and $\alpha \in \mathbb{N}_0^4$ by

$$\mathcal{B}_{0,\alpha}(\varepsilon) := \Big\{ \{\pi_{\alpha_1}, B(\varepsilon) - b_0(\varepsilon)\mathbf{1}_{\mathcal{H}_\mathrm{f}}\}_{\alpha_2}, \pi_{\alpha_3} \Big\}$$

and

$$\mathcal{B}_{j,\alpha}(\varepsilon) := -\Big\{ \{\pi_{\alpha_1}, b_j(\varepsilon)\}_{\alpha_2}, \pi_{\alpha_3} \Big\} \text{ for } 1 \leq j \leq N\,.$$

By the induction hypothesis (3.29), it holds that for every $m \in \mathbb{N}_0$ with $m \leq N$ and every $\beta \in \mathbb{N}_0^4$

$$\begin{aligned} &\sum_{j=0}^{m} \sum_{\substack{\alpha \in \mathbb{N}_0^4, \\ |\alpha| = m-j}} \Big\{ \{\pi_{\beta_1}, \mathcal{B}_{j,\alpha}(\varepsilon)\}_{\beta_2}, \pi_{\beta_3} \Big\}_{\beta_4} \\ &\quad = \{\{\pi_{\beta_1}, \sum_{j=0}^{m} \sum_{\substack{\alpha \in \mathbb{N}_0^4, \\ |\alpha| = m-j}} \mathcal{B}_{j,\alpha}(\varepsilon)\}_{\beta_2}, \pi_{\beta_3}\}_{\beta_4} = 0\,. \end{aligned} \tag{3.30}$$

Hence, Lemma A.8 yields

$$\begin{aligned} \sum_{j=0}^{N} \sum_{\substack{\alpha \in \mathbb{N}_0^4, \\ |\alpha| = N+1-j}} \mathcal{B}_{j,\alpha}(\varepsilon) &= \sum_{j=0}^{N} \sum_{\substack{\alpha,\beta \in \mathbb{N}_0^4, \\ |\alpha|+|\beta| = N+1-j}} \Big\{ \{\pi_{\beta_1}, \mathcal{B}_{j,\alpha}(\varepsilon)\}_{\beta_2}, \pi_{\beta_3} \Big\}_{\beta_4} \\ &= \sum_{j=0}^{N} \sum_{\substack{\alpha \in \mathbb{N}_0^4, \\ |\alpha| = N+1-j}} P_0\, \mathcal{B}_{j,\alpha}(\varepsilon)\, P_0 \\ &\quad + \sum_{i=1}^{N} \sum_{\substack{\beta \in \mathbb{N}_0^4, \\ |\beta| = i}} \sum_{j=0}^{N+1-i} \sum_{\substack{\alpha \in \mathbb{N}_0^4, \\ |\alpha| = N+1-i-j}} \Big\{ \{\pi_{\beta_1}, \mathcal{B}_{j,\alpha}(\varepsilon)\}_{\beta_2}, \pi_{\beta_3} \Big\}_{\beta_4} \\ &= \sum_{j=0}^{N} \sum_{\substack{\alpha \in \mathbb{N}_0^4, \\ |\alpha| = N+1-j}} P_0\, \mathcal{B}_{j,\alpha}(\varepsilon)\, P_0 \end{aligned} \tag{3.31}$$

where the last equation follows directly from (3.30) with $m = N+1-i$. Applying (2.15) results in

$$\sum_{j=0}^{N} \sum_{\substack{\alpha \in \mathbb{N}_0^4, \\ |\alpha| = N+1-j}} P_0\, \mathcal{B}_{j,\alpha}(\varepsilon)\, P_0 = \sum_{j=0}^{N} \sum_{\substack{\alpha \in \mathbb{N}_0^4, \\ |\alpha| = N+1-j}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\, \mathcal{B}_{j,\alpha}(\varepsilon))\, P_0 = b_{N+1}(\varepsilon)\, P_0\,. \tag{3.32}$$

Combining (3.31) and (3.32) we get

$$\sum_{j=0}^{N} \sum_{\substack{\alpha\in\mathbb{N}_0^4,\\ |\alpha|=N+1-j}} \mathcal{B}_{j,\alpha}(\varepsilon) = b_{N+1}(\varepsilon)\, P_0 \tag{3.33}$$

and thus

$$\begin{aligned}\sum_{\substack{\alpha\in\mathbb{N}_0^4,\\ |\alpha|=N+1}} \Big\{\{\pi_{\alpha_1}\,, B(\varepsilon)\}_{\alpha_2}\,, \pi_{\alpha_3}\Big\}_{\alpha_4} - \sum_{j=0}^{N+1} \sum_{\substack{\alpha\in\mathbb{N}_0^4,\\ |\alpha|=N+1-j}} \Big\{\{\pi_{\alpha_1}\,, b_j(\varepsilon)\}_{\alpha_2}\,, \pi_{\alpha_3}\Big\}_{\alpha_4}\\ = b_{N+1}(\varepsilon)\, P_0 - b_{N+1}(\varepsilon)\, P_0 = 0\,.\end{aligned}$$

In the next step, we apply (3.33) to the asymptotic expansion of $\pi \,\#\, B \,\#\, \pi$ given by the induction hypothesis (3.28). We obtain

$$\begin{aligned}\pi \,\#\, (B - b^{(N)}\mathbf{1}_{\mathcal{H}_\mathrm{f}}) \,\#\, \pi \asymp \sum_{i=N+1}^{\infty} \varepsilon^i \sum_{j=0}^{N} \sum_{\substack{\alpha\in\mathbb{N}_0^4,\\ |\alpha|=i-j}} \mathcal{B}_{j,\alpha}(\varepsilon)\\ = -\,\varepsilon^{N+1}\, b_{N+1}(\varepsilon)\, P_0 + \sum_{i=N+2}^{\infty} \varepsilon^i \sum_{j=0}^{N} \sum_{\substack{\alpha\in\mathbb{N}_0^4,\\ |\alpha|=i-j}} \mathcal{B}_{j,\alpha}(\varepsilon)\,.\end{aligned} \tag{3.34}$$

By the expansion of the Moyal product (2.4), $\pi(\varepsilon) \,\#\, b_{N+1}(\varepsilon) \,\#\, \pi(\varepsilon)$ has an asymptotic expansion given by

$$\begin{aligned}\pi \,\#\, b_{N+1} \,\#\, \pi \asymp b_{N+1}(\varepsilon)\, P_0 + \sum_{i=1}^{\infty} \varepsilon^i \sum_{\substack{\alpha\in\mathbb{N}_0^4,\\ |\alpha|=i}} \Big\{\{\pi_{\alpha_1}\,, b_{N+1}(\varepsilon)\}_{\alpha_2}\,, \pi_{\alpha_3}\Big\}_{\alpha_4}\\ = b_{N+1}(\varepsilon)\, P_0\\ + \varepsilon^{-(N+1)} \sum_{i=N+2}^{\infty} \varepsilon^i \sum_{\substack{\alpha\in\mathbb{N}_0^4,\\ |\alpha|=i-N-1}} \Big\{\{\pi_{\alpha_1}\,, b_{N+1}(\varepsilon)\}_{\alpha_2}\,, \pi_{\alpha_3}\Big\}_{\alpha_4}\,.\end{aligned} \tag{3.35}$$

Then, combining (3.34) and (3.35) yields

$$\begin{aligned}
&\pi \# (B - b^{(N)}\mathbf{1}_{\mathcal{H}_\mathrm{f}}) \# \pi - \pi \# b^{(N+1)} \# \pi \\
&\asymp \sum_{i=N+2}^{\infty} \varepsilon^i \Bigg( \sum_{\substack{\alpha\in\mathbb{N}_0^4,\\ |\alpha|=i}} \left\{ \{\pi_{\alpha_1}, B(\varepsilon)\}_{\alpha_2}, \pi_{\alpha_3} \right\}_{\alpha_4} \\
&\qquad - \sum_{j=0}^{N+1} \sum_{\substack{\alpha\in\mathbb{N}_0^4,\\ |\alpha|=i-j}} \left\{ \{\pi_{\alpha_1}, b_j(\varepsilon)\}_{\alpha_2}, \pi_{\alpha_3} \right\}_{\alpha_4} \Bigg)
\end{aligned}$$

which finishes the proof. □

Combining Proposition 3.28 and the continuity of the Moyal remainder (2.6) we get that $\pi \# (B - b^{(N)}\mathbf{1}_{\mathcal{H}_\mathrm{f}}) \# \pi$ is of order $\varepsilon^{N+1}$ in $S^k(\varepsilon)$ for every $N \in \mathbb{N}_0$. In addition, applying the Calderon-Vaillancourt theorem (2.2) the result about symbols can be turned into a statement about operators, i.e.

$$\|\hat{\pi}^\varepsilon \, \hat{B}^\varepsilon \, \hat{\pi}^\varepsilon - \hat{\pi}^\varepsilon \, \hat{b}^\varepsilon \, \hat{\pi}^\varepsilon\| = \mathcal{O}(\varepsilon^\infty) \, .$$

By Proposition 3.2 $\hat{\Pi}^\varepsilon = \hat{\pi}^\varepsilon + \mathcal{O}(\varepsilon^\infty)$ which implies

$$\|\hat{\Pi}^\varepsilon \, \hat{B}^\varepsilon \, \hat{\Pi}^\varepsilon - \hat{\Pi}^\varepsilon \, \hat{b}^\varepsilon \, \hat{\Pi}^\varepsilon\| = \mathcal{O}(\varepsilon^\infty) \, .$$

In Chapter 4 we will derive semiclassical approximations for expectation values of thermodynamic equilibrium distribution, i.e. terms of the form

$$\mathrm{tr}_{\mathcal{H}} \left( \hat{\Pi}^\varepsilon f(\hat{H}^\varepsilon) \hat{A}^\varepsilon \right) \, .$$

For this derivation similar statement as (3.25) but for trace class operators $\hat{B}^\varepsilon \in \mathcal{J}(\mathcal{H})$ will be of big importance i.e. that

$$\mathrm{tr}_{\mathcal{H}} \left( \left( \hat{B}^\varepsilon - \widehat{b^{(N)}}^\varepsilon \right) \hat{\Pi}^\varepsilon \right) = \mathcal{O}(\varepsilon^{N+1-n} \sup_{\varepsilon\in[0,\varepsilon_B)} \|B\|_{L^1})$$

where the more precise error estimate will be crucial when taking a thermodynamic limit.

**Theorem 3.6** *Let $N \in \mathbb{N}_0$ and $B$ be a symbol in $S^k(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f}))$, $k \geq 0$ with effective symbol $b \in S^k(\varepsilon, \mathbb{C})$ given by (3.26). Then*

$$\pi \# B \# \pi - \pi \# b \# \pi = \mathcal{O}(\varepsilon^\infty) \quad \text{in} \quad S^k(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f})) \tag{3.36}$$

*and*

$$\|\hat{\Pi}^\varepsilon \, \hat{B}^\varepsilon \, \hat{\Pi}^\varepsilon - \hat{\Pi}^\varepsilon \, \hat{b}^\varepsilon \, \hat{\Pi}^\varepsilon\| = \mathcal{O}(\varepsilon^\infty). \tag{3.37}$$

*Also, there exist $\tilde{r} \in N_0$ and $C_r < \infty$ for every $r \in \mathbb{N}_0$ such that*

$$\|\pi \# B \# \pi - \pi \# b^{(N)} \# \pi\|_{k,r}^{\varepsilon} \leq C_r \, \varepsilon^{N+1} \, \|B\|_{k,\tilde{r}}^{\varepsilon} \,. \tag{3.38}$$

*If additionally $k > 2n$ then it holds for every $R \in S^0(\varepsilon, \mathcal{J}(\mathcal{H}_\mathrm{f}))$ that*

$$\mathrm{tr}_{\mathcal{H}} \left( \widehat{b^{(N)}}^{\,\varepsilon} \, \hat{R}^{\varepsilon} \right) = \mathcal{O}\Big( \varepsilon^{-n} \, \|R\|_{0,j,1}^{\varepsilon} \, \|B\|_{L^1}^{\varepsilon} \Big) \tag{3.39}$$

*and*

$$\mathrm{tr}_{\mathcal{H}} \left( \widehat{b^{(N)}}^{\,\varepsilon} \, \hat{\Pi}^{\varepsilon} \right) = \mathcal{O}\Big( \varepsilon^{-n} \, \|B\|_{L^1}^{\varepsilon} \Big) \,. \tag{3.40}$$

*Furthermore,*

$$\mathrm{tr}_{\mathcal{H}} \left( \left( \hat{B}^{\varepsilon} - \widehat{b^{(N)}}^{\,\varepsilon} \right) \hat{\pi}^{\varepsilon} \right) = \mathcal{O}\Big( \varepsilon^{N+1-n} \, \|B\|_{L^1}^{\varepsilon} \Big) \tag{3.41}$$

*and*

$$\mathrm{tr}_{\mathcal{H}} \left( \left( \hat{B}^{\varepsilon} - \widehat{b^{(N)}}^{\,\varepsilon} \right) \hat{\Pi}^{\varepsilon} \right) = \mathcal{O}\Big( \varepsilon^{N+1-n} \, \|B\|_{L^1}^{\varepsilon} \Big) \,. \tag{3.42}$$

PROOF Let $N \in \mathbb{N}_0$, $B \in S^k(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f}))$, $k \geq 0$ and $b \in S^k(\varepsilon, \mathbb{C})$ the associated effective symbol. Clearly, (3.36) and (3.37) hold by the previous discussion. Also, (3.36) is a direct consequence of (3.38). Hence, we will start our prove by showing (3.38). By Proposition 3.5 we have

$$\begin{aligned} \pi \# (B - b^{(N)} \mathbf{1}_{\mathcal{H}_\mathrm{f}}) \# \pi \asymp \sum_{i=N+1}^{\infty} \varepsilon^i \Bigg( & \sum_{\substack{\alpha \in \mathbb{N}_0^4, \\ |\alpha| = i}} \Big\{ \{\pi_{\alpha_1} , B(\varepsilon)\}_{\alpha_2} \, , \pi_{\alpha_3} \Big\}_{\alpha_4} \\ & - \sum_{j=0}^{N} \sum_{\substack{\alpha \in \mathbb{N}_0^4, \\ |\alpha| = i-j}} \Big\{ \{\pi_{\alpha_1} , b_j(\varepsilon)\}_{\alpha_2} \, , \pi_{\alpha_3} \Big\}_{\alpha_4} \Bigg) \,. \end{aligned}$$

Thus, for $r \in \mathbb{N}_0$ we have

$$\begin{aligned} & \Big\| \pi \# (B - b^{(N)} \mathbf{1}_{\mathcal{H}_\mathrm{f}}) \# \pi \Big\|_{k,r} \\ & \quad \leq \Bigg\| \pi \# B \# \pi - \sum_{i=0}^{N} \varepsilon^i \sum_{\substack{\alpha \in \mathbb{N}_0^4, \\ |\alpha| = i}} \Big\{ \{\pi_{\alpha_1} , B(\varepsilon)\}_{\alpha_2} \, , \pi_{\alpha_3} \Big\}_{\alpha_4} \Bigg\|_{k,r} \\ & \qquad + \sum_{j=0}^{N} \varepsilon^j \Bigg\| \pi \# b_j \# \pi - \sum_{i=0}^{N-j} \varepsilon^i \sum_{\substack{\alpha \in \mathbb{N}_0^4, \\ |\alpha| = i}} \Big\{ \{\pi_{\alpha_1} , b_j(\varepsilon) \mathbf{1}_{\mathcal{H}_\mathrm{f}}\}_{\alpha_2} \, , \pi_{\alpha_3} \Big\}_{\alpha_4} \Bigg\|_{k,r} \,. \end{aligned} \tag{3.43}$$

By the continuity of the Moyal remainders (2.6) there exists $r_1 \in N_0$ and a constant $C_1 < \infty$ for every $r \in \mathbb{N}_0$ such that

$$\Big\| \pi \# B \# \pi - \sum_{i=0}^{N} \varepsilon^i \sum_{\substack{\alpha \in \mathbb{N}_0^4, \\ |\alpha| = i}} \Big\{ \{\pi_{\alpha_1}, B(\varepsilon)\}_{\alpha_2}, \pi_{\alpha_3} \Big\}_{\alpha_4} \Big\|_{k,r} \leq \varepsilon^{N+1} C_1 \, \|B(\varepsilon)\|_{k,\tilde{r}}$$

and (3.44)

$$\Big\| \pi \# b_j \# \pi - \sum_{i=0}^{N-j} \varepsilon^i \sum_{\substack{\alpha \in \mathbb{N}_0^4, \\ |\alpha| = i}} \Big\{ \{\pi_{\alpha_1}, b_j(\varepsilon)\}_{\alpha_2}, \pi_{\alpha_3} \Big\}_{\alpha_4} \Big\|_{k,r} \leq \varepsilon^{N-j+1} C_1 \, \|b_j(\varepsilon)\|_{k,\tilde{r}}$$

for every $0 \leq j \leq N$. Of course, the $C_1$s and $r_1$s may be different in each inequality but taking the maximum of all these constants the inequalities are still true. In addition, by (3.27) there exist $\tilde{r} \in N_0$ and $C_r < \infty$ such that

$$\|B(\varepsilon)\|_{k,r_0} \leq (N+2)^{-1} \, C_1^{-1} \, C_r \, \|B\|^{\varepsilon}_{k,\tilde{r}}$$

and (3.45)

$$\|b_j(\varepsilon) \mathbf{1}_{\mathcal{H}_\mathrm{f}}\|_{k,r_0} \leq (N+2)^{-1} \, C_1^{-1} \, C_r \, \|B\|^{\varepsilon}_{k,\tilde{r}}$$

for every $0 \leq j \leq N$. Then, our claim (3.38) follows directly by combining (3.43)- (3.45).

Now we additionally assume $k > 2n$. Prior to proving (3.39) - (3.41) we reformulate the $b_j$s. By Lemma A.9 there exist $Q_\alpha^{j,r} \in S^0(\mathcal{J}(\mathcal{H}_\mathrm{f}))$, $0 \leq r \leq j$ and $\alpha \in \{1, \ldots, 2n\}^r$ for any $j \in \mathbb{N}_0$ such that

$$b_j(\varepsilon) = \sum_{r=0}^{j} \sum_{\alpha \in \{1,\ldots,2n\}^r} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(Q_\alpha^{j,r} \, \nabla_\alpha^r B(\varepsilon)) \, . \tag{3.46}$$

Let $R \in S^0(\varepsilon, \mathcal{J}(\mathcal{H}_\mathrm{f}))$ then an integration by parts shows

$$\begin{aligned} \Big| \int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(Q_\alpha^{j,r} \, \nabla_\alpha^r B(\varepsilon))(z) \, \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(R(\varepsilon))(z) \, \mathrm{d}z \Big| \\ = \Big| \int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\nabla_\alpha^r (\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(R(\varepsilon)) \, Q_\alpha^{j,r}) \, B(\varepsilon))(z) \, \mathrm{d}z \Big| \\ \leq \|Q_\alpha^{j,r}\|_{0,r,1} \, \|R(\varepsilon)\|_{0,r,1} \int_{\mathbb{R}^{2n}} \|B(\varepsilon, z)\| \, \mathrm{d}z \\ \leq \|Q_\alpha^{j,r}\|_{0,j,1} \, \|R\|^{\varepsilon}_{0,j,1} \, \|B\|^{\varepsilon}_{L^1} \end{aligned} \tag{3.47}$$

for any $j \geq 0$, $0 \leq r \leq j$ and $\alpha \in \{1, \dots, 2n\}^r$. Combining (3.46) and (3.47) there exists a constant $C_j > 0$ for each $j \in \mathbb{N}_0$

$$\left| \int_{\mathbb{R}^{2n}} b_j(\varepsilon, z) \operatorname{tr}_{\mathcal{H}_\mathrm{f}}(R(\varepsilon, z)) \,\mathrm{d}z \right| \leq C_j \, \|R\|^{\varepsilon}_{0,j,1} \, \|B\|^{\varepsilon}_{L^1} . \tag{3.48}$$

Then, (3.39) directly follows by (3.48) and the trace formula (2.12). Moreover, replacing $R \in S^0(\varepsilon, \mathcal{J}(\mathcal{H}_\mathrm{f}))$ by $\pi \in S^0(\varepsilon, \mathcal{J}(\mathcal{H}_\mathrm{f}))$ in (3.39) we get

$$\operatorname{tr}_{\mathcal{H}} \left( \widehat{b^{(N)}}^{\varepsilon} \, \hat{\pi}^{\varepsilon} \right) = \mathcal{O}\Big( \varepsilon^{-n} \, \|\pi\|^{\varepsilon}_{0,j,1} \, \|B\|^{\varepsilon}_{L^1} \Big) .$$

Then, (3.40) follows from the above equation and (3.10).

To prove (3.41), we again use the reformulated form of the $b_j$s (3.46). By Proposition A.10 we have for any $m \in \mathbb{N}_0$

$$\begin{aligned} &\int_{\mathbb{R}^{2n}} \operatorname{tr}_{\mathcal{H}_\mathrm{f}} \Big( \pi \,\#\, B \,\#\, \pi \Big)(\varepsilon, z) \,\mathrm{d}z \\ &\qquad = \sum_{i=0}^{m} \varepsilon^i \sum_{\substack{\alpha \in \mathbb{N}_0^4, \\ |\alpha| = i}} \int_{\mathbb{R}^{2n}} \operatorname{tr}_{\mathcal{H}_\mathrm{f}} \Big( \big\{ \{ \pi_{\alpha_1} , B(\varepsilon) \}_{\alpha_2} , \pi_{\alpha_3} \big\}_{\alpha_4} \Big)(z) \,\mathrm{d}z \\ &\qquad\quad + \mathcal{O}\Big( \varepsilon^{m+1} \, \|B\|^{\varepsilon}_{L^1} \Big) \end{aligned} \tag{3.49}$$

and

$$\begin{aligned} &\int_{\mathbb{R}^{2n}} \operatorname{tr}_{\mathcal{H}_\mathrm{f}} \Big( \pi \,\#\, \operatorname{tr}_{\mathcal{H}_\mathrm{f}}(Q^{j,r}_{\alpha} \, \partial^{\alpha}_{z} B) \,\#\, \pi \Big)(\varepsilon, z) \,\mathrm{d}z \\ &\quad = \sum_{i=0}^{m} \varepsilon^i \sum_{\substack{\alpha \in \mathbb{N}_0^4, \\ |\alpha| = i}} \int_{\mathbb{R}^{2n}} \operatorname{tr}_{\mathcal{H}_\mathrm{f}} \Big( \Big\{ \Big\{ \pi_{\alpha_1} , \operatorname{tr}_{\mathcal{H}_\mathrm{f}}(Q^{j,r}_{\alpha} \, \partial^{\alpha}_{z} B(\varepsilon)) \Big\}_{\alpha_2} , \pi_{\alpha_3} \Big\}_{\alpha_4} \Big)(z) \,\mathrm{d}z \\ &\quad\quad + \mathcal{O}\Big( \varepsilon^{m+1} \, \|B\|^{\varepsilon}_{L^1} \Big) \end{aligned} \tag{3.50}$$

for any $j \geq 0$, $0 \leq r \leq j$, $\alpha \in \{1, \dots, 2n\}^r$. Combining (3.46) with (3.50) we see

$$\begin{aligned} &\int_{\mathbb{R}^{2n}} \operatorname{tr}_{\mathcal{H}_\mathrm{f}} (\pi \,\#\, b_j \,\#\, \pi)(\varepsilon, z) \,\mathrm{d}z \\ &\qquad = \sum_{i=0}^{N-j} \varepsilon^i \sum_{\substack{\alpha \in \mathbb{N}_0^4, \\ |\alpha| = i}} \int_{\mathbb{R}^{2n}} \operatorname{tr}_{\mathcal{H}_\mathrm{f}} \Big( \big\{ \{ \pi_{\alpha_1} , b_j(\varepsilon) \}_{\alpha_2} , \pi_{\alpha_3} \big\}_{\alpha_4} \Big)(z) \,\mathrm{d}z \\ &\qquad\quad + \mathcal{O}\Big( \varepsilon^{N-j+1} \, \|B\|^{\varepsilon}_{L^1} \Big) \end{aligned} \tag{3.51}$$

for each $0 \leq j \leq N$. Subtracting (3.51) and (3.49) we conclude

$$\begin{aligned}
&\int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\pi \# (B - b^{(N)} \mathbf{1}_{\mathcal{H}_\mathrm{f}}) \# \pi)(\varepsilon, z)\, \mathrm{d}z \\
&\quad = \sum_{i=0}^{N} \varepsilon^i \sum_{\substack{\alpha \in \mathbb{N}_0^4, \\ |\alpha| = i}} \int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}} \Big( \big\{ \{\pi_{\alpha_1}, B(\varepsilon)\}_{\alpha_2}, \pi_{\alpha_3} \big\}_{\alpha_4} \Big)(z)\, \mathrm{d}z \\
&\qquad - \sum_{j=0}^{N} \varepsilon^j \sum_{i=0}^{N-j} \varepsilon^i \sum_{\substack{\alpha \in \mathbb{N}_0^4, \\ |\alpha| = i}} \int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}} \Big( \big\{ \{\pi_{\alpha_1}, b_j(\varepsilon)\}_{\alpha_2}, \pi_{\alpha_3} \big\}_{\alpha_4} \Big)(z)\, \mathrm{d}z \\
&\qquad + \mathcal{O}\Big( \varepsilon^{N+1} \, \|B\|^{\varepsilon}_{L^1} \Big) .
\end{aligned} \tag{3.52}$$

Finally, applying Lemma 3.5 to the previous equation (3.52)

$$\int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\pi \# (B - b^{(N)} \mathbf{1}_{\mathcal{H}_\mathrm{f}}) \# \pi)(z)\, \mathrm{d}z = \mathcal{O}\Big( \varepsilon^{N+1} \, \|B\|^{\varepsilon}_{L^1} \Big) . \tag{3.53}$$

Then (3.41) directly follows by (3.53) and the trace formula (2.12). To finish the proof, we apply (3.10) to (3.41) which proves (3.42). □

To finalize this section, we consider classical symbols $B \in S^k(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f}))$, as in the beginning of this section. Imagine that in an application one may only be interested in the leading order of the effective symbol $b_0$. Until this point one would have to compute $b_0 = \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0 \, B(\varepsilon))$ in order to get the needed error estimates provided by Theorem 3.6. But $b_0$ is obviously a classical symbol and contains higher order terms one may actually not be interested in. Thus we provide the respective error estimates for such a case in the following proposition.

**Proposition 3.7** *Let $N \in \mathbb{N}_0$ and $B$ be a classical symbol in $S^k(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f}))$, $k \geq 0$ with effective symbol $b \in S^k(\varepsilon, \mathbb{C})$. Then $b_j$ is a classical symbols for every $j \in \mathbb{N}_0$ with asymptotic expansion*

$$b_j(\varepsilon) \asymp \sum_{i=0}^{\infty} \varepsilon^i \, b_{j,i} \, .$$

*Defining*

$$\tilde{b}^{(N)}(\varepsilon) := \sum_{j=0}^{N} \sum_{i=0}^{N-j} \varepsilon^{i+j} \, b_{j,i}$$

*we have*

$$\pi \# B \# \pi - \pi \# \tilde{b}^{(N)} \# \pi = \mathcal{O}(\varepsilon^\infty) \quad \text{in} \quad S^k(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f})) \tag{3.54}$$

*and*

$$\|\hat{\Pi}^{\varepsilon}\,\hat{B}^{\varepsilon}\,\hat{\Pi}^{\varepsilon} - \hat{\Pi}^{\varepsilon}\,\mathrm{op}_{\varepsilon}\left(\tilde{b}^{(N)}\right)\,\hat{\Pi}^{\varepsilon}\| = \mathcal{O}(\varepsilon^{\infty}). \tag{3.55}$$

*Also, there exist* $\tilde{r} \in N_0$ *and* $C_r < \infty$ *for every* $r \in \mathbb{N}_0$ *such that*

$$\left\|\pi \,\#\, (B - \tilde{b}^{(N)}\,\mathbf{1}_{\mathcal{H}_{\mathrm{f}}}) \,\#\, \pi\right\|_{k,r} \leq C_r\,\varepsilon^{N+1}\left(\|B\|^{\varepsilon}_{k,\tilde{r}} + \sum_{i=0}^{N}\left\|\varepsilon^{-(i+1)}\,(B - B^{(i)})\right\|^{\varepsilon}_{k,\tilde{r}}\right). \tag{3.56}$$

*If additionally* $k > 2n$ *then it holds for every* $R \in S^0(\varepsilon, \mathcal{J}(\mathcal{H}_{\mathrm{f}}))$ *that*

$$\mathrm{tr}\left(\mathrm{op}_{\varepsilon}\left(\tilde{b}^{(N)}\right)\,\hat{R}^{\varepsilon}\right) = \mathcal{O}\Big(\varepsilon^{-n}\,\|R\|^{\varepsilon}_{0,N,1}\,\sum_{i=0}^{N}\|B_i\|_{L^1}\Big) \tag{3.57}$$

*and*

$$\mathrm{tr}\left(\mathrm{op}_{\varepsilon}\left(\tilde{b}^{(N)}\right)\,\hat{\Pi}^{\varepsilon}\right) = \mathcal{O}\Big(\varepsilon^{-n}\,\sum_{i=0}^{N}\|B_i\|_{L^1}\Big). \tag{3.58}$$

*Furthermore,*

$$\mathrm{tr}\left(\left(\widehat{b^{(N)}}^{\,\varepsilon} - \widehat{\tilde{b}^{(N)}}^{\,\varepsilon}\right)\hat{R}^{\varepsilon}\right) = \mathcal{O}\Big(\varepsilon^{N+1-n}\,\|R\|^{\varepsilon}_{0,N,1}\,\Big(\sum_{i=0}^{N}\|\varepsilon^{-(i+1)}\,(B - B^{(i)})\|^{\varepsilon}_{L^1}\Big)\Big) \tag{3.59}$$

*Thus,*

$$\mathrm{tr}\left(\left(\hat{B}^{\varepsilon} - \widehat{\tilde{b}^{(N)}}^{\,\varepsilon}\right)\hat{\pi}^{\varepsilon}\right) = \mathcal{O}\Big(\varepsilon^{N+1-n}\,\Big(\|B\|_{L^1} + \sum_{i=0}^{N}\|\varepsilon^{-(i+1)}\,(B - B^{(i)})\|^{\varepsilon}_{L^1}\Big)\Big) \tag{3.60}$$

*and*

$$\mathrm{tr}\left(\left(\hat{B}^{\varepsilon} - \widehat{\tilde{b}^{(N)}}^{\,\varepsilon}\right)\hat{\Pi}^{\varepsilon}\right) = \mathcal{O}\Big(\varepsilon^{N+1-n}\,\Big(\|B\|^{\varepsilon}_{L^1} + \sum_{i=0}^{N}\|\varepsilon^{-(i+1)}\,(B - B^{(i)})\|^{\varepsilon}_{L^1}\Big)\Big). \tag{3.61}$$

PROOF Since $\pi \,\#\, (b - \tilde{b}^{(N)}) \,\#\, \pi$ is clearly of order $\varepsilon^{N+1}$ in $S^k(\varepsilon, \mathcal{H}_{\mathrm{f}})$, (3.54) follows by (3.36). As in the proof of Theorem 3.6, (3.55) follows by (3.54), the Calderon-Vaillancourt theorem (2.2) and the fact that $\hat{\Pi}^{\varepsilon} = \hat{\pi}^{\varepsilon} + \mathcal{O}(\varepsilon^{\infty})$.

Using the reformulation of the $b_j$s (3.46) we find that there are $Q^{j,r}_{\alpha} \in S^0(\mathcal{J}(\mathcal{H}_{\mathrm{f}}))$, $0 \leq r \leq j$ and $\alpha \in \{1, \ldots, 2n\}^r$ for any $j \in \mathbb{N}_0$ such that

$$b_{j,i} = \sum_{r=0}^{j}\sum_{\alpha \in \{1,\ldots,2n\}^r}\mathrm{tr}_{\mathcal{H}_{\mathrm{f}}}(Q^{j,r}_{\alpha}\,\nabla^r_{\alpha}B_i) \tag{3.62}$$

and

$$
\begin{aligned}
b_j(\varepsilon) - \sum_{i=0}^{N-j} \varepsilon^i \, b_{j,i} \\
= \varepsilon^{N+1-j} \sum_{r=0}^{j} \sum_{\alpha \in \{1,\dots,2n\}^r} \mathrm{tr}_{\mathcal{H}_\mathrm{f}} \Big( Q_\alpha^{j,r} \, \nabla_\alpha^r \varepsilon^{-(N+1-j)} \big( B(\varepsilon) - B^{(N-j)}(\varepsilon) \big) \Big) \,. 
\end{aligned} \tag{3.63}
$$

Thus, there exist $\tilde{r} \in N_0$ and $C_r < \infty$ for every $r \in \mathbb{N}_0$ such that

$$
\|\pi \,\#\, (b^{(N)} - \tilde{b}^{(N)}) \,\#\, \pi\|_{k,r} \le C_r \, \varepsilon^{N+1} \left( \sum_{i=0}^{N} \|\varepsilon^{-(i+1)} (B - B^{(i)})\|_{k,\tilde{r}}^{\varepsilon} \right)
$$

which, together with (3.38) shows (3.56).

Similar to (3.47)

$$
\begin{aligned}
\left| \int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}} (Q_\alpha^{j,r} \, \nabla_\alpha^r B_i)(z) \, \mathrm{tr}_{\mathcal{H}_\mathrm{f}} (R(\varepsilon, z)) \, \mathrm{d}z \right| &\le \|Q_\alpha^{j,r}\|_{0,j,1} \, \|R\|_{0,j,1}^{\varepsilon} \, \|B_i\|_{L^1} \\
&\le \|Q_\alpha^{j,r}\|_{0,j,1} \, \|R\|_{0,j,1}^{\varepsilon} \, \sum_{i=0}^{N} \|B_i\|_{L^1}
\end{aligned}
$$

for every $i, j \in \mathbb{N}_0$, $j \le N$, $i \le N - j$. This, together with the trace formula (2.12) and the reformulation of $b_{j,i}$ (3.62) implies (3.57). With the same argument as in the proof of Theorem 3.6, (3.58) follows from (3.57).

Applying Proposition A.10 with $N = -1$ we have

$$
\begin{aligned}
\varepsilon^{N-j} \int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}} \Big( \pi \,\#\, \mathrm{tr}_{\mathcal{H}_\mathrm{f}} \Big( Q_\alpha^{j,r} \, \partial_z^\alpha (\varepsilon^{-(N-j)} (B - B^{(N-j)})) \Big) \,\#\, \pi \Big)(z) \, \mathrm{d}z \\
= \mathcal{O}\Big( \varepsilon^{N+1-j} \, \|\varepsilon^{-(N+1-j)} (B - B^{(N-j)})\|_{L^1}^{\varepsilon} \Big)
\end{aligned}
$$

for each $j \in \mathbb{N}_0$, $j \le N$. This, together with the trace formula (2.12) and the reformulation of $b_{j,i}$ (3.63) implies (3.59). Then, (3.60) follows by additionally using the result for general $B \in S^k(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f}))$ (3.41). With the same argument as in the proof of Theorem 3.6, (3.61) follows from (3.60). □

# 3.3 The Classical Hamiltonian System

We derive a classical Hamiltonian system $(\mathbb{R}^{2n}, \omega^\varepsilon, h)$ which, up to additional quantum corrections, approximates quantum expectation values to higher orders in $\varepsilon$. We begin with the derivation of the classical Hamiltonian $h : \mathbb{R}^{2n} \to \mathbb{R}$. Since we are interested in semiclassical approximations inside the adiabatic subspace $\hat{\Pi}^\varepsilon \mathcal{H}$, our goal is to derive a real valued, $\varepsilon$-dependent function whose quantization approximates the action of the full Hamiltonian $\hat{H}^\varepsilon$ restricted to the adiabatic subspace. Thus, we want to define $h(z)$ as the effective Symbol of $H(z)$ using Theorem 3.6. Because of the linear part $\xi \cdot z$ the Hamiltonian does not fulfill the assumptions of Theorem 3.6. On the other hand $\xi \cdot z$ is a scalar function already. Thus, the solution is to define the classical Hamiltonian as $h(z) := \tilde{h}(z) + \xi \cdot z$ where $\tilde{h}$ is the effective symbol of $H(z) - \xi \cdot z$. In addition, we will compute the expansion of the classical Hamiltonian up to the second order in $\varepsilon$.

**Corollary 3.8** *Let Assumption 2.10 and 2.11 hold. Then, there exists a classical symbol* $\tilde{h} \in S^0(\varepsilon, \mathbb{R})$ *such that* $h(z) := \tilde{h}(z) + \xi \cdot z$ *satisfies*

$$\pi \# H \# \pi - \pi \# h \# \pi = \mathcal{O}(\varepsilon^\infty) \quad \textit{in} \quad S^0(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f}))$$

*and thus*

$$\|\hat{\Pi}^\varepsilon \hat{H}^\varepsilon \hat{\Pi}^\varepsilon - \hat{\Pi}^\varepsilon \hat{h}^\varepsilon \hat{\Pi}^\varepsilon\| = \mathcal{O}(\varepsilon^\infty)\,. \tag{3.64}$$

*In addition, for* $\Omega_0, W, M \in S^0(\mathbb{R}^{2n\times 2n})$ *and* $M^{op}_{ij} \in S^0(\mathcal{J}(\mathcal{H}_\mathrm{f}))$, $1 \le i, j \le 2n$ *defined by*

$$\Omega_0^{ij} = -\mathrm{i}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\,[\partial_i P_0, \partial_j P_0])\,,$$

$$W_{ij} := \mathrm{tr}_{\mathcal{H}_\mathrm{f}}([\,\partial_i P_0 \,|\, (H_0 - e_0)^{-1} \,|\, \partial_j P_0\,]_+)\,,$$

$$M_{ij} := \tfrac{\mathrm{i}}{2}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\partial_i P_0\,(H_0 - e_0)\,\partial_j P_0)$$

*and*

$$M^{op}_{ij} = -\tfrac{\mathrm{i}}{2}\,\partial_i P_0\,\partial_j (H_0 - e_0),$$

*we have*

$$
\begin{aligned}
h(z) = {} & e_0(z) + \xi \cdot z + \varepsilon \Big(\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(H^1\, P_0) + \mathrm{Tr}_{2n}(\omega^0\, M)\Big) \Big(1 - \tfrac{1}{4}\,\varepsilon\, \mathrm{Tr}_{2n}(\omega^0\, \Omega_0)\Big) \\
& + \varepsilon^2 \Big[ \tfrac{1}{2} \,\langle\, \omega^0\, (\nabla e_0 + \xi)\,,\, W\, \omega^0\, (\nabla e_0 + \xi)\,\rangle \\
& - \mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big( (\,\mathrm{Tr}_{2n}(\omega^0\, M^{op}) + H^1\,)\, (H_0 - e_0)^{-1}\, (\,\mathrm{Tr}_{2n}((\omega^0\, M^{op})^*\,) + H^1\,)\, P_0\Big) \\
& - \tfrac{\mathrm{i}}{2}\, \mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big( \langle\, \omega^0\, \nabla \mathrm{Tr}_{2n}(\omega^0\, M^{op})\,,\, \nabla P_0\,\rangle\, P_0\Big) \\
& + \tfrac{1}{8}\, \mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big( \mathrm{Tr}_{2n}(\,\omega^0\, \nabla^2 P_0\, \omega^0\, \nabla^2 (H_0 - e_0)\,)\, P_0 - \tfrac{\mathrm{i}}{2} \langle\, \omega^0\, \nabla P_0\,,\, \nabla H^1\,\rangle P_0\Big) \\
& - \tfrac{\mathrm{i}}{2}\, \mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big( \langle\, \omega^0\, \nabla P_0\,,\, H^1\, \nabla P_0\,\rangle P_0 - \tfrac{\mathrm{i}}{2}\, \langle\, \omega^0\, \nabla H^1\,,\, \nabla P_0\,\rangle P_0\Big)\Big] + \mathcal{O}(\varepsilon^3)
\end{aligned}
\tag{3.65}
$$

PROOF The existence of $\tilde{h} \in S^0(\varepsilon, \mathbb{R})$ follows by applying Theorem 3.6 to $H(z) - \xi \cdot z$. So, the only thing left to proof is that $h^{(2)}(z) - \xi \cdot z$ given by (3.65) coincides with the effective Symbol of $H(z) - \xi \cdot z$ defined by (3.26). We define $v(z) = \xi \cdot z$ such that $H - v = H_0 + \varepsilon\, H^1$. Since $P_0$ is the rank-one projection to the eigenspace associated to the eigenvalue $e_0$ of $H_0$

$$
\mathrm{tr}_{\mathcal{H}_\mathrm{f}}\,((H - v)_0 P_0) = \mathrm{tr}_{\mathcal{H}_\mathrm{f}}\,(H_0\, P_0) = e_0 = \tilde{h}_0\,.
$$

Before we proceed with the computations for $h_1$ note that

$$
0 = \partial_j (P_0\, (H_0 - e_0)) = \partial_j P_0\, (H_0 - e_0) + P_0\, \partial_j (H_0 - e_0)
$$

so that

$$
\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(M^{op}_{ij}\, P_0) = -\mathrm{tr}_{\mathcal{H}_\mathrm{f}}((M^{op})^*_{ij}\, P_0) = \tfrac{\mathrm{i}}{2}\, \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\partial_i P_0\, (H_0 - e_0)\, \partial_j P_0) = M_{ij}\,.
\tag{3.66}
$$

Regarding $h_1$, note that

$$
\begin{aligned}
(H - v - e_0) \,\#\, \pi = {} & (H_0 - e_0)\, P_0 + \varepsilon\, (H_0 - e_0)\, \pi_1 + \varepsilon\, H_0^1\, P_0 \\
& + \varepsilon\, \{H_0 - e_0\,,\, P_0\}_1 + \mathcal{O}(\varepsilon^2) \\
= {} & \varepsilon\, (H_0 - e_0)\, \pi_1 + \varepsilon\, H_0^1\, P_0 + \varepsilon\, \{H_0 - e_0\,,\, P_0\}_1 \\
& + \mathcal{O}(\varepsilon^2)\,.
\end{aligned}
$$

Thus a simple computation using (3.66) results in

$$
\mathrm{tr}_{\mathcal{H}_\mathrm{f}}\,((\pi \,\#\, (H - v - e_0) \,\#\, \pi)_1\, P_0) = \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\, H_0^1\, P_0) + \varepsilon\, \mathrm{Tr}_{2n}(\omega^0\, M) = h_1\,.
$$

Since the scalar symbol $h_1$ commutes with any operator-valued symbol and $\partial_j P_0$ is off-diagonal with respect to $P_0$

$$\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\{h_1\,,P_0\}_1\,P_0) = 0 = \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\{P_0\,,h_1\}_1\,P_0)\,. \tag{3.67}$$

In addition

$$0 = \{P_0\,(H_0-e_0)\,,\pi_1\}_1 = \{\pi_1\,|H_0-e_0\,|\,P_0\}_1 + P_0\,\{H_0-e_0\,,\pi_1\}_1 \tag{3.68}$$

as well as

$$0 = \{\pi_1\,,(H_0-e_0)\,P_0\}_1 = \{\pi_1\,|H_0-e_0\,|\,P_0\}_1 + \{\pi_1\,,H_0-e_0\}_1\;P_0\,. \tag{3.69}$$

Then, the explicit expansion of the triple Moyal product (2.8) combined with (3.67)-(3.69) yields

$$\begin{aligned}
&(\pi\,\#\,(H-v-e_0-\varepsilon h_1)\,\#\,\pi)_2\\
&\qquad = \pi_1\,(H_0-e_0)\,\pi_1 + \pi_1\,\{H_0-e_0\,,P_0\}_1 + \{P_0\,,H_0-e_0\}_1\,\pi_1\\
&\qquad\quad + \{\{P_0\,,H_0-e_0\}_1\;,P_0\}_1 + \{P_0\,,H_0-e_0\}_2\\
&\qquad\quad + \pi_1\,H_0^1\,P_0 + P_0\,H_0^1\,\pi_1 + \left\{P_0\,,H_0^1\right\}_1 P_0 + \left\{P_0\,\middle|H_0^1\middle|\,P_0\right\}_1\\
&\qquad\quad + P_0\left\{H_0^1\,,P_0\right\}_1 - h_1\,\pi_1\,P_0 - h_1\,P_0\,\pi_1 - h_1\,\{P_0\,,P_0\}_1 + P_0\,H_1^1\,P_0\,.
\end{aligned}$$

By definition we have

$$\{P_0\,,H_0-e_0\}_1 = \mathrm{Tr}_n(\omega^0\,M^{op}) \quad \text{and} \quad \{H_0-e_0\,,P_0\}_1 = \mathrm{Tr}_n((\omega^0\,M^{op})^*)\,.$$

This and a simple computation using the definition of $\pi_1$ as well as (3.66) leads to

$$\begin{aligned}
&\mathrm{tr}_{\mathcal{H}_\mathrm{f}}((\pi\,\#\,(H-v-e_0-\varepsilon h_1)\,\#\,\pi)_2\,P_0)\\
&\quad = \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(H_1^1\,P_0) - \tfrac14\,\mathrm{Tr}_{2n}(\omega^0\,M)\mathrm{Tr}_{2n}(\omega^0\,\Omega_0) - \tfrac14\,\mathrm{Tr}_{2n}(\omega^0\,\Omega_0)\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(H_0^1\,P_0)\\
&\qquad - \mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big((\,\mathrm{Tr}_{2n}(\omega^0\,M^{op}) + H_0^1\,)\,(H_0-e_0)^{-1}\,(\,\mathrm{Tr}_{2n}((\omega^0\,M^{op})^*\,) + H_0^1\,)\,P_0\Big)\\
&\qquad + \mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big(\langle\,\nabla e_0+\xi\,,\,\omega^0\,\nabla P_0\,\rangle\,(H_0-e_0)^{-1}\langle\,\omega^0\,\nabla P_0\,,\,\nabla e_0+\xi\,\rangle P_0\Big)\\
&\qquad + \mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big(\{\mathrm{Tr}_{2n}(\omega^0\,M^{op})\,,P_0\,\}_1\,P_0 + \{P_0\,,H_0-e_0\}_2\;P_0\Big)\\
&\qquad + \mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big(\{P_0\,,H_0^1\,\}_1 P_0 + \{P_0\,|\,H_0^1\,|\,P_0\,\}_1 P_0 + \{H_0^1\,,P_0\,\}_1 P_0\Big)\,.
\end{aligned}$$

Using the definition of the generalized Poisson bracket $\{\cdot\,,\cdot\}_j$ finishes the proof. □

What is left in the derivation of the Hamiltonian system is the symplectic form $\omega^\varepsilon$. Similarly to [ST13][Section 5], we define $\omega^\varepsilon := \omega^0 + \varepsilon\,\Omega^\varepsilon$ where $\omega^0 = \begin{pmatrix} 0 & \mathbf{1}_n \\ -\mathbf{1}_n & 0 \end{pmatrix}$ is the canonical symplectic form. Up to the factor $\mathrm{i}$, $\Omega^\varepsilon$ is given as the curvature form of the Berry connection where we replace the eigenprojection $P_0$ by the modified projection $\mathcal{P}^\varepsilon$ in the derivation of the Berry connection.

Regarding the modified Berry connection we define the Hilbert bundle $E : \mathbb{R}^{2n} \times \mathcal{H}_\mathrm{f} \overset{P_E}{\to} \mathbb{R}^{2n}$ with $P_E$ the projection onto the first component and equipped with a canonical flat connection where for $\phi \in \Gamma(E)$ and $X \in \Gamma(T\mathbb{R}^{2n})$, $(\nabla_X\phi)(z) = X^j\,\partial_j\phi(z)$. Then, the symbol $H_0 : \mathbb{R}^{2n} \to \mathcal{B}(\mathcal{H}_\mathrm{f})$ can be seen as a section in the endomorphism bundle of $E$, i.e. $H_0 \in \Gamma(\mathrm{End}(E))$ acting on sections $\phi \in \Gamma(E)$. By Proposition 3.2 we associate a rank-one projection $\mathcal{P}^\varepsilon : \mathbb{R}^{2n} \to \mathcal{B}(\mathcal{H}_\mathrm{f})$ with an isolated eigenvalue $e_0 : \mathbb{R}^{2n} \to \mathbb{R}$ of $H_0$. The projection $\mathcal{P}^\varepsilon$ can also be seen as $\mathcal{P}^\varepsilon \in \Gamma(\mathrm{End}(E))$. With this we can define a sub vector bundle $L^\varepsilon := \{(z,\phi)\,|\,\phi(z) \in \mathcal{P}^\varepsilon(z)\,\mathcal{H}_\mathrm{f}\}$ of $E$. The connection of $E$ then induces a connection on $L$ by projection, i.e. $\nabla^\varepsilon_X\,\phi := \mathcal{P}^\varepsilon\nabla_X\,\phi$ for $\phi \in \Gamma(L) \subset \Gamma(E)$ and $X \in \Gamma(T\mathbb{R}^{2n})$. For the curvature form $R^\varepsilon$ of the modified Berry connection $\nabla^\varepsilon$ the following result holds.

**Proposition 3.9** *The curvature form $R^\varepsilon$ of the modified Berry connection $\nabla^\varepsilon$ is $\frac{1}{2}R^\varepsilon_{ij}\,\mathrm{d}z^i \wedge \mathrm{d}z^j$, where*

$$R^\varepsilon_{ij} = \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\mathcal{P}^\varepsilon\,[\partial_i\mathcal{P}^\varepsilon, \partial_j\mathcal{P}^\varepsilon]).$$

Proof Let $X, Y \in \Gamma(T\mathbb{R}^{2n})$ and $\phi \in \Gamma(L^\varepsilon)$. Then

$$\begin{aligned}
&\nabla^\varepsilon_X\nabla^\varepsilon_Y\,\phi - \nabla^\varepsilon_Y\nabla^\varepsilon_X\,\phi \\
&\qquad = \mathcal{P}^\varepsilon X^i\,\partial_i(\mathcal{P}^\varepsilon\,Y^j\,\partial_j\phi) - \mathcal{P}^\varepsilon\,Y^j\,\partial_j(\mathcal{P}^\varepsilon X^i\,\partial_i\phi) \\
&\qquad = \mathcal{P}^\varepsilon X^i\,Y^j\,\partial_i(\mathcal{P}^\varepsilon\,\partial_j\phi) + \mathcal{P}^\varepsilon X^i\,\partial_i Y^j\,\partial_j\phi \\
&\qquad\quad - \mathcal{P}^\varepsilon\,Y^j\,\partial_j X^i\,\partial_i\phi - \mathcal{P}^\varepsilon X^i\,Y^j\,\partial_j(\mathcal{P}^\varepsilon\,\partial_i\phi) \\
&\qquad = X^i\,Y^j\,[\mathcal{P}^\varepsilon\,\partial_i\mathcal{P}^\varepsilon\,\partial_j\phi - \mathcal{P}^\varepsilon\,\partial_j\mathcal{P}^\varepsilon\,\partial_i\phi] + \nabla^\varepsilon_{[X,Y]}\phi\,.
\end{aligned}$$

Since $\mathcal{P}^\varepsilon$ is a projection of rank-one and $\phi = \mathcal{P}^\varepsilon\,\phi$, (2.15) yields

$$\mathcal{P}^\varepsilon\,[\partial_i\mathcal{P}^\varepsilon, \partial_j\mathcal{P}^\varepsilon]\phi = \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\mathcal{P}^\varepsilon\,[\partial_i\mathcal{P}^\varepsilon, \partial_j\mathcal{P}^\varepsilon])\phi\,.$$

Additionally using that $\partial_i \mathcal{P}^\varepsilon$ is off diagonal with respect to $\mathcal{P}^\varepsilon$ we obtain

$$\begin{aligned}
R^\varepsilon(X,Y)\phi :=& (\nabla^\varepsilon_X \nabla^\varepsilon_Y - \nabla^\varepsilon_Y \nabla^\varepsilon_X - \nabla^\varepsilon_{[X,Y]})\phi \\
=& X^i\, Y^j \,[\mathcal{P}^\varepsilon\, \partial_i \mathcal{P}^\varepsilon\, \partial_j \phi - \mathcal{P}^\varepsilon\, \partial_j \mathcal{P}^\varepsilon\, \partial_i \phi] \\
=& X^i\, Y^j \,[\mathcal{P}^\varepsilon\, \partial_i \mathcal{P}^\varepsilon\, \partial_j (\mathcal{P}^\varepsilon \phi) - \mathcal{P}^\varepsilon\, \partial_j \mathcal{P}^\varepsilon\, \partial_i (\mathcal{P}^\varepsilon \phi)] \\
=& X^i\, Y^j \,[\mathcal{P}^\varepsilon\, \partial_i \mathcal{P}^\varepsilon\, \partial_j \mathcal{P}^\varepsilon\, \phi - \mathcal{P}^\varepsilon\, \partial_j \mathcal{P}^\varepsilon\, \partial_i \mathcal{P}^\varepsilon\, \phi \\
&\quad + \mathcal{P}^\varepsilon\, \partial_i \mathcal{P}^\varepsilon\, \mathcal{P}^\varepsilon\, \partial_j \phi - \mathcal{P}^\varepsilon\, \partial_j \mathcal{P}^\varepsilon\, \mathcal{P}^\varepsilon\, \partial_i \phi] \\
=& X^i\, Y^j\, \mathcal{P}^\varepsilon\, [\partial_i \mathcal{P}^\varepsilon, \partial_j \mathcal{P}^\varepsilon]\, \phi \\
=& X^i\, Y^j\, \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\mathcal{P}^\varepsilon\, [\partial_i \mathcal{P}^\varepsilon, \partial_j \mathcal{P}^\varepsilon])\, \phi\,.
\end{aligned}$$

□

We then define the symplectic form $\omega^\varepsilon$ of the Hamiltonian system $(h, \omega^\varepsilon)$ as

$$\omega^\varepsilon = \omega^0 + \varepsilon\, \Omega^\varepsilon$$

where $\omega^0$ is the standard symplectic form on $\mathbb{R}^{2n}$ and $\Omega^\varepsilon$ a two form with coefficients

$$\Omega^\varepsilon_{ij} = -\mathrm{i}\, R^\varepsilon_{ij} = -\mathrm{i}\, \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\mathcal{P}^\varepsilon\, [\partial_i \mathcal{P}^\varepsilon, \partial_j \mathcal{P}^\varepsilon])\,.$$

Clearly, the fact that $\mathcal{P}^\varepsilon \in S^0(\varepsilon, \mathcal{J}_\mathrm{sa}(\mathcal{H}_\mathrm{f}))$ (see Proposition 3.2) implies that $\mathcal{P}^\varepsilon\,[\partial_i \mathcal{P}^\varepsilon, \partial_j \mathcal{P}^\varepsilon]$ is skew-symmetric. Therefore, the coefficients of $\Omega^\varepsilon$ are symbols in $S^0(\varepsilon, \mathbb{R})$. What is left is to show that $\omega^\varepsilon$ actually defines a symplectic form.

**Proposition 3.10** *For $\varepsilon$ small enough the two form $\omega^\varepsilon$ defines a symplectic form on the phase space $\mathbb{R}^{2n}$.*

PROOF The matrix $\Omega^\varepsilon_{ij}$ is skew-symmetric and bounded by definition. Thus $\omega^\varepsilon$ is non-degenerate since $\det \omega^\varepsilon \neq 0$ for $\varepsilon$ small enough. In addition a simple computation shows that $\omega^\varepsilon$ is closed, see [ST13, Proposition 4] and replace $\pi_0$ by $\mathcal{P}^\varepsilon$. □

Note that by (3.9) we have

$$\mathcal{P}^\varepsilon(z) = P(z) + \mathcal{O}(\varepsilon^\infty) = P_0(z) + \varepsilon\, P_1(z) + \mathcal{O}(\varepsilon^2)\,.$$

Therefore, the symplectic form $\omega^\varepsilon$ has an asymptotic expansion where

$$\omega^\varepsilon_{ij} = \omega^0_{ij} + \varepsilon\, \Omega^\varepsilon_{ij} = \omega^0_{ij} + \varepsilon\, \Omega^{ij}_0 + \varepsilon^2\, \Omega^{ij}_1 + \mathcal{O}(\varepsilon^3) \tag{3.70}$$

where

$$\Omega^{ij}_0 = -\mathrm{i}\, \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\, [\partial_i P_0, \partial_j P_0])$$

and

$$\Omega_1^{ij} = -\mathrm{i}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_1\,[\partial_i P_0, \partial_j P_0]) - \mathrm{i}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\,[\partial_i P_1, \partial_j P_0]) - \mathrm{i}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\,[\partial_i P_0, \partial_j P_1])\,.$$

Since $P_1$ is off-diagonal with respect to $P_0$ we obtain

$$\begin{aligned}\Omega_1^{ij} &= -\mathrm{i}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\,[\partial_i P_1, \partial_j P_0]) - \mathrm{i}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\,[\partial_i P_0, \partial_j P_1]) \\ &= -\mathrm{i}\,\partial_i \mathrm{tr}_{\mathcal{H}_\mathrm{f}}([\,P_1\,, \partial_j P_0\,]\,P_0) + \mathrm{i}\,\partial_j \mathrm{tr}_{\mathcal{H}_\mathrm{f}}([\,P_1\,, \partial_i P_0\,]\,P_0) \\ &= 2\,\partial_i \mathfrak{Im}(\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_1\,\partial_j P_0\,P_0)) - 2\,\partial_j \mathfrak{Im}(\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_1\,\partial_i P_0\,P_0))\,.\end{aligned} \tag{3.71}$$

Hence, we can reformulate $\Omega_1$ as the exterior derivative of the one form $S$ with coefficients

$$S_j = -\mathrm{i}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}([\,P_1\,, \partial_j P_0\,]\,P_0) = 2\,\mathfrak{Im}(\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_1\,\partial_j P_0\,P_0))$$

leading to

$$\omega^\varepsilon = \omega^0 - \tfrac{\mathrm{i}}{2}\,\varepsilon\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\,[\partial_i P_0, \partial_j P_0])\,\mathrm{d}z^i \wedge \mathrm{d}z^j + \varepsilon^2\,\mathrm{d}S + \mathcal{O}(\varepsilon^3)\,.$$

In addition to the symplectic form $\omega^\varepsilon$ we can associate a Fubini-Study metric $g^\varepsilon$ to the phase space $\mathbb{R}^{2n}$ with coefficients

$$g^\varepsilon_{ij} = \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\mathcal{P}^\varepsilon\,[\partial_i \mathcal{P}^\varepsilon, \partial_j \mathcal{P}^\varepsilon]_+)\,.$$

Similarly to $\Omega^\varepsilon$, the Fubini-Study metric $g^\varepsilon$ has an asymptotic expansion starting with

$$g^\varepsilon_{ij} = \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\,[\partial_i P_0, \partial_j P_0]_+) + \mathcal{O}(\varepsilon) =: g_0^{ij} + \mathcal{O}(\varepsilon)\,. \tag{3.72}$$

In addition, we define

$$\mathcal{T}^\varepsilon_{ij} := \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\mathcal{P}^\varepsilon\,\partial_i \mathcal{P}^\varepsilon\,\partial_j \mathcal{P}^\varepsilon) = \tfrac{1}{2}(g^\varepsilon_{ij} + \mathrm{i}\,\Omega^\varepsilon_{ij})\,. \tag{3.73}$$

The Liouville measure of $\omega^\varepsilon$ will be very important when we derive semiclassical approximations for thermodynamic equilibrium states in Section 4. By Proposition 2.7 we obtain that the Liouville measure of $\omega^\varepsilon$ is given by

$$\lambda^\varepsilon = \nu^\varepsilon\,\mathrm{d}q^1 \wedge \cdots \wedge \mathrm{d}p^n = \Big(1 + \sum_{k=1}^{n} \varepsilon^k\,\nu^\varepsilon_k\Big)\,\mathrm{d}q^1 \wedge \cdots \wedge \mathrm{d}p^n \tag{3.74}$$

with

$$\nu_k^\varepsilon = \sum_{\substack{\alpha\in\mathbb{N}_0^k,\\ \sum_{i=1}^k i\,\alpha_i = k}} \left(-\tfrac{1}{2}\right)^{|\alpha|} \prod_{j=1}^{k} (j^{\alpha_j}\,\alpha_j!)^{-1}\,\mathrm{Tr}_{2n}\Big((\omega^0\,\Omega^\varepsilon)^j\Big)^{\alpha_j}\,.$$

for $1 \le k \le n$. In particular, applying Corollary 2.8 shows

$$\nu^\varepsilon = 1 - \tfrac{1}{2}\,\varepsilon\,\mathrm{Tr}_{2n}(\omega^0\,\Omega^\varepsilon)) + \tfrac{1}{8}\,\varepsilon^2\,\mathrm{Tr}_{2n}(\omega^0\,\Omega^\varepsilon)^2 - \tfrac{1}{4}\,\varepsilon^2\,\mathrm{Tr}_{2n}(\omega^0\,\Omega^\varepsilon\,\omega^0\,\Omega^\varepsilon) + \mathcal{O}(\varepsilon^3)\,. \tag{3.75}$$

# 4 Semiclassical Approximations for Stationary States

For an equilibrium state $f(\hat{H}^\varepsilon)$ in $\hat{\Pi}^\varepsilon \mathcal{H}$ the expectation value with respect to an observable $\hat{A}^\varepsilon$ is given by

$$\operatorname{tr}\left(\hat{\Pi}^\varepsilon f(\hat{H}^\varepsilon)\hat{A}^\varepsilon\right) .$$

One can think of $f$ being a distribution function like a Fermi-Dirac or Boltzmann distribution. In this section we develop a formalism to derive semiclassical approximations of such equilibrium expectations. The approximation is given as phase space integrals over symbols that can be explicitly expressed in terms of $f$, the observable $A$, an isolated eigenband $e_0$, the associated eigenprojection $P_0$, effective Hamiltonian $h$ as well as the reduced resolvent $(H_0 - e_0)^{-1}$ on $\hat{\Pi}^{\varepsilon\perp}\mathcal{H}_\mathrm{f}$ and their derivatives. As already mentioned in the introduction, even in the special case of a purely semiclassical system it is not possible to express the second-order terms of an equilibrium expectation value in terms of a classical system, see (1.4). Hence, this will not be possible in the general case either. Nevertheless, we will show how to express the terms obtained from the second order semiclassical approximation by the $\varepsilon$-dependent Hamiltonian system $(\mathbb{R}^{2n}, \omega^\varepsilon, h)$ derived in Section 3.3 plus quantum corrections of order $\varepsilon^2$.

We begin with some formal computations that aim to give the reader an overview over the approach. First, we introduce a tool that is used throughout this section, the Helffer-Sjöstrand formula. For $\hat{R}$ a self-adjoint operator acting on the separable Hilbert space $\mathcal{H}$ and

$$f \in \mathcal{A} := \{f \in C^\infty(\mathbb{R}) |\, \exists \beta > 0 : \sup_{x\in\mathbb{R}} |\langle x\rangle^{(n+\beta)} f^{(n)}(x)| < \infty \;\forall n \in \mathbb{N}_0\}$$

with almost analytic extension $\tilde{f}$ we have

$$f(\hat{R}) = \tfrac{1}{\pi} \int_{\mathbb{R}^2} \partial_{\bar{\zeta}} \tilde{f}(\zeta)\, (\hat{R} - \zeta)^{-1}\, \mathrm{d}x\, \mathrm{d}y\,, \quad \text{see e.g. [Dav95]}\,.$$

The Hamiltonian $\hat{H}^\varepsilon$ almost commutes with the super-adiabatic projection $\hat{\Pi}^\varepsilon$. Therefore, the resolvent $(\hat{H}^\varepsilon - \zeta)^{-1}$ almost commutes with $\hat{\Pi}^\varepsilon$ for any $\zeta \in \mathbb{C} \setminus \mathbb{R}$. Then, the Hellfer-Sjöstrand formula suggests that $f(\hat{H}^\varepsilon)$ almost commutes with $\hat{\Pi}^\varepsilon$. Hence,

$$\operatorname{tr}_{\mathcal{H}}\left(\hat{\Pi}^\varepsilon f\left(\hat{H}^\varepsilon\right) \hat{A}^\varepsilon\right) \approx \operatorname{tr}_{\mathcal{H}}\left(\hat{\Pi}^\varepsilon f\left(\hat{H}^\varepsilon\right) \hat{\Pi}^\varepsilon \hat{A}^\varepsilon \hat{\Pi}^\varepsilon\right) .$$

For now, assume the existence of an $\varepsilon$-dependent scalar symbol $f^\varepsilon(\varepsilon, z)$ whose quantization approximates the action of the equilibrium state $f(\hat{H}^\varepsilon)$ restricted to the almost-invariant subspace, i.e. $\hat{\Pi}^\varepsilon f(\hat{H}^\varepsilon) \hat{\Pi}^\varepsilon \approx \hat{\Pi}^\varepsilon \operatorname{op}_\varepsilon(f^\varepsilon) \hat{\Pi}^\varepsilon$. Then,

$$\operatorname{tr}_{\mathcal{H}}\left(\hat{\Pi}^\varepsilon f\left(\hat{H}^\varepsilon\right) \hat{\Pi}^\varepsilon \hat{A}^\varepsilon \hat{\Pi}^\varepsilon\right) \approx \operatorname{tr}_{\mathcal{H}}\left(\hat{\Pi}^\varepsilon \operatorname{op}_\varepsilon(f^\varepsilon) \hat{\Pi}^\varepsilon \hat{A}^\varepsilon \hat{\Pi}^\varepsilon\right) .$$

In the next step we replace $\hat{A}^\varepsilon$ by its effective operator $\hat{a}^\varepsilon$ defined in Section 3.2. In addition, a simple computation using the fact that $\hat{\Pi}^\varepsilon$ is a projection yields

$$\hat{\Pi}^\varepsilon \operatorname{op}_\varepsilon(f^\varepsilon) \hat{\Pi}^\varepsilon \hat{a}^\varepsilon = \hat{\Pi}^\varepsilon \operatorname{op}_\varepsilon(f^\varepsilon) \hat{a}^\varepsilon - \mathrm{i}\,\varepsilon\, \hat{\Pi}^\varepsilon \tfrac{\mathrm{i}}{\varepsilon}\left[\operatorname{op}_\varepsilon(f^\varepsilon), \hat{\Pi}^\varepsilon\right] \hat{a}^\varepsilon .$$

Thus,

$$\begin{aligned}
\operatorname{tr}_{\mathcal{H}}\left(\hat{\Pi}^\varepsilon \operatorname{op}_\varepsilon(f^\varepsilon) \hat{\Pi}^\varepsilon \hat{A}^\varepsilon \hat{\Pi}^\varepsilon\right) &\approx \operatorname{tr}_{\mathcal{H}}\left(\hat{\Pi}^\varepsilon \operatorname{op}_\varepsilon(f^\varepsilon) \hat{\Pi}^\varepsilon \hat{a}^\varepsilon \hat{\Pi}^\varepsilon\right) \\
&= \operatorname{tr}_{\mathcal{H}}\left(\hat{\Pi}^\varepsilon \operatorname{op}_\varepsilon(f^\varepsilon) \hat{a}^\varepsilon\right) \\
&\quad - \mathrm{i}\,\varepsilon \operatorname{tr}_{\mathcal{H}}\left(\hat{\Pi}^\varepsilon \tfrac{\mathrm{i}}{\varepsilon}\left[\operatorname{op}_\varepsilon(f^\varepsilon), \hat{\Pi}^\varepsilon\right] \hat{a}^\varepsilon\right)
\end{aligned}$$

By the trace formula (2.13)

$$\begin{aligned}
&\operatorname{tr}_{\mathcal{H}}\left(\hat{\Pi}^\varepsilon \operatorname{op}_\varepsilon(f^\varepsilon) \hat{a}^\varepsilon\right) - \mathrm{i}\,\varepsilon \operatorname{tr}_{\mathcal{H}}\left(\hat{\Pi}^\varepsilon \tfrac{\mathrm{i}}{\varepsilon}\left[\operatorname{op}_\varepsilon(f^\varepsilon), \hat{\Pi}^\varepsilon\right] \hat{a}^\varepsilon\right) \\
&\quad\approx (2\pi\varepsilon)^{-n} \int_{\mathbb{R}^{2n}} \left(\operatorname{tr}_{\mathcal{H}_\mathrm{f}}(\pi) \# f^\varepsilon\right)(\varepsilon, z)\, a(\varepsilon, z)\, \mathrm{d}z \\
&\quad\quad - \mathrm{i}\,\varepsilon\, (2\pi\varepsilon)^{-n} \int_{\mathbb{R}^{2n}} \operatorname{tr}_{\mathcal{H}_\mathrm{f}}(\pi \# \tfrac{\mathrm{i}}{\varepsilon}[\, f^\varepsilon, \pi\,]_\#)(\varepsilon, z)\, a(\varepsilon, z)\, \mathrm{d}z .
\end{aligned}$$

Combining the statements above leads to

$$\begin{aligned}
\operatorname{tr}_{\mathcal{H}}\left(\hat{\Pi}^\varepsilon f\left(\hat{H}^\varepsilon\right) \hat{A}^\varepsilon\right) &\approx (2\pi\varepsilon)^{-n} \int_{\mathbb{R}^{2n}} \left(\operatorname{tr}_{\mathcal{H}_\mathrm{f}}(\pi) \# f^\varepsilon\right)(z)\, a(z)\, \mathrm{d}z \\
&\quad - \mathrm{i}\,\varepsilon\, (2\pi\varepsilon)^{-n} \int_{\mathbb{R}^{2n}} \operatorname{tr}_{\mathcal{H}_\mathrm{f}}(\pi \# \tfrac{\mathrm{i}}{\varepsilon}[\, f^\varepsilon, \pi\,]_\#)(z)\, a(z)\, \mathrm{d}z .
\end{aligned}$$

Note that the basic strategy displayed above in due to Stiepan and Teufel [ST13][Theorem 1]. At this point all the statements above can be made rigorous quite easily using the tools we have developed in the previous chapters. Nevertheless, we will present the proofs in Section 4.2. However, we only assumed the existence of an effective symbol $f^\varepsilon(z)$ of the equilibrium state $f(\hat{H}^\varepsilon)$. This is the main issue remaining in deriving a semiclassical expansion of expectation values in thermodynamic equilibrium. We explain our solution for this problem in the following section.

## 4.1 Effective Operators of Stationary States

We derive an effective symbol of a stationary state $f(\hat{H}^\varepsilon)$ restricted to the almost-invariant subspace, i.e. a symbol $f^\varepsilon \in S^0(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f}))$ such that

$$\hat{\Pi}^\varepsilon f(\hat{H}^\varepsilon)\,\hat{\Pi}^\varepsilon = \hat{\Pi}^\varepsilon \operatorname{op}_\varepsilon(f^\varepsilon)\,\hat{\Pi}^\varepsilon + \mathcal{O}(\varepsilon^\infty)\,.$$

By Helffer and Sjöstrand's formula we have

$$\hat{\Pi}^\varepsilon f(\hat{H}^\varepsilon)\,\hat{\Pi}^\varepsilon = \tfrac{1}{\pi}\int_{\mathbb{R}^2} \partial_{\bar\zeta}\tilde{f}(\zeta)\,\hat{\Pi}^\varepsilon\,(\hat{H}^\varepsilon-\zeta)^{-1}\,\hat{\Pi}^\varepsilon\,\mathrm{d}x\,\mathrm{d}y \tag{4.1}$$

with $\tilde{f}$ being an almost analytic extension of $f \in \mathcal{A}$. Hence, the key problem is to approximate the resolvent $(\hat{H}^\varepsilon-\zeta)^{-1}$ restricted to the adiabatic subspace $\hat{\Pi}^\varepsilon\mathcal{H}$.

This approximation divides into a three step procedure. First, we 'push' the adiabatic projection into the resolvent

$$\hat{\Pi}^\varepsilon\,(\hat{H}^\varepsilon-\zeta)^{-1}\,\hat{\Pi}^\varepsilon = \hat{\Pi}^\varepsilon\,(\hat{\Pi}^\varepsilon\,\hat{H}^\varepsilon\,\hat{\Pi}^\varepsilon-\zeta)^{-1}\,\hat{\Pi}^\varepsilon + \mathcal{O}(\varepsilon^\infty)\,,$$

see e.g. [ST13, Theorem 1], or rather [ST13, Appendix Lemma 1]. Although the above statement was proven already, we give a proof as part of Proposition 4.3, the main Proposition of this section. The next step is to replace the full Hamiltonian $\hat{H}^\varepsilon$ by the effective Hamiltonian $\hat{h}^\varepsilon$ defined in Section 3.3. By (3.64) we have $\|\hat{\Pi}^\varepsilon\hat{H}^\varepsilon\hat{\Pi}^\varepsilon - \hat{\Pi}^\varepsilon\hat{h}^\varepsilon\hat{\Pi}^\varepsilon\| = \mathcal{O}(\varepsilon^\infty)$. Additionally, making use of the fact that for self-adjoint operators $R$, $B$ and $\zeta \in \mathbb{C}\setminus\mathbb{R}$

$$\|(R-\zeta)^{-1}-(B-\zeta)^{-1}\| = \|(R-\zeta)^{-1}\,(B-R)\,(B-\zeta)^{-1}\| \le \frac{\|B-R\|}{|\mathfrak{Im}(\zeta)|^2} \tag{4.2}$$

we obtain

$$\hat{\Pi}^\varepsilon\,(\hat{\Pi}^\varepsilon\,\hat{H}^\varepsilon\,\hat{\Pi}^\varepsilon-\zeta)^{-1}\,\hat{\Pi}^\varepsilon = \hat{\Pi}^\varepsilon\,(\hat{\Pi}^\varepsilon\,\hat{h}^\varepsilon\,\hat{\Pi}^\varepsilon-\zeta)^{-1}\,\hat{\Pi}^\varepsilon + \mathcal{O}(\varepsilon^\infty)\,.$$

The final and most elaborate step is to derive an effective symbol whose Weyl-quantization approximates $(\hat{\Pi}^\varepsilon\,\hat{h}^\varepsilon\,\hat{\Pi}^\varepsilon - \zeta)^{-1}$ restricted to the almost-invariant subspace. The main idea here is to derive an operator that approximates $(\hat{\Pi}^\varepsilon\,\hat{h}^\varepsilon\,\hat{\Pi}^\varepsilon - \zeta)^{-1}$ and is admissible to semiclassical approximations.

**Lemma 4.1** *Let $B$ be a self-adjoint operator on $\mathcal{H}$ with domain $D(B)$ and $\Pi \in \mathcal{B}(\mathcal{H})$ an orthogonal projection satisfying $\Pi\, D(B) \subset D(B)$ and*

$$\|\,[\Pi\,,B]\,\| \leq d$$

*for some $d < \infty$. Then*

$$\left\| \Pi \left( (\Pi\, B\, \Pi - \zeta)^{-1} - \sum_{l=0}^{N} \Big(G(\zeta)\Big)^{l} (B-\zeta)^{-1} \right) \Pi \right\| \leq \frac{d^{\,2(N+1)}}{|\mathfrak{Im}(\zeta)|^{2N+3}}$$

*for any $N \in \mathbb{N}_0$ and $\zeta \in \mathbb{C} \setminus \mathbb{R}$ where*

$$G(\zeta) := (B-\zeta)^{-1}\ [B,\Pi]\ (B-\zeta)^{-1}\ [B,\Pi]\,\Pi\,.$$

Proof Let $\zeta \in \mathbb{C} \setminus \mathbb{R}$ and $N \in \mathbb{N}_0$. By assumption $B$ is self-adjoint. As a consequence, $\|(B-\zeta)^{-1}\| \leq \frac{1}{|\mathfrak{Im}(\zeta)|}$ and

$$\|G(\zeta)\| \leq \frac{d^2}{|\mathfrak{Im}(\zeta)|^2}\,. \tag{4.3}$$

In addition, $\Pi\, B\, \Pi$ is self-adjoint on $\Pi\, D(B) \oplus \Pi^{\perp}\, \mathcal{H}$ which implies

$$\|(\Pi\, B\, \Pi - \zeta)^{-1}\| \leq |\mathfrak{Im}(\zeta)|^{-1} \ \text{ and } \ \|\Pi\, (\Pi\, B\, \Pi - \zeta)^{-1}\, \Pi\| \leq |\mathfrak{Im}(\zeta)|^{-1}\,. \tag{4.4}$$

Moreover, $\zeta$ commutes with $\Pi$ so that $[B,\Pi] = [B-\zeta,\Pi]$ and $\Pi\,(B-\zeta)\,\Pi = \Pi\,(\Pi\, B\, \Pi - \zeta)$. Therefore,

$$\begin{aligned}
G(\zeta) =&(B-\zeta)^{-1}\ [B,\Pi]\ (B-\zeta)^{-1}\ [B,\Pi]\,\Pi \\
=&+(B-\zeta)^{-1}\,(B-\zeta)\,\Pi\,(B-\zeta)^{-1}\,(B-\zeta)\,\Pi\,\Pi \\
&-(B-\zeta)^{-1}\,\Pi\,(B-\zeta)\,(B-\zeta)^{-1}\,(B-\zeta)\,\Pi\,\Pi \\
&-(B-\zeta)^{-1}\,(B-\zeta)\,\Pi\,(B-\zeta)^{-1}\,\Pi\,(B-\zeta)\,\Pi \\
&+(B-\zeta)^{-1}\,\Pi\,(B-\zeta)\,(B-\zeta)^{-1}\,\Pi\,(B-\zeta)\,\Pi \\
=&-\Pi\,(B-\zeta)^{-1}\,\Pi\,(\Pi\, B\, \Pi - \zeta) + \Pi\,.
\end{aligned}$$

Since $G(\zeta) = G(\zeta)\,\Pi$, we conclude

$$\Pi\,(\Pi\,B\,\Pi - \zeta)^{-1}\Pi = \Pi\,(B-\zeta)^{-1}\,\Pi + \Pi\,G(\zeta)\,\Pi\,(\Pi\,B\,\Pi - \zeta)^{-1}\,\Pi\,. \tag{4.5}$$

Repeatedly substituting (4.5) into itself we obtain

$$\begin{aligned}\Pi\,(\Pi\,B\,\Pi - \zeta)^{-1}\Pi = &\sum_{l=0}^{N} \Pi\,\Big(G(\zeta)\,\Pi\Big)^{l}\,(B-\zeta)^{-1}\,\Pi \\ &+ \Pi\,\Big(G(\zeta)\,\Pi\Big)^{N+1}\,(\Pi\,B\,\Pi-\zeta)^{-1}\,\Pi\,.\end{aligned}$$

By $G(\zeta) = G(\zeta)\,\Pi$, the above equation turns into

$$\begin{aligned}\Pi\,(\Pi\,B\,\Pi - \zeta)^{-1}\Pi = &\sum_{l=0}^{N} \Pi\,\Big(G(\zeta)\Big)^{l}\,(B-\zeta)^{-1}\,\Pi \\ &+ \Pi\,\Big(G(\zeta)\Big)^{N+1}\,(\Pi\,B\,\Pi-\zeta)^{-1}\,\Pi\,.\end{aligned} \tag{4.6}$$

Applying the estimates (4.3) and (4.4)

$$\Big\|\Pi\,G^{N+1}(\zeta)\,(\Pi\,B\,\Pi-\zeta)^{-1}\,\Pi\Big\| \leq \frac{d^{2(N+1)}}{|\mathfrak{Im}(z)|^{2N+3}} \tag{4.7}$$

Then, combining (4.6) and (4.7) finishes the proof. □

Note that for the special case where $N = 1$, Lemma 4.1 was previously shown in [ST13, Appendix, Lemma 1].

In [DS99, Chapter 8] Dimassi and Sjöstrand derived a symbol $r(\varepsilon, z)$ whose quantization approximates $(\hat{h}^{\varepsilon} - \zeta)^{-1}$ to any order in $\varepsilon$. Therefore, by applying Lemma 4.1 to $(\hat{\Pi}^{\varepsilon}\,\hat{h}^{\varepsilon}\,\hat{\Pi}^{\varepsilon} - \zeta)^{-1}$ it is easy to see that

$$\begin{aligned}&\bigg\|\hat{\Pi}^{\varepsilon}\,\Big(\Big(\hat{\Pi}^{\varepsilon}\,\hat{h}^{\varepsilon}\,\hat{\Pi}^{\varepsilon}-\zeta\Big)^{-1} - \mathrm{op}_{\varepsilon}\Big(\sum_{l=0}^{N}\overbrace{G^{\varepsilon}(\zeta)\,\#\,\ldots\,\#\,G^{\varepsilon}(\zeta)}^{l\text{-times}}\,\#\,r\Big)\Big)\,\hat{\Pi}^{\varepsilon}\bigg\| \\ &\quad = \mathcal{O}(\varepsilon^{2(N+1)})\end{aligned}$$

where

$$G(\zeta) := r\,\#\,(h\,\#\,\pi - \pi\,\#\,h)\,\#\,r\,\#\,(h\,\#\,\pi - \pi\,\#\,h)\,\#\,\pi\,.$$

Which is what we are aiming for. The derivation of $r(\varepsilon, z)$ is a very important and non-trivial step. In addition, we aim for a special representation of $r(\varepsilon, z)$. Hence, we derive $r(\varepsilon, z)$ in the following Lemma with some slight variations compared to [DS99, Chapter 8].

**Lemma 4.2** *Let* $\xi \in \mathbb{R}^{2n}$ *and* $b(\varepsilon, z) = b_0(z) + \varepsilon\, \tilde{b}_1(\varepsilon, z)$ *where* $b_0(z) - \xi \cdot z$ *belongs to* $S^0(\mathbb{R})$ *and* $\tilde{b}_1$ *is a classical symbol in* $S^0(\varepsilon, \mathbb{R})$*. Then, there exists a classical symbol* $r(\zeta) \in S^0(\varepsilon, \mathbb{C})$ *for every* $\zeta \in \mathbb{C} \setminus \mathbb{R}$ *such that*

$$r(\zeta)\#(b-\zeta) = 1 + \mathcal{O}(\varepsilon^\infty) \quad \textit{and} \quad (b-\zeta)\#r(\zeta) = 1 + \mathcal{O}(\varepsilon^\infty)\,.$$

*In addition, there exist classical symbols* $\tilde{q}_{l,j}(b) \in S^0(\varepsilon, \mathbb{R})$*,* $l \in \mathbb{N}_0$*,* $0 \le j \le 2l$ *such that*

$$r(\zeta) \asymp \sum_{l=0}^{\infty} \varepsilon^l \frac{q_l(\zeta)}{(b_0-\zeta)^{2l+1}}$$

*with*

$$q_l(\zeta) = \Big(-b_1\,(b_0-\zeta)\Big)^l + \sum_{j=0}^{2l} \tilde{q}_{l,j}(b)\,(b_0-\zeta)^j.$$

*The* $\tilde{q}_{l,j}(b)$*s can be expressed explicitly in terms of* $b_0, \tilde{b}_1$ *and their derivatives where*

$$\begin{aligned}
&\tilde{q}_{0,0}(b) = \tilde{q}_{1,0}(b) = \tilde{q}_{1,1}(b) = \tilde{q}_{1,2}(b) = \tilde{q}_{2,0}(b) = \tilde{q}_{2,3}(b) = \tilde{q}_{2,4}(b) = 0,\\
&\tilde{q}_{2,1}(b) = \tfrac{1}{4}\,\langle\,\omega^0\,\nabla b_0\,,\ \nabla^2 b_0\,\omega^0\,\nabla b_0\,\rangle + \mathcal{O}(\varepsilon)
\end{aligned} \tag{4.8}$$

*and*

$$\tilde{q}_{2,2}(b) = \tfrac{1}{8}\,\mathrm{Tr}_{2n}(\omega^0\,\nabla^2 b_0\,\omega^0\,\nabla^2 b_0) + \mathcal{O}(\varepsilon)$$

*Hence,*

$$\begin{aligned}
r(\zeta) =& (b_0-\zeta)^{-1} - \varepsilon\,\tilde{b}_1\,(b_0-\zeta)^{-2} + \varepsilon^2\,\tilde{b}_1^2\,(b_0-\zeta)^{-3}\\
&+ \tfrac{1}{4}\,\varepsilon^2\,\langle\,\omega^0\,\nabla b_0\,,\ \nabla^2 b_0\,\omega^0\,\nabla b_0\,\rangle\,(b_0-\zeta)^{-4}\\
&+ \tfrac{1}{8}\,\varepsilon^2\,\mathrm{Tr}_{2n}(\omega^0\,\nabla^2 b_0\,\omega^0\,\nabla^2 b_0)\,(b_0-\zeta)^{-3} + \mathcal{O}(\varepsilon^3)\,.
\end{aligned}$$

PROOF We will mainly follow the procedure developed in [DS99, Chapter 8]. Fix $\zeta \in \mathbb{C} \setminus \mathbb{R}$. We make the ansatz

$$r(\zeta) \asymp \sum_{j=0}^{\infty} \varepsilon^j \frac{q_j(\zeta)}{(b_0-\zeta)^{2j+1}} = \sum_{j\ge 0} \varepsilon^j\, r_j(\zeta)\,.$$

Then, $r(\zeta)\#(b-\zeta)$ has an asymptotic expansion given by

$$\begin{aligned}
r(\zeta)\#(b-\zeta) \asymp& \sum_{l=0}^{\infty} \varepsilon^l \Big( \sum_{k=0}^{l} \tfrac{1}{(2\mathrm{i})^k}\,\{r_{l-k}(\zeta)\,, b_0-\zeta\}_k + \sum_{k=0}^{l-1} \tfrac{1}{(2\mathrm{i})^k}\{r_{l-k-1}(\zeta)\,, \tilde{b}_1\,\}_k \Big)\\
=:& \sum_{l=0}^{\infty} \varepsilon^l\, C_l^\varepsilon(\zeta)\,.
\end{aligned}$$

Then

$$C_0^\varepsilon(\zeta) = \frac{q_0(\zeta)}{(b_0-\zeta)}\,(b_0-\zeta) = q_0(\zeta) \tag{4.9}$$

and

$$\begin{aligned}
C_l^\varepsilon(\zeta) &= \sum_{k=0}^{l} \tfrac{1}{(2\mathrm{i})^k}\,\{r_{l-k}(\zeta)\,, b_0-\zeta\}_k + \sum_{k=0}^{l-1} \tfrac{1}{(2\mathrm{i})^k}\{r_{l-k-1}(\zeta)\,, \tilde{b}_1\,\}_k \\
&= r_l(\zeta)\,(b_0-\zeta) + r_{l-1}(\zeta)\,\tilde{b}_1 \\
&\quad + \sum_{k=1}^{l} \tfrac{1}{(2\mathrm{i})^k}\,\{r_{l-k}(\zeta)\,, b_0-\zeta\}_k + \sum_{k=1}^{l-1} \tfrac{1}{(2\mathrm{i})^k}\{r_{l-k-1}(\zeta)\,, \tilde{b}_1\,\}_k \\
&= \frac{q_l(\zeta)}{(b_0-\zeta)^{2l+1}}\,(b_0-\zeta) + \frac{q_{l-1}(\zeta)}{(b_0-\zeta)^{2l-1}}\,\tilde{b}_1 \\
&\quad + \sum_{k=1}^{l} \tfrac{1}{(2\mathrm{i})^k} \left\{ \frac{q_{l-k}(\zeta)}{(b_0-\zeta)^{2(l-k)+1}}\,, b_0-\zeta \right\}_k \\
&\quad + \sum_{k=1}^{l-1} \tfrac{1}{(2\mathrm{i})^k} \left\{ \frac{q_{l-k-1}(\zeta)}{(b_0-\zeta)^{2(l-k)-1}}\,, \tilde{b}_1 \right\}_k
\end{aligned}$$

for $l \geq 1$. Thus, defining $q_0 := 1$ and $q_l$ for $l \geq 1$ recursively by

$$\begin{aligned}
q_l(\zeta) :=& -q_{l-1}(\zeta)\,\tilde{b}_1\,(b_0-\zeta) \\
&- \sum_{k=1}^{l} \tfrac{1}{(2\mathrm{i})^k} \left\{ \frac{q_{l-k}(\zeta)}{(b_0-\zeta)^{2(l-k)+1}}\,, b_0-\zeta \right\}_k (b_0-\zeta)^{2l} \\
&- \sum_{k=1}^{l-1} \tfrac{1}{(2\mathrm{i})^k} \left\{ \frac{q_{l-k-1}(\zeta)}{(b_0-\zeta)^{2(l-k)-1}}\,, \tilde{b}_1 \right\}_k (b_0-\zeta)^{2l}
\end{aligned} \tag{4.10}$$

yields

$$r^{(N)}(\zeta)\#(b-\zeta) = 1 + \mathcal{O}(\varepsilon^{N+1})$$

for any $N \in \mathbb{N}_0$. In addition, since

$$\partial_{z_i}(b_0-\zeta)^{-m} = -m\,(b_0-\zeta)^{-(m+1)}\,\partial_{z_i} b_0$$

one can easily see that $q_l(\zeta)$, $l \geq 0$ can be written in the form

$$q_l(\zeta) = \Big(-\tilde{b}_1\,(b_0-\zeta)\Big)^l + \sum_{j=0}^{2l} \tilde{q}_{l,j}(b)\,(b_0-\zeta)^j.$$

The boundedness of the $\tilde{q}_{l,j}$s and their derivatives is obvious since none of these terms depends on $b_0$ directly but just on its derivatives. It follows that

$r_j(\zeta)$ are classical symbols in $S^0(\varepsilon, \mathbb{C})$. A resummation (Lemma 2.1) shows the existence of $r(\zeta)$ with

$$r(\zeta)\#(b-\zeta) = 1 + \mathcal{O}(\varepsilon^\infty)\,.$$

Note that one can construct $r_R(\zeta)$ with $(b-\zeta)\,\#\,r_R(\zeta) = 1 + \mathcal{O}(\varepsilon^\infty)$ analogously. By the associativity of the Moyal product it follows that

$$\begin{aligned} r_R(\zeta) &= (r(\zeta)\#(b-\zeta))\,\#\,r_R(\zeta) + \mathcal{O}(\varepsilon^\infty) = r(\zeta)\,\#\,((b-\zeta)\,\#\,r_R(\zeta)) + \mathcal{O}(\varepsilon^\infty) \\ &= r(\zeta) + \mathcal{O}(\varepsilon^\infty)\,. \end{aligned}$$

Regarding the explicit formulas (4.8), note $q_0(\zeta) = 1$ by (4.9) and $q_1(\zeta) = -\tilde{b}_1\,(b_0-\zeta)$ by (4.10) and

$$\begin{aligned} &\sum_{\substack{j+k=1\\k\geq 1}} \tfrac{1}{(2\mathrm{i})^k}\Big(\Big\{\frac{q_j(\zeta)}{(b_0-\zeta)^{2j+1}}\,,\,b_0\Big\}_k + \Big\{\frac{q_{j-1}(\zeta)}{(b_0-\zeta)^{2j-1}}\,,\,\tilde{b_1}\Big\}_k\Big)(b_0-\zeta)^2 \\ &\qquad = \tfrac{1}{(2\mathrm{i})}\Big\{\frac{1}{(b_0-\zeta)}\,,\,b_0\Big\}(b_0-\zeta)^2 = -\tfrac{1}{(2\mathrm{i})}\{\,b_0\,,\,b_0\,\} = 0\,. \end{aligned}$$

In addition, a simple computation shows

$$\begin{aligned} &-\sum_{\substack{j+k=2\\k\geq 1}} \tfrac{1}{(2\mathrm{i})^k}\Big(\Big\{\frac{q_j(\zeta)}{(h_0-\zeta)^{2j+1}}\,,\,b_0\Big\}_k + \Big\{\frac{q_{j-1}(\zeta)}{(b_0-\zeta)^{2j-1}}\,,\,\tilde{h_1}\Big\}_k\Big)(b_0-\zeta)^4 \\ &\qquad = +\tfrac{1}{4}\,\omega^0_{ij}\,\omega^0_{lm}\,\partial_j b_0\,\partial_m b_0\,\partial^2_{il} b_0\,(b_0-\zeta) \\ &\qquad\quad -\tfrac{1}{8}\,\omega^0_{ij}\,\omega^0_{lm}\,\partial^2_{jm} b_0\,\partial^2_{il} b_0\,(b_0-\zeta)^2 + \mathcal{O}(\varepsilon) \end{aligned}$$

which implies

$$\begin{aligned} q_2(\zeta) = {} & \tilde{b}_1^2\,(b_0-\zeta)^2 + \tfrac{1}{4}\,\varepsilon^2\,\langle\,\omega^0\,\nabla b_0\,,\,\nabla^2 b_0\,\omega^0\,\nabla b_0\,\rangle\,(b_0-\zeta) \\ & + \tfrac{1}{8}\,\varepsilon^2\,\mathrm{Tr}_{2n}(\omega^0\,\nabla^2 b_0\,\omega^0\,\nabla^2 b_0)\,(b_0-\zeta)^2 + \mathcal{O}(\varepsilon)\,. \end{aligned}$$

□

We now have all the tools needed to derive the effective symbol of $f(\hat{H}^\varepsilon)$.

**Proposition 4.3** *Let Assumptions 2.10 and 2.11 hold. Moreover, let $f \in \mathcal{A}$ and $h$ be the effective hamiltonian as defined in Corollary 3.8. Then, there exist classical symbols $f^{\mathrm{sc}}(h)$ and $f^{\mathrm{adi}}(\pi, h)$ in $S^0(\varepsilon, \mathbb{R})$ such that*

$$\Big\|\hat{\Pi}^\varepsilon\,\Big(f(\hat{H}^\varepsilon) - \widehat{f(h)}^\varepsilon - \varepsilon^2\,\mathrm{op}_\varepsilon(\,f^{\mathrm{sc}}(h)\,) - \varepsilon^2\,\mathrm{op}_\varepsilon(\,f^{\mathrm{adi}}(\pi, h)\,)\Big)\,\hat{\Pi}^\varepsilon\Big\| = \mathcal{O}(\varepsilon^\infty)\,. \tag{4.11}$$

*The expansion of $f^{\mathrm{sc}}(h)$ is given explicitly in terms of $f$, $h$ and their derivatives with*

$$\begin{aligned} f^{\mathrm{sc}}(h) &= -\tfrac{1}{24}\, f'''(h_0)\, \langle\, \omega^0\, \nabla h_0\,,\, \nabla^2 h_0\, \omega^0\, \nabla h_0\, \rangle \\ &\quad + \tfrac{1}{16}\, f''(h_0)\, \mathrm{Tr}_{2n}(\omega^0\, \nabla^2 h_0\, \omega^0\, \nabla^2 h_0) + \mathcal{O}(\varepsilon) \\ &= -\tfrac{1}{24}\, \mathrm{Tr}_{2n}\Big(\omega^0\, \nabla (f''(h_0)\, \nabla^2 h_0\, \omega^0\, \nabla h_0)\Big) \\ &\quad + \tfrac{1}{48}\, f''(h_0)\, \mathrm{Tr}_{2n}\Big((\omega^0\, \nabla^2 h_0)^2\Big) + \mathcal{O}(\varepsilon) \end{aligned} \tag{4.12}$$

*and the expansion of $f^{\mathrm{adi}}(h,\pi)$ is given explicitly in terms of $f$, $h$, $\pi$ and their derivatives with*

$$f^{\mathrm{adi}}(h,\pi) = -\tfrac{1}{4}\, f''(h_0)\, \|\omega^0\, \nabla h_0\|_g^2 + \mathcal{O}(\varepsilon)\,. \tag{4.13}$$

PROOF Let $\zeta \in \mathbb{C}\setminus\mathbb{R}$ and $N \in \mathbb{N}_0$. By (3.7) the full Hamiltonian $\hat{H}^{\varepsilon}$ and the adiabatic projection $\hat{\Pi}^{\varepsilon}$ almost commute. Hence, applying Lemma 4.1 (with $N = 0$) yields

$$\Big\|\hat{\Pi}^{\varepsilon}\,\Big((\hat{H}^{\varepsilon} - \zeta)^{-1} - (\hat{\Pi}^{\varepsilon}\, \hat{H}^{\varepsilon}\, \hat{\Pi}^{\varepsilon} - \zeta)^{-1}\Big)\,\hat{\Pi}^{\varepsilon}\Big\| = |\mathfrak{Im}(\zeta)|^{-3}\, \mathcal{O}(\varepsilon^{\infty})\,. \tag{4.14}$$

By (3.64) the effective Hamiltonian operator $\hat{h}^{\varepsilon}$ approximates the action of $\hat{H}^{\varepsilon}$ restricted to the adiabatic subspace to any order in $\varepsilon$, i.e.

$$\|\hat{\Pi}^{\varepsilon}\hat{H}^{\varepsilon}\hat{\Pi}^{\varepsilon} - \hat{\Pi}^{\varepsilon}\hat{h}^{\varepsilon}\hat{\Pi}^{\varepsilon}\| = \mathcal{O}(\varepsilon^{\infty})\,.$$

This and the estimate (4.2) imply

$$\Big\|\hat{\Pi}^{\varepsilon}\,\Big((\hat{\Pi}^{\varepsilon}\, \hat{H}^{\varepsilon}\, \hat{\Pi}^{\varepsilon} - \zeta)^{-1} - (\hat{\Pi}^{\varepsilon}\, \hat{h}^{\varepsilon}\, \hat{\Pi}^{\varepsilon} - \zeta)^{-1}\Big)\,\hat{\Pi}^{\varepsilon}\Big\| = |\mathfrak{Im}(\zeta)|^{-2}\, \mathcal{O}(\varepsilon^{\infty})\,. \tag{4.15}$$

The symbol of $\hat{\Pi}^{\varepsilon}\, \hat{h}^{\varepsilon}\, \hat{\Pi}^{\varepsilon}$ is operator-valued. Thus, we cannot approximate $(\hat{\Pi}^{\varepsilon}\, \hat{h}^{\varepsilon}\, \hat{\Pi}^{\varepsilon} - \zeta)^{-1}$ using Lemma 4.2 directly. We first want to remove the projections from this resolvent, followed by an application of Lemma 4.2which leads us to an effective symbol of $(\hat{\Pi}^{\varepsilon}\, \hat{h}^{\varepsilon}\, \hat{\Pi}^{\varepsilon} - \zeta)^{-1}$. Since $h$ is real valued, $\hat{h}^{\varepsilon}$ is self-adjoint on $\mathcal{H}$ with domain $D(\hat{H}^{\varepsilon})$. Moreover, we have $[\,\hat{h}^{\varepsilon}, \hat{\Pi}^{\varepsilon}\,] = [\,\hat{h}^{\varepsilon}, \hat{\pi}^{\varepsilon}\,] + \mathcal{O}(\varepsilon^{\infty}) = \mathcal{O}(\varepsilon)$. Hence, Lemma 4.1 shows

$$\begin{aligned} &\Big\|\,\hat{\Pi}^{\varepsilon}\,\Big((\hat{\Pi}^{\varepsilon}\, \hat{h}^{\varepsilon}\, \hat{\Pi}^{\varepsilon} - \zeta)^{-1} - (\hat{h}^{\varepsilon} - \zeta)^{-1} - \sum_{l=1}^{\lfloor N/2 \rfloor} G^{l}(\zeta)\, \hat{\Pi}^{\varepsilon}\, (\hat{h}^{\varepsilon} - \zeta)^{-1}\Big)\, \hat{\Pi}^{\varepsilon}\,\Big\| \\ &\qquad = |\mathfrak{Im}(\zeta)|^{-(N+3)}\, \mathcal{O}(\varepsilon^{N+1}) \end{aligned} \tag{4.16}$$

where

$$G(\zeta) := (\hat{h}^\varepsilon - \zeta)^{-1} \left[\hat{h}^\varepsilon, \hat{\Pi}^\varepsilon\right] (\hat{h}^\varepsilon - \zeta)^{-1} \left[\hat{h}^\varepsilon, \hat{\Pi}^\varepsilon\right] \hat{\Pi}^\varepsilon .$$

Moreover, by Lemma 4.2 there exist classical symbols $r(\zeta) \in S^0(\varepsilon, \mathbb{C})$ and $\tilde{q}_{l,j}(h) \in S^0(\varepsilon, \mathbb{R})$ for $l \in \mathbb{N}_0$, $0 \le j \le 2l$ such that

$$r(\zeta) \# (h - \zeta) = 1 + \mathcal{O}(\varepsilon^\infty) \quad \text{and} \quad (h - \zeta) \# r(\zeta) = 1 + \mathcal{O}(\varepsilon^\infty) \tag{4.17}$$

and

$$r(\zeta) \asymp \sum_{l \ge 0} \varepsilon^l \left( (-\tilde{h}_1)^l (h_0 - \zeta)^{-(l+1)} + \sum_{j=0}^{2l} \tilde{q}_{l,j} (h_0 - \zeta)^{-(2l+1)+j} \right). \tag{4.18}$$

where $\tilde{h}_1(z) := h(z) - e_0(z) - \xi \cdot z$. Then, replacing $\hat{\Pi}^\varepsilon$ by $\hat{\pi}^\varepsilon$ (3.8) and applying (4.17) yields

$$\left\| \hat{\Pi}^\varepsilon \Big( \sum_{l=0}^{\lfloor N/2 \rfloor} G^l(\zeta) (\hat{h}^\varepsilon - \zeta)^{-1} - \sum_{l=0}^{\lfloor N/2 \rfloor} \mathrm{op}_\varepsilon \left( G^\varepsilon(\zeta)^l_\# \# r^{(N)}(\zeta) \right) \Big) \hat{\Pi}^\varepsilon \right\| = \mathcal{O}(\varepsilon^{N+1}) \tag{4.19}$$

where

$$G^\varepsilon(\zeta) := -\varepsilon^2 r^{(N)}(\zeta) \# \tfrac{\mathrm{i}}{\varepsilon} [h, \pi]_\# \# r^{(N)}(\zeta) \# \tfrac{\mathrm{i}}{\varepsilon} [h, \pi]_\# \# \pi .$$

and $G^\varepsilon(\zeta)^l_\#$ denotes $\overbrace{G^\varepsilon(\zeta) \# \cdots \# G^\varepsilon(\zeta)}^{l-\text{times}}$.

Combining (4.14)-(4.16) and (4.19) yields

$$\begin{aligned} &\left\| \hat{\Pi}^\varepsilon \left( (\hat{H}^\varepsilon - \zeta)^{-1} - \sum_{l=0}^{\lfloor N/2 \rfloor} \mathrm{op}_\varepsilon \left( G^\varepsilon(\zeta)^l_\# \# r^{(N)}(\zeta) \right) \right) \hat{\Pi}^\varepsilon \right\| \\ &\qquad = |\mathfrak{Im}(\zeta)|^{-(N+3)} \mathcal{O}(\varepsilon^{N+1}) \end{aligned} \tag{4.20}$$

Now let $\tilde{f}$ be an almost analytic extension of $f$ with $|\partial_{\bar{\zeta}} \tilde{f}(\zeta)| \le C |\mathfrak{Im}(\zeta)|^{N+3}$ (see e.g. [Mar02, Chapter 2, Exercise 23]). Since $\hat{H}^\varepsilon$ is self-adjoint with domain $D(\hat{H}^\varepsilon)$ and $\hat{\Pi}^\varepsilon D(\hat{H}^\varepsilon) \subset D(\hat{H}^\varepsilon)$ we apply the Helffer-Sjöstrand formula leading to

$$\hat{\Pi}^\varepsilon f(\hat{H}^\varepsilon) \hat{\Pi}^\varepsilon = \frac{1}{\pi} \int_{\mathbb{R}^2} \partial_{\bar{\zeta}} \tilde{f}(\zeta) \hat{\Pi}^\varepsilon (\hat{H}^\varepsilon - \zeta)^{-1} \hat{\Pi}^\varepsilon \, \mathrm{d}x \, \mathrm{d}y .$$

Then, (4.20) leads to

$$
\begin{aligned}
&\left\| \hat{\Pi}^{\varepsilon} \left( f(\hat{H}^{\varepsilon}) - \tfrac{1}{\pi} \int_{\mathbb{R}^2} \partial_{\bar{\zeta}} \tilde{f}(\zeta)\, \mathrm{op}_{\varepsilon}\Big( \sum_{l=0}^{\lfloor N/2 \rfloor} G^{\varepsilon}(\zeta)^{l}_{\#} \# r^{(N)}(\zeta) \Big) \,\mathrm{d}x\,\mathrm{d}y \right) \hat{\Pi}^{\varepsilon} \right\| \\
&\quad = \left\| \tfrac{1}{\pi} \int_{\mathbb{R}^2} \partial_{\bar{\zeta}} \tilde{f}(\zeta)\, \hat{\Pi}^{\varepsilon} \Big( (\hat{H}^{\varepsilon} - \zeta)^{-1} \right. \\
&\qquad \left. - \sum_{l=0}^{\lfloor N/2 \rfloor} \mathrm{op}_{\varepsilon} \Big( G^{\varepsilon}(\zeta)^{l}_{\#} \# r^{(N)}(\zeta) \Big) \Big) \hat{\Pi}^{\varepsilon} \,\mathrm{d}x\,\mathrm{d}y \right\| \\
&\quad \le \tfrac{1}{\pi} \int_{\mathbb{R}^2} |\partial_{\bar{\zeta}} \tilde{f}(\zeta)| \left\| \hat{\Pi}^{\varepsilon} \Big( (\hat{H}^{\varepsilon} - \zeta)^{-1} \right. \\
&\qquad \left. - \sum_{l=0}^{\lfloor N/2 \rfloor} \mathrm{op}_{\varepsilon} \Big( G^{\varepsilon}(\zeta)^{l}_{\#} \# r^{(N)}(\zeta) \Big) \Big) \hat{\Pi}^{\varepsilon} \right\| \mathrm{d}x\,\mathrm{d}y \\
&\quad = \mathcal{O}(\varepsilon^{N+1}) \,.
\end{aligned}
\tag{4.21}
$$

By Taylor's formula

$$
f(h) = f(h_0 + \varepsilon\, \tilde{h}_1) = \sum_{l=0}^{N} \frac{1}{l!} (\varepsilon\, \tilde{h}_1)^l \, \tfrac{\mathrm{d}^l}{\mathrm{d}x^l} f(h_0) + \mathcal{O}(\varepsilon^{N+1}) \,.
$$

Then, the fact that

$$
\tfrac{\mathrm{d}^m}{\mathrm{d}x^m} f(h_0) = \tfrac{1}{\pi} \int_{\mathbb{R}^2} \partial_{\bar{\zeta}} \partial_{\zeta}^m \tilde{f}(\zeta)\, (h_0 - \zeta)^{-1} \,\mathrm{d}x\,\mathrm{d}y \tag{4.22}
$$

for any $m \in \mathbb{N}_0$ (see e.g. [Mar02, Chapter 2, Exercise 24]) and integration by parts leads to

$$
\begin{aligned}
f(h) &= \sum_{l=0}^{N} \frac{1}{l!} (\varepsilon\, \tilde{h}_1)^l \, \tfrac{1}{\pi} \int_{\mathbb{R}^2} \partial_{\bar{\zeta}} \partial_{\zeta}^l \tilde{f}(\zeta)\, (h_0 - \zeta)^{-1} \,\mathrm{d}x\,\mathrm{d}y + \mathcal{O}(\varepsilon^{N+1}) \\
&= \tfrac{1}{\pi} \int_{\mathbb{R}^2} \partial_{\bar{\zeta}} \tilde{f}(\zeta) \sum_{l=0}^{N} (-\varepsilon\, \tilde{h}_1)^l \, (h_0 - \zeta)^{-(l+1)} \,\mathrm{d}x\,\mathrm{d}y + \mathcal{O}(\varepsilon^{N+1}) \\
&=: f(h)^{(N)} + \mathcal{O}(\varepsilon^{N+1}) \,.
\end{aligned}
\tag{4.23}
$$

Moreover, we define

$$
f^{\mathrm{sc},(N)}(h) := \frac{1}{\pi\, \varepsilon^2} \int_{\mathbb{R}^2} \partial_{\bar{\zeta}} \tilde{f}(\zeta) \sum_{l=0}^{N} \varepsilon^l \sum_{j=0}^{2l} \tilde{q}_{l,j}(h)\, (h_0 - \zeta)^{-(2l+1)+j} \,\mathrm{d}x\,\mathrm{d}y \tag{4.24}
$$

and

$$
F^{\mathrm{adi},(N)}(h, \pi) := \frac{1}{\pi \varepsilon^2} \sum_{l=1}^{\lfloor N/2 \rfloor} \int_{\mathbb{R}^2} \partial_{\bar{\zeta}} \tilde{f}(\zeta)\, G^{\varepsilon}(\zeta)^{l}_{\#} \# r^{(N)}(\zeta) \,\mathrm{d}x\,\mathrm{d}y \,. \tag{4.25}
$$

Combining (4.23)- (4.25), (4.21) and (4.18) leads to

$$\begin{aligned}
&\left\| \hat{\Pi}^{\varepsilon} \left( f(\hat{H}^{\varepsilon}) - \mathrm{op}_{\varepsilon} \left( f^{(N)}(h) + \varepsilon^2 f^{\mathrm{sc},(N)}(h) + \varepsilon^2 F^{\mathrm{adi},(N)}(h,\pi) \right) \right) \hat{\Pi}^{\varepsilon} \right\| \\
&\quad = \left\| \hat{\Pi}^{\varepsilon} \left( f(\hat{H}^{\varepsilon}) - \tfrac{1}{\pi} \int_{\mathbb{R}^2} \partial_{\bar{\zeta}} \tilde{f}(\zeta)\, \mathrm{op}_{\varepsilon}\Big( + \sum_{l=0}^{\lfloor N/2 \rfloor} G^{\varepsilon}(\zeta)^{l}_{\#} \# r^{(N)}(\zeta) \Big) \right) \hat{\Pi}^{\varepsilon} \right\| \\
&\quad = \mathcal{O}(\varepsilon^{N+1}) .
\end{aligned} \tag{4.26}$$

Note, for any $\alpha \in \mathbb{N}_0^{2n}$

$$|\partial_z^{\alpha} r_j(\zeta)| = \mathcal{O}(|\mathfrak{Im}(\zeta)|^{-(2j+1+|\alpha|)}) .$$

Thus, the corrections to the equilibrium density $f^{\mathrm{sc},(N)}(h)$ and $F^{\mathrm{adi},(N)}(h,\pi)$ are classical symbols in $S^0(\varepsilon,\mathbb{R})$ and $S^0(\varepsilon,\mathcal{J}(\mathcal{H}_{\mathrm{f}}))$, respectively. In addition, it is easy to see that $F^{\mathrm{adi},(N)}(h,\pi)$ takes value in the self-adjoint operators on $\mathcal{H}_{\mathrm{f}}$. By a resummation there exist classical symbols $f^{\mathrm{sc}}(h) \in S^0(\varepsilon,\mathbb{R})$ and $F^{\mathrm{adi}}(h,\pi) \in S^0(\varepsilon,\mathcal{J}_{\mathrm{sa}}(\mathcal{H}_{\mathrm{f}}))$ such that

$$f^{\mathrm{sc}}(h) \asymp f^{\mathrm{sc},(\infty)}(h)$$

and

$$F^{\mathrm{adi}}(h,\pi) \asymp F^{\mathrm{adi},(\infty)}(h,\pi) .$$

Then, (4.26) yields

$$\left\| \hat{\Pi}^{\varepsilon} \left( f(\hat{H}^{\varepsilon}) - \mathrm{op}_{\varepsilon} \left( f(h) + \varepsilon^2 f^{\mathrm{sc}}(h) + \varepsilon^2 F^{\mathrm{adi}}(h,\pi) \right) \right) \hat{\Pi}^{\varepsilon} \right\| = \mathcal{O}(\varepsilon^{N+1}) .$$

By Proposition 3.7 the scalar symbol $f^{\mathrm{adi}}(h,\pi) \in S^0(\varepsilon,\mathbb{R})$ of $F^{\mathrm{adi}}(h,\pi)$ defined by (3.26) satisfies

$$\left\| \hat{\Pi}^{\varepsilon} \left( \mathrm{op}_{\varepsilon} \left( F^{\mathrm{adi}}(h,\pi) \right) - \mathrm{op}_{\varepsilon} \left( f^{\mathrm{adi}}(h,\pi) \right) \right) \hat{\Pi}^{\varepsilon} \right\| = \mathcal{O}(\varepsilon^{\infty}) .$$

Clearly, $f^{\mathrm{adi}}(h,\pi)$ is a classical symbol by the definition of effective symbols and since $F^{\mathrm{adi}}(h,\pi)$ is a classical symbol. This completes the proof of (4.11).

What is left is to proof that the coefficients in the asymptotic expansions of $f^{\mathrm{sc}}(h)$ and $f^{\mathrm{adi}}(h,\pi)$ can be expressed explicitly in terms of $f$, $h$, $\pi$ and their derivatives where the expansions start with (4.12) and (4.13), respectively. We start by reformulating $f^{\mathrm{sc},(N)}(h)$.

An integration by parts and (4.22) yield

$$f^{\mathrm{sc},(N)}(h) = \sum_{l=0}^{N} \varepsilon^{l-2} \sum_{j=0}^{2l} \frac{(-1)^{2l-j}}{(2l-j)!}\, \tilde{q}_{l,j}(h)\, \tfrac{1}{\pi} \int_{\mathbb{R}^2} \partial_{\bar{\zeta}} \partial_{\zeta}^{2l-j} \tilde{f}(\zeta)\, (h_0-\zeta)^{-1}\, \mathrm{d}x\, \mathrm{d}y$$
$$= \sum_{l=0}^{N} \varepsilon^{l-2} \sum_{j=0}^{2l} \frac{(-1)^{2l-j}}{(2l-j)!}\, \tilde{q}_{l,j}(h)\, \tfrac{\mathrm{d}^{2l-j}}{\mathrm{d}x^{2l-j}} f(h_0)\,.$$

Then, replacing the $\tilde{q}_{l,j}(h)$s by their explicit formulas (4.8) yields

$$f^{\mathrm{sc}}(h) = -\tfrac{1}{24}\, f'''(h_0)\, \langle\, \omega^0\, \nabla h_0\,,\ \nabla^2 h_0\, \omega^0\, \nabla h_0\, \rangle$$
$$+ \tfrac{1}{16}\, f''(h_0)\, \mathrm{Tr}_{2n}(\omega^0\, \nabla^2 h_0\, \omega^0\, \nabla^2 h_0) + \mathcal{O}(\varepsilon)\,.$$

Regarding $f^{\mathrm{adi},N}(h)$, note $\partial_{z_j}(h_0-\zeta)^{-l} = -l\,(h_0-\zeta)^{-(l+1)}\,\partial_{z_j} h_0$. Therefore, it is easy to see that the expansion of

$$\varepsilon^{-2} \sum_{i=1}^{\lfloor N/2 \rfloor} (G^{\varepsilon}(\zeta))^{i}_{\#} \# \pi \# r^{(N)}(\zeta)$$

can be reformulated as a polynomial in $(h_0 - \zeta)^{-1}$ with coefficients in $S^0(\varepsilon, \mathcal{J}_{\mathrm{sa}}(\mathcal{H}_{\mathrm{f}}))$, i.e. there exist $m_l \in \mathbb{N}$ for $l = 0, \ldots, N-2$ and symbols $c_{lj}(\pi, h) \in S^0(\varepsilon, \mathcal{J}_{\mathrm{sa}}(\mathcal{H}_{\mathrm{f}}))$ for $l = 0, \ldots, N-2$ and $j = 0, \ldots, m_l$ depending on $\pi$ and $h$ as well as their derivatives up to order $N$ such that

$$\varepsilon^{-2} \sum_{k=1}^{\lfloor N/2 \rfloor} (G(\zeta))^{i}_{\#} \# \pi \# r^{(N)}(\zeta) = \sum_{l=0}^{N-2} \varepsilon^{l} \sum_{j=0}^{m_l} c_{lj}(\pi, h)\, (h_0-\zeta)^{-(j+1)} + \mathcal{O}(\varepsilon^{N-1})\,.$$

An integration by parts together with (4.22) yields

$$\sum_{l=0}^{N-2} \varepsilon^{l} \sum_{j=0}^{m_l} \tfrac{1}{\pi} \int_{\mathbb{R}^2} \partial_{\bar{\zeta}} \tilde{f}(\zeta)\, c_{lj}(\pi,h)\, (h_0-\zeta)^{-(j+1)}\, \mathrm{d}x\, \mathrm{d}y$$
$$= \sum_{l=0}^{N-2} \varepsilon^{l} \sum_{j=0}^{m_l} \frac{1}{\pi\, j!} \int_{\mathbb{R}^2} \partial_{\bar{\zeta}} \partial_{\zeta}^{j} \tilde{f}(\zeta)\, c_{lj}(\pi,h)\, (h_0-\zeta)^{-1}\, \mathrm{d}x\, \mathrm{d}y$$
$$= \sum_{l=0}^{N-2} \varepsilon^{l} \sum_{j=0}^{m_l} \frac{1}{j!} \partial_{\zeta}^{j} f(h_0)\, c_{lj}(\pi,h)$$

Hence,

$$F^{\mathrm{adi},N}(h,\pi) = \sum_{l=0}^{N-2} \varepsilon^{l} \sum_{j=0}^{m_l} \frac{1}{j!} \partial_{\zeta}^{j} f(h_0)\, c_{lj}(\pi,h) + \mathcal{O}(\varepsilon^{N-1})\,.$$

In addition, by using the definition of effective symbols (3.26) it is easy to see that the coefficients in the expansion of $f^{\mathrm{adi}}(h,\pi)$ can be expressed explicitly in terms of $f$, $h$, $\pi$. Moreover,

$$\varepsilon^{-2}\sum_{k=1}^{\lfloor N/2\rfloor}(G(\zeta))^{i}_{\#}\,\#\,\pi\,\#\,r^{(N)}(\zeta)=-(h_0-\zeta)^{-3}\,\{h\,,P_0\}\,\{h\,,P_0\}\,P_0+\mathcal{O}(\varepsilon)$$

for $N\geq 2$. This implies $m_0=2$, $c_{0,0}=c_{0,1}=0$ and

$$c_{0,2}=\{h\,,P_0\}\,\{P_0\,,h\}\,P_0$$

leading to

$$F^{\mathrm{adi}}(h,\pi)=-\frac{1}{2}\,f''(h_0)\,\{h_0\,,P_0\}\,\{h_0\,,P_0\}\,P_0+\mathcal{O}(\varepsilon)$$

Thus, by definition of the effective symbols (3.26) the expansion of $f^{\mathrm{adi}}(h,\pi)$ starts with

$$f^{\mathrm{adi}}(h,\pi)=-\frac{1}{2}\,f''(h_0)\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\{h_0\,,P_0\}\,\{h_0\,,P_0\}\,P_0)+\mathcal{O}(\varepsilon)\,.$$

Finally, a simple computation shows

$$\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\{h_0\,,P_0\}\,\{h_0\,,P_0\}\,P_0)=\tfrac{1}{2}\,\langle\,\omega^0\,\nabla h_0\,,\,g\,\omega^0\,\nabla h_0\,\rangle=\tfrac{1}{2}\|\omega^0\,\nabla h_0\|_g^2$$

which completes the proof. □

## 4.2 Expectation Values for Stationary States

With all the preparatory work done in the previous sections we are now at the point to prove one of the main theorems on this thesis, the semiclassical approximation of quantum mechanical expectation values of thermodynamic equilibrium state

$$\mathrm{tr}\Big(\hat{\Pi}^{\varepsilon}f(\hat{H}^{\varepsilon})\hat{A}^{\varepsilon}\Big)\,.$$

The expectation value of the classical thermodynamic system with $\varepsilon$-dependent classical Hamiltonian system $(\mathbb{R}^{2n},\omega^{\varepsilon},h)$ defined in Section 3.3, classical $\varepsilon$-dependent observable $a(\varepsilon,z)$ given as the effective symbol of $A(\varepsilon,z)$ and density $f(h)$ is given by the phase space integral

$$\int_{\mathbb{R}^{2n}}f(h(\varepsilon,z))\,a(\varepsilon,z)\,\lambda^{\varepsilon}$$

where $\lambda^\varepsilon$ is the Liouville measure associated to $\omega^\varepsilon$. We will show that, up to quantum corrections of order $\varepsilon^2$, the semiclassical approximations up to errors of order $\varepsilon^3$ can be represented as the classical expectation value above.

**Theorem 4.4** *Let Assumption 2.10 and 2.11 hold. In addition, assume $f \in \mathcal{A}$ and $A \in S^k(\varepsilon, \mathcal{B}_{\mathrm{sa}}(\mathcal{H}_\mathrm{f}))$ Then*

$$
\begin{aligned}
\mathrm{tr}_{\mathcal{H}} \Big( f(\hat{H}^\varepsilon)\, \hat{A}^\varepsilon\, \hat{\Pi}^\varepsilon \Big) =& (2\pi\varepsilon)^{-n} \int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\pi) \,\#\, f^\varepsilon(h,\pi)\, a^{(N)}\, \mathrm{d}z \\
& - \mathrm{i}\, \varepsilon\, (2\pi\varepsilon)^{-n} \int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\pi \,\#\, \tfrac{\mathrm{i}}{\varepsilon}\, [\, f^\varepsilon(h,\pi)\,,\pi\,]_\#)\, a^{(N)}\, \mathrm{d}z \\
& + \mathcal{O}\Big(\varepsilon^{-n+N+1}\, \|A\|^\varepsilon_{L^1}\Big)
\end{aligned}
\tag{4.27}
$$

*for every $N \in \mathbb{N}_0$. Here $a \in S^k(\varepsilon, \mathbb{R})$ is the effective symbol of $A(\varepsilon, z)$ with asymptotic expansion $a \asymp \sum_{j=0}^\infty a_j(\varepsilon, z)$ defined by (3.26). The effective symbol of the stationary state $f(\hat{H}^\varepsilon)$ is*

$$
f^\varepsilon(h,\pi) = f(h) + \varepsilon^2\, f^{\mathrm{sc}}(h) + \varepsilon^2\, f^{\mathrm{adi}}(h,\pi) \tag{4.28}
$$

*with $f^{\mathrm{sc}}(h)$ and $f^{\mathrm{adi}}(\pi, h)$ given by (4.12) and (4.13), respectively. The effective Hamiltonian $h(\varepsilon, z)$ is defined in Corollary 3.8.*

*Moreover, if $A(\varepsilon, z)$ is a classical symbol. Then, $a_j$ is a classical symbol for every $j \in \mathbb{N}_0$ with asymptotic expansion*

$$
a_j(\varepsilon) \asymp \sum_{i=0}^\infty \varepsilon^i\, a_{j,i}
$$

*and*

$$
\begin{aligned}
&\mathrm{tr}_{\mathcal{H}} \Big( f(\hat{H}^\varepsilon)\, \hat{A}^\varepsilon\, \hat{\Pi}^\varepsilon \Big) \\
&\quad = (2\pi\varepsilon)^{-n} \Big( \int_{\mathbb{R}^{2n}} f^\varepsilon(h,\pi)\, \tilde{a}^{(2)}\, \lambda^\varepsilon + \varepsilon^2 \int_{\mathbb{R}^{2n}} Q(h_0, g_0)\, \tilde{a}^{(2)}\, \mathrm{d}z \Big) \\
&\quad + \mathcal{O}\Big( \varepsilon^{3-n} \Big( \|A\|^\varepsilon_{L^1} + \sum_{i=0}^2 \Big( \|A_i\|_{L^1} + \|\varepsilon^{-(i+1)} (A - A^{(i)})\|^\varepsilon_{L^1} \Big) \Big) \Big)
\end{aligned}
\tag{4.29}
$$

*where $\lambda^\varepsilon$ is the Liouville measure (3.74) associated to the Hamiltonian system $(\mathbb{R}^{2n}, \omega^\varepsilon, h)$. The effective symbol of the observable is*

$$
\tilde{a}^{(2)}(\varepsilon) := \sum_{j=0}^{2} \sum_{i=0}^{2-j} \varepsilon^{i+j}\, a_{j,i}\,,
$$

*and the quantum correction*

$$Q(h_0, g_0) = \tfrac{1}{2}\,\mathrm{Tr}_{2n}(\omega^0\,\nabla(f'(h_0)\,g_0\,\omega^0\,\nabla h_0)\,)\,. \tag{4.30}$$

PROOF Fix $N \in \mathbb{N}_0$. By (2.14) we have that $\mathrm{tr}_{\mathcal{H}}\Big(\hat{A}^{\varepsilon}\,\hat{\Pi}^{\varepsilon}\Big) = \mathcal{O}(\varepsilon^{-n}\|A\|^{\varepsilon}_{L^1})$. For $B \in \mathcal{B}(\mathcal{H})$ this implies

$$\mathrm{tr}_{\mathcal{H}}\Big(B\,\hat{A}^{\varepsilon}\,\hat{\Pi}^{\varepsilon}\Big) = \mathcal{O}(\varepsilon^{-n}\,\|B\|\,\|A\|^{\varepsilon}_{L^1})\,. \tag{4.31}$$

By Theorem 3.6

$$\mathrm{tr}_{\mathcal{H}}\left(\widehat{a^{(N)}}^{\,\varepsilon}\,\hat{\Pi}^{\varepsilon}\right) = \mathcal{O}\Big(\varepsilon^{-n}\|A\|^{\varepsilon}_{L^1}\Big)$$

and

$$\mathrm{tr}_{\mathcal{H}}\left(\Big(\hat{A}^{\varepsilon} - \widehat{a^{(N)}}^{\,\varepsilon}\Big)\,\hat{\Pi}^{\varepsilon}\right) = \mathcal{O}\Big(\varepsilon^{N+1-n}\|A\|^{\varepsilon}_{L^1}\Big)\,.$$

Hence,

$$\mathrm{tr}_{\mathcal{H}}\left(B\,\widehat{a^{(N)}}^{\,\varepsilon}\,\hat{\Pi}^{\varepsilon}\right) = \mathcal{O}\Big(\varepsilon^{-n}\,\|B\|\,\|A\|^{\varepsilon}_{L^1}\Big) \tag{4.32}$$

and

$$\mathrm{tr}_{\mathcal{H}}\left(B\,\Big(\hat{A}^{\varepsilon} - \widehat{a^{(N)}}^{\,\varepsilon}\Big)\,\hat{\Pi}^{\varepsilon}\right) = \mathcal{O}\Big(\varepsilon^{N+1-n}\,\|B\|\|A\|^{\varepsilon}_{L^1}\Big) \tag{4.33}$$

for any $B \in \mathcal{B}(\mathcal{H})$.

By (3.7) the resolvent $(\hat{H}^{\varepsilon} - \zeta)^{-1}$ almost commutes with the adiabatic projection $\hat{\Pi}^{\varepsilon}$ for any $\zeta \in \mathbb{C} \setminus \mathbb{R}$. In addition, since $\hat{H}^{\varepsilon}$ is self-adjoint on $\mathcal{H}$ with domain $D(\hat{H}^{\varepsilon})$ the Helffer-Sjöstrand formula (4.1) together with (4.31) and the cyclicity of the trace imply

$$\mathrm{tr}_{\mathcal{H}}\left(f(\hat{H}^{\varepsilon})\,\hat{A}^{\varepsilon}\,\hat{\Pi}^{\varepsilon}\right) = \mathrm{tr}_{\mathcal{H}}\left(\hat{\Pi}^{\varepsilon}\,f(\hat{H}^{\varepsilon})\,\hat{\Pi}^{\varepsilon}\,\hat{A}^{\varepsilon}\,\hat{\Pi}^{\varepsilon}\right) + \mathcal{O}\Big(\varepsilon^{N+1}\,\|A\|^{\varepsilon}_{L^1}\Big)\,. \tag{4.34}$$

By Proposition 4.3 there exist classical symbols $f^{\mathrm{sc}}(h)$ and $f^{\mathrm{adi}}(\pi, h)$ in $S^0(\varepsilon, \mathbb{R})$ such that

$$\left\|\hat{\Pi}^{\varepsilon}\left(f(\hat{\Pi}^{\varepsilon}\,\hat{h}^{\varepsilon}\,\hat{\Pi}^{\varepsilon}) - \mathrm{op}_{\varepsilon}\left(f(h) - \varepsilon^2\,f^{\mathrm{sc}}(h) - \varepsilon^2\,f^{\mathrm{adi}}(\pi, h)\Big)\right)\hat{\Pi}^{\varepsilon}\right\| = \mathcal{O}(\varepsilon^{N+1})\,.$$

Combining this with (4.31) yields

$$\begin{aligned}\mathrm{tr}_{\mathcal{H}}\left(\hat{\Pi}^{\varepsilon}\,f(\hat{H}^{\varepsilon})\,\hat{\Pi}^{\varepsilon}\,\hat{A}^{\varepsilon}\,\hat{\Pi}^{\varepsilon}\right) &= \mathrm{tr}_{\mathcal{H}}\left(\hat{\Pi}^{\varepsilon}\mathrm{op}_{\varepsilon}(\,f^{\varepsilon}(h, \pi)\,)\,\hat{\Pi}^{\varepsilon}\,\hat{A}^{\varepsilon}\,\hat{\Pi}^{\varepsilon}\right)\\ &\quad + \mathcal{O}\Big(\varepsilon^{N+1}\,\|A\|^{\varepsilon}_{L^1}\Big)\,.\end{aligned} \tag{4.35}$$

where $f^\varepsilon(h,\pi) := f(h) + \varepsilon^2 f^{\rm sc}(h) + \varepsilon^2 f^{\rm adi}(\pi,h)$. By (4.33) replacing the observable $\hat{A}^\varepsilon$ by is effective operator $\widehat{a^{(N)}}^{\,\varepsilon}$ yields

$$\begin{aligned}\mathrm{tr}_{\mathcal{H}}\Big(\hat{\Pi}^\varepsilon \mathrm{op}_\varepsilon(\, f^\varepsilon(h,\pi)\,)\, \hat{\Pi}^\varepsilon\, \hat{A}^\varepsilon\, \hat{\Pi}^\varepsilon\Big) &= \mathrm{tr}_{\mathcal{H}}\Big(\hat{\Pi}^\varepsilon \mathrm{op}_\varepsilon(\, f^\varepsilon(h,\pi)\,)\, \hat{\Pi}^\varepsilon\, \widehat{a^{(N)}}^{\,\varepsilon}\, \hat{\Pi}^\varepsilon\Big)\\ &\quad + \mathcal{O}\Big(\varepsilon^{N-n+1} \sum_{i=0}^m \|A_i\|_{L^1}\Big)\,.\end{aligned} \tag{4.36}$$

A simple computation using that $\hat{\Pi}^\varepsilon$ is a projection leads to

$$\begin{aligned}&\mathrm{tr}_{\mathcal{H}}\Big(\hat{\Pi}^\varepsilon \mathrm{op}_\varepsilon(\, f^\varepsilon(h,\pi)\,)\, \hat{\Pi}^\varepsilon\, \widehat{a^{(N)}}^{\,\varepsilon}\, \hat{\Pi}^\varepsilon\Big)\\ &\quad = \mathrm{tr}_{\mathcal{H}}\Big(\hat{\Pi}^\varepsilon \mathrm{op}_\varepsilon(\, f^\varepsilon(h,\pi)\,)\, \widehat{a^{(N)}}^{\,\varepsilon}\Big)\\ &\qquad - \mathrm{i}\,\varepsilon\, \mathrm{tr}_{\mathcal{H}}\Big(\hat{\Pi}^\varepsilon\, \tfrac{\mathrm{i}}{\varepsilon}\Big[\,\mathrm{op}_\varepsilon(\, f^\varepsilon(h,\pi)\,)\,, \hat{\Pi}^\varepsilon\Big]\, \widehat{a^{(N)}}^{\,\varepsilon}\Big)\,.\end{aligned} \tag{4.37}$$

Combining (3.10) with (4.32) we obtain

$$\begin{aligned}&\mathrm{tr}_{\mathcal{H}}\Big(\hat{\Pi}^\varepsilon \mathrm{op}_\varepsilon(\, f^\varepsilon(h,\pi)\,)\, \widehat{a^{(N)}}^{\,\varepsilon}\Big) - \mathrm{i}\,\varepsilon\, \mathrm{tr}_{\mathcal{H}}\Big(\hat{\Pi}^\varepsilon\, \tfrac{\mathrm{i}}{\varepsilon}\Big[\,\mathrm{op}_\varepsilon(\, f^\varepsilon(h,\pi)\,)\,, \hat{\Pi}^\varepsilon\Big]\, \widehat{a^{(N)}}^{\,\varepsilon}\Big)\\ &\quad = \mathrm{tr}_{\mathcal{H}}\Big(\hat{\pi}^\varepsilon \mathrm{op}_\varepsilon(\, f^\varepsilon(h,\pi)\,)\, \widehat{a^{(N)}}^{\,\varepsilon}\Big) - \mathrm{i}\,\varepsilon\, \mathrm{tr}_{\mathcal{H}}\Big(\hat{\Pi}^\varepsilon\, \tfrac{\mathrm{i}}{\varepsilon}\,[\,\mathrm{op}_\varepsilon(\, f^\varepsilon(h,\pi)\,)\,, \hat{\pi}^\varepsilon\,]\, \widehat{a^{(N)}}^{\,\varepsilon}\Big)\\ &\qquad + \mathcal{O}\Big(\varepsilon^{N-n+1}\,\|A\|^\varepsilon_{L^1}\Big)\,.\end{aligned} \tag{4.38}$$

Then, the trace formula (2.13) implies

$$\begin{aligned}&\mathrm{tr}_{\mathcal{H}}\Big(\hat{\pi}^\varepsilon \mathrm{op}_\varepsilon(\, f^\varepsilon(h,\pi)\,)\, \widehat{a^{(N)}}^{\,\varepsilon}\Big) - \mathrm{i}\,\varepsilon\, \mathrm{tr}_{\mathcal{H}}\Big(\hat{\Pi}^\varepsilon\, \tfrac{\mathrm{i}}{\varepsilon}\,[\,\mathrm{op}_\varepsilon(\, f^\varepsilon(h,\pi)\,)\,, \hat{\pi}^\varepsilon\,]\, \widehat{a^{(N)}}^{\,\varepsilon}\Big)\\ &\quad = (2\pi\varepsilon)^{-n}\int_{\mathbb{R}^{2n}} \Big(\mathrm{tr}_{\mathcal{H}_{\rm f}}(\pi)\,\#\, f^\varepsilon(h,\pi)\Big)(\varepsilon,z)\, a^{(N)}(\varepsilon,z)\,\mathrm{d}z\\ &\qquad - \mathrm{i}\,\varepsilon\,(2\pi\varepsilon)^{-n}\int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_{\rm f}}\Big(\pi\,\#\,\tfrac{\mathrm{i}}{\varepsilon}\,[\, f^\varepsilon(h,\pi)\,,\pi\,]_\#\Big)(\varepsilon,z)\, a^{(N)}(\varepsilon,z)\,\mathrm{d}z\,.\end{aligned} \tag{4.39}$$

Finally, (4.34)-(4.39) shows (4.27).

What is left is to proof (4.29). So, let $A \in S^k(\varepsilon, \mathcal{B}_{\rm sa}(\mathcal{H}_{\rm f}))$ be a classical symbol.

We begin by proving that the Liouville measure $\lambda^\varepsilon$ given by (3.74) satisfies

$$\lambda^\varepsilon = (\mathrm{tr}_{\mathcal{H}_{\rm f}}(\pi) + \mathcal{O}(\varepsilon^3))\,\mathrm{d}q_1 \wedge \cdots \wedge \mathrm{d}p_n\,. \tag{4.40}$$

Since $P_0$ takes value in the rank-one projections and $P_1$ is off-diagonal with respect to $P_0$ (see Equation 3.18) we have

$$\mathrm{tr}_{\mathcal{H}_{\rm f}}(\pi) = 1 + \varepsilon\,\mathrm{tr}_{\mathcal{H}_{\rm f}}(\tilde{\pi}_0) + \varepsilon^2\,\mathrm{tr}_{\mathcal{H}_{\rm f}}(P_2) + \varepsilon^2\,\mathrm{tr}_{\mathcal{H}_{\rm f}}(\tilde{\pi}_1) + \mathcal{O}(\varepsilon^3)\,. \tag{4.41}$$

By the fact that

$$\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0^\perp\,[\partial_j P_0, \partial_i P_0]) = \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\,[\partial_i P_0, \partial_j P_0])$$

and

$$\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\Omega^{op}_{0,ij}\,P_0) = -\mathrm{i}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}([\,\partial_i P_0\,,\partial_j P_0\,]\;P_0) = \Omega_{0,ij}\,.$$

we get

$$\begin{aligned}\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\tilde{\pi}_0) &= -\tfrac{1}{4}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\,\mathrm{Tr}_{2n}(\omega^0\,\Omega_0^{op})) + \tfrac{1}{4}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0^\perp\,\mathrm{Tr}_{2n}(\omega^0\,\Omega_0^{op}))\\ &= -\tfrac{1}{2}\,\mathrm{Tr}_{2n}(\omega^0\,\Omega_0)\,.\end{aligned} \tag{4.42}$$

By definition, $\Omega^{op}_{0,ij}$ is diagonal with respect to $P_0$ (3.14) and

$$\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\Omega^{op}_{1,ij}\,P_0) = -\mathrm{i}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}([\,\partial_i P_1\,,\partial_j P_0\,]\;P_0) - \mathrm{i}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}([\,\partial_i P_0\,,\partial_j P_1\,]\;P_0) = \Omega_{1,ij}\,.$$

Thus, (3.15) and (3.16) yield

$$\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\tilde{\pi}_1) = -\tfrac{1}{2}\,\mathrm{Tr}_{2n}(\omega^0\,\Omega_1) + \tfrac{1}{8}\,\mathrm{Tr}_{2n}(\omega^0\,\Omega_0)^2 - \tfrac{1}{4}\;\mathrm{Tr}_{2n}(\omega^0\,\Omega_0\,\omega^0\,\Omega_0)\,. \tag{4.43}$$

By the cyclicity of the trace

$$\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_2) = -\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\,P_1\,P_0^\perp\,P_1\,P_0) - \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0^\perp\,P_1\,P_0\,P_1\,P_0^\perp) = 0\,. \tag{4.44}$$

Combining (4.41)-(4.44) we conclude

$$\begin{aligned}\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\pi) = 1 &- \tfrac{1}{2}\,\varepsilon\,\mathrm{Tr}_{2n}(\omega^0\,\Omega^\varepsilon) + \tfrac{1}{8}\,\varepsilon^2\,\mathrm{Tr}_{2n}(\omega^0\,\Omega^\varepsilon)^2 - \tfrac{1}{4}\,\varepsilon^2\,\mathrm{Tr}_{2n}(\omega^0\,\Omega^\varepsilon\,\omega^0\,\Omega^\varepsilon)\\ &+ \mathcal{O}(\varepsilon^3)\end{aligned}$$

which shows (4.40).

Combining estimate (3.59) and the trace formula (2.13) we obtain

$$\begin{aligned}&\int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\pi)\,\#\,f^\varepsilon(h,\pi)\,a^{(2)}\,\mathrm{d}z\\ &\quad - \mathrm{i}\,\varepsilon\int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\pi\,\#\,\tfrac{\mathrm{i}}{\varepsilon}\,[\,f^\varepsilon(h,\pi)\,,\pi\,]_\#)\,a^{(2)}\,\mathrm{d}z\\ &\qquad = \int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\pi)\,\#\,f^\varepsilon(h,\pi)\,\tilde{a}^{(2)}\,\mathrm{d}z\\ &\qquad\quad - \mathrm{i}\,\varepsilon\int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\pi\,\#\,\tfrac{\mathrm{i}}{\varepsilon}\,[\,f^\varepsilon(h,\pi)\,,\pi\,]_\#)\,\tilde{a}^{(2)}\,\mathrm{d}z\\ &\qquad\quad + \mathcal{O}\Big(\varepsilon^{N+1}\,\|A\|^\varepsilon_{L^1} + \sum_{i=0}^{2}\|\varepsilon^{-(i+1)}(A - A^{(i)})\|^\varepsilon_{L^1}\Big)\end{aligned} \tag{4.45}$$

In what follows we will repeatedly use that by (3.57) and (2.13)

$$\Big| \int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(R)\, \tilde{a}^{(2)}\ \mathrm{d}z \Big| = \mathcal{O}\Big( \|R\|^{\varepsilon}_{0,2,1} \sum_{i=0}^{2} \|A_i\|_{L^1} \Big)$$

for any $R \in S^0(\varepsilon, J(\mathcal{H}_\mathrm{f}))$.

Clearly, $f^\varepsilon(h,\pi) = f(h) + \mathcal{O}(\varepsilon^2)$ and $\partial_i\, \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0) = 0$. Thus,

$$\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\pi) \,\#\, f^\varepsilon(h,\pi)\, \tilde{a}^{(2)} = \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\pi)\, f^\varepsilon(h,\pi)\, a^{(2)} + \varepsilon^2\ \{\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\pi_1)\,,f(h)\}_1\ \tilde{a}^{(2)} + \mathcal{O}(\varepsilon^3)$$

Since $P_1$ is off-diagonal with respect to $P_0$ and (4.42) we have

$$\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\pi_1) = \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\tilde{\pi}_0) = 2\, \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\, \pi_1)\,.$$

Therefore, Lemma A.11 leads to

$$\begin{aligned} &\int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\pi) \,\#\, f^\varepsilon(h,\pi)\, \tilde{a}^{(2)}\, \mathrm{d}z \\ &\qquad = \int_{\mathbb{R}^{2n}} f^\varepsilon(h,\pi)\, \tilde{a}^{(2)}\, \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\pi)\, \mathrm{d}z + 2\,\varepsilon^2 \int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\, \pi_1)\, \{f(h)\,,\tilde{a}^{(2)}\,\}_1\, \mathrm{d}z \\ &\qquad\quad + \mathcal{O}(\varepsilon^3\ \sum_{i=0}^{2} \|A_i\|_{L^1})\,. \end{aligned} \tag{4.46}$$

By $f^\varepsilon(h,\pi) = f(h) + \mathcal{O}(\varepsilon^2)$ we have

$$\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\pi \,\#\, \tfrac{\mathrm{i}}{\varepsilon}\, [\, f^\varepsilon(h,\pi)\,,\pi\,]_\#) = \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\pi \,\#\, \tfrac{\mathrm{i}}{\varepsilon}\, [\, f(h)\,,\pi\,]_\#) + \mathcal{O}(\varepsilon^2)\,. \tag{4.47}$$

Since $f(h)$ is scalar and $\partial_j P_0$ is off-diagonal with respect to $P_0$ we conclude

$$\begin{aligned} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\pi \,\#\, \tfrac{\mathrm{i}}{\varepsilon}\, [\, f(h)\,,\pi\,]_\#) = {}& 2\,\mathrm{i}\,\varepsilon\, \mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big(\pi_1\, \{f(h)\,,P_0\}_1) + P_0\, \{f(h)\,,\pi_1\}_1 \\ & + \{P_0\,,\{f(h)\,,P_0\}_1\}_1\Big) + \mathcal{O}(\varepsilon^2) \end{aligned}$$

By Lemma A.11 and the product rule

$$\begin{aligned} \int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\, \{f(h)\,,\pi_1\}_1)\, \tilde{a}^{(2)}\, \mathrm{d}z = {}& - \int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\pi_1\, \{f(h)\,,P_0\}_1)\, \tilde{a}^{(2)}\, \mathrm{d}z \\ & - \int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\, \pi_1)\, \{f(h)\,,\tilde{a}^{(2)}\,\}_1\, \mathrm{d}z \end{aligned} \tag{4.48}$$

By (4.46) - (4.48) we get

$$\begin{aligned}&\int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\pi) \,\#\, f^\varepsilon(h,\pi)\, \tilde{a}^{(2)}\, \mathrm{d}z - \mathrm{i}\,\varepsilon \int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\pi \,\#\, \tfrac{\mathrm{i}}{\varepsilon}\,[\, f^\varepsilon(h,\pi)\,,\pi\,]_\#)\, \tilde{a}^{(2)}\, \mathrm{d}z \\ &\quad = \int_{\mathbb{R}^{2n}} f^\varepsilon(h,\pi)\, \tilde{a}^{(2)}\, \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\pi)\, \mathrm{d}z + 2\,\varepsilon^2 \int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\{P_0\,,\{f(h)\,,P_0\}_1\}_1)\, \tilde{a}^{(2)}\, \mathrm{d}z \\ &\qquad + \mathcal{O}(\varepsilon^3 \sum_{i=0}^{2} \|A_i\|_{L^1})\,. \end{aligned} \tag{4.49}$$

Then, combining (4.45), (4.49) and the fact that $f(h(z)) = f(h_0) + \mathcal{O}(\varepsilon)$ with (4.27) we obtain

$$\begin{aligned}&\mathrm{tr}_\mathcal{H}\left(f(\hat{H}^\varepsilon)\,\hat{A}^\varepsilon\,\hat{\Pi}^\varepsilon\right) \\ &\quad = (2\pi\varepsilon)^{-n} \int_{\mathbb{R}^{2n}} f^\varepsilon(h,\pi)\, \tilde{a}^{(2)}\, \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\pi)\, \mathrm{d}z \\ &\qquad + 2\,\varepsilon^2\,(2\pi\varepsilon)^{-n} \int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\{P_0\,,\{f(h_0)\,,P_0\}_1\}_1)\, \tilde{a}^{(2)}\, \mathrm{d}z \\ &\qquad + \mathcal{O}\Big(\varepsilon^{3-n}\left(\|A\|^\varepsilon_{L^1} + \sum_{i=0}^{2}\left(\|A_i\|_{L^1} + \|\varepsilon^{-(i+1)}(A - A^{(i)})\|^\varepsilon_{L^1}\right)\right)\Big)\end{aligned}$$

Replacing $\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\pi)\,\mathrm{d}z$ by $\lambda^\varepsilon$ (4.40) and a simple computation yields

$$\begin{aligned}\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\{P_0\,,\{f(h_0)\,,P_0\}_1\}_1) &= -\tfrac{1}{4}\,\omega^0_{ij}\,\partial_i\Big(\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\partial_j P_0\,\partial_l P_0)\, f'(h_0)\,\omega^0_{lr}\,\partial_r h_0\Big) \\ &= \tfrac{1}{4}\,\omega^0_{ji}\,\partial_i(f'(h_0)\, g_{0,jl}\,\omega^0_{lr}\,\partial_r h_0) \\ &= \tfrac{1}{4}\,\mathrm{Tr}_{2n}(\omega^0\,\nabla(f'(h_0)\,g_0\,\omega^0\,\nabla h_0)\,)\end{aligned}$$

finishes the proof. □

REMARK 4.5 It is easy to validate that in the special case of particles subject to a potential the quantum correction $f^\mathrm{sc}(h)$ (4.30) coincides with the corrections derived by Wigner (see Equation 1.4). In addition, one can conclude from a comparison of those two results that the $\varepsilon$-dependent Hamiltonian system incorporates many of the terms emerging from the adiabatic approximation. But there are additional quantum corrections appearing, namely $Q(h,\pi)$ (4.30) and $f^\mathrm{adi}(h,\pi)$ (4.13). The correction $\varepsilon^2\,(f^\mathrm{sc}(h) + f^\mathrm{adi}(h,\pi))$ can be interpreted as quantum correction to the density $f(h)$. The term $Q(h,\pi)$ does not allow such an interpretation and is thus simply considered as a quantum correction to the expectation value.

If we assume the Liouville measure $\lambda^\varepsilon$ to satisfy

$$\lambda^\varepsilon = \Big(\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\pi) + \mathcal{O}(\varepsilon^\infty)\Big)\,\mathrm{d}z\,, \tag{4.50}$$

then we can also express the higher order semiclassical approximations (4.27) as classical expectation with respect to the Hamiltonian system $(h, \omega^\varepsilon)$ and corrected density $f^\varepsilon(h,\pi)$ plus quantum correction $Q^\varepsilon(h,\pi)$, i.e.

$$\begin{aligned}\operatorname{tr}_{\mathcal{H}}\left(f(\hat{H}^\varepsilon)\,\hat{A}^\varepsilon\,\hat{\Pi}^\varepsilon\right) =&(2\pi\varepsilon)^{-n}\Big(\int_{\mathbb{R}^{2n}} f^\varepsilon(h,\pi)\,a^{(N)}\,\lambda^\varepsilon + \int_{\mathbb{R}^{2n}} Q^\varepsilon(h,\pi)\,a^{(N)}\,\mathrm{d}z\Big)\\ &+ \mathcal{O}\Big(\varepsilon^{-n+N+1}\,\|A\|^\varepsilon_{L^1}\Big)\,.\end{aligned}$$

Nevertheless, at this point it is not clear whether (4.50) holds.

# 5 An Egorov Type Theorem

The goal of this chapter is to approximate expectation values of non-stationary states $\rho(t) = \mathrm{e}^{-\mathrm{i}\hat{H}^\varepsilon t/\varepsilon}\,\rho_0\,\mathrm{e}^{\mathrm{i}\hat{H}^\varepsilon t/\varepsilon}$ with initial state $\rho_0$ satisfying $\rho = \hat{\Pi}^\varepsilon\,\rho_0\,\hat{\Pi}^\varepsilon$, i.e.

$$\mathrm{tr}_{\mathcal{H}}(\rho(t)\,\hat{A}^\varepsilon).$$

Here, $\hat{A}^\varepsilon$ is an observable given as Weyl quantization of an operator-valued symbol taking values in the self-adjoint operators acting on $\mathcal{H}_\mathrm{f}$. Then $\rho_0 = \hat{\Pi}^\varepsilon\rho_0\hat{\Pi}^\varepsilon$ and consequently

$$\begin{aligned}\mathrm{tr}_{\mathcal{H}}(\rho(t)\,\hat{A}^\varepsilon) &= \mathrm{tr}_{\mathcal{H}}(\mathrm{e}^{-\mathrm{i}\hat{H}^\varepsilon t/\varepsilon}\,\hat{\Pi}^\varepsilon\,\rho_0\,\hat{\Pi}^\varepsilon\,\mathrm{e}^{\mathrm{i}\hat{H}^\varepsilon t/\varepsilon}\,\hat{A}^\varepsilon)\\ &= \mathrm{tr}_{\mathcal{H}}(\rho_0\,\hat{\Pi}^\varepsilon\,\mathrm{e}^{\mathrm{i}\hat{H}^\varepsilon t/\varepsilon}\,\hat{A}^\varepsilon\,\mathrm{e}^{-\mathrm{i}\hat{H}^\varepsilon t/\varepsilon}\,\hat{\Pi}^\varepsilon) =: \mathrm{tr}_{\mathcal{H}}(\rho_0\,\hat{\Pi}^\varepsilon\,\hat{A}^\varepsilon(t)\,\hat{\Pi}^\varepsilon)\,.\end{aligned}$$

It is known that in the case where the symbol of the observable $\hat{A}^\varepsilon$ is a scalar multiple of the identity on $\mathcal{H}_\mathrm{f}$ one can approximate the quantum evolution $\hat{A}^\varepsilon(t)$ restricted to the almost-invariant subspace up to errors of order $\varepsilon^2$ by evolving the symbol $A(z)$ by an $\varepsilon$-dependent classical flow $\Phi^t_\varepsilon$, see e.g. [ST13, Theorem 2]. This is known as Egorov's theorem. As we have seen in the introduction already, even in the case of a purely semiclassical system there is no classical system whose flow approximates the quantum evolution up to errors of order $\varepsilon^3$. But, there are quantum corrections to the classically evolved observable that lead to an approximation of the quantum evolution up to errors of order $\varepsilon^3$, see (1.1). In Section 5.1 we prove that even in the case of Hamiltonian and observable having operator-valued symbols a similar result as (1.1) holds, when restricting the initial state $\rho_0$ to the super-adiabatic subspace $\hat{\Pi}^\varepsilon\mathcal{H}$. We show that, up to explicitly given quantum corrections, the classical evolution according to the $\varepsilon$-dependent classical system $(\mathbb{R}^{2n}, \omega^\varepsilon, h)$ (see Section 3.3) approximates the quantum evolution to errors of order $\varepsilon^3$. Moreover, we show how to derive semiclassical approximations for the quantum evolution restricted to the super-adiabatic subspace up to arbitrary order in $\varepsilon$.

In [LR10] Lasser and Röblitz developed a numerical scheme to approximate quantum mechanical expectation values $\langle\phi_t, \hat{a}^\varepsilon\,\psi_t\rangle$ for particles subject to a potential up to errors of order $\varepsilon^2$. This approach was extended in [GL14] to approximations up to errors of order three in $\varepsilon$. In Section 5.2 we explain how one can use the results of Section 5.1 to generalize this numerical scheme to Hamiltonians $\hat{H}^\varepsilon$ and observables $\hat{A}^\varepsilon$ with operator values symbols.

# 5.1 The Corrections to Egorov's Theorem

One of the crucial steps in deriving semiclassical approximation for the quantum evolution of observables is the semiclassical approximation of the commutator $\frac{\mathrm{i}}{\varepsilon}\left[\hat{H}^\varepsilon, \hat{a}^\varepsilon\right]$ restricted to the super-adiabatic subspace.

**Proposition 5.1** *Let Assumptions 2.10 and 2.11 hold and $a$ a scalar symbol in $S^0(\varepsilon,\mathbb{R})$. Then, with $h$ the effective Hamiltonian given by Corollary 3.8 the Hamiltonian vector field $X_h^{\varepsilon,\alpha} = -(\omega^\varepsilon)^{-1}_{\alpha\beta}\,\partial_\beta h$ is a symbol in $S^0(\varepsilon,\mathbb{R}^{2n})$. In addition, for any $N\in\mathbb{N}_0$ there exists a linear map $\mathfrak{A}_h^{c,N} : S^0(\varepsilon,\mathbb{R}) \to S^0(\varepsilon,\mathbb{R})$ satisfying that there is a $r\in\mathbb{N}_0$ such that*

$$\left\|\hat{\Pi}^\varepsilon\left(\frac{\mathrm{i}}{\varepsilon}\left[\hat{H}^\varepsilon, \hat{a}^\varepsilon\right] - \mathrm{op}_\varepsilon(X_h^\varepsilon\cdot\nabla a) - \varepsilon^2\,\mathrm{op}_\varepsilon(\mathfrak{A}_h^{c,N}(a)\right)\hat{\Pi}^\varepsilon\right\| = \mathcal{O}(\varepsilon^{N+1}\|a\|^\varepsilon_{0,r})\,. \tag{5.1}$$

*Moreover, there exists a constant $C_r<\infty$ and a $\tilde{r}\in\mathbb{N}_0$ for every $r\in\mathbb{N}_0$ such that*

$$\|\mathfrak{A}_h^{c,N}(a)\|^\varepsilon_{0,r} \le C_r\,\|a\|^\varepsilon_{0,\tilde{r}}\,. \tag{5.2}$$

*Furthermore, there is a $r\in\mathbb{N}_0$ such that*

$$\mathfrak{A}_h^{c,N}(a) = 2\,\mathrm{i}\,\{h_0\,, a\}_3 - \tfrac{1}{2}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\{\{h_0\,,P_0\}\,,\{a\,,P_0\}\}) + \mathcal{O}(\varepsilon\,\|a\|^\varepsilon_{0,r})\,. \tag{5.3}$$

PROOF We start our proof by reformulating $(\omega^\varepsilon)^{-1}$ for $\varepsilon$ small enough by use of a Neumann series. We get

$$\begin{aligned}(\omega^\varepsilon)^{-1} =&(\omega^0+\varepsilon\,\Omega^\varepsilon)^{-1} = (\omega^0)^{-1}(1-(-\varepsilon\,\Omega^\varepsilon\,(\omega^0)^{-1}))^{-1}\\ =&(\omega^0)^{-1}(1-(\varepsilon\,\Omega^\varepsilon\,\omega^0\,))^{-1} = -\omega^0\sum_{j=0}^\infty \varepsilon^j(\Omega^\varepsilon\,\omega^0)^j\,.\end{aligned} \tag{5.4}$$

Therefore, the fact that $\Omega^\varepsilon_{ij}$, $0\le i,j\le 2n$ and $\partial_\beta h$ are a symbols in $S^0(\varepsilon,\mathbb{R})$ (see Section 3.3) implies that $X_h^{\varepsilon,\alpha}$ is a symbol in $S^0(\varepsilon,\mathbb{R}^{2n})$. To show (5.1) we start by replacing the Hamiltonian by its effective Operator (see Corollary 3.8) and obtain

$$\begin{aligned}
&\hat{\Pi}^{\varepsilon}\,\tfrac{\mathrm{i}}{\varepsilon}\left[\,\hat{H}^{\varepsilon}\,,\hat{a}^{\varepsilon}\,\right]\,\hat{\Pi}^{\varepsilon} \\
&\quad = \hat{\Pi}^{\varepsilon}\,\tfrac{\mathrm{i}}{\varepsilon}\left[\,\hat{\Pi}^{\varepsilon}\,\hat{H}^{\varepsilon}\,\hat{\Pi}^{\varepsilon}\,,\hat{\Pi}^{\varepsilon}\,\hat{a}^{\varepsilon}\,\hat{\Pi}^{\varepsilon}\,\right]\,\hat{\Pi}^{\varepsilon} + \mathcal{O}(\varepsilon^{\infty}\,\|\hat{a}^{\varepsilon}\|) \\
&\quad = \hat{\Pi}^{\varepsilon}\,\tfrac{\mathrm{i}}{\varepsilon}\left[\,\hat{\Pi}^{\varepsilon}\,\hat{h}^{\varepsilon}\,\hat{\Pi}^{\varepsilon}\,,\hat{\Pi}^{\varepsilon}\,\hat{a}^{\varepsilon}\,\hat{\Pi}^{\varepsilon}\,\right]\,\hat{\Pi}^{\varepsilon} + \mathcal{O}(\varepsilon^{\infty}\,\|\hat{a}^{\varepsilon}\|)\,.
\end{aligned} \tag{5.5}$$

where in the first equation we used that the Hamiltonian $\hat{H}^{\varepsilon}$ almost commutes with the adiabatic projection $\hat{\Pi}^{\varepsilon}$ (see Proposition 3.2). Since $\hat{\Pi}^{\varepsilon}$ is a projection

$$\begin{aligned}
&\hat{\Pi}^{\varepsilon}\,\tfrac{\mathrm{i}}{\varepsilon}\left[\,\hat{\Pi}^{\varepsilon}\,\hat{h}^{\varepsilon}\,\hat{\Pi}^{\varepsilon}\,,\hat{\Pi}^{\varepsilon}\,\hat{a}^{\varepsilon}\,\hat{\Pi}^{\varepsilon}\,\right]\,\hat{\Pi}^{\varepsilon} \\
&\quad = \hat{\Pi}^{\varepsilon}\left(\tfrac{\mathrm{i}}{\varepsilon}[\,\hat{h}^{\varepsilon}\,,\hat{a}^{\varepsilon}\,] - \mathrm{i}\,\varepsilon\,\left[\,\tfrac{\mathrm{i}}{\varepsilon}[\,\hat{h}^{\varepsilon}\,,\hat{\Pi}^{\varepsilon}\,]\,,\tfrac{\mathrm{i}}{\varepsilon}[\,\hat{a}^{\varepsilon}\,,\hat{\Pi}^{\varepsilon}\,]\,\right]\right)\hat{\Pi}^{\varepsilon}
\end{aligned} \tag{5.6}$$

An application of Proposition 3.2 to replace $\hat{\Pi}^{\varepsilon}$ by $\hat{\pi}^{\varepsilon}$ and the definition of the Moyal product yield

$$\begin{aligned}
&\hat{\Pi}^{\varepsilon}\left(\tfrac{\mathrm{i}}{\varepsilon}[\,\hat{h}^{\varepsilon}\,,\hat{a}^{\varepsilon}\,] - \mathrm{i}\,\varepsilon\,\left[\,\tfrac{\mathrm{i}}{\varepsilon}[\,\hat{h}^{\varepsilon}\,,\hat{\Pi}^{\varepsilon}\,]\,,\tfrac{\mathrm{i}}{\varepsilon}[\,\hat{a}^{\varepsilon}\,,\hat{\Pi}^{\varepsilon}\,]\,\right]\right)\hat{\Pi}^{\varepsilon} \\
&\quad = \hat{\Pi}^{\varepsilon}\left(\tfrac{\mathrm{i}}{\varepsilon}[\,\hat{h}^{\varepsilon}\,,\hat{a}^{\varepsilon}\,] - \mathrm{i}\,\varepsilon\,\left[\,\tfrac{\mathrm{i}}{\varepsilon}[\,\hat{h}^{\varepsilon}\,,\hat{\pi}^{\varepsilon}\,]\,,\tfrac{\mathrm{i}}{\varepsilon}[\,\hat{a}^{\varepsilon}\,,\hat{\pi}^{\varepsilon}\,]\,\right]\right)\hat{\Pi}^{\varepsilon} + \mathcal{O}(\varepsilon^{\infty}\,\|\hat{a}^{\varepsilon}\|) \\
&\quad = \hat{\Pi}^{\varepsilon}\,\mathrm{op}_{\varepsilon}\left(\tfrac{\mathrm{i}}{\varepsilon}[\,h\,,a\,]_{\#} - \mathrm{i}\,\varepsilon\,\left[\,\tfrac{\mathrm{i}}{\varepsilon}[\,h\,,\pi\,]_{\#}\,,\tfrac{\mathrm{i}}{\varepsilon}[\,a\,,\pi\,]_{\#}\,\right]_{\#}\right)\hat{\Pi}^{\varepsilon} + \mathcal{O}(\varepsilon^{\infty}\,\|\hat{a}^{\varepsilon}\|)\,.
\end{aligned} \tag{5.7}$$

Here, we use the notation of the Moyal commutator $[\,h\,,\pi\,]_{\#} := h\,\#\,\pi - \pi\,\#\,h$. As scalar symbols, $a$ and $h$ commute with any operator-valued symbol. We define $B_j^{h,a}(\varepsilon) \in S^0(\varepsilon,\mathbb{R})$ and $B_j^{a,\pi}(\varepsilon), B_j^{h,\pi}(\varepsilon) \in S^0(\varepsilon,\mathcal{J}(\mathcal{H}_{\mathrm{f}}))$ for $j \in \mathbb{N}_0$ by

$$\begin{aligned}
\tfrac{\mathrm{i}}{\varepsilon}\,[\,h\,,a\,]_{\#}\,(\varepsilon) &\asymp \sum_{j=0}^{\infty} \varepsilon^{2j}\,2\,\mathrm{i}\,\{h(\varepsilon)\,,a(\varepsilon)\}_{2j+1} =: \sum_{j=0}^{\infty} \varepsilon^{j}\,B_j^{h,a}(\varepsilon)\,, \\
\tfrac{\mathrm{i}}{\varepsilon}\,[\,a\,,\pi\,]_{\#}\,(\varepsilon) &\asymp \sum_{j=0}^{\infty} \varepsilon^{2j}\,2\,\mathrm{i}\,\{a(\varepsilon)\,,\pi(\varepsilon)\}_{2j+1} =: \sum_{j=0}^{\infty} \varepsilon^{j}\,B_j^{a,\pi}(\varepsilon)
\end{aligned} \tag{5.8}$$

and

$$\tfrac{\mathrm{i}}{\varepsilon}\,[\,h\,,\pi\,]_{\#}\,(\varepsilon) \asymp \sum_{j=0}^{\infty} \varepsilon^{2j}\,2\,\mathrm{i}\,\{h(\varepsilon)\,,\pi(\varepsilon)\}_{2j+1} =: \sum_{j=0}^{\infty} \varepsilon^{j}\,B_j^{h,\pi}(\varepsilon)\,.$$

where we used the expansion of the Moyal product (2.4) and the identity (2.7) to obtain the above asymptotic expansions.

Again using (2.4) yields

$$\begin{aligned}
&\tfrac{\mathrm{i}}{\varepsilon}[\,h\,,a\,]_{\#} - \mathrm{i}\,\varepsilon\,\Big[\,\tfrac{\mathrm{i}}{\varepsilon}\,[\,h\,,\pi\,]_{\#}\,,\tfrac{\mathrm{i}}{\varepsilon}[\,a\,,\pi\,]_{\#}\,\Big]_{\#} \\
&\asymp \sum_{j=0}^{\infty} \varepsilon^{j}\,\Big( B_j^{h,a}(\varepsilon) - \mathrm{i}\,\varepsilon \sum_{\substack{\alpha\in\mathbb{N}_0^3,\\ |\alpha|=j}} \Big( \Big\{ B_{\alpha_1}^{h,\pi}(\varepsilon)\,, B_{\alpha_2}^{a,\pi}(\varepsilon) \Big\}_{\alpha_3} - \Big\{ B_{\alpha_2}^{a,\pi}(\varepsilon)\,, B_{\alpha_1}^{h,\pi}(\varepsilon) \Big\}_{\alpha_3} \Big)\Big) \\
&=: \sum_{j=0}^{\infty} \varepsilon^{j}\, B_j^{H,a}(\varepsilon)\,.
\end{aligned} \tag{5.9}$$

Now fix $N \in \mathbb{N}_0$. Combining the continuity of the Moyal product (2.3), the continuity of the Moyal remainder (2.6), the fact that $\partial_j h \in S^0(\varepsilon, \mathbb{R}), 1 \le j \le 2n$ and the previous result (5.9) there is a constant $C > 0$ and a $\tilde{r} \in \mathbb{N}_0$ for every $r \in \mathbb{N}_0$ such that

$$\Big\| \tfrac{\mathrm{i}}{\varepsilon}[\,h\,,a\,]_{\#} - \mathrm{i}\,\varepsilon\,\Big[\,\tfrac{\mathrm{i}}{\varepsilon}\,[\,h\,,\pi\,]_{\#}\,,\tfrac{\mathrm{i}}{\varepsilon}[\,a\,,\pi\,]_{\#}\,\Big]_{\#} - \sum_{j=0}^{N} \varepsilon^{j}\, B_j^{H,a} \Big\|_{0,r} \le C\,\varepsilon^{N+1}\,\|a\|_{0,\tilde{r}}^{\varepsilon}\,.$$

Hence, applying Calderon-Vaillancourt's Theorem (2.2) there is a $r_1 \in \mathbb{N}_0$ such that

$$\begin{aligned}
&\hat{\Pi}^{\varepsilon}\,\mathrm{op}_{\varepsilon}\Big(\tfrac{\mathrm{i}}{\varepsilon}[\,h\,,a\,]_{\#} - \mathrm{i}\,\varepsilon\,\Big[\,\tfrac{\mathrm{i}}{\varepsilon}\,[\,h\,,\pi\,]_{\#}\,,\tfrac{\mathrm{i}}{\varepsilon}[\,a\,,\pi\,]_{\#}\,\Big]_{\#}\Big)\,\hat{\Pi}^{\varepsilon} \\
&\qquad = \hat{\Pi}^{\varepsilon}\,\mathrm{op}_{\varepsilon}\Big(\sum_{j=0}^{N} \varepsilon^{j}\, B_j^{H,a}(\varepsilon)\Big)\,\hat{\Pi}^{\varepsilon} + \mathcal{O}\Big(\varepsilon^{N+1}\,\|a\|_{0,r_1}^{\varepsilon}\Big)\,.
\end{aligned} \tag{5.10}$$

Following Section 3.2, there exists a linear map $b_{h,\varepsilon}^{(N)} : S^0(\varepsilon, \mathbb{R}) \to S^0(\varepsilon, \mathbb{R})$ which maps $a \in S^0(\varepsilon, \mathbb{R})$ to the $N$th order effective symbol of $\sum_{j=0}^{N} \varepsilon^j\, B_j^{H,a}(\varepsilon)$. Hence, it follows from Theorem 3.6 that there is a constant $C > 0$ and a $\tilde{r} \in \mathbb{N}_0$ for every $r \in \mathbb{N}_0$ such that

$$\Big\| \pi \,\#\, \Big( \sum_{j=0}^{N} \varepsilon^{j}\, B_j^{H,a}(\varepsilon) - b_{h,\varepsilon}^{(N)}(a(\varepsilon)) \Big) \,\#\, \pi \,\Big\|_{0,r} \le C\,\varepsilon^{N+1}\,\|a\|_{0,\tilde{r}}^{\varepsilon}\,.$$

As above, the Calderon-Vaillancourt Theorem (2.2) yields

$$\hat{\Pi}^{\varepsilon}\,\mathrm{op}_{\varepsilon}\Big(\sum_{j=0}^{N} \varepsilon^{j}\, B_j^{H,a}(\varepsilon)\Big)\,\hat{\Pi}^{\varepsilon} = \hat{\Pi}^{\varepsilon}\,\mathrm{op}_{\varepsilon}\Big(b_{h,\varepsilon}^{(N)}(a(\varepsilon))\Big)\,\hat{\Pi}^{\varepsilon} + \mathcal{O}\Big(\varepsilon^{N+1}\,\|a\|_{0,r_2}^{\varepsilon}\Big) \tag{5.11}$$

for a $r_2 \in \mathbb{N}_0$ large enough.

Combining (5.5)-(5.7) with (5.10) and (5.11) there is a $r_3 \in \mathbb{N}_0$ such that

$$\hat{\Pi}^{\varepsilon}\, \tfrac{\mathrm{i}}{\varepsilon} \Big[ \hat{H}^{\varepsilon} , \hat{a}^{\varepsilon} \Big]\, \hat{\Pi}^{\varepsilon} = \hat{\Pi}^{\varepsilon}\, \mathrm{op}_{\varepsilon}\Big( b^{(N)}_{h,\varepsilon}(a(\varepsilon)) \Big)\, \hat{\Pi}^{\varepsilon} + \mathcal{O}\Big( \varepsilon^{N+1} \, \|a\|^{\varepsilon}_{0,r_3} \Big) . \tag{5.12}$$

In the next step we compute $b^{(N)}_{h,\varepsilon}(a(\varepsilon))$ up to the contributions of second order in $\varepsilon$. For this, let $N \geq 2$. By (5.8) and the definition of $B^{H,a}$ (5.9) we have

$$\begin{aligned} B^{H,a}_0(\varepsilon) &= 2\,\mathrm{i}\, \{h(\varepsilon) , a(\varepsilon)\}_1 = \{h(\varepsilon) , a(\varepsilon)\} = \Big\langle \omega^0 \, \nabla h \, , \, \nabla a \Big\rangle \, , \\ B^{H,a}_1(\varepsilon) &= -\,\mathrm{i}\, \varepsilon \; [\, \{h(\varepsilon) , \pi(\varepsilon)\} \; , \{a(\varepsilon) , \pi(\varepsilon)\} \,] \end{aligned}$$

and

$$\begin{aligned} B^{H,a}_2(\varepsilon) &= 2\,\mathrm{i}\, \{h(\varepsilon) , a(\varepsilon)\}_3 - \mathrm{i}\, \varepsilon \Big\{ \{h(\varepsilon) , \pi(\varepsilon)\} \; , \{a(\varepsilon) , \pi(\varepsilon)\} \Big\}_1 \\ &\quad + \mathrm{i}\, \varepsilon \Big\{ \{a(\varepsilon) , \pi(\varepsilon)\} \; , \{h(\varepsilon) , \pi(\varepsilon)\} \Big\}_1 . \end{aligned}$$

Hence, Lemma B.3 and B.4 imply that the expansion of the effective symbol $b^{(N)}_{h,\varepsilon}(a(\varepsilon))$ starts with

$$\begin{aligned} b^{(N)}_{h,\varepsilon}(a(\varepsilon)) = &\Big\langle \omega^0 \, \nabla h(\varepsilon) \, , \, \nabla a(\varepsilon) \Big\rangle + 2\,\mathrm{i}\, \varepsilon^2 \; \{h(\varepsilon) , a(\varepsilon)\}_3 \\ &+ \varepsilon \; \Big\langle \omega^0 \, \Omega^{\varepsilon} \, \omega^0 \, \nabla h(\varepsilon) \, , \, \nabla a(\varepsilon) \Big\rangle + \varepsilon^2 \; \Big\langle \omega^0 \, (\Omega^{\varepsilon} \, \omega^0)^2 \, \nabla h(\varepsilon) \, , \, \nabla a(\varepsilon) \Big\rangle \\ &- \tfrac{1}{2} \, \varepsilon^2 \, \mathrm{tr}_{\mathcal{H}_{\mathrm{f}}}(\{\{h(\varepsilon) , P_0\} \; , \{a(\varepsilon) , P_0\}\}) + \mathcal{O}(\varepsilon^3 \, \|a\|^{\varepsilon}_{0,r_4}) \end{aligned}$$

for some $r_4 \in \mathbb{N}_0$ large enough. Comparing the above result with the Neumann series (5.4) shows

$$\begin{aligned} b^{(N)}_{h,\varepsilon}(a(\varepsilon)) = &\Big\langle -(\omega^{\varepsilon})^{-1} \, \nabla h(\varepsilon) \, , \, \nabla a(\varepsilon) \Big\rangle + 2\,\mathrm{i}\, \varepsilon^2 \; \{h(\varepsilon) , a(\varepsilon)\}_3 \\ &- \tfrac{1}{2} \, \varepsilon^2 \, \mathrm{tr}_{\mathcal{H}_{\mathrm{f}}}(\{\{h(\varepsilon) , P_0\} \; , \{a(\varepsilon) , P_0\}\}) + \mathcal{O}(\varepsilon^3) \\ = &X^{\varepsilon}_h \cdot \nabla a(\varepsilon) + 2\,\mathrm{i}\, \varepsilon^2 \; \{h(\varepsilon) , a(\varepsilon)\}_3 \\ &- \tfrac{1}{2} \, \varepsilon^2 \, \mathrm{tr}_{\mathcal{H}_{\mathrm{f}}}(\{\{h(\varepsilon) , P_0\} \; , \{a(\varepsilon) , P_0\}\}) + \mathcal{O}(\varepsilon^3 \, \|a\|^{\varepsilon}_{0,r_4}) \end{aligned} \tag{5.13}$$

Then (5.1) follows by combining (5.12) and (5.13) and defining

$$\mathfrak{A}^{c,N}_{h,\varepsilon}(a(\varepsilon)) := \varepsilon^{-2} \Big( b^{(N)}_{h,\varepsilon}(a(\varepsilon)) - X^{\varepsilon}_h \cdot \nabla a(\varepsilon) \Big) . \tag{5.14}$$

In addition, by (3.27) and the continuity of the Moyal product there is a constant $\tilde{C} > 0$ and a $\tilde{r} \in \mathbb{N}_0$ for every $r \in \mathbb{N}_0$ such that

$$\| b^{(N)}_{h,\varepsilon}(a(\varepsilon)) \|_{0,r} \leq \tilde{C} \, \|a\|^{\varepsilon}_{0,\tilde{r}}$$

and thus

$$\|\mathfrak{A}^{c,N}_{h,\varepsilon}(a(\varepsilon)))\|_{0,r} \leq C\, \|a\|^{\varepsilon}_{0,\tilde{r}}$$

for a constant $C \geq \tilde{C}$. To finish the proof, notice that (5.3) follows by combining (5.13) and (5.14). □

Notice that extending the proposition above to observables with operator-valued symbols is fairly simple. Nevertheless, as we will see in the proof of Theorem 5.2 that this generalization is unnecessary to derive semiclassical approximations of the quantum evolution of observables with operator-valued symbols.

**Theorem 5.2** *Let Assumptions 2.10 and 2.11 hold. In addition, assume $A \in S^0(\varepsilon, \mathcal{B}_{\mathrm{sa}}(\mathcal{H}_{\mathrm{f}}))$ with effective Operator $\hat{a}^\varepsilon \in S^0(\varepsilon, \mathbb{R})$. Then, the Hamiltonian flow $\Phi^t_\varepsilon$ of $(\mathbb{R}^{2n}, \omega^\varepsilon, h)$ exists globally. Moreover, for any $N \in \mathbb{N}_0$ and $t \in \mathbb{R}$ there exists a constant $C > 0$ and a $r \in \mathbb{N}_0$ such that*

$$\left\|\hat{\Pi}^\varepsilon \left(\hat{A}^\varepsilon(t) - \mathrm{op}_\varepsilon\left(a^{(N)}(\Phi^t_\varepsilon) + \varepsilon^2\, \mathfrak{A}^N(t)\right)\right)\hat{\Pi}^\varepsilon\right\| \leq C\, \varepsilon^{N+1}\, \|A\|^{\varepsilon}_{0,r} \sum_{j=0}^{N+3} |t|^j \tag{5.15}$$

*where*

$$\hat{A}^\varepsilon(t) := \mathrm{e}^{\mathrm{i}\hat{H}^\varepsilon t/\varepsilon}\hat{A}^\varepsilon \mathrm{e}^{-\mathrm{i}\hat{H}^\varepsilon t/\varepsilon}$$

*and $\mathfrak{A}^N(t) = \sum_{j=0}^{\lfloor N/2 \rfloor} \varepsilon^{2j}\, \mathfrak{A}^N_{2j}(t)$ with $\mathfrak{A}^N_{2j}(t) \in S^0(\varepsilon, \mathbb{R})$ inductively given by*

$$\mathfrak{A}^N_0(t) := \int_0^t \mathfrak{A}^{c,N}_{h,\varepsilon}(a^{(N)}(\Phi^\tau_\varepsilon)) \circ \Phi^{t-\tau}_\varepsilon\, \mathrm{d}\tau$$

*and*

$$\mathfrak{A}^N_{2j}(t) := \int_0^t \mathfrak{A}^{c,N}_{h,\varepsilon}(\mathfrak{A}^N_{2(j-1)}(\tau)) \circ \Phi^{t-\tau}_\varepsilon\, \mathrm{d}\tau \quad \textit{for } j \geq 1\,.$$

*with $\mathfrak{A}^{c,N}_{h,\varepsilon}(a)(z)$ defined by (5.14). Moreover, there exists a $r \in \mathbb{N}_0$ such that*

$$\begin{aligned}\mathfrak{A}^2_0(t) = {} & 2\,\mathrm{i}\int_0^t \{h_0\,, a_0(\Phi^\tau_\varepsilon)\}_3 \circ \Phi^{t-\tau}_\varepsilon\, \mathrm{d}\tau \\ & - \tfrac{1}{2}\int_0^t \mathrm{tr}_{\mathcal{H}_{\mathrm{f}}}(\{\{h_0\,, P_0\}\ , \{a_0(\Phi^\tau_\varepsilon)\,, P_0\}\}) \circ \Phi^{t-\tau}_\varepsilon\, \mathrm{d}\tau + \mathcal{O}(\varepsilon\, \|A\|^\varepsilon_{0,r}\, |t|)\,.\end{aligned} \tag{5.16}$$

Proof Fix $N \in \mathbb{N}_0$. By Proposition 5.1 the Hamiltonian vector field $X^\varepsilon_h$ is a classical symbol in $S^0(\varepsilon, \mathbb{R}^{2n})$. This implies that the Hamiltonian flow $\Phi^t_\varepsilon$ of $(h, \omega^\varepsilon)$ exists globally and $\Phi^t_\varepsilon \in S^0(\varepsilon, \mathbb{R}^{2n})$ for $t$ fixed. By (3.27) there exists a constant $\tilde{C} > 0$ and a $\tilde{r} \in \mathbb{N}_0$ for every $r \in \mathbb{N}_0$ and $t \in \mathbb{R}$ such that

$$\|a^{(N)}(\Phi^t_\varepsilon)\|^\varepsilon_{0,r} \leq \tilde{C}\, \|A\|^\varepsilon_{0,\tilde{r}}\,.$$

Moreover, by (5.2) we have for every $r \in \mathbb{N}_0$ and $t \in \mathbb{R}$ that

$$\|\mathfrak{A}_0^N(t)\|_{0,r}^\varepsilon \leq \int_0^{|t|} \| \mathfrak{A}_{h,\varepsilon}^{c,N}(a^{(N)}(\Phi_\varepsilon^\tau)) \circ \Phi_\varepsilon^{t-\tau} \|_{0,r}^\varepsilon \, \mathrm{d}\tau$$
$$\leq \tilde{C}_2 \, |t| \, \|a^{(N)}(\Phi_\varepsilon^\tau)\|_{0,\tilde{r}_2}^\varepsilon \leq \tilde{C} \, |t| \, \|A\|_{0,\tilde{r}}^\varepsilon$$

for large enough $\tilde{C} > \tilde{C}_2 > 0$ and $\tilde{r}, \tilde{r}_2 \in \mathbb{N}_0$. From the definition of $\mathfrak{A}^N(t)$ and the results above it is easy to see that there is a constant $\tilde{C} > 0$ and a $\tilde{r} \in \mathbb{N}_0$ for every $r \in \mathbb{N}_0$ and $t \in \mathbb{R}$ such that

$$\left\| \, a^{(N)}(\Phi_\varepsilon^t) + \varepsilon^2 \, \mathfrak{A}^N(t) \, \right\|_{0,r}^\varepsilon \leq \tilde{C} \, \|A\|_{0,\tilde{r}}^\varepsilon \sum_{j=0}^{N+1} |t|^j \, . \tag{5.17}$$

Defining

$$a^N(t) := a^{(N)}(\Phi_\varepsilon^t) + \varepsilon^2 \, \mathfrak{A}^N(t)$$

it directly follows that $a^N(t) \in S^0(\varepsilon, \mathbb{R})$ for fixed $t$. In addition, $a^N(t)$ depends smoothly on $t$ and is uniformly bounded on bounded time intervals. By Calderon-Vaillancourt's theorem (2.2) and Corollary 3.4

$$\hat{\Pi}^\varepsilon \, \mathrm{e}^{\mathrm{i}\hat{H}^\varepsilon t/\varepsilon} \, \hat{A}^\varepsilon \, \mathrm{e}^{-\mathrm{i}\hat{H}^\varepsilon t/\varepsilon} \, \hat{\Pi}^\varepsilon = \mathrm{e}^{\mathrm{i}\hat{H}^\varepsilon t/\varepsilon} \, \hat{\Pi}^\varepsilon \, \hat{A}^\varepsilon \, \hat{\Pi}^\varepsilon \, \mathrm{e}^{-\mathrm{i}\hat{H}^\varepsilon t/\varepsilon} + \mathcal{O}(\varepsilon^\infty \, \|A\|_{0,2n+1}^\varepsilon \, |t|) \, . \tag{5.18}$$

By (2.2) and the estimate (3.38) there exists a $r_1 \in \mathbb{N}_0$ such that

$$\mathrm{e}^{\mathrm{i}\hat{H}^\varepsilon t/\varepsilon} \, \hat{\Pi}^\varepsilon \, \hat{A}^\varepsilon \, \hat{\Pi}^\varepsilon \, \mathrm{e}^{-\mathrm{i}\hat{H}^\varepsilon t/\varepsilon} = \mathrm{e}^{\mathrm{i}\hat{H}^\varepsilon t/\varepsilon} \, \hat{\Pi}^\varepsilon \, \mathrm{op}_\varepsilon\left(a^{(N)}\right) \, \hat{\Pi}^\varepsilon \, \mathrm{e}^{-\mathrm{i}\hat{H}^\varepsilon t/\varepsilon} + \mathcal{O}(\varepsilon^{N+1} \, \|A\|_{0,r_1}^\varepsilon) \, . \tag{5.19}$$

Moreover, combining (2.2), Corollary 3.4 and the estimate (3.27) there is a $r_2 \in \mathbb{N}_0$ such that

$$\begin{aligned} &\mathrm{e}^{\mathrm{i}\hat{H}^\varepsilon t/\varepsilon} \, \hat{\Pi}^\varepsilon \, \mathrm{op}_\varepsilon\left(a^{(N)}\right) \, \hat{\Pi}^\varepsilon \, \mathrm{e}^{-\mathrm{i}\hat{H}^\varepsilon t/\varepsilon} \\ &\quad = \hat{\Pi}^\varepsilon \mathrm{e}^{\mathrm{i}\hat{H}^\varepsilon t/\varepsilon} \, \mathrm{op}_\varepsilon\left(a^{(N)}\right) \, \mathrm{e}^{-\mathrm{i}\hat{H}^\varepsilon t/\varepsilon} \hat{\Pi}^\varepsilon + \mathcal{O}(\varepsilon^\infty \, \|A\|_{0,r_2}^\varepsilon \, |t|) \, . \end{aligned} \tag{5.20}$$

By a standard Duhamel argument and the fact that $a^N(0) = a$

$$
\begin{aligned}
&\hat{\Pi}^\varepsilon \left( \mathrm{e}^{\mathrm{i}\hat{H}^\varepsilon t/\varepsilon} \operatorname{op}_\varepsilon \left( a^{(N)} \right) \mathrm{e}^{-\mathrm{i}\hat{H}^\varepsilon t/\varepsilon} - \operatorname{op}_\varepsilon \left( a^N(t) \right) \right) \hat{\Pi}^\varepsilon \\
&\quad = \int_0^t \tfrac{\mathrm{d}}{\mathrm{d}s} \hat{\Pi}^\varepsilon \, \mathrm{e}^{\mathrm{i}\hat{H}^\varepsilon s/\varepsilon} \operatorname{op}_\varepsilon \left( a^N(t-s) \right) \mathrm{e}^{-\mathrm{i}\hat{H}^\varepsilon s/\varepsilon} \, \hat{\Pi}^\varepsilon \, \mathrm{d}s \\
&\quad = \int_0^t \mathrm{e}^{\mathrm{i}\hat{H}^\varepsilon s/\varepsilon} \, \hat{\Pi}^\varepsilon \, \tfrac{\mathrm{i}}{\varepsilon} \left[ \hat{H}^\varepsilon, \operatorname{op}_\varepsilon \left( a^N(t-s) \right) \right] \hat{\Pi}^\varepsilon \, \mathrm{e}^{-\mathrm{i}\hat{H}^\varepsilon s/\varepsilon} \\
&\qquad\quad - \mathrm{e}^{\mathrm{i}\hat{H}^\varepsilon s/\varepsilon} \, \hat{\Pi}^\varepsilon \operatorname{op}_\varepsilon \left( \tfrac{\mathrm{d}}{\mathrm{d}t} a^N(t-s) \right) \Big) \hat{\Pi}^\varepsilon \, \mathrm{e}^{-\mathrm{i}\hat{H}^\varepsilon s/\varepsilon} \, \mathrm{d}s \\
&\qquad + \mathcal{O}\Big( \varepsilon^\infty \, t^2 \sup_{s \in [0,t]} \left\| \operatorname{op}_\varepsilon \left( a^N(s) \right) \right\| \Big)
\end{aligned}
$$

where we applied Corollary 3.4 at the last equality. In addition, applying Calderon-Vaillancourt's theorem (2.2) and the estimate (5.17) to the previous result we get that there is a $r_3 \in \mathbb{N}_0$ such that

$$
\begin{aligned}
&\hat{\Pi}^\varepsilon \left( \mathrm{e}^{\mathrm{i}\hat{H}^\varepsilon t/\varepsilon} \operatorname{op}_\varepsilon \left( a^{(N)} \right) \mathrm{e}^{-\mathrm{i}\hat{H}^\varepsilon t/\varepsilon} - \operatorname{op}_\varepsilon \left( a^N(t) \right) \right) \hat{\Pi}^\varepsilon \\
&\quad = \int_0^t \mathrm{e}^{\mathrm{i}\hat{H}^\varepsilon s/\varepsilon} \, \hat{\Pi}^\varepsilon \, \tfrac{\mathrm{i}}{\varepsilon} \left[ \hat{H}^\varepsilon, \operatorname{op}_\varepsilon \left( a^N(t-s) \right) \right] \hat{\Pi}^\varepsilon \, \mathrm{e}^{-\mathrm{i}\hat{H}^\varepsilon s/\varepsilon} \\
&\qquad\quad - \mathrm{e}^{\mathrm{i}\hat{H}^\varepsilon s/\varepsilon} \, \hat{\Pi}^\varepsilon \operatorname{op}_\varepsilon \left( \tfrac{\mathrm{d}}{\mathrm{d}t} a^N(t-s) \right) \hat{\Pi}^\varepsilon \, \mathrm{e}^{-\mathrm{i}\hat{H}^\varepsilon s/\varepsilon} \, \mathrm{d}s \\
&\qquad + \mathcal{O}\Big( \varepsilon^\infty \, \|A\|^\varepsilon_{0,r_3} \sum_{j=2}^{N+3} |t|^j \Big) .
\end{aligned}
\tag{5.21}
$$

Now, note that $\frac{\mathrm{d}}{\mathrm{d}t} a^{(N)}(\Phi^t_\varepsilon) = X^\varepsilon_h \cdot \nabla a^{(N)}(\Phi^t_\varepsilon)$ as well as

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t} \mathfrak{A}^N_0(t) &= \frac{\mathrm{d}}{\mathrm{d}t} \int_0^t \mathfrak{A}^{c,N}_{h,\varepsilon} (a^{(N)}(\Phi^\tau_\varepsilon)) \circ \Phi^{t-\tau}_\varepsilon \, \mathrm{d}\tau \\
&= \mathfrak{A}^{c,N}_{h,\varepsilon} (a^{(N)}(\Phi^t_\varepsilon)) + X^\varepsilon_h \cdot \nabla \int_0^t \mathfrak{A}^{c,N}_{h,\varepsilon} (a^{(N)}(\Phi^\tau_\varepsilon)) \circ \Phi^{t-\tau}_\varepsilon \, \mathrm{d}\tau \\
&= \mathfrak{A}^{c,N}_{h,\varepsilon} h (a^{(N)}(\Phi^t_\varepsilon)) + X^\varepsilon_h \cdot \nabla \mathfrak{A}^N_0(t)
\end{aligned}
$$

and similarly

$$
\frac{\mathrm{d}}{\mathrm{d}t} \mathfrak{A}^N_{2j}(t) = \mathfrak{A}^{c,N}_{h,\varepsilon} (\mathfrak{A}^N_{2(j-1)}(t)) + X^\varepsilon_h \cdot \nabla \mathfrak{A}^N_{2j}(t) .
$$

Hence,

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t} a^N(t) = {} & X^\varepsilon_h \cdot \nabla a^{(N)}(\Phi^t_\varepsilon) + \varepsilon^2 \, \mathfrak{A}^{c,N}_{h,\varepsilon} (a^{(N)}(\Phi^t_\varepsilon)) \\
& + \sum_{j=0}^{\lfloor N/2 \rfloor} \varepsilon^{2(j+1)} \Big( X^\varepsilon_h \cdot \nabla \mathfrak{A}^N_{2j}(t) + \varepsilon^2 \, \mathfrak{A}^{c,N}_{h,\varepsilon} (\mathfrak{A}^N_{2j}(t)) \Big) .
\end{aligned}
\tag{5.22}
$$

At the same time, by Proposition 5.1 we have that

$$
\begin{aligned}
&\hat{\Pi}^{\varepsilon}\, \tfrac{\mathrm{i}}{\varepsilon} \Big[\, \hat{H}^{\varepsilon} , \mathrm{op}_{\varepsilon}\Big(a^N(t)\Big) \Big]\, \hat{\Pi}^{\varepsilon} \\
&\quad = \hat{\Pi}^{\varepsilon}\, \mathrm{op}_{\varepsilon}\Big( X_h^{\varepsilon} \cdot \nabla a^{(N)}(\Phi_{\varepsilon}^t) + \varepsilon^2\, \mathfrak{A}_{h,\varepsilon}^{c,N}(a^{(N)}(\Phi_{\varepsilon}^t)) \\
&\qquad + \sum_{j=0}^{\lfloor N/2 \rfloor} \varepsilon^{2(j+1)} \Big( X_h^{\varepsilon} \cdot \nabla \mathfrak{A}_{2j}^N(t) + \varepsilon^2\, \mathfrak{A}_{h,\varepsilon}^{c,N}(\mathfrak{A}_{2j}^N(t)) \Big) \Big)\, \hat{\Pi}^{\varepsilon} \\
&\qquad + \mathcal{O}(\varepsilon^{N+1} \| a^N(t) \|_{0,r_3}^{\varepsilon})
\end{aligned}
\tag{5.23}
$$

for some $r_3 \in \mathbb{N}_0$ large enough. Combining (5.22), (5.23) and the estimate (5.17) there exists a $r_4 \in \mathbb{N}_0$ such that

$$
\begin{aligned}
&\int_0^t \mathrm{e}^{\mathrm{i}\hat{H}^{\varepsilon} s/\varepsilon}\, \hat{\Pi}^{\varepsilon} \Big( \tfrac{\mathrm{i}}{\varepsilon} \Big[\, \hat{H}^{\varepsilon} , \mathrm{op}_{\varepsilon}\Big(a^N(t-s)\Big) \Big] - \mathrm{op}_{\varepsilon}\Big(\tfrac{\mathrm{d}}{\mathrm{d}t} a^N(t-s)\Big) \Big)\, \hat{\Pi}^{\varepsilon}\, \mathrm{e}^{-\mathrm{i}\hat{H}^{\varepsilon} s/\varepsilon}\, \mathrm{d}s \\
&\quad = \mathcal{O}\Big( \varepsilon^{N+1}\, \|A\|_{0,r_4}^{\varepsilon} \sum_{j=1}^{N+2} |t|^j \Big) .
\end{aligned}
\tag{5.24}
$$

Finally, combining (5.18)- (5.21) and (5.24) shows (5.15).

What is left is to show (5.16). By (5.3) one can easily see that

$$
\begin{aligned}
\mathfrak{A}_0^2(t) &= 2\,\mathrm{i} \int_0^t \Big\{ h_0 \,, a^{(2)}(\Phi_{\varepsilon}^{\tau}) \Big\}_3 \circ \Phi_{\varepsilon}^{t-\tau}\, \mathrm{d}\tau \\
&\quad - \tfrac{1}{2} \int_0^t \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\Big\{ \{h_0 \,, P_0\} \,, \Big\{ a^{(2)}(\Phi_{\varepsilon}^{\tau}) \,, P_0 \Big\} \Big\}) \circ \Phi_{\varepsilon}^{t-\tau}\, \mathrm{d}\tau + \mathcal{O}\Big( \varepsilon\, |t|\, \|A\|_{0.r}^{\varepsilon} \Big)
\end{aligned}
$$

for $r \in \mathbb{N}_0$ large enough. Then, applying (3.27) to the above equation finishes the proof. □

REMARK 5.3 Comparing the result of Theorem 5.2 to the result for semiclassical systems (1.1) one can see that including the second order in $\varepsilon$ the $\varepsilon$-dependent Hamiltonian system incorporates most additional terms of the semiclassical expansion. But there appears an additional quantum correction that one has to take into account, namely

$$
-\tfrac{1}{2} \int_0^t \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\{\{h_0 \,, P_0\} \,, \{a_0(\Phi_{\varepsilon}^{\tau}) \,, P_0\}\}) \circ \Phi_{\varepsilon}^{t-\tau}\, \mathrm{d}\tau \,.
$$

We expect that for higher orders the $\varepsilon$-dependent Hamiltonian system incorporates parts of the semiclassical expansion. In more detail, we expect that parts of $b_{h,\varepsilon}^{(N)}(a(\varepsilon))$ are canceled by subtracting $X_h^{\varepsilon} \cdot \nabla a(\varepsilon)$ and thus no additional error is produced defining $\mathfrak{A}_{h,\varepsilon}^{c,N}(a(\varepsilon))$ by (5.14). But this is not clear at this point.

To end this section we show how to apply our results to approximate the dynamics of quantum mechanical expectation values using Wigner functions. The expectation value of an observable $\hat{A}^\varepsilon$, $A \in S^0(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f}))$ with respect to a wave function $\psi \in \hat{\Pi}^\varepsilon \mathcal{H} = \hat{\Pi}^\varepsilon L^2(\mathbb{R}^n, \mathcal{H}_\mathrm{f})$ is given by

$$\langle \psi, \hat{A}^\varepsilon \psi \rangle_\mathcal{H} = \mathrm{tr}_\mathcal{H}(\hat{\rho}^\psi \, \hat{A}^\varepsilon) \,.$$

For $\psi \in \mathcal{H}$ the corresponding Wigner transform $W^\psi : \mathbb{R}^{2n} \to \mathcal{B}(\mathcal{H}_\mathrm{f})$ is defined by

$$W^\psi(q,p) = \tfrac{1}{(2\pi)^n} \int_{\mathbb{R}^n} \mathrm{e}^{\mathrm{i} p \cdot x} \psi(q - \tfrac{\varepsilon}{2} x) \otimes \psi^*(q + \tfrac{\varepsilon}{2} x) \, \mathrm{d}x \,.$$

A well known result for Wigner transforms is that the quantum expectation value with respect to a state $\hat{\rho}^\psi$ and an observable $\hat{A}^\varepsilon$ can be expressed as

$$\mathrm{tr}_\mathcal{H}(\hat{\rho}^\psi \, \hat{A}^\varepsilon) = \int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(W^\psi \, A)(z) \, \mathrm{d}z \,. \tag{5.25}$$

**Corollary 5.4** *Let the assumptions of Theorem 5.2 hold and assume the initial wave function $\psi_0$ to satisfy $\psi_0 \in \hat{\Pi}^\varepsilon \mathcal{H}$. Then, the quantum mechanical expectation value at time $t > 0$ with respect to the observable $\hat{A}^\varepsilon$ satisfies*

$$\mathrm{tr}_\mathcal{H}(\hat{\rho}^{\psi_t} \, \hat{A}^\varepsilon) = \int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(W^{\psi_0})(z) \, \Big( a(\Phi^t_\varepsilon) + \varepsilon^2 \, \mathfrak{A}^N(t) \Big)(z) \, \mathrm{d}z + \mathcal{O}(\varepsilon^{N+1})$$

*where* $\psi_t := \mathrm{e}^{-\mathrm{i} \hat{H}^\varepsilon t/\varepsilon} \, \psi_0$.

Proof By assumption, $\hat{\rho}^{\psi_t} = \mathrm{e}^{-\mathrm{i} \hat{H}^\varepsilon t/\varepsilon} \, \hat{\rho}^{\psi_0} \, \mathrm{e}^{\mathrm{i} \hat{H}^\varepsilon t/\varepsilon}$ and $\psi_0 = \hat{\Pi}^\varepsilon \psi_0$. Therefore,

$$\mathrm{tr}_\mathcal{H}(\hat{\rho}^{\psi_t} \, \hat{A}^\varepsilon) = \mathrm{tr}_\mathcal{H}(\mathrm{e}^{-\mathrm{i} \hat{H}^\varepsilon t/\varepsilon} \, \hat{\Pi}^\varepsilon \, \hat{\rho}^{\psi_0} \, \hat{\Pi}^\varepsilon \, \mathrm{e}^{\mathrm{i} \hat{H}^\varepsilon t/\varepsilon} \hat{A}^\varepsilon) = \mathrm{tr}_\mathcal{H}(\hat{\rho}^{\psi_0} \, \hat{\Pi}^\varepsilon \, \hat{A}^\varepsilon(t) \, \hat{\Pi}^\varepsilon) \,.$$

Then, Theorem 5.2 yields

$$\begin{aligned}
&\mathrm{tr}_\mathcal{H}(\hat{\rho}^{\psi_0} \, \hat{\Pi}^\varepsilon \, \hat{A}^\varepsilon(t) \, \hat{\Pi}^\varepsilon) \\
&\quad = \mathrm{tr}_\mathcal{H}\Big(\hat{\rho}^{\psi_0} \, \hat{\Pi}^\varepsilon \, \mathrm{op}_\varepsilon \Big(a(\Phi^t_\varepsilon) + \varepsilon^2 \, \mathfrak{A}^N(t)\Big) \, \hat{\Pi}^\varepsilon\Big) + \mathcal{O}(\varepsilon^{N+1}) \\
&\quad = \mathrm{tr}_\mathcal{H}\Big(\hat{\rho}^{\psi_0} \, \mathrm{op}_\varepsilon \Big(a(\Phi^t_\varepsilon) + \varepsilon^2 \, \mathfrak{A}^N(t)\Big) \Big) + \mathcal{O}(\varepsilon^{N+1}) \\
&\quad = \int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(W^{\psi_0})(z) \, \Big(a(\Phi^t_\varepsilon) + \varepsilon^2 \, \mathfrak{A}^N(t)\Big)(z) \, \mathrm{d}z + \mathcal{O}(\varepsilon^{N+1})
\end{aligned}$$

where in the last equality we applied (5.25) and used that $a(\Phi^t_\varepsilon) + \varepsilon^2 \, \mathfrak{A}^N(t)$ is scalar. □

## 5.2 How to get from Egorov's Theorem to a Numerical Scheme

In this section we explain a general scheme to derive numerical approximation schemes for the time evolution of quantum mechanical expectation values $\mathrm{tr}_{\mathcal{H}}(\hat\rho^{\psi_t}\,\hat A^{\varepsilon})$ with initial wave function $\psi_0 \in \hat\Pi^{\varepsilon}\mathcal{H}$. Hereto, we adopt the general scheme for the case of semiclassical operators developed in [LR10] that was extended to higher order approximations in [GL14]. The main idea is the following. By Corollary 5.4 we have

$$\mathrm{tr}_{\mathcal{H}}(\hat\rho^{\psi_t}\,\hat A^{\varepsilon}) = \int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(W^{\psi_0})(z)\,\Big(a(\Phi^t_\varepsilon) + \varepsilon^2\,\mathfrak{A}^N(t)\Big)(z)\,\mathrm{d}z + \mathcal{O}(\varepsilon^{N+1})\,.$$

Splitting the scalar Wigner function $\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(W^{\psi_0})(z)$ into its positive and negative part $\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(W^{\psi_0})(z) = w_+^{\psi_0}(z) - w_-^{\psi_0}(z)$ and sampling $w_+^{\psi_0}(z)$ and $w_-^{\psi_0}(z)$ by sufficiently many phase space points $z_1^{\pm},\dots,z_M^{\pm}\in\mathbb{R}^{2n}$ the expectation values $\mathrm{tr}_{\mathcal{H}}(\hat\rho^{\psi_t}\,\hat A^{\varepsilon})$ are approximated by

$$\begin{aligned}
\mathrm{tr}_{\mathcal{H}}(\hat\rho^{\psi_t}\,\hat A^{\varepsilon}) &= \int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(W^{\psi_0})(z)\,\Big(a(\Phi^t_\varepsilon) + \varepsilon^2\,\mathfrak{A}^N(t)\Big)(z)\,\mathrm{d}z + \mathcal{O}(\varepsilon^{N+1})\\
&\approx \frac{1}{M}\sum_{i=0}^{M}\Big(a(\Phi^t_\varepsilon) + \varepsilon^2\,\mathfrak{A}^N(t)\Big)(z_i^+) - \frac{1}{M}\sum_{i=0}^{M}\Big(a(\Phi^t_\varepsilon) + \varepsilon^2\,\mathfrak{A}^N(t)\Big)(z_i^-)\\
&=: I^M\Big(a(\Phi^t_\varepsilon) + \varepsilon^2\,\mathfrak{A}^N(t)\Big)\\
&= I^M(a(\Phi^t_\varepsilon)) + \sum_{j=0}^{\lfloor N/2\rfloor}\varepsilon^{2(j+1)}\,I^M(\mathfrak{A}^N_{2j}(t))\,.
\end{aligned} \tag{5.26}$$

where we used Corollary 5.4 in the first equality. Then, approximating the classical flow $\Phi^t_\varepsilon(z)$ by $\Psi^t(z)$ and $\mathfrak{A}^N_{2j}(t,z)$ by $\aleph^t_{2j}(z)$ for $j = 0,\dots,\lfloor N/2\rfloor$

$$\mathrm{tr}_{\mathcal{H}}(\hat\rho^{\psi_t}\,\hat A^{\varepsilon}) \approx I^M(a(\Psi^t)) + \sum_{j=0}^{\lfloor N/2\rfloor}\varepsilon^{2(j+1)}\,I^M(\aleph^t_{2j})\,. \tag{5.27}$$

Treating each summand in (5.27) independently has a big impact in the computational effort of the numerical scheme. Here, the prefactor $\varepsilon^j$ allows the descretization of the more complex higher order terms to be rather coarsely with the same overall accuracy. The computational work in the above procedure lies in the sampling of the scalar Wigner functions and the approximation of the classical flow $\Phi^t_\varepsilon(z)$ as well as of $\mathfrak{A}^N_{2j}(t,z)$ for each sampling point. In what follows we will focus on the latter where we will show a procedure with which one can derive systems of initial value problems whose respective flows give the corrections $\mathfrak{A}^N_{2j}(t)$ for any $N \in \mathbb{N}$ and $j = 0, \dots, \lfloor N/2 \rfloor$. Note that this is a generalization of [GL14] where quite similar IVPs for the second order correction in the special case of a scalar Hamiltonian $h(z)$ were derived.

To derive the IVPs we take the following steps. For fixed $N \in \mathbb{N}_0$ we reformulate the corrections $\mathfrak{A}^N_j(t)$ leading to

$$\sum_{j=0}^{\lfloor N/2 \rfloor} \varepsilon^{2(j+1)}\, \mathfrak{A}^N_{2j}(t,z) = \sum_{i=0}^{N} \varepsilon^j \sum_{k=0}^{l_j} \Gamma_{j,k}(t,z,D^{m_{j,k}} a \circ \Phi^t_\varepsilon(z)) \tag{5.28}$$

where

$$\Gamma_{j,k}(t,z) : \mathbb{R}^{\overbrace{2d \times \cdots \times 2d}^{m_{j,k} \text{ times}}} \to \mathbb{R}$$

are explicitly defined linear mappings from the space of $m_{j,k}$-tensors to the real numbers that are independent of $a$. Then we derive a first order system of initial value problems for the components of $\Gamma^{j,k}(t,z)$ such that the vectorization of this system can be written as

$$\frac{\partial}{\partial t}\vec{\Gamma}(t,z) = N(t,z)\,\vec{\Gamma}(t,z) + b(t,z), \qquad \vec{\Gamma}(0,z) = 0$$

where the components of the Matrix $N(t,z)$ and the vector $b(t,z)$ are given explicitly in terms of the classical Hamiltonian $h$, the symbol of the adiabatic projection $\pi$ as well as their derivatives, evaluated along the classical flow $\Phi^t_\varepsilon$.

We start by bringing the corrections into the form (5.28). By definition, $\mathfrak{A}^{c,N}_{h,\varepsilon}(a^{(N)})$ is the effective symbol of a function that consists only of Moyal products of $a$ with other functions (see (5.11) and (5.14)). Thus, similar to Lemma A.9 one can prove that $\mathfrak{A}^{c,N}_h(a^{(N)})$ can be reformulated as sum over terms of the form $\varepsilon^k B_{i_1,\dots,i_m} \partial^m_{i_1,\dots,i_m} a(\Phi^t_\varepsilon)$ with $B_{i_1,\dots,i_m} \in S^0(\varepsilon, \mathbb{C}), i_1, \dots, i_m = 1, \dots, 2n, m \in \mathbb{N}$. So $\mathfrak{A}^N_{2j}(t)$ can be expanded as a sum where each summand is of the form

$$\begin{aligned}\varepsilon^k \int_0^t \Bigg( & B^1_{i^1_1,\dots,i^1_{m_1}}\, \partial^{m_1}_{i^1_1,\dots,i^1_{m_1}} \int_0^{\tau_1} \Big( B^2_{i^2_1,\dots,i^2_{m_2}}\, \partial^{m_2}_{i^2_1,\dots,i^2_{m_2}} \\ & \cdots \int_0^{\tau_j} (B^{j+1}_{i^{j+1}_1,\dots,i^{j+1}_{m_{j+1}}}\, \partial^{m_{j+1}}_{i^{j+1}_1,\dots,i^{j+1}_{m_{j+1}}} a(\Phi^{\tau_{j+1}}_\varepsilon)) \circ \Phi^{\tau_j - \tau_{j+1}}_\varepsilon \, \mathrm{d}\tau_{j+1} \cdots \\ & \Big) \circ \Phi^{\tau_1-\tau_2}_\varepsilon \, \mathrm{d}\tau_2 \Bigg) \circ \Phi^{t-\tau_1}_\varepsilon \, \mathrm{d}\tau_1 \,. \end{aligned} \tag{5.29}$$

To obtain the desired form (5.28) the idea is to 'pull out' $a(\Phi_\varepsilon^{\tau_{j+1}})$ from the integrals using the chain rule together with the semi-group property of the Hamiltonian flow. This of course has to be done for every summand.

For a general term of the form (5.29) the procedure to 'pull out' the observable $a$ is very technical. Since the procedure is very similar for any term of the form (5.29) we will only show it for a special case $\{j = 0, m_1 = 2\}$, i.e.

$$\int_0^t (B_{i_1 i_2}\, \partial^2_{i_1 i_2}\, a(\Phi^\tau_\varepsilon)) \circ \Phi^{t-\tau}_\varepsilon \, \mathrm{d}\tau\,.$$

Applying the chain rule and the semi-group property of the Hamiltonian flow yields

$$\begin{aligned}
&\int_0^t (B_{i_1 i_2}\, \partial^2_{i_1 i_2}\, a(\Phi^\tau_\varepsilon)) \circ \Phi^{t-\tau}_\varepsilon \, \mathrm{d}\tau \\
&\quad = \int_0^t \Big(B_{i_1 i_2}\, \partial_{i_2} \Phi^\tau_{\varepsilon, j_2}\, \partial_{i_1} \Phi^\tau_{\varepsilon, j_1}\, \partial^2_{j_1 j_2 \nu} a \circ \Phi^\tau_\varepsilon\Big) \circ \Phi^{t-\tau}_\varepsilon \, \mathrm{d}\tau \\
&\qquad + \int_0^t \Big(B_{i_1 i_2}\, \partial_{i_1 i_2} \Phi^\tau_{\varepsilon, j}\, \partial_j a \circ \Phi^\tau_\varepsilon\Big) \circ \Phi^{t-\tau}_\varepsilon \, \mathrm{d}\tau && (5.30) \\
&\quad = \partial^2_{j_1 j_2} a \circ \Phi^t_\varepsilon \int_0^t \Big(B_{i_1 i_2}\, \partial_{i_2} \Phi^\tau_{\varepsilon, j_2}\, \partial_{i_1} \Phi^\tau_{\varepsilon, j_1}\Big) \circ \Phi^{t-\tau}_\varepsilon \, \mathrm{d}\tau \\
&\qquad + \partial_j a \circ \Phi^t_\varepsilon \int_0^t \Big(B_{i_1 i_2}\, \partial_{i_1 i_2} \Phi^\tau_{\varepsilon, j}\Big) \circ \Phi^{t-\tau}_\varepsilon \, \mathrm{d}\tau && (5.31) \\
&\quad =: \Gamma^1(t, z, \nabla^2 a \circ \Phi^t) + \Gamma^2(t, z, \nabla a \circ \Phi^t\,)\,.
\end{aligned}$$

With this one can easily see how one can reformulate $\mathfrak{A}^N(t)$ to obtain the desired form (5.28).

Next, we want to derive coupled systems of IVPs whose solutions are given by the coefficients of the tensors $\Gamma(t, z, \cdot)$. Similar to above, the general derivation of the IVPs is very technical so we want continue with the previous example and derive the IVPs that are solved by $\Gamma^1_{j_1, j_2}(t, z)$ and $\Gamma^2_j(t, z)$, respectively. Obviously, the initial value for $t = 0$ will be zero for all of the terms. So we want to compute the time derivative of $\Gamma^1_{j_1, j_2}(t, z)$ and $\Gamma^2_j(t, z)$. The idea here is to 'push' the time derivative through the integrals and end up with terms as

$$\int_0^t \Big(B_{i_1 i_2}\, \tfrac{\mathrm{d}}{\mathrm{d}\tau} \partial_{i_1 i_2} \Phi^\tau_j\Big) \circ \Phi^{t-\tau} \, \mathrm{d}\tau\,.$$

We will show this step in detail later. Then using the Hamiltonian equation

$$\frac{\mathrm{d}}{\mathrm{d}\tau} \Phi^\tau = \Big( -(\omega^\varepsilon)^{-1} \nabla h\Big) \circ \Phi^\tau_\varepsilon$$

yields

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}\tau}\partial_i\Phi_j^\tau &= -\,\partial_l\Big((\omega^\varepsilon)^{-1}\,\nabla h\Big)_j \circ \Phi_\varepsilon^\tau\,\partial_i\Phi_l^\tau \\
\frac{\mathrm{d}}{\mathrm{d}\tau}\partial_{i_1i_2}^2\Phi_j^\tau &= -\,\partial_{l_1l_2}^2\Big((\omega^\varepsilon)^{-1}\,\nabla h\Big)_j \circ \Phi^\tau\,\partial_{i_1}\Phi_{l_1}^\tau\,\partial_{i_2}\Phi_{l_2}^\tau \\
&\quad -\,\partial_l\Big((\omega^\varepsilon)^{-1}\,\nabla h\Big)_j \circ \Phi^\tau\,\partial_{i_1i_2}\Phi_l^\tau\,.
\end{aligned}$$

Therefore,

$$\begin{aligned}
&\int_0^t \Big(B_{i_1i_2}\,\tfrac{\mathrm{d}}{\mathrm{d}\tau}\partial_{i_1i_2}\Phi_j^\tau\Big)\circ\Phi^{t-\tau}\,\mathrm{d}\tau \\
&\qquad = -\int_0^t \Big(B_{i_1i_2}\,\partial_{l_1l_2}^2\Big((\omega^\varepsilon)^{-1}\,\nabla h\Big)_j \circ \Phi^\tau\,\partial_{i_1}\Phi_{l_1}^\tau\,\partial_{i_2}\Phi_{l_2}^\tau\Big)\circ\Phi^{t-\tau}\,\mathrm{d}\tau \\
&\qquad\quad -\int_0^t \Big(B_{i_1i_2}\,\partial_l\Big((\omega^\varepsilon)^{-1}\,\nabla h\Big)_j \circ \Phi^\tau\,\partial_{i_1i_2}\Phi_l^\tau\Big)\circ\Phi^{t-\tau}\,\mathrm{d}\tau
\end{aligned}$$

which coincides with (5.30), replacing $-(\omega^\varepsilon)^{-1}\,\nabla h$ by $a$. So, we again want to 'pull out' this term in front of the integrals leading to terms similar to (5.31). Doing the same thing for $\Gamma^1(t)$ would thus lead to a system IVPs of the form

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\Gamma^2(t) &= -\partial_{l_1l_2}^2\Big((\omega^\varepsilon)^{-1}\,\nabla h\Big)\circ\Phi^t\,\Gamma^1_{l_1l_2}(t) - \partial_{l_1}\Big((\omega^\varepsilon)^{-1}\,\nabla h\Big)\circ\Phi^t\,\Gamma^2_{l_1}(t) \\
\frac{\mathrm{d}}{\mathrm{d}t}\Gamma^1(t)_{j_1j_2} &= -\partial_l\Big((\omega^\varepsilon)^{-1}\,\nabla h\Big)_{j_1}\circ\Phi^t\,\Gamma^1_{lj_2}(t) - \partial_l\Big((\omega^\varepsilon)^{-1}\,\nabla h\Big)_{j_2}\circ\Phi^t\,\Gamma^1_{j_1l}(t)
\end{aligned}$$

It's easy to see that a similar procedure can be applied to every term of the form (5.29). This simply holds since pulling out $a(\Phi^t)$ or $(-(\omega^\varepsilon)^{-1}\,\nabla h)\circ\Phi^t$ just produce the same type of terms. Now, the only question left is how to push the time derivative into the integral. The following observation gives an answer, namely: for $b:\mathbb{R}^{2n}\to\mathbb{R}$ and $f:\mathbb{R}\times\mathbb{R}^{2n}\to\mathbb{R}$ smooth we have that

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_0^t (bf(\tau))\circ\Phi^{t-\tau}\,\mathrm{d}\tau = \int_0^t (b\frac{\mathrm{d}}{\mathrm{d}\tau}f(\tau))\circ\Phi^{t-\tau}\,\mathrm{d}\tau + (b\,f(0))\circ\Phi^t\,.$$

see [GL14, Lemma 2.2] for a proof.

Applying the above to $\Gamma^1(t)_{j_1 j_2}$ leads to

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\Gamma^1(t)_{j_1j_2} =& \frac{\mathrm{d}}{\mathrm{d}t}\int_0^t \Big( B_{i_1i_2}\,\partial_{i_2}\Phi^\tau_{j_2}\,\partial_{i_1}\Phi^\tau_{j_1}\Big)\circ\Phi^{t-\tau}\,\mathrm{d}\tau \\
=& \int_0^t \Big( B_{i_1i_2}\,\frac{\mathrm{d}}{\mathrm{d}\tau}(\partial_{i_2}\Phi^\tau_{j_2})\,\partial_{i_1}\Phi^\tau_{j_1}\Big)\circ\Phi^{t-\tau}\,\mathrm{d}\tau \\
&+ \int_0^t \Big( B_{i_1i_2}\,\partial_{i_2}\Phi^\tau_{j_2}\,\frac{\mathrm{d}}{\mathrm{d}\tau}(\partial_{i_1}\Phi^\tau_{j_1})\Big)\circ\Phi^{t-\tau}\,\mathrm{d}\tau \\
&+ \Big( B_{i_1i_2}\,\partial_{i_2}\Phi^0_{j_2}\,\partial_{i_1}\Phi^0_{j_1}\Big)\circ\Phi^t \\
=& \int_0^t \Big( B_{i_1i_2}\,\frac{\mathrm{d}}{\mathrm{d}\tau}(\partial_{i_2}\Phi^\tau_{j_2})\,\partial_{i_1}\Phi^\tau_{j_1}\Big)\circ\Phi^{t-\tau}\,\mathrm{d}\tau \\
&+ \int_0^t \Big( B_{i_1i_2}\,\partial_{i_2}\Phi^\tau_{j_2}\,\frac{\mathrm{d}}{\mathrm{d}\tau}(\partial_{i_1}\Phi^\tau_{j_1})\Big)\circ\Phi^{t-\tau}\,\mathrm{d}\tau \\
&+ \Big( B_{i_1i_2}\,\delta_{i_1j_1}\,\delta_{i_1j_1}\Big)\circ\Phi^t\,.
\end{aligned}$$

So, the procedure of 'pushing' the time derivative into the integral produces an additional term. In the above example this extra term is given by $\Big( B_{i_1i_2}\,\delta_{i_1j_1}\,\delta_{i_1j_1}\Big)\circ\Phi^t$. Notice that $\partial^m_{ij}\Phi^0 = 0$ for any $i,j\in\{1,\dots,2n\}$ and $m\geq 2$. Therefore, this additional term is non-zero only if all derivatives acting on $\Phi^t$ are of first order. It is easy to see that the above procedure can be applied to any term of the form (5.29). The only difference is that terms of lower order may be reproduced and thus need to be included in the system of IVPs.

REMARK 5.5 In certain situations it is useful to reformulate the assertion of Theorem 5.2 by neglecting the additional structure leading to the full $\varepsilon$-dependent classical System $(\mathbb{R}^{2n},\omega^\varepsilon,h)$ and base the result on $(\mathbb{R}^{2n},\omega^0,h)$. Using the Neumann series for $(\omega^\varepsilon)^{-1}$ (5.4) we define

$$(\omega^\varepsilon)^{-1} = (\omega^0)^{-1} - \omega^0\sum_{j=1}^\infty \varepsilon^j(\Omega^\varepsilon\,\omega^0)^j =: (\omega^0)^{-1} + \varepsilon\,\omega_{cor}\,.$$

Then, we can reformulate (5.1) leading to the assertion that there is a constant $C>0$ and a $r\in\mathbb{N}_0$ such that

$$\begin{aligned}
&\Big\|\,\hat{\Pi}^\varepsilon\,\Big(\tfrac{\mathrm{i}}{\varepsilon}\Big[\hat{H}^\varepsilon,\hat{a}^\varepsilon\Big] - \mathrm{op}_\varepsilon(X^0_{h_0}\cdot\nabla a) - \varepsilon\,\mathrm{op}_\varepsilon(\widetilde{\mathfrak{A}}^{c,N}_{h,\varepsilon}(a)\Big)\,\hat{\Pi}^\varepsilon\,\Big\| \\
&\quad\leq C\,\varepsilon^{N+1}\,\|a\|^\varepsilon_{0,r}
\end{aligned}$$

where $X^0_{h_0} = -(\omega^0)^{-1}\,\nabla h_0 = \omega^0\,\nabla h_0$ and

$$\widetilde{\mathfrak{A}}^{c,N}_{h,\varepsilon}(a) = -\langle\,\omega^\varepsilon\,\nabla(h-h_0)\,,\,\nabla a\,\rangle - \langle\,\omega^{(N)}_{cor}\,\nabla h\,,\,\nabla a\,\rangle + \varepsilon\,\mathfrak{A}^{c,N}_{h,\varepsilon}(a)\,.$$

Then, defining $\widetilde{\mathfrak{A}}^N(t) = \sum_{j=0}^N \varepsilon^j\, \widetilde{\mathfrak{A}}_j^N(t)$ with $\widetilde{\mathfrak{A}}_j^N(t) \in S^0(\varepsilon, \mathbb{R})$ by

$$\widetilde{\mathfrak{A}}_0^N(t) := \int_0^t \widetilde{\mathfrak{A}}_{h,\varepsilon}^{c,N}(a(\Phi_0^\tau)) \circ \Phi_0^{t-\tau}\, \mathrm{d}\tau$$

and

$$\widetilde{\mathfrak{A}}_j^N(t) := \int_0^t \widetilde{\mathfrak{A}}_{h,\varepsilon}^{c,N}(\widetilde{\mathfrak{A}}_{j-1}^N(\tau)) \circ \Phi_0^{t-\tau}\, \mathrm{d}\tau \quad \text{for } j \geq 1$$

one can proof analogously to the proof of Theorem 5.2 that for any $N \in \mathbb{N}_0$ and $t \in \mathbb{R}$ there exists a constant $C > 0$ and a $r \in \mathbb{N}_0$ such that

$$\left\| \hat{\Pi}^\varepsilon \left( \hat{A}^\varepsilon(t) - \mathrm{op}_\varepsilon \left( a(\Phi_0^t) + \varepsilon\, \widetilde{\mathfrak{A}}^N(t) \right) \right) \hat{\Pi}^\varepsilon \right\| \leq C\, \varepsilon^{N+1}\, \|A\|_{0,r}^\varepsilon \sum_{j=0}^{N+3} |t|^j\,.$$

At first sight it may seem that this formulation is less complex since the terms only depend on the Hamiltonian flow associated to the canonical symplectic form $\omega^0$ rather than $\omega^\varepsilon$ but $\widetilde{\mathfrak{A}}^N(t)$ contains many more terms than $\mathfrak{A}^N(t)$. Then, why is this formulation useful? Similar to (5.26), expectation values $\mathrm{tr}_{\mathcal{H}}(\hat{\rho}^{\psi_t}\, \hat{A}^\varepsilon)$ for an initial wave function $\psi_0 \in \hat{\Pi}^\varepsilon \mathcal{H}$ are approximated by

$$\begin{aligned}
\mathrm{tr}_{\mathcal{H}}(\hat{\rho}^{\psi_t}\, \hat{A}^\varepsilon) &= \int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(W^{\psi_0})(z) \left( a(\Phi_0^t) + \varepsilon\, \widetilde{\mathfrak{A}}^N(t) \right)(z)\, \mathrm{d}z + \mathcal{O}(\varepsilon^{N+1}) \\
&\approx \tfrac{1}{M} \sum_{i=0}^M \left( a(\Phi_0^t) + \varepsilon\, \widetilde{\mathfrak{A}}^N(t) \right)(z_i^+) - \tfrac{1}{M} \sum_{i=0}^M \left( a(\Phi_0^t) + \varepsilon\, \widetilde{\mathfrak{A}}^N(t) \right)(z_i^-) \\
&=: I^M(a(\Phi_0^t) + \varepsilon\, \widetilde{\mathfrak{A}}^N(t)) \\
&= I^M(a(\Phi_0^t)) + \sum_{j=0}^N \varepsilon^{j+1}\, I^M(\widetilde{\mathfrak{A}}_j^N(t))\,.
\end{aligned} \tag{5.32}$$

Now, assume $\varepsilon$ to be small, take $\varepsilon = 10^{-3}$ as an example. Then, the term $\varepsilon\, I^M(\widetilde{\mathfrak{A}}_0^N(t))$ can already be discretized rather coarsely given a fixed overall accuracy. Thus, the biggest computational effort lies in the approximation of the term $I^M(a(\Phi_0^t))$. On the other hand, if we base our numerical scheme on (5.26) then the biggest computational effort lies in the approximation of the term $I^M(a(\Phi_\varepsilon^t))$. Clearly, to be able to reach the same overall accuracy in both approaches one needs the same accuracy in the approximation of $I^M(a(\Phi_0^t))$ and $I^M(a(\Phi_\varepsilon^t))$. Now, the point is that there are several very effective numerical methods to approximate the Hamiltonian flow of classical Hamiltonian systems with canonical symplectic form $\omega^0$ and classical Hamiltonian of the form $h(q,p) = |p|^2 + V(q)$ as for example high order symplectic splitting methods, see e.g. [Yos90]. For the case of a $\varepsilon$-dependent symplectic form $\omega^\varepsilon$

there are in general no such effective integrators making the approximation of the Hamiltonian flow $\Phi_\varepsilon^t$ more costly and so for every sampling point $z_i^\pm$.

# 6 Application: The Hofstadter Model

In the following chapter we apply the theory developed in Chapters 2 - 5 to a gas of non-interacting fermionic particles in the tight binding approximation on the lattice $\mathbb{Z}^2$ subject to a strong constant magnetic field and an additional electro-magnetic field with slowly varying potentials. The main goal is to approximate the free energy per unit area of such a gas at inverse temperature $\beta$ and chemical potential $\mu$ up to errors of order $\varepsilon^3$ where here $\varepsilon$ represents the scale on which the potentials of the electro-magnetic field vary. From the free energy one can deduce many important physical properties of solids where we will focus on the magnetic susceptibility. In addition, we will derive an Egorov type theorem to approximate the quantum evolution of observables restricted to adiabatic subspace associated to magnetic Bloch bands. Last but not least we will apply the Egorov theorem to approximate the evolution of quantum mechanical expectation values for initial states that are in some, to a magnetic Bloch band associated, adiabatic subspace.

The single particle Hamiltonian is

$$H^{A^\varepsilon} = \sum_{|\alpha|=1} T_\alpha^{A^\varepsilon} + \phi^\varepsilon \tag{6.1}$$

acting as bounded self-adjoint operator on $\ell^2(\mathbb{Z}^2)$. The magnetic translations $T_\alpha^{A^\varepsilon}$ are defined by

$$(T_\alpha^{A^\varepsilon}\psi)_\beta = \mathrm{e}^{-\mathrm{i}\langle \alpha\,,\,A^\varepsilon(\beta)\rangle}\psi_{\beta-\alpha} \quad \text{for} \quad \psi \in \ell^2(\mathbb{Z}^2) \quad \text{and} \quad \alpha,\beta \in \mathbb{Z}^2\,.$$

Here, the magnetic vector potential $A^\varepsilon : \mathbb{R}^2 \to \mathbb{R}^2$ is given by

$$A^\varepsilon(r) = -\tfrac{1}{2}\mathbf{B}_0\, r + A(\varepsilon\, r) \qquad \text{where} \qquad A(r) = A_b(r) - \tfrac{1}{2}\mathbf{b}\, r$$

with $\mathbf{B}_0 = \left(\begin{smallmatrix} 0 & B_0 \\ -B_0 & 0 \end{smallmatrix}\right)$, $B_0 \in \mathbb{R}$, $\mathbf{b} = \left(\begin{smallmatrix} 0 & b \\ -b & 0 \end{smallmatrix}\right)$, $b \in \mathbb{R}$ and $A_b : \mathbb{R}^2 \to \mathbb{R}^2$ smooth and bounded together with all its derivatives. The electric potential $\phi^\varepsilon$ is a multiplication operator defined by

$$(\phi^\varepsilon\psi)_\beta = \phi(\varepsilon\beta)\psi_\beta \quad \text{for} \quad \psi \in \ell^2(\mathbb{Z}^2), \beta \in \mathbb{Z}^2 \quad \text{where} \quad \phi(r) = \phi_b(r) + \mathcal{E}\cdot r$$

with $\mathcal{E} \in \mathbb{R}^2$ and $\phi_b : \mathbb{R}^2 \to \mathbb{R}$ smooth and bounded with all its derivatives.

Clearly, our approach is not directly applicable here. Hence, we first transform the above system to a setup where our approach is applicable. To begin with, assume $A^\varepsilon = \phi^\varepsilon = 0$. Clearly, the translation operators $T_\alpha^{A^\varepsilon=0}$, $\alpha \in \mathbb{Z}^2$ commute and thus form a unitary representation of the group $\mathbb{Z}^2$. Moreover, the Hamiltonian $H^0 = \sum_{|\alpha|=1} T_\alpha^{A^\varepsilon=0}$ commutes with the translation operator $T_\alpha^{A^\varepsilon=0}$ for every $\alpha \in \mathbb{Z}^2$. Hence, $H^0$ is diagonalized by the Fourier transform

$$\mathcal{F} : \ell^2(\mathbb{Z}^2) \to L^2(\mathbb{R}^2 \,/\, (2\,\pi\,\mathbb{Z}^2)), \quad \psi \mapsto (\mathcal{F}\psi)(k) = \sum_{\gamma \in \mathbb{Z}^2} \mathrm{e}^{\mathrm{i}\langle k\,,\,\gamma\rangle} (T_\gamma^{A^\varepsilon=0}\psi)_0$$

where the Hamiltonian $H^0$ transforms to a multiplication operator with the function $e(k) = 2\,(\cos(k_1) + \cos(k_2))$. Next, we assume only $B_0$ to be zero. In this case, we have that $\mathcal{F}\,H^{A^\varepsilon, B_0=0}\,\mathcal{F}^* = e(k + A(\mathrm{i}\,\varepsilon\,\nabla_k^{\mathrm{per}})) + \phi(\mathrm{i}\,\varepsilon\,\nabla_k^{\mathrm{per}}) = h^0(\mathrm{i}\,\varepsilon\,\nabla_k^{\mathrm{per}}, k)$. Here, $\nabla_k^{\mathrm{per}}$ denotes the derivative with periodic boundary conditions. Note, that we cannot apply Weyl calculus here directly since $h^0(\mathrm{i}\,\varepsilon\,\nabla_k^{\mathrm{per}}, k)$ is an operator acting on $L^2(\mathbb{R}^2 \,/\, (2\,\pi\,\mathbb{Z}^2))$ rather than $L^2(\mathbb{R}^2)$. This problem can easily be solved by associating functions in $L^2(\mathbb{R}^2 \,/\, (2\,\pi\,\mathbb{Z}^2))$ with $2\,\pi$-periodic function in $L^2_{\mathrm{loc}}(\mathbb{R}^2)$ and restricting to $2\,\pi$-periodic symbols. We conclude that in the case where the strong magnetic field $B_0$ is zero the Fourier transform $\mathcal{F}$ transforms $(6.1)$ into a semiclassical system.

As a next step we consider particles subject to the strong magnetic field represented by $\mathbf{B}_0$ where $B_0$ is a rational multiple of $2\,\pi$, i.e. $A = 0$, $\phi = 0$ and $B_0 = 2\,\pi\,\frac{p}{q}$, $p \in \mathbb{Z}$, $q \in \mathbb{N}$. Then, the Hamiltonian is

$$H^{B_0} = \sum_{|\alpha|=1} T_\alpha^{B_0}$$

with magnetic translations

$$(T_\alpha^{B_0}\psi)_\beta = \mathrm{e}^{\frac{\mathrm{i}}{2}\langle \alpha\,,\,\mathbf{B}_0\,\beta\rangle}\psi_{\beta-\alpha} \quad \text{for } \psi \in \ell^2(\mathbb{Z}^2) \text{ and } \alpha, \beta \in \mathbb{Z}^2\,.$$

The associated dual magnetic translations are given as

$$(\bar{T}_\alpha^{B_0}\psi)_\beta = \mathrm{e}^{-\frac{\mathrm{i}}{2}\langle \alpha\,,\,\mathbf{B}_0\,\beta\rangle}\psi_{\beta-\alpha} \quad \text{for} \quad \alpha, \beta \in \mathbb{Z}^2\,.$$

Analogously to the case where $A^\varepsilon = \phi^\varepsilon = 0$ the Hamiltonian $H^{B_0}$ in invariant under dual magnetic translations. But $\bar{T}_{(1,0)}^{B_0}\,\bar{T}_{(0,1)}^{B_0} = \mathrm{e}^{\mathrm{i}\,B_0}\,\bar{T}_{(0,1)}^{B_0}\,\bar{T}_{(1,0)}^{B_0}$ so that the $\bar{T}_\alpha^{B_0}$s do not form a unitary representation of $\mathbb{Z}^2$. On the other hand, the dual magnetic translations can be extended to a unitary representation of the subgroup $\Gamma_q = \{\gamma \in \mathbb{Z}^2 : \gamma_1 \in q\,\mathbb{Z}\}$ of $\mathbb{Z}^2$ by

$$\widetilde{T}^{B_0}_{\gamma} := \left(\bar{T}^{B_0}_{(1,0)}\right)^{\gamma_1} \left(\bar{T}^{B_0}_{(0,1)}\right)^{\gamma_2} .$$

In addition, for $R_q := \{(m,0) : m \in \{1,\dots,q-1\}\}$ we represent the state space $\ell^2(\mathbb{Z}^2)$ as $\ell^2(\mathbb{Z}^2) \cong \ell^2(\Gamma_q \times R_q) \cong \ell^2(\Gamma_q) \otimes \ell^2(R_q) \cong \ell^2(\Gamma_q) \otimes \mathbb{C}^q$ and apply a Fourier transform to the first component, replacing the ordinary translations $T^{A^\varepsilon=0}_{\gamma}$ by the extended dual magnetic translations $\widetilde{T}^{B_0}_{\gamma}$. The resulting transformation is known as magnetic Bloch-Floquet transform, sometimes also referred to as Zak transform [Zak68]. For technical reasons we introduce an additional factor to the magnetic Bloch-Floquet transform leading to

$$\begin{aligned} \mathcal{U}^{B_0} &: \ell^2(\mathbb{Z}^2) \to L^2(M_q, \mathbb{C}^q), \\ &\psi \mapsto \mathrm{e}^{-\mathrm{i}k_1 m}((\mathcal{F}_{\mathrm{Magn}} \otimes \mathbf{1}_{\mathbb{C}^q})\,\psi)_m = \mathrm{e}^{-\mathrm{i}k_1 m} \sum_{\gamma\in\Gamma_q} \mathrm{e}^{\mathrm{i}\langle k\,,\gamma\rangle} (\widetilde{T}^{B_0}_{\gamma}\psi)_{(m,0)} \qquad (6.2) \\ &\qquad \text{for } m = 0,\dots,q-1 \end{aligned}$$

where $M_q := [0, 2\,\pi/q) \times [0, 2\,\pi)$ is the reduced Brillouin zone. From the definition of $\mathcal{U}^{B_0}$ (6.2) it is easy to see that for every $\gamma^*$ in the dual lattice $\Gamma^*_q := \{(\gamma^*_1, \gamma^*_2) \in \mathbb{R}^2 \,|\, \gamma^*_1 \in \frac{2\pi}{q}\,\mathbb{Z}, \gamma^*_2 \in 2\pi\,\mathbb{Z}\}$ we have

$$\begin{aligned} (\mathcal{U}^{B_0}\,\psi)(k+\gamma^*) &= \mathrm{diag}(1, \mathrm{e}^{-\mathrm{i}\gamma*}, \dots, \mathrm{e}^{-\mathrm{i}(q-1)\gamma*})(\mathcal{U}^{B_0}\,\psi)(k) \\ &=: \tau(\gamma^*)(\mathcal{U}^{B_0}\,\psi)(k) \,. \end{aligned}$$

Hereto, we say that a function $f : \mathbb{R}^2 \to \mathbb{C}^q$ is $\tau$-equivariant if

$$f(k+\gamma^*) = \tau(\gamma^*) f(k) := \mathrm{diag}(1, \mathrm{e}^{-\mathrm{i}\gamma*}, \dots, \mathrm{e}^{-\mathrm{i}(q-1)\gamma*}) f(k) \quad \text{for all } \gamma^* \in \Gamma^*_q \,.$$

It follows, that functions in the range of $\mathcal{U}^{B_0}$ can be extended to $\tau$-equivariant functions in $L^2_{\mathrm{loc}}(\mathbb{R}^2, \mathbb{C}^q)$. For general results on Floquet theory, see e.g. [Kuc82]. The magnetic Bloch-Floquet transform $\mathcal{U}^{B_0}\,H^{B_0}\,U^{B_0*}$ of the Hamiltonian $H^{B_0}$ acts on $L^2(M_q, \mathbb{C}^q)$ as matrix valued multiplication operator

$$H_0(k) = \begin{pmatrix} 2\cos(k_2) & \mathrm{e}^{-\mathrm{i}k_1} & 0 & \cdots & \mathrm{e}^{\mathrm{i}k_1} \\ \mathrm{e}^{\mathrm{i}k_1} & 2\cos(k_2+B_0) & \mathrm{e}^{-\mathrm{i}k_1} & \ddots & 0 \\ 0 & \mathrm{e}^{\mathrm{i}k_1} & 2\cos(k_2+2B_0) & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & & & & \mathrm{e}^{-\mathrm{i}k_1} \\ \mathrm{e}^{-\mathrm{i}k_1} & 0 & \cdots & \mathrm{e}^{\mathrm{i}k_1} & 2\cos(k_2+(q-1)B_0) \end{pmatrix} . \qquad (6.3)$$

For $q$ odd, $H_0$ has $q$ real-analytic isolated eigenvalues $e^{(1)}(k) < \ldots < e^{(q)}(k)$ where $e^{(m)}(M_q) \cap \{e^{(l)}(k)\} = \emptyset$ for $m \neq l$, $k \in M_q$. If $q$ is even, it is known that the two middle bands touch at $q$ points. Other than that the rest of the bands are real-analytic and isolated.

Finally we consider the full Hamiltonian $H^{A^\varepsilon}$, see (6.1). Analogously to the case where $B_0 = 0$, an application of the magnetic Bloch-Floquet transform to $H^{A^\varepsilon}$ yields

$$\hat{H}^\varepsilon = \mathcal{U}^{B_0} H^{A^\varepsilon} \mathcal{U}^{B_0 *} = H_0(k - A(\mathrm{i}\varepsilon\nabla_k^\tau)) + \phi(\mathrm{i}\varepsilon\nabla_k^\tau) \tag{6.4}$$

acting on $L^2(M_q, \mathbb{C}^q)$ where the matrix entries of $H_0(k - A(\mathrm{i}\varepsilon\nabla_k^\tau))$ are defined by the functional calculus for self-adjoint operators and $\partial_{k_j}^\tau$ denotes the derivative with $\tau$-equivariant boundary conditions. Also here, we cannot apply Weyl calculus directly since $\hat{H}^\varepsilon$ acts on $L^2(M_q, \mathbb{C}^q)$ and not $L^2(\mathbb{R}^2, \mathbb{C}^q)$. The overcome this problem we use the fact that $H_0(k)$ is $\tau$-equivariant, i.e.

$$H_0(k + \gamma^*) = \tau(\gamma^*)\, H_0(k)\, \tau(-\gamma^*) \quad \text{for every} \quad \gamma^* \in \Gamma^* \,.$$

It follows, that for any fixed $r \in \mathbb{R}^2$ the symbol

$$H(r, k) = H_0(k - A(r)) + \phi(r) \,.$$

is $\tau$-equivariant. Now, we identify $L^2(M_q, \mathbb{C}^q)$ with the space $L^2_\tau := \{f \in L^2_{\mathrm{loc}}(\mathbb{R}^2, \mathbb{C}^q) : f \text{ is } \tau\text{-equivariant}\}$ with norm $\|f\|_\tau^2 = \frac{q}{(2\pi)^2} \int_{M_q} |f(k)|^2 \mathrm{d}k$ and restrict to $\tau$-equivariant symbols. Then, $\hat{H}^\varepsilon$ can be reinterpreted as the Weyl quantization of $H(r, k)$ and all results of Chapters 2 - 5 hold with the same proofs, for details see [PST03a] or [Teu03, Appendix B].

## 6.1 The Classical Hamiltonian System

In what follows we will derive the classical Hamiltonian system $(T^*\mathbb{T}^2, \omega^\varepsilon, h)$ associated to $H(r, k)$ and an eigenvalue $e$ of $H$. Note here, in our notation $k$ denotes elements of the torus $\mathbb{T}^2$ and $r \in \mathbb{R}^2$. Nevertheless, since $r$ takes the part of $q$ as used in the previous chapters we will keep the ordering of the parameters as above for readability reasons. So, let $e^{(m)}$, $1 \leq m \leq q$ be an isolated eigenvalue of $H_0(k)$ with $P_0^{(m)}(k)$ the associated spectral projection. Then,

$$\tilde{e}^{(m)}(r, k) := e^{(m)}(k - A(r)) + \phi(r)$$

is an isolated eigenvalue of $H(r,k)$ with spectral projection

$$\tilde{P}_0^{(m)}(r,k) = P_0^{(m)}(k - A(r)) .$$

Throughout this chapter we will represented the magnetic field by the matrix

$$\mathbf{B}(r) = \nabla A(r) - (\nabla A)^T(r) = B(r)\, \mathrm{J}_2 \tag{6.5}$$

where

$$B(r) := \nabla \times A(r) = \partial_1 A_2(r) - \partial_2 A_1(r)$$

and

$$\mathrm{J}_2 := \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} .$$

In addition, we denote

$$v^\perp = \mathrm{J}_2\, v \quad \text{for any} \quad v \in \mathbb{R}^2$$

as well as

$$\nabla^\perp = \mathrm{J}_2\, \nabla \quad \text{and} \quad \nabla^{2\,\perp} = \mathrm{J}_2\, \nabla^2.$$

The classical system $(\tilde{h}, \tilde{\omega})$, Liouville measure $\lambda^\varepsilon$ and equations of motion associated to $H(r,k)$ with eigenvalue $\tilde{e}^{(m)}$ follow directly from Lemma B.7. Here, we will focus on the Hamiltonian system that results from a change of coordinates to kinetic momentum $\kappa = k - A(r)$.

By (B.60) the modified Berry curvature for the $m$-th band is given by

$$\Omega^{(m)}(r,\kappa) = \Omega_0^{(m)}(r,\kappa) + \varepsilon\, \Omega_1^{(m)}(r,\kappa). \tag{6.6}$$

Here,

$$\Omega_0^{(m)}(\kappa) = \mathfrak{Im}\, \mathrm{tr}_{\mathbb{C}^q}\Big(\nabla P_0^{(m)} \times \nabla P_0^{(m)}\, P_0^{(m)}\Big)(\kappa) ,$$

is the well known Berry curvature. The order $\varepsilon$ correction $\Omega_1^{(m)}(r,\kappa)$ to the Berry curvature satisfies

$$\Omega_1^{(m)}(r,\kappa) = \ \partial_\kappa \times \left(B(r)\, S^{(m)}(\kappa) + W^{(m)}(\kappa)\, \nabla\phi(r)\right)$$

with

$$S_j^{(m)}(\kappa) = -\mathfrak{Re}\, \mathrm{tr}_{\mathbb{C}^q}\Big(\nabla P_0^{(m)}(\kappa) \times \nabla(H_0 + e^{(m)})(\kappa) \\ (H_0 - e^{(m)})^{-1}(\kappa)\, \partial_j P_0^{(m)}(\kappa)\, P_0^{(m)}(\kappa)\Big) .$$

and

$$W_{ij}^{(m)}(\kappa) := 2\,\mathfrak{Re}\,\mathrm{tr}_{\mathbb{C}^q}\Big(\partial_i P_0^{(m)}\,(H_0 - e^{(m)})^{-1}\,\partial_j P_0^{(m)}\Big)(\kappa)\,.$$

As is easy to see, the leading order of the Fubini-Study metric $g_0^{(m)}$ satisfies

$$g_{0,ij}^{(m)}(\kappa) = 2\,\mathfrak{Re}\,\mathrm{tr}_{\mathbb{C}^q}\Big(\partial_i P_0^{(m)}\,\partial_j P_0^{(m)}\,P_0\Big)(\kappa)\,.$$

Moreover, by Lemma B.8 and a straight forward computations using (6.5) the classical Hamiltonian is

$$\begin{aligned}
h^{(m)}(r,\kappa) = {} & e^{(m)}(\kappa) + \phi(r) + \varepsilon\,B(r)\,\mathcal{M}^{(m)}(\kappa)\,\Big(1 + \tfrac{1}{2}\,\varepsilon\,B(r)\,\Omega_0^{(m)}(\kappa)\Big)\\
& + \varepsilon^2\Big(\,\tfrac{1}{2}\langle\,\mathcal{F}_{\mathrm{Lor}}^{(m)}(r,\kappa)\,,\,W^{(m)}(\kappa)\,\mathcal{F}_{\mathrm{Lor}}^{(m)}(r,\kappa)\,\rangle\\
& - B(r)^2\,\mathrm{tr}_{\mathbb{C}^q}\Big(\mathcal{M}_{op}^{(m)}(\kappa)\,(H_0 - e^{(m)})^{-1}(\kappa)\,\mathcal{M}_{op}^{*(m)}(\kappa)\,P_0^{(m)}(\kappa)\Big)\\
& + \tfrac{\mathrm{i}}{2}\,B(r)^2\,\mathrm{tr}_{\mathbb{C}^q}\Big(\nabla\mathcal{M}_{op}^{(m)}(\kappa)\times\nabla P_0^{(m)}(\kappa)\,P_0^{(m)}(\kappa)\Big)\\
& + \tfrac{\mathrm{i}}{2}\,\mathrm{tr}_{\mathbb{C}^q}\Big(\mathcal{M}_{op}^{(m)}(\kappa)\,\langle\,\nabla B(r)\,,\,\nabla P_0^{(m)}(\kappa)\,\rangle\,P_0^{(m)}(\kappa)\Big)\\
& + \tfrac{1}{8}\,B(r)^2\,\mathrm{tr}_{\mathbb{C}^q}\Big(\mathrm{Tr}_2(\,\nabla^{2\perp}P_0^{(m)}(\kappa)\,\nabla^{2\perp}(H_0 - e^{(m)})(\kappa)\,)\,P_0^{(m)}(\kappa)\Big)\\
& + \tfrac{1}{8}\,\mathrm{tr}_{\mathbb{C}^q}\Big(\mathrm{Tr}_2(\,\nabla^2 P_0^{(m)}(\kappa)\,(\nabla^2 A(r)\,\nabla^2(H_0 - e^{(m)})(\kappa))\,)\,P_0^{(m)}(\kappa)\Big)\\
& + \tfrac{1}{8}\,\mathrm{tr}_{\mathbb{C}^q}\Big(\mathrm{Tr}_2(\,(\nabla^2 A(r)\,\nabla^2 P_0^{(m)}(\kappa))\,\nabla^2(H_0 - e^{(m)})(\kappa)\,)\,P_0^{(m)}(\kappa)\Big)
\end{aligned} \tag{6.7}$$

with Lorentz force

$$\mathcal{F}_{\mathrm{Lor}}^{(m)}(r,\kappa) = -\nabla\phi(r) + \mathbf{B}(r)\,\nabla e^{(m)}(\kappa)\,,$$

effective magnetic moment

$$\mathcal{M}^{(m)}(\kappa) = \mathfrak{Im}\,\mathrm{tr}_{\mathbb{C}^q}\Big(\partial_1 P_0^{(m)}\,(H_0 - e^{(m)})\,\partial_2 P_0^{(m)}\Big)(\kappa)$$

as well as

$$\mathcal{M}_{op}^{(m)}(\kappa) = \tfrac{\mathrm{i}}{2}\,\nabla P_0^{(m)}(\kappa)\times\nabla(H_0 - e^{(m)})(\kappa)\,.$$

Then, the coefficient matrix defining the system's symplectic form is

$$\omega_{\mathrm{KM}}^{(m)}(r,\kappa) = \begin{pmatrix} -\mathbf{B}(r) & \mathbf{1}_2\\ -\mathbf{1}_2 & \varepsilon\,\mathbf{\Omega}^{(m)}(r,\kappa)\end{pmatrix} + \varepsilon^2\,\begin{pmatrix} 0 & \mathbf{L}^{(m)}(r,\kappa)\\ -(\mathbf{L}^{(m)})^T(r,\kappa) & 0\end{pmatrix} \tag{6.8}$$

where

$$\mathbf{L}_{ij}^{(m)}(r,\kappa) = \partial_{il}^2\phi(r)\,W_{lj}^{(m)}(\kappa) + \partial_i B(r)\,S_j^{(m)}(\kappa) \tag{6.9}$$

and

$$\mathbf{\Omega}^{(m)}(r,\kappa) = \Omega^{(m)}(r,\kappa)\,\mathrm{J}_2. \tag{6.10}$$

By the fact that

$$\mathbf{B}(r)\,\mathbf{\Omega}_0^{(m)}(\kappa) = B(r)\,\Omega_0^{(m)}(\kappa)\,\mathrm{J}_2\,\mathrm{J}_2 = -B(r)\,\Omega_0^{(m)}(\kappa)\,\mathbf{1}_2 \tag{6.11}$$

we have

$$\tfrac{1}{8}\,\varepsilon^2\,\mathrm{Tr}_2\Big(\mathbf{B}(r)\,\mathbf{\Omega}_0^{(m)}(\kappa)\Big)^2 - \tfrac{1}{4}\,\varepsilon^2\,\mathrm{Tr}_2\Big(\mathbf{B}(r)\,\mathbf{\Omega}_0^{(m)}(\kappa)\,\mathbf{B}(r)\,\mathbf{\Omega}_0^{(m)}(\kappa)\Big) = 0\,.$$

Hence, the Liouville measure of $\omega_{\mathrm{KM}}^{(m)}(r,\kappa)$ given by (B.61) simplifies to

$$\lambda_\varepsilon^{(m)} = \Big(\nu^{(m)}(r,\kappa) + \mathcal{O}(\varepsilon^3)\Big)\,\mathrm{d}r_1 \wedge \cdots \wedge \mathrm{d}\kappa_n \tag{6.12}$$

with

$$\nu^{(m)}(r,\kappa) = 1 + \varepsilon\,B(r)\,\Omega^{(m)}(\kappa) + \varepsilon^2\,\mathrm{Tr}_2\Big(\mathbf{L}^{(m)}(r,\kappa)\Big)\,.$$

In the next step we simplify the Hamiltonian equations (B.57). Combining (6.5),(6.10) and (6.11) we get

$$\begin{aligned}(\omega_{\mathrm{KM}}^{(m)})^{-1} =& \Big(1 - \varepsilon\,\Omega^{(m)}\,B + \varepsilon^2\,(\Omega^{(m)}\,B)^2\Big)\begin{pmatrix}\varepsilon\,\mathbf{\Omega}^{(m)} & -\mathbf{1}_2\\ \mathbf{1}_2 & -\mathbf{B}\end{pmatrix}\\ &+ \varepsilon^2\begin{pmatrix}0 & (\mathbf{L}^{(m)})^T\\ -\mathbf{L}^{(m)} & \mathbf{B}\,(\mathbf{L}^{(m)})^T + \mathbf{L}^{(m)}\,\mathbf{B}\end{pmatrix} + \mathcal{O}(\varepsilon^3)\,.\end{aligned} \tag{6.13}$$

On the other hand,

$$\begin{aligned}(\nu^{(m)})^{-1} =& \Big[1 - \Big(-\varepsilon\,B\,\Omega^{(m)} - \varepsilon^2\,\mathrm{Tr}_2(\mathbf{L}^{(m)})\Big)\Big]^{-1}\\ =& \sum_{j=0}^{\infty}\Big(-\varepsilon\,B\,\Omega^{(m)} - \varepsilon^2\,\mathrm{Tr}_2(\mathbf{L}^{(m)})\Big)^j\\ =& 1 - \varepsilon\,B\,\Omega^{(m)} - \varepsilon^2\,\mathrm{Tr}_2(\mathbf{L}^{(m)}) + \varepsilon^2\,(B\,\Omega^{(m)})^2 + \mathcal{O}(\varepsilon^3)\end{aligned}$$

for $\varepsilon$ small enough. Hence,

$$\begin{aligned}\frac{1}{\nu^{(m)}}\begin{pmatrix}\varepsilon\,\mathbf{\Omega}^{(m)} & -\mathbf{1}_2\\ \mathbf{1}_2 & -\mathbf{B}\end{pmatrix} =& \Big(1 - \varepsilon\,B\,\Omega^{(m)} + \varepsilon^2\,(B\,\Omega^{(m)})^2\Big)\begin{pmatrix}\varepsilon\,\mathbf{\Omega}^{(m)} & -\mathbf{1}_2\\ \mathbf{1}_2 & -\mathbf{B}\end{pmatrix}\\ &+ \varepsilon^2\begin{pmatrix}0 & \mathrm{Tr}_2(\mathbf{L}^{(m)})\,\mathbf{1}_2\\ -\mathrm{Tr}_2(\mathbf{L}^{(m)})\,\mathbf{1}_2 & B\,\mathrm{Tr}_2(\mathbf{L}^{(m)})\,\mathrm{J}_2\end{pmatrix} + \mathcal{O}(\varepsilon^3)\,.\end{aligned} \tag{6.14}$$

In addition,

$$\mathbf{L}^{(m)} - \mathrm{Tr}_2(\mathbf{L}^{(m)})\,\mathbf{1}_2 = \mathrm{J}_2\,\mathbf{L}^{(m)}\,\mathrm{J}_2$$

as well as

$$\mathrm{J}_2\,(\mathbf{L}^{(m)})^T + \mathbf{L}^{(m)}\,\mathrm{J}_2 - \mathrm{Tr}_2(\mathbf{L}^{(m)})\,\mathrm{J}_2 = 0\,.$$

Comparing (6.13) and (6.14) and making use of the two identities above we conclude that the Hamiltonian equation simplify to

$$\begin{aligned}\begin{pmatrix}\dot r\\ \dot\kappa\end{pmatrix} &= -\left(\omega^{(m)}_{\mathrm{KM}}\right)^{-1}\begin{pmatrix}\partial_r h^{(m)}\\ \partial_\kappa h^{(m)}\end{pmatrix}\\ &= \frac{1}{\nu^{(m)}}\left[\begin{pmatrix}-\varepsilon\,\boldsymbol{\Omega}^{(m)} & \mathbf{1}_2\\ -\mathbf{1}_2 & \mathbf{B}\end{pmatrix} + \varepsilon^2\begin{pmatrix}0 & -\mathrm{J}_2\,(\mathbf{L}^{(m)})^T\,\mathrm{J}_2\\ \mathrm{J}_2\,\mathbf{L}^{(m)}\,\mathrm{J}_2 & 0\end{pmatrix}\right]\begin{pmatrix}\partial_r h^{(m)}\\ \partial_\kappa h^{(m)}\end{pmatrix}.\end{aligned} \tag{6.15}$$

Note, for $A_b(r) = 0$ the magnetic field is constant with $\mathbf{B}(r) = \mathbf{b}$ and $\partial^2_{ij}A_l(r) = 0$. If the electric field $\phi$ is zero as well then the classical Hamiltonian system simplifies significantly. We get

$$\begin{aligned} h^{(m)}(\kappa) = {}& e^{(m)}(\kappa) + \varepsilon\, b\,\mathcal{M}^{(m)}(\kappa) + \tfrac{1}{2}\,(\varepsilon\, b)^2\,\mathcal{M}^{(m)}(\kappa)\,\Omega^{(m)}_0(\kappa)\\ & + (\varepsilon\, b)^2\Big(\tfrac{1}{2}\,\langle\,\nabla^\perp e^{(m)}\,,\,W^{(m)}\,\nabla^\perp e^{(m)}\,\rangle(\kappa)\\ & - \mathrm{tr}_{\mathbb{C}^q}\Big(\mathcal{M}^{(m)}_{op}\,(H_0 - e^{(m)})^{-1}\,\mathcal{M}^{*(m)}_{op}\,P^{(m)}_0\Big)(\kappa)\\ & + \tfrac{\mathrm{i}}{2}\,\mathrm{tr}_{\mathbb{C}^q}\Big(\nabla\mathcal{M}^{(m)}_{op}\times\nabla P^{(m)}_0\,P^{(m)}_0\Big)(\kappa)\\ & + \tfrac{1}{8}\,\mathrm{tr}_{\mathbb{C}^q}\Big(\mathrm{Tr}_2(\nabla^{2\,\perp}P^{(m)}_0\,\nabla^{2\,\perp}(H_0 - e^{(m)})\,)\,P^{(m)}_0\Big)(\kappa)\end{aligned} \tag{6.16}$$

with modified Berry curvature

$$\Omega^{(m)}(\kappa) = \Omega^{(m)}_0(\kappa) + \varepsilon\,\Omega^{(m)}_1(\kappa)$$

where

$$\Omega^{(m)}_1(\kappa) := b\,\nabla\times S^{(m)}(\kappa)$$

with

$$S^{(m)}_j(\kappa) = -\mathfrak{Re}\,\mathrm{tr}_{\mathbb{C}^q}\Big(\nabla P^{(m)}_0\times\nabla(H_0 + e^{(m)})\,(H_0 - e^{(m)})^{-1}\,\partial_j P^{(m)}_0\,P^{(m)}_0\Big)(\kappa)\,.$$

The symplectic form simplifies to

$$\omega^{(m)}_{\mathrm{KM}}(\kappa) = \begin{pmatrix}-\mathbf{b} & \mathbf{1}_2\\ -\mathbf{1}_2 & \varepsilon\,\boldsymbol{\Omega}^{(m)}(\kappa)\end{pmatrix}$$

which results in Hamiltonian equations

$$\begin{pmatrix} \dot{r} \\ \dot{\kappa} \end{pmatrix} = \frac{1}{\nu^{(m)}(\kappa)} \begin{pmatrix} -\varepsilon\, \mathbf{\Omega}^{(m)}(\kappa) & \mathbf{1}_2 \\ -\mathbf{1}_2 & \mathbf{b} \end{pmatrix} \begin{pmatrix} \partial_r h^{(m)}(\kappa) \\ \partial_\kappa h^{(m)}(\kappa) \end{pmatrix} .$$

The Liouville measure is

$$\lambda_\varepsilon^{(m)} = \left(\nu^{(m)}(\kappa) + \mathcal{O}(\varepsilon^3)\right) \mathrm{d}r_1 \wedge \cdots \wedge \mathrm{d}\kappa_n$$

with

$$\nu^{(m)}(\kappa) = 1 + \varepsilon\, b\, \Omega(\kappa) = 1 + \varepsilon\, b\, \Omega_0(\kappa) + \varepsilon^2\, b\, \Omega_1(\kappa)\,. \tag{6.17}$$

## 6.2 Equilibrium Expectations, Free Energy and the Magnetic Susceptibility

In this section we first derive the second order semiclassical approximation of thermodynamic equilibrium expectations. Clearly, our theory allows to extend the below result to semiclassical approximation of arbitrary order in $\varepsilon$. Nevertheless, within the context of Bloch electrons we will focus on second order approximations. We will then use the results on steady states to compute the free energy per unit area of a gas of Hofstadter electrons up to errors of order $\varepsilon^3$. This result will then lead us to an explicit formula for the magnetic susceptibility.

**Proposition 6.1** *Let $\varepsilon > 0$ small enough, $B_0 = 2\pi \frac{p}{q}$, $p \in \mathbb{Z}$, $q$ odd and $f \in \mathcal{A}$. In addition, let $\hat{R}$ be a self-adjoint operator acting on $\ell^2(\mathbb{Z}^2)$ such that $\hat{O}^\varepsilon = \mathcal{U}^{B_0}\, \hat{R}\, \mathcal{U}^{B_0 *}$ is a Weyl operator with $\tau$-equivariant symbol in $S^0(\mathcal{B}_{\mathrm{sa}}(\mathbb{C}^q))$. Then, the effective symbol $\tilde{o}^{(m)} \in S^0(\mathbb{R})$ of $O$ is $\tau$-equivariant and*

$$\begin{aligned} \mathrm{tr}_{\ell^2(\mathbb{Z}^2)}\big(\hat{R}\, f(H^{A^\varepsilon})\big) = & \frac{1}{(2\,\pi\,\varepsilon)^2} \sum_{m=1}^{q} \bigg( \int_{\mathbb{R}^2 \times M_q} o^{(m)}\, f^\varepsilon(h^{(m)}, \pi^{(m)})\, \lambda^{\varepsilon,(m)} \\ & \qquad + \int_{\mathbb{R}^2 \times M_q} o^{(m)}\, Q(h_0^{(m)}, g_0^{(m)})\, \mathrm{d}r\, \mathrm{d}\kappa \bigg) \\ & + \mathcal{O}(\varepsilon\, \|O\|_{L^1}) \end{aligned}$$

*where $M_q := [0, 2\,\pi/q) \times [0, 2\,\pi)$ is the reduced Brillouin zone. The second order effective symbol in kinetic momentum representation is $o^{(m)}(r,\kappa) := \sum_{i=0}^{2} \varepsilon^i\, \tilde{o}_i^{(m)}(r, \kappa + A(r))$. The classical Hamiltonian is given by (6.7) and $\lambda^{\varepsilon,(m)}$ is the Liouville measure (6.12) of the symplectic form $\omega_{\mathrm{KM}}^{(m)}(r,\kappa)$ (6.8). The* *effective equilibrium state $f^\varepsilon(h^{(m)},\pi^{(m)})$ is given by (B.67) and the quantum correction $Q(h_0^{(m)},g_0^{(m)})$ by (B.65).*

PROOF We begin with the following observation. The effective symbol $\tilde{o}^{(m)}$ of the observable $\hat{O}^\varepsilon$ depends only on $\tau$-equvariant symbols and their derivatives and is therefore $\tau$-equvariant as well.

By the unitarity of the Bloch-Floquet transform and (6.4)

$$\begin{aligned}\mathrm{tr}_{\ell^2(\mathbb{Z}^2)}\left(\hat{R}\,f(H^{A^\varepsilon})\right) &= \mathrm{tr}_{L^2(M_q,\mathbb{C}^q)}\left(\mathcal{U}^{B_0}\,\hat{R}\,\mathcal{U}^{B_0\,*}\,\mathcal{U}^{B_0}\,f(H^{A^\varepsilon})\,\mathcal{U}^{B_0\,*}\right)\\ &= \mathrm{tr}_{L^2(M_q,\mathbb{C}^q)}\left(\hat{O}^\varepsilon\,f(\hat{H}^\varepsilon)\right)\,.\end{aligned}$$

Since $q$ is odd we already know that all $q$ eigenbands $e^{(m)}$ of $H_0$ are non-degenerate, real-analytic and isolated. Hence,

$$\mathrm{tr}_{L^2(M_q,\mathbb{C}^q)}\left(\hat{O}^\varepsilon\,f(\hat{H}^\varepsilon)\right) = \sum_{m=1}^{q}\mathrm{tr}_{L^2(M_q,\mathbb{C}^q)}\left(\hat{O}^\varepsilon\,f(\hat{H}^\varepsilon)\,\hat{\Pi}^{\varepsilon(m)}\right)$$

where $\hat{\Pi}^{\varepsilon(m)}$ is the super-adiabatic projection associated to the $m$-th eigenband $e^{(m)}$ of $H_0(\kappa)$ as defined in Proposition 3.2. An application of Theorem 4.4 yields

$$\begin{aligned}\mathrm{tr}_{L^2(M_q,\mathbb{C}^q)}\left(\hat{O}^\varepsilon\,f(\hat{H}^\varepsilon)\,\hat{\Pi}^{\varepsilon(m)}\right) =& \tfrac{1}{(2\pi\varepsilon)^2}\sum_{m=1}^{q}\bigg(\int_{\mathbb{R}^2\times M_q}\tilde{o}^{(2),(m)}\,\tilde{f}^\varepsilon(\tilde{h}^{(m)},\tilde{\pi}^{(m)})\,\tilde{\lambda}^{\varepsilon,(m)}\\ &+\int_{\mathbb{R}^2\times M_q}\tilde{o}^{(2),(m)}\,\tilde{Q}(\tilde{h}_0^{(m)},\tilde{g}_0^{(m)})\,\mathrm{d}r\,\mathrm{d}k\bigg)\\ &+\mathcal{O}(\varepsilon\,\|O\|_{L^1})\end{aligned}$$

where $\tilde{Q}(\tilde{h}^{(m)},\tilde{g}_0^{(m)})(r,k)$ is given by (4.30) and

$$\tilde{f}^\varepsilon(\tilde{h}^{(m)},\tilde{\pi}^{(m)}) = f(\tilde{h}^{(m)}) + \varepsilon^2\,\tilde{f}^{\mathrm{sc}}(\tilde{h}^{(m)}) + \varepsilon^2\,\tilde{f}^{\mathrm{adi}}(\tilde{h}^{(m)},\tilde{\pi}^{(m)})$$

with $\tilde{f}^{\mathrm{sc}}(\tilde{h})$ and $\tilde{f}^{\mathrm{adi}}(\tilde{h},\tilde{\pi})$ given by (4.12) and (4.13), respectively. The classical Hamiltonian is $\tilde{h}^{(m)}(r,k) = h^{(m)}(k-A(r))$ where $h^{(m)}(\kappa)$ is given by (6.7). The Liouville measure $\tilde{\lambda}^{\varepsilon,(m)}$ is defined in (6.12).

Then, a change of coordinates to kinetic momentum $\kappa = k - A(r)$ and application of Lemma B.9 yields

$$\begin{aligned}&\int_{\mathbb{R}^2\times M_q}\tilde{o}^{(2),(m)}\,\tilde{f}^\varepsilon(\tilde{h}^{(m)},\tilde{\pi}^{(m)})\,\tilde{\lambda}^{\varepsilon,(m)} + \int_{\mathbb{R}^2\times M_q}\tilde{o}^{(2),(m)}\,\tilde{Q}(\tilde{h}_0^{(m)},\tilde{g}_0^{(m)})\,\mathrm{d}r\,\mathrm{d}k\\ &\quad= \int_{\mathbb{R}^2\times M_q}o^{(m)}\,f^\varepsilon(h^{(m)},\pi^{(m)})\,\lambda^{\varepsilon,(m)} + \int_{\mathbb{R}^2\times M_q}o^{(m)}\,Q(h_0^{(m)},g_0^{(m)})\,\mathrm{d}r\,\mathrm{d}\kappa\,.\end{aligned}$$

Combining the above results finishes the proof. □

Now we compute the free energy per unit area also known as pressure of a gas of non-interacting fermionic particles on the lattice $\mathbb{Z}^2$ at inverse temperature $\beta$ and chemical potential $\mu$ subject to a constant magnetic field.

**Proposition 6.2** *Let $q$ odd, $B_0 = 2\pi\frac{p}{q}$ and $A_b(r) = \phi(r) = 0$, i.e. $A^\varepsilon(r) = -\frac{1}{2}\begin{pmatrix} 0 & B^\varepsilon \\ -B^\varepsilon & 0 \end{pmatrix} r$ with $B^\varepsilon = B_0 + \varepsilon\, b$, $b \in \mathbb{R}$. In addition, let $\chi_j : \mathbb{R}^2 \to [0,1]$ be a sequence of smooth cutoff functions supported in $\Lambda_j := [-j,j]^2$ such that $\chi_j(z) = 1$ for all $z \in \Lambda_{j-1}$ where with an abuse of notation we define $|\Lambda_j| = \|\chi_j\|_{L^1}$. Then, for $\varepsilon > 0$ small enough, $\beta > 0$ and $\mu \in \mathbb{R}$, the limit*

$$p(B^\varepsilon,\beta,\mu) := \tfrac{1}{\beta}\lim_{j\to\infty}\frac{\varepsilon^2}{|\Lambda_j|}\mathrm{tr}_{\ell^2(\mathbb{Z}^2)}\left(\chi_j(\varepsilon x)\,\ln\left(1+\mathrm{e}^{-\beta(H^{A^\varepsilon}-\mu)}\right)\right)$$

*exists and it holds that*

$$p(B^\varepsilon,\beta,\mu) = -\tfrac{q}{(2\pi)^2}\sum_{m=1}^{q}\left(\int_{\mathbb{T}_q} F_{\beta,\mu}(h^{(m)}(\kappa))\,\nu^{(m)}(\kappa)\,\mathrm{d}\kappa - \varepsilon^2\int_{\mathbb{T}_q} Q^{(m)}_{\mathrm{pr}}(\kappa)\,\mathrm{d}\kappa\right) + \mathcal{O}(\varepsilon^3) \tag{6.18}$$

*where $\mathbb{T}_q$ is the torus $[0,\frac{2\pi}{q})^2$, $F_{\beta,\mu}(x) = -\beta^{-1}\ln\left(1+e^{-\beta(x-\mu)}\right)$ is the anti-derivative of the Fermi-Dirac distribution $f_{\beta,\mu}(x) = (1+\mathrm{e}^{\beta(x-\mu)})^{-1}$ and*

$$Q^{(m)}_{\mathrm{pr}} = b^2\, f'_{\beta,\mu}(e^{(m)})\left(\tfrac{1}{24}\det\left(\nabla^2 e^{(m)}\right) + \tfrac{1}{4}\,\|\nabla e^{(m)\perp}\|^2_{g_0^{(m)}}\right). \tag{6.19}$$

PROOF We begin our proof with the observation that

$$\mathcal{U}^{B_0}\,\chi_j(\varepsilon x)\,U^{B_0 *} = \chi_j(\mathrm{i}\varepsilon\nabla_k^\tau) = \mathrm{op}_\varepsilon\left(\chi_j(r)\right).$$

Then, applying Proposition 6.1 with observable $\hat{R} = \chi_j(\varepsilon x)$ and equilibrium distribution $f(x) = -F_{\beta,\mu}(x)$ yields

$$\begin{aligned}
&\frac{\varepsilon^2}{\beta\,|\Lambda_j|}\,\mathrm{tr}_{\ell^2(\mathbb{Z}^2)}\left(\chi_j(\varepsilon x)\,\ln\left(1+\mathrm{e}^{-\beta(H^{A^\varepsilon}-\mu)}\right)\right)\\
&\quad= \frac{1}{(2\,\pi)^2\,|\Lambda_j|}\sum_{m=1}^{q}\left(\int_{\mathbb{R}^2\times M_q}\chi_j(r)\,f^\varepsilon(h^{(m)},\pi^{(m)})(\kappa)\,\nu^{(m)}(\kappa)\,\mathrm{d}r\,\mathrm{d}\kappa\right.\\
&\qquad\left. + \varepsilon^2\int_{\mathbb{R}^2\times M_q}\chi_j(r)\,Q(h_0^{(m)},g_0^{(m)})(\kappa)\,\mathrm{d}r\,\mathrm{d}\kappa\right) + \mathcal{O}(\varepsilon^3)\\
&\quad= \frac{1}{(2\,\pi)^2}\sum_{m=1}^{q}\left(\int_{M_q} f^\varepsilon(h^{(m)},\pi^{(m)})(\kappa)\,\nu^{(m)}(\kappa)\,\mathrm{d}\kappa\right.\\
&\qquad\left. + \varepsilon^2\int_{M_q} Q(h_0^{(m)},g_0^{(m)})(\kappa)\,\mathrm{d}\kappa\right) + \mathcal{O}(\varepsilon^3).
\end{aligned} \tag{6.20}$$

where

$$Q(h_0^{(m)}, g_0^{(m)})(\kappa) = -\tfrac{1}{2}\mathrm{Tr}_2\Big(\partial_\kappa \mathcal{N}_1^{Q,(m)}(\kappa) + \tfrac{1}{2}\,\mathbf{b}\;\partial_\kappa \mathcal{N}_2^{Q,(m)}(\kappa)\Big)$$

and

$$\begin{aligned} f^\varepsilon(h^{(m)}, \pi^{(m)})(\kappa) = \; & - F_{\beta,\mu}(h^{(m)}(\kappa)) + \tfrac{1}{4}\,\varepsilon^2\, f'_{\beta,\mu}(e^{(m)}(\kappa))\, \|\mathbf{b}\nabla e^{(m)}\|^2_{g_0^{(m)}}(\kappa) \\ & - \tfrac{1}{48}\,\varepsilon^2\, f'_{\beta,\mu}(e^{(m)}(\kappa))\,\mathrm{Tr}_2(\mathbf{b}\,\nabla^2 e^{(m)}\,\mathbf{b}\,\nabla^2 e^{(m)})(\kappa) \\ & + \tfrac{1}{24}\,\varepsilon^2\,\mathrm{Tr}_2\Big(\partial_\kappa \mathcal{N}_1^{\mathrm{sc},(m)} + \tfrac{1}{2}\,\mathbf{b}\,\partial_\kappa \mathcal{N}_2^{\mathrm{sc},(m)}\Big)(\kappa) \\ & + \mathcal{O}(\varepsilon^3)\,. \end{aligned}$$

For the definition of $\mathcal{N}^Q$ and $\mathcal{N}^{\mathrm{sc},(m)}$ see (B.66) and (B.69), respectively.

Note, by the $\tau$-equivariance of $H_0$, the integrand in (6.20) is periodic with respect to $\Gamma_q^*$ in $\kappa$. Moreover, by the symmetry of the original problem it is even periodic with respect to $\frac{2\pi}{q}\,\mathbb{Z}^2$. Hence, we can restrict to an integration over the torus $\mathbb{T}_q$ resulting in a factor $q$. Moreover, we have

$$\mathrm{Tr}_2(\mathbf{b}\,\nabla^2 e^{(m)}\,\mathbf{b}\,\nabla^2 e^{(m)})(\kappa) = -2\,b^2\,\det(\nabla^2 e^{(m)})(\kappa) \tag{6.21}$$

In addition, by the fact that the torus $\mathbb{T}_q$ has no boundary and $\nu_\varepsilon^{(m)}(\kappa) = 1 + \mathcal{O}(\varepsilon)$ we have

$$\int_{\mathbb{T}_q} \mathrm{Tr}_2\Big(\partial_\kappa \mathcal{N}_1^{\mathrm{sc},(m)} + \tfrac{1}{2}\,\mathbf{b}\,\partial_\kappa \mathcal{N}_2^{\mathrm{sc},(m)}\Big)(\kappa)\,\nu^{(m)}(\kappa)\,\mathrm{d}\kappa = \mathcal{O}(\varepsilon) \tag{6.22}$$

as well as (6.23)

$$\int_{\mathbb{T}_q} \mathrm{Tr}_2\Big(\partial_\kappa \mathcal{N}_1^{Q,(m)}(\kappa) + \tfrac{1}{2}\,\mathbf{b}\,\partial_\kappa \mathcal{N}_2^{Q,(m)}(\kappa)\Big)(\kappa)\,\mathrm{d}\kappa = 0\,. \tag{6.24}$$

Hence, we conclude that

$$\begin{aligned} & \int_{M_q} f^\varepsilon(h_0^{(m)}, P_0^{(m)})(\kappa)\,\nu^{(m)}(\kappa)\,\mathrm{d}\kappa + \varepsilon^2 \int_{M_q} Q(h_0^{(m)}, g_0^{(m)})(\kappa)\,\mathrm{d}\kappa \\ & \quad = -q \int_{\mathbb{T}_q} F_{\beta,\mu}(h^{(m)}(\kappa))\,\nu^{(m)}(\kappa)\,\mathrm{d}\kappa + q\,\varepsilon^2 \int_{\mathbb{T}_q} Q_{\mathrm{pr}}^{(m)}(\kappa)\,\mathrm{d}\kappa + \mathcal{O}(\varepsilon^3)\,. \end{aligned} \tag{6.25}$$

Combining (6.20)-(6.25) finishes the proof. □

With the thermodynamic pressure in hand we are now able to compute many physically interesting quantities, where the magnetic susceptibility $\mathcal{S}(B^\varepsilon, \beta, \mu) = \partial^2_{B^\varepsilon} p(B^\varepsilon, \beta, \mu)$ is of our main interest.

**Corollary 6.3** *Let $q$ odd, $B_0 = 2\pi\frac{p}{q}$ and $A_b(r) = \phi(r) = 0$. Then for $0 < \beta < \infty$ and $\mu \in \mathbb{R}$ the magnetic susceptibility is*

$$\begin{aligned}
&\mathcal{S}(B_0, \beta, \mu) \\
&\quad = \partial^2_{B^\varepsilon} p\,(B_0, \beta, \mu) \\
&\quad = -\frac{q}{(2\pi)^2} \sum_{m=1}^{q} \int_{\mathbb{T}_q} f_{\beta,\mu}(e^{(m)}(\kappa)) \Big( 2\, S^{(m)} \times \nabla e^{(m)} + 3\, \mathcal{M}^{(m)}\, \Omega_0 \\
&\qquad\quad + \langle\, \nabla^{\perp} e^{(m)} \,,\, W^{(m)}\, \nabla^{\perp} e^{(m)} \,\rangle - 2\, \mathrm{tr}_{\mathbb{C}^q} \Big( \mathcal{M}^{(m)}_{op}\, (H_0 - e^{(m)})^{-1}\, \mathcal{M}^{*(m)}_{op}\, P_0^{(m)} \Big) \\
&\qquad\quad + \mathrm{i}\, \mathrm{tr}_{\mathbb{C}^q} \Big( \nabla \mathcal{M}^{(m)}_{op} \times \nabla P_0^{(m)}\, P_0^{(m)} \Big) \\
&\qquad\quad + \tfrac{1}{4}\, \mathrm{tr}_{\mathbb{C}^q} \Big( \mathrm{Tr}_2 ( \nabla^{2\,\perp} P_0^{(m)}\, \nabla^{2\,\perp} (H_0 - e^{(m)})\,)\, P_0^{(m)} \Big) \Big)(\kappa) \\
&\qquad + f'_{\beta,\mu}(e^{(m)}(\kappa)) \Big( (\mathcal{M}^{(m)})^2 - \tfrac{1}{12}\, \det \Big( \nabla^2 e^{(m)} \Big) - \tfrac{1}{2}\, \| \nabla e^{(m)\,\perp} \|^2_{g_0^{(m)}} \Big)(\kappa)\, \mathrm{d}\kappa\,.
\end{aligned}$$

*where $f_{\beta,\mu}(x)$ is the Fermi-Dirac distribution $(1 + \mathrm{e}^{\beta(x-\mu)})^{-1}$.*

PROOF We start with the following observations. Clearly we have

$$\partial^2_{B^\varepsilon} p\,(B_0, \beta, \mu) = b^{-2}\, \partial^2_\varepsilon p\,(B^\varepsilon, \beta, \mu) \Big|_{\varepsilon=0}\,.$$

Replacing $p\,(B^\varepsilon, \beta, \mu)$ by our result for the free energy (6.18) we obtain

$$\begin{aligned}
\mathcal{S}(B_0, \beta, \mu) &= \partial^2_{B^\varepsilon} p\,(B_0, \beta, \mu) \\
&= -\frac{q}{(2\pi\, b)^2} \sum_{m=1}^{q} \partial^2_\varepsilon \Big( \int_{\mathbb{T}_q} F_{\beta,\mu}(h^{(m)}(\kappa))\, \nu^{(m)}(\kappa)\, \mathrm{d}\kappa \\
&\qquad\qquad - \varepsilon^2 \int_{\mathbb{T}_q} Q^{(m)}_{\mathrm{pr}}(\kappa)\, \mathrm{d}\kappa + \mathcal{O}(\varepsilon^3) \Big) \Big|_{\varepsilon=0}
\end{aligned}$$

where

$$F_{\beta,\mu}(x) := -\beta^{-1} \ln \Big( 1 + e^{-\beta(x-\mu)} \Big)\,.$$

is the anti-derivative of the Fermi-Dirac distribution $f_{\beta,\mu}(x)$. Then, a simple computation shows

$$\begin{aligned}
\mathcal{S}(B_0, \beta, \mu) = -\frac{q}{(2\pi\, b)^2} \sum_{m=1}^{q} \int_{\mathbb{T}_q} &2\, F_{\beta,\mu}(e^{(m)}(\kappa))\, \nu_2^{(m)}(\kappa) \\
&+ 2\, f_{\beta,\mu}(e^{(m)}(\kappa))\, (h_1^{(m)}\, \nu_1^{(m)} + h_2^{(m)})(\kappa) \\
&+ f'_{\beta,\mu}(e^{(m)}(\kappa))\, (h_1^{(m)})^2(\kappa) - 2\, Q^{(m)}_{\mathrm{pr}}(\kappa)\, \mathrm{d}\kappa\,.
\end{aligned}$$

Replacing the density, the effective Hamiltonian and the quantum corrections to the pressure by the expressions (6.16), (6.17) and (6.19) leads to

$$
\begin{aligned}
&\mathcal{S}(B_0,\beta,\mu)\\
&\quad= -\frac{q}{(2\pi)^2}\sum_{m=1}^{q}\int_{\mathbb{T}_q} 2\,F_{\beta,\mu}(e^{(m)}(\kappa))\,\nabla\times S^{(m)}\\
&\qquad\quad f_{\beta,\mu}(e^{(m)}(\kappa))\Big(2\,S^{(m)}\times\nabla e^{(m)} + 3\,\mathcal{M}^{(m)}\,\Omega_0\\
&\qquad\quad + \langle\,\nabla^{\perp}e^{(m)}\,,\,W^{(m)}\,\nabla^{\perp}e^{(m)}\,\rangle - 2\,\mathrm{tr}_{\mathbb{C}^q}\Big(\mathcal{M}_{op}^{(m)}\,(H_0-e^{(m)})^{-1}\,\mathcal{M}_{op}^{*(m)}\,P_0^{(m)}\Big)\\
&\qquad\quad + \mathrm{i}\,\mathrm{tr}_{\mathbb{C}^q}\Big(\nabla\mathcal{M}_{op}^{(m)}\times\nabla P_0^{(m)}\,P_0^{(m)}\Big)\\
&\qquad\quad + \tfrac{1}{4}\,\mathrm{tr}_{\mathbb{C}^q}\Big(\mathrm{Tr}_2(\nabla^{2\,\perp}P_0^{(m)}\,\nabla^{2\,\perp}(H_0-e^{(m)})\,)\,P_0^{(m)}\Big)\Big)(\kappa)\\
&\qquad + f'_{\beta,\mu}(e^{(m)}(\kappa))\Big((\mathcal{M}^{(m)})^2 - \tfrac{1}{12}\,\det\Big(\nabla^2 e^{(m)}\Big) - \tfrac{1}{2}\,\|\nabla e^{(m)\,\perp}\|^2_{g_0^{(m)}}\Big)(\kappa)\,\mathrm{d}\kappa\,.
\end{aligned}
$$

By the divergence theorem and the fact that the torus $\mathbb{T}_q$ has no boundary we have

$$
\begin{aligned}
0 &= \int_{\mathbb{T}_q}\mathrm{div}(F_{\beta,\mu}(e^{(m)})\,\left(\begin{smallmatrix}0&1\\-1&0\end{smallmatrix}\right)S^{(m)})(\kappa)\,\mathrm{d}\kappa\\
&= \int_{\mathbb{T}_q} f_{\beta,\mu}(e^{(m)})(\kappa)\,\Big(\nabla e^{(m)}\times S^{(m)}\Big)(\kappa) + F_{\beta,\mu}(e^{(m)})(\kappa)\,\Big(\nabla\times S^{(m)}\Big)(\kappa)\,\mathrm{d}\kappa\,,
\end{aligned}
$$

which finishes the proof. □

# 6.3 An Egorov Type Theorem

To end this chapter on the Hofstadter Model we derive an Egorov type theorem to approximate the quantum evolution of observables restricted to adiabatic subspaces associated to magnetic Bloch bands. In the subsequent corollary we then apply the result to approximate the evolution of quantum mechanical expectation values for initial states that are in a magnetic Bloch band's associated adiabatic subspace.

**Proposition 6.4** *Let $\varepsilon > 0$ small enough, $A_b(r) = 0$, $B_0 = 2\pi\frac{p}{q}$, $p \in \mathbb{Z}$, $q \in \mathbb{N}$ and $m \in \{1,\dots,q\}$ for $q$ odd or $m \in \{1,\dots,q\}\setminus\{q/2, q/2+1\}$ for $q$ even. In addition, let $\hat{R}$ be a self-adjoint operator acting on $\ell^2(\mathbb{Z}^2)$ such that*

*$\hat{O}^{\varepsilon} = \mathcal{U}^{B_0}\,\hat{R}\,\mathcal{U}^{B_0*}$ is a Weyl operator with $\tau$-equivariant symbol in $S^0(\mathcal{B}_{\mathrm{sa}}(\mathbb{C}^q))$. Then, the effective symbol $\tilde{o}^{(m)} \in S^0(\mathbb{R})$ of $O$ is $\tau$-equivariant and*

$$\begin{aligned}
&\hat{\Pi}^{\varepsilon(m)}\,\mathcal{U}^{B_0}\,\mathrm{e}^{\mathrm{i}\,H^{A^\varepsilon}t/\varepsilon}\,\hat{R}\,\mathrm{e}^{-\mathrm{i}\,H^{A^\varepsilon}t/\varepsilon}\,U^{B_0*}\,\hat{\Pi}^{\varepsilon(m)} \\
&\quad = \hat{\Pi}^{\varepsilon(m)}\,\mathrm{op}_\varepsilon\Big(\Big(o^{(m)}(\Phi_t^{(m)}) + \varepsilon^2\,\mathfrak{A}^{(m)}(t)\Big)(r, k + \tfrac{1}{2}\,\mathbf{b}\,r)\Big)\,\hat{\Pi}^{\varepsilon(m)} \\
&\qquad + \mathcal{O}\Big(\varepsilon^{N+1}\,\|O\|^{\varepsilon}_{0,r}\,\sum_{j=0}^{5}|t|^j\Big)
\end{aligned}$$

*where the second order effective symbol in kinetic momentum representation is $o^{(m)}(r,\kappa) := \sum_{i=0}^{2}\varepsilon^i\,\tilde{o}_i^{(m)}(r, \kappa - \frac{1}{2}\,\mathbf{b}\,r)$ and the Hamiltonian flow $\Phi_t^{(m)}$ is the flow of the Hamiltonian system $(\omega_{\mathrm{KM}}^{(m)}, h^{(m)})$ (see Equations 6.7 and 6.8).*
*The second order quantum correction $\mathfrak{A}^{(m)}(t)$ satisfies*

$$\mathfrak{A}^{(m)}(t) := \int_0^t \mathfrak{A}^{c,(m)}\big(o^{(m)}(\Phi_\tau^{(m)})\big)\circ\Phi^{t-\tau}\,\mathrm{d}\tau \tag{6.26}$$

*where for $a \in S^0(\varepsilon, \mathbb{C})$*

$$\begin{aligned}
&\mathfrak{A}^{c,(m)}(a)(r,\kappa) \\
&\quad = -\tfrac{1}{2}\Big\langle \mathcal{M}^{\mathbf{b}}\,\nabla\mathcal{F}^{(m)}_{\mathrm{Lor},i}\,,\ \nabla\mathcal{D}^{\mathbf{b}}_j a\Big\rangle(r,\kappa)\,g_0^{(m),ij}(\kappa) \\
&\qquad - \tfrac{1}{4}\Big\langle \mathcal{D}^{\mathbf{b}}_i\mathcal{F}^{(m)}_{\mathrm{Lor},j}\,\mathcal{D}^{\mathbf{b}}a\,,\ \nabla g_0^{(m),ij}\Big\rangle(r,\kappa) \\
&\qquad + \tfrac{1}{4}\Big\langle \mathcal{D}^{\mathbf{b}}_i\mathcal{D}^{\mathbf{b}}_j a\,\mathcal{F}^{(m)}_{\mathrm{Lor}}\,,\ \nabla g_0^{(m),ij}\Big\rangle(r,\kappa) \\
&\qquad - \tfrac{1}{2}\,\mathrm{tr}_{\mathbb{C}^q}\Big(\Big\langle \nabla^2 P_0^{(m)}\,\mathbf{b}\,\nabla^2 P_0^{(m)}\,\mathcal{F}^{(m)}_{\mathrm{Lor}}\,,\ \mathcal{D}^{\mathbf{b}}a\Big\rangle\Big)(r,\kappa) \\
&\qquad + \tfrac{1}{12}\,\partial^3_{ijk}\phi(r)\,\partial^3_{\kappa_i\kappa_j\kappa_k}a(r,\kappa) \\
&\qquad - \tfrac{1}{12}\,\partial^3_{ijk}e^{(m)}(\kappa)\,\partial^3_{r_ir_jr_k}a(r,\kappa)
\end{aligned}$$

*with*

$$\mathcal{M}^{\mathbf{b}} := \begin{pmatrix} 0 & \mathbf{1}_n \\ -\mathbf{1}_n & \mathbf{b} \end{pmatrix}$$

*and $\mathcal{D}^{\mathbf{b}} = (\mathcal{D}^{\mathbf{b}}_i)_{i=1,\ldots,n} : S^0(\varepsilon,\mathbb{C}) \to S^0(\varepsilon,\mathbb{C}^n)$ is a differential operators defined by*

$$\mathcal{D}^{\mathbf{b}}a(r,\kappa) = \mathbf{b}\,\partial_\kappa a(r,\kappa) - \partial_r a(r,\kappa)$$

*for $a \in S^0(\varepsilon,\mathbb{C})$.*

REMARK 6.5 Note that the assumption $A_b(r) = 0$ in the above preposition is only technical and simplifies the computations for the explicit expressions. In addition, here we only present the result to errors of order $\varepsilon^3$. Clearly, our theory allows the derivation of an Egorov Type theorem to errors of arbitrary order in $\varepsilon$.

PROOF We begin with the following observation. The effective symbol $\tilde{o}^{(m)}$ of the observable $\hat{O}^\varepsilon$ depends only on $\tau$-equvariant symbols and their derivatives and is therefore $\tau$-equvariant as well.

Combining, the fact that the Bloch-Floquet transform $\mathcal{U}^{B_0}$ is unitary and (6.4) yields

$$\begin{aligned}
&\hat{\Pi}^{\varepsilon(m)} \mathcal{U}^{B_0} \, \mathrm{e}^{\mathrm{i}\, H^{A^\varepsilon} t/\varepsilon} \, \hat{R} \, \mathrm{e}^{-\mathrm{i}\, H^{A^\varepsilon} t/\varepsilon} \, U^{B_0 *} \, \hat{\Pi}^{\varepsilon(m)} \\
&\quad = \hat{\Pi}^{\varepsilon(m)} \mathcal{U}^{B_0} \, \mathrm{e}^{\mathrm{i}\, H^{A^\varepsilon} t/\varepsilon} \mathcal{U}^{B_0 *} \mathcal{U}^{B_0} \, \hat{R} \, \mathcal{U}^{B_0 *} \mathcal{U}^{B_0} \, \mathrm{e}^{-\mathrm{i}\, H^{A^\varepsilon} t/\varepsilon} \, U^{B_0 *} \, \hat{\Pi}^{\varepsilon(m)} \\
&\quad = \hat{\Pi}^{\varepsilon(m)} \, \mathrm{e}^{\mathrm{i}\, \hat{H}^\varepsilon t/\varepsilon} \, \hat{O}^\varepsilon \, \mathrm{e}^{-\mathrm{i}\, \hat{H}^\varepsilon t/\varepsilon} \, \hat{\Pi}^{\varepsilon(m)} \, .
\end{aligned}$$

By Theorem 5.2 and Lemma B.10 we have

$$\begin{aligned}
&\hat{\Pi}^{\varepsilon(m)} \, \mathrm{e}^{\mathrm{i}\, \hat{H}^\varepsilon t/\varepsilon} \, \hat{O}^\varepsilon \, \mathrm{e}^{-\mathrm{i}\, \hat{H}^\varepsilon t/\varepsilon} \, \hat{\Pi}^{\varepsilon(m)} \\
&\quad = \hat{\Pi}^{\varepsilon(m)} \, \mathrm{op}_\varepsilon \Big( \Big( o^{(m)}(\Phi^{(m)}_t) + \varepsilon^2 \, \mathfrak{A}^{(m)}(t) \Big)(r, k + \tfrac{1}{2} \, \mathbf{b} \, r) \Big) \, \hat{\Pi}^{\varepsilon(m)} \\
&\qquad + \mathcal{O}\Big( \varepsilon^{N+1} \, \| O \|^\varepsilon_{0,r} \, \sum_{j=0}^{5} |t|^j \Big)
\end{aligned}$$

with

$$\begin{aligned}
&\mathfrak{A}^{c,(m)}\big(o^{(m)}(\Phi^{(m)}_\tau)\big)(r,\kappa) \\
&\quad = -\tfrac{1}{2} \mathrm{tr}_{\mathbb{C}^q} \Big( \Big( \Big\langle \mathcal{M}^{\mathbf{b}} \, \nabla(\mathcal{D}^{\mathbf{b}}_i h^{(m)}_0) \, , \, \nabla(\mathcal{D}^{\mathbf{b}}_j o^{(m)}(\Phi^{(m)}_\tau)) \Big\rangle_{2n} \, \partial_{\kappa_i} P^{(m)}_0 \, \partial_{\kappa_j} P^{(m)}_0 \\
&\qquad + \Big\langle (\mathcal{D}^{\mathbf{b}})^2 h^{(m)}_0 \, \nabla P^{(m)}_0 \, , \, \nabla^2 P^{(m)}_0 \, \mathcal{D}^{\mathbf{b}} o^{(m)}(\Phi^{(m)}_\tau) \Big\rangle_n \\
&\qquad - \Big\langle \nabla^2 P^{(m)}_0 \, \mathcal{D}^{\mathbf{b}} h^{(m)}_0 \, , \, (\mathcal{D}^{\mathbf{b}})^2 o^{(m)}(\Phi^{(m)}_\tau) \, \nabla_\kappa P^{(m)}_0 \Big\rangle_n \\
&\qquad + \Big\langle \mathbf{b} \, \nabla^2 P^{(m)}_0 \, \mathcal{D}^{\mathbf{b}} h^{(m)}_0 \, , \, \nabla^2 P^{(m)}_0 \, \mathcal{D}^{\mathbf{b}} o^{(m)}(\Phi^{(m)}_\tau) \Big\rangle_n \Big)(r,\kappa) \\
&\qquad - \tfrac{1}{12} \, \mathcal{M}^{\mathbf{b}}_{\alpha_1\beta_1} \, \mathcal{M}^{\mathbf{b}}_{\alpha_2\beta_2} \, \mathcal{M}^{\mathbf{b}}_{\alpha_3\beta_3} \, \partial^3_{\beta_1\beta_2\beta_3} h^{(m)}_0(r,\kappa) \, \partial^3_{\alpha_1\alpha_2\alpha_3} o^{(m)}(\Phi^{(m)}_t)(r,\kappa) \, .
\end{aligned}$$

Then, by definition

$$\mathcal{D}^{\mathbf{b}} h^{(m)}_0 = \mathcal{F}^{(m)}_{\mathrm{Lor}}$$

as well as

$$\nabla^2_{r_i\kappa_j} h^{(m)}_0(r,\kappa) = 0, \qquad \nabla^3_{r_i r_j r_l} h^{(m)}_0(r,\kappa) = \partial^3_{ijl}\phi(r)$$

and

$$\nabla^3_{\kappa_i\kappa_j\kappa_l} h^{(m)}_0(r,\kappa) = \partial^3_{ijl} e^{(m)}(\kappa) \, .$$

We finish the proof using

$$\mathrm{tr}_{\mathbb{C}^q}\Big( \partial_i P^{(m)}_0 \, \partial_j P^{(m)}_0 \Big)(\kappa) = g^{(m),ij}_0(\kappa)$$

and that for any symmetric matrix $M \in \mathbb{C}^{n\times n}$ and vector $c \in \mathbb{C}^n$ we have

$$\begin{aligned}\Big\langle M_{ij}\, c\,,\, \nabla g_0^{(m),ij} \Big\rangle_n &= M_{ij}\, c_l\, \partial_l \operatorname{tr}_{\mathbb{C}^q}\Big(\partial_i P_0^{(m)}\, \partial_j P_0^{(m)}\Big)\\ &= M_{ij}\, c_l\, \Big(\operatorname{tr}_{\mathbb{C}^q}\Big(\partial^2_{il} P_0^{(m)}\, \partial_j P_0^{(m)}\Big) + \operatorname{tr}_{\mathbb{C}^q}\Big(\partial_i P_0^{(m)}\, \partial^2_{jl} P_0^{(m)}\Big)\Big)\\ &= 2\, M_{ij}\, c_l \operatorname{tr}_{\mathbb{C}^q}\Big(\partial^2_{il} P_0^{(m)}\, \partial_j P_0^{(m)}\Big)\\ &= 2 \operatorname{tr}_{\mathbb{C}^q}\Big(\Big\langle \nabla^2 P_0^{(m)}\, c\,,\, M\, \nabla P_0^{(m)} \Big\rangle\Big)\\ &= 2 \operatorname{tr}_{\mathbb{C}^q}\Big(\Big\langle M\, \nabla P_0^{(m)}\,,\, \nabla^2 P_0^{(m)}\, c \Big\rangle\Big)\,.\end{aligned}$$

□

**Corollary 6.6** *Let the assumptions of Proposition 6.4 hold. In addition, assume* $\rho_t := |\psi_t\rangle\langle\psi_t|$ *with* $\psi_t = \mathrm{e}^{-\mathrm{i}\, H^{A^\varepsilon} t/\varepsilon}\, \psi_0$ *where the initial state* $\psi_0 \in \ell^2(\mathbb{Z}^2)$ *satisfies* $\mathcal{U}^{B_0}\, \psi_0 = \widetilde{\psi}_0 \in \hat{\Pi}^{\varepsilon(m)} L^2(M_q, \mathbb{C}^q)$*. Then,*

$$\operatorname{tr}_{\ell^2(\mathbb{Z}^2)}\Big(\rho_t\, \hat{R}\Big) = \operatorname{tr}_{L^2(M_q,\mathbb{C}^q)}\Big(\widetilde{\rho}_0\, \operatorname{op}_\varepsilon\Big(\Big(o^{(m)}(\Phi_t^{(m)}) + \varepsilon^2\, \mathfrak{A}^{(m)}(t)\Big)(r, k + \tfrac{1}{2}\, \mathbf{b}\, r)\Big)\Big) + \mathcal{O}(\varepsilon^3)$$

*where* $\widetilde{\rho}_0 = |\widetilde{\psi}_0\rangle\langle\widetilde{\psi}_0|$.

Proof By definition

$$\begin{aligned}\operatorname{tr}_{\ell^2(\mathbb{Z}^2)}\Big(\rho_t\, \hat{R}\Big) &= \operatorname{tr}_{\ell^2(\mathbb{Z}^2)}\Big(\mathrm{e}^{-\mathrm{i}\, H^{A^\varepsilon} t/\varepsilon}\, \rho_0\, \mathrm{e}^{\mathrm{i}\, H^{A^\varepsilon} t/\varepsilon}\, \hat{R}\Big)\\ &= \operatorname{tr}_{\ell^2(\mathbb{Z}^2)}\Big(\mathrm{e}^{-\mathrm{i}\, H^{A^\varepsilon} t/\varepsilon}\, U^{B_0 *}\, \hat{\Pi}^{\varepsilon(m)}\, \widetilde{\rho}_0\, \hat{\Pi}^{\varepsilon(m)}\, \mathcal{U}^{B_0}\, \mathrm{e}^{\mathrm{i}\, H^{A^\varepsilon} t/\varepsilon}\, \hat{R}\Big)\,.\end{aligned}$$

By the unitarity of the Bloch-Floquet transform together with the cyclicity of the trace we have

$$\begin{aligned}&\operatorname{tr}_{\ell^2(\mathbb{Z}^2)}\Big(\mathrm{e}^{-\mathrm{i}\, H^{A^\varepsilon} t/\varepsilon}\, U^{B_0 *}\, \hat{\Pi}^{\varepsilon(m)}\, \widetilde{\rho}_0\, \hat{\Pi}^{\varepsilon(m)}\, \mathcal{U}^{B_0}\, \mathrm{e}^{\mathrm{i}\, H^{A^\varepsilon} t/\varepsilon}\, \hat{R}\Big)\\ &\quad = \operatorname{tr}_{L^2(M_q,\mathbb{C}^q)}\Big(\widetilde{\rho}_0\, \hat{\Pi}^{\varepsilon(m)}\, \mathcal{U}^{B_0}\, \mathrm{e}^{\mathrm{i}\, H^{A^\varepsilon} t/\varepsilon}\, \hat{R}\, \mathrm{e}^{-\mathrm{i}\, H^{A^\varepsilon} t/\varepsilon}\, U^{B_0 *}\, \hat{\Pi}^{\varepsilon(m)}\Big)\end{aligned}$$

Then, applying Proposition 6.4 finishes the proof. □

# 7 Application: Born-Oppenheimer Type Hamiltonian

In this section we aim to apply the theory developed in Chapter 2 - 5 to the paradigmatic system of adiabatic perturbation theory, namely to Born-Oppenheimer type Hamiltonians. Hereto, we consider the Hamiltonian operator

$$\hat{H}^{\varepsilon} = \tfrac{\varepsilon^2}{2}(-\mathrm{i}\,\nabla_x - A(x))^2 + V(x)$$

acting on $\mathcal{H} = L^2(\mathbb{R}^n) \otimes \mathcal{H}_{\mathrm{f}}$ for $\mathcal{H}_{\mathrm{f}}$ some separable Hilbert space. The magnetic vector potential $A : \mathbb{R}^n \to \mathbb{R}^n$ is assumed to be smooth and bounded and $V(x) \in S_0(\mathbb{R}^n, \mathcal{B}_{\mathrm{sa}}(\mathcal{H}_{\mathrm{f}}))$. In addition, we assume $V(x)$ to have a non-degenerate eigenvalue $e_v(x)$ with eigenprojection $P_0(q)$ such that $e_v : \mathbb{R}^n \to \mathbb{R}$ is continuous and satisfies the uniform gap condition

$$\mathrm{dist}(e_v(x), \sigma(V(x))\backslash\{e_v(x)\}) \geq g > 0 \tag{7.1}$$

for every $x \in \mathbb{R}^n$. Since $-\mathrm{i}\,\nabla_x$ is infinitesimally operator bounded with respect to $\Delta_x$, the operator $\frac{\varepsilon^2}{2}(-\mathrm{i}\,\nabla_x - A(x))^2$ is self-adjoint on the Sobolev space $H^2(\mathbb{R}^n)$. Hence, $\hat{H}^{\varepsilon}$ is self-adjoint on $H^2(\mathbb{R}^n) \otimes \mathcal{H}_{\mathrm{f}}$. The Born-Oppenheimer type Hamiltonian $\hat{H}^{\varepsilon}$ can be represented as Weyl-operator with symbol

$$H(q,p) = \tfrac{1}{2}\,|p - \varepsilon\,A(q)|^2\,\mathbf{1}_{\mathcal{H}_f} + V(q), \qquad \text{for} \quad (q,p) = z \in \mathbb{R}^{2n} \tag{7.2}$$

satisfying the gap condition Assumption 2.11 with eigenvalue

$$e(q,p) = \tfrac{1}{2}\,|p - \varepsilon\,A(q)|^2 + e_v(q)$$

and eigenprojection $P_0(q)$. Nevertheless, the Weyl symbol $H(q,p)$ is unbounded in $p$ and so does not fulfill Assumption 2.10. This prevents us from applying our results to $\hat{H}^{\varepsilon}$ directly. Therefore, we introduce the Hamiltonian

$H_\lambda(q,p)$ by replacing $|p - \varepsilon\, A(q)|^2$ by a function that flattens at large kinetic momentum $|p - \varepsilon\, A(q)|$ depending on a parameter $\lambda$, i.e.

$$H_\lambda := \tfrac{1}{2}\, \chi_\lambda\Big(|\, p - \varepsilon\, A(q)\, |^2\Big) + V(q)$$

where $\chi_\lambda : \mathbb{R} \to \mathbb{R}$ is a smooth and monotonically non-decreasing function satisfying that $\chi_\lambda(x) = x$ for $x \le \lambda$ and $\chi_\lambda(x)$ is constant for $x \ge \lambda + 1$. Clearly, $\hat{H}^\varepsilon_\lambda$ satisfies Assumption 2.10 and 2.11 with eigenvalue

$$e_\lambda(q,p) := \tfrac{1}{2}\, \chi_\lambda\Big(|\, p - \varepsilon\, A(q)\, |^2\Big) + e_v(q)$$

and eigenprojection $P_0(q)$.

## 7.1 The Classical Hamiltonian System

We start with the derivation of the Hamiltonian system $(h^\lambda, \omega^\varepsilon_\lambda)$ associated to $H_\lambda$ with eigenvalue $e_\lambda$. By (B.25) the associated classical Hamiltonian is

$$\begin{aligned} h^\lambda(q,p) = \tfrac{1}{2}\, \chi_\lambda(|p - \varepsilon\, A(q)|^2) + e_v(q) \\ + \tfrac{1}{2}\, \varepsilon^2\, \chi'_\lambda(|p - \varepsilon\, A(q)|^2)^2\, \|p - \varepsilon\, A(q)\|^2_{W(q)} + \mathcal{O}(\varepsilon^3) \end{aligned} \tag{7.3}$$

with

$$W_{ij}(q) := \mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big(\big[\, \partial_i P_0\, |\, (V - e_v)^{-1}\, |\, \partial_j P_0\, \big]_+\Big)(q)\,.$$

Note here, the second order correction to the classical Hamiltonian can be reformulated to

$$\begin{aligned} \tfrac{1}{2}\, \|\kappa\|^2_{W(q)} &= \tfrac{1}{2}\, \kappa_i\, \mathrm{tr}_{\mathcal{H}_\mathrm{f}}([\, \partial_i P_0\, |\, (V - e_v)^{-1}\, |\, \partial_j P_0\, ]_+)(q)\, \kappa_j \\ &= \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\langle \kappa\, ,\, \nabla P_0(q)\rangle\, (V(q) - e_v(q))^{-1}\, \langle \nabla P_0(q)\, ,\, \kappa\rangle)\,. \end{aligned}$$

By (B.26) the coefficients of the symplectic form are

$$\begin{aligned} \omega^\varepsilon_\lambda(q,p) = \omega^0 + \varepsilon\, \mathbf{\Omega}_0(q) + \varepsilon^2\, \chi'_\lambda(|p - \varepsilon\, A(q)|^2)\, \mathbf{\Omega}_1(q,p) \\ + \varepsilon^2\, \chi''_\lambda(|p - \varepsilon\, A(q)|^2)\, \mathbf{\Omega}_\mathrm{cut}(q,p) + \mathcal{O}(\varepsilon^3) \end{aligned}$$

where

$$\mathbf{\Omega}_0(q) = \begin{pmatrix} \Omega_0(q) & 0 \\ 0 & 0 \end{pmatrix} \quad \text{with} \quad \Omega_0(q) = -\mathrm{i}\, \mathrm{tr}_{\mathcal{H}_\mathrm{f}}([\, \partial_i P_0\, ,\, \partial_j P_0\, ]\, P_0)(q) \tag{7.4}$$

and

$$\boldsymbol{\Omega}_1(q,p) = \begin{pmatrix} \Omega_1(q, p - \varepsilon\, A(q)) & W(q) \\ -W(q) & 0 \end{pmatrix} \tag{7.5}$$

with

$$\Omega_1^{ij}(q,\kappa) := -(\partial_i W_{jl}(q) - \partial_j W_{il}(q))\, \kappa_l$$

and

$$\boldsymbol{\Omega}_{\mathrm{cut}}(q,p) := \begin{pmatrix} 0 & \Omega_{\mathrm{cut}}^T(q,p) \\ -\Omega_{\mathrm{cut}}(q,p) & 0 \end{pmatrix}$$

where $\Omega_{\mathrm{cut}}(q,p) = (p - \varepsilon\, A(q)) \otimes \Big(W(q)\,(p - \varepsilon\, A(q))\Big)$. By (B.27) the associated Liouville measure satisfies $\lambda_\lambda^\varepsilon = \nu_\lambda^\varepsilon(q,p)\, \mathrm{d}q_1 \wedge \cdots \wedge \mathrm{d}p_n$ with

$$\begin{aligned} \nu_\lambda^\varepsilon(q,p) =& 1 + \varepsilon^2\, \chi_\lambda'(|p - \varepsilon\, A(q)|^2)\, \mathrm{Tr}_n(W)(q) \\ &+ \varepsilon^2\, \chi_\lambda''(|p - \varepsilon\, A(q)|^2)\, \|p - \varepsilon\, A(q)\|^2_{W(q)} + \mathcal{O}(\varepsilon^3)\,. \end{aligned} \tag{7.6}$$

By Lemma B.6 the Hamiltonian equations of motion are

$$\begin{pmatrix} \dot{q} \\ \dot{p} \end{pmatrix} = -\, \omega_\lambda^\varepsilon(q,p)^{-1} \begin{pmatrix} \partial_q h(q,p) \\ \partial_p h(q,p) \end{pmatrix}$$

where

$$\begin{aligned} (\omega_\lambda^\varepsilon)^{-1}(q,p) = & \begin{pmatrix} 0 & -\mathbf{1}_n \\ \mathbf{1}_n & \varepsilon\, \Omega_\lambda(q,p) \end{pmatrix} + \varepsilon^2\, \chi_\lambda'(|p - \varepsilon\, A(q)|^2) \begin{pmatrix} 0 & W(q) \\ -W(q) & 0 \end{pmatrix} \\ & + \varepsilon^2\, \chi_\lambda''(|p - \varepsilon\, A(q)|^2) \begin{pmatrix} 0 & \Omega_{\mathrm{cut}}(q,p) \\ -\Omega_{\mathrm{cut}}^T(q,p) & 0 \end{pmatrix} + \mathcal{O}(\varepsilon^3) \end{aligned}$$

with

$$\Omega_\lambda(q,p) = \Omega_0(q) + \varepsilon\, \chi_\lambda'(|p - \varepsilon\, A(q)|^2)\, \Omega_1(q, p - \varepsilon\, A(q))$$

The Hamiltonian equation can be represented as

$$\dot{q} \ = \chi_\lambda'(|p - \varepsilon\, A(q)|^2)\ (p - \varepsilon\, A(q)) + \mathcal{O}(\varepsilon^3)$$

and

$$
\begin{aligned}
\dot{p}_i = &- \partial_i e_v(q) + \varepsilon\, \chi'_\lambda(|p - \varepsilon\, A(q)|^2)\ \langle \partial_i A(q)\, ,\, p - \varepsilon\, A(q)\rangle \\
&- \varepsilon\, \chi'_\lambda(|p - \varepsilon\, A(q)|^2)\ \Omega^{ij}_\lambda(q,p)\, (p - \varepsilon\, A(q))_j \\
&- \tfrac{1}{2}\, \varepsilon^2\, \chi'_\lambda(|p - \varepsilon\, A(q)|^2)^2\ \langle p - \varepsilon\, A(q)\, ,\, \partial_i W(q)\, (p - \varepsilon\, A(q))\rangle \\
&+ \varepsilon^2\, \chi'_\lambda(|p - \varepsilon\, A(q)|^2)\ W_{ij}(q)\, \partial_j e_v(q) \\
&+ \varepsilon^2\, \chi''_\lambda(|p - \varepsilon\, A(q)|^2)\ \langle p - \varepsilon\, A(q)\, ,\, \nabla e_v(q)\rangle\ W_{ij}(q)\, (p - \varepsilon\, A(q))_j \\
&+ \mathcal{O}(\varepsilon^3)\, .
\end{aligned}
$$

As is easy to see, the associated Fubini-Study metric $\mathbf{g}^\varepsilon$ (3.72) satisfies

$$
\mathbf{g}^\varepsilon(q,p) = \mathbf{g}_0(q) + \mathcal{O}(\varepsilon) = \begin{pmatrix} g_0(q) & 0 \\ 0 & 0 \end{pmatrix} + \mathcal{O}(\varepsilon)
$$

where (7.7)

$$
g^{ij}_0(q) = \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\, [\partial_i P_0(q), \partial_j P_0(q)]_+)\, .
$$

REMARK 7.1 Assume $\psi(q)$ to be a eigenfunction of $V(q)$ depending smoothly on $q$, i.e. $P_0(q) = |\, \psi(q)\, \rangle\langle\, \psi(q)\, |$. Then, a straightforward computation leads

$$
\mathrm{Tr}_n(g_0)(q) = 2\left( \langle\, \partial_i\psi(q)\,|\, P_0^\perp(q)\, \partial_i\psi(q)\,\rangle + \sum_{i=1}^{n} \mathfrak{Re}\langle\, \partial_i\psi(q)\,|\,\psi(q)\,\rangle^2 \right).
$$

Here, the first term on the right hand side is known as the Born-Huang potential and the second is closely related the Berry connection $\mathcal{A}(q) = \mathrm{i}\,\langle\, \nabla\psi(q)\,|\,\psi(q)\,\rangle$, see e.g. [PST07]. Note, when deriving an effective Hamiltonian whose quantum evolution approximates the quantum evolution of the full Hamiltonian $\hat{H}^\varepsilon_\lambda$ then the Born-Huang potential and Berry connection are part of the effective Hamiltonian, see e.g. [WL93] or [PST07]. Since we do not compute an effective Hamiltonian in that sense but yield to directly approximate the dynamics through semiclassical approximations it is not surprising that our effective/classical Hamiltonian does not coincide with the effective Hamiltonian derived in [PST07]. Nevertheless, we will see later in this section that by altering the coefficients of the symplectic form as well as the quantum corrections one can reformulate the semiclassical approximations in the dynamic case leading to a classical Hamiltonian the coincides with the one stated in [PST07].

REMARK 7.2 Note that in the case where $V(q)$ is a real operator, with $\psi(q)$ also $\psi^*(q)$ is an eigenfunction of $V(q)$ to the eigenvalue $e_v$. Thus, $\psi_0(q) = \frac{\psi(q)+\psi^*(q)}{2}$ is an eigenfunction of $V(q)$ to the eigenvalue $e_v$ taking value in the real numbers. Moreover, since $e_v$ is assumed to be non-degenerate $\psi(q)$ is of the form $e^{i f(q)} \psi_0(q)$ where $f(q)$ is a real function. Clearly, the eigenprojection $P_0(q)$ is gauge invariant, i.e. $P_0(q) = |\,\psi(q)\,\rangle\langle\,\psi(q)\,| = |\,\psi_0(q)\,\rangle\langle\,\psi_0(q)\,|$. We conclude

$$\Omega_0^{ij}(q) = 2\,\mathfrak{Im}\Big(\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\partial_i P_0(q)\,\partial_j P_0(q)\,P_0)\Big) = 0\,.$$

Therefore, the second order corrections are the leading order quantum corrections to the canonical classical Hamiltonian system $(e_\lambda, \omega^0)$.

## 7.2 Expectation Values of Equilibrium States

Now, we are ready to apply our main results where we begin with the semiclassical approximation of expectation values in thermodynamic equilibrium. Note that here and also in the subsequent proposition we will only show the result for the semiclassical approximation up the errors of order $\varepsilon^3$. The only reasons for this are that we want to present the result in a specific way and only compute the explicit expressions for the corrections up to second order. Rather than that one gets semiclassical approximations to any order in $\varepsilon$ with the same arguments just by including the additional corrections as given by Theorem 4.4 or Theorem 5.2, respectively.

**Proposition 7.3** *Let $\varepsilon$ small enough, $\lambda > 0$ and $\hat{\Pi}^\varepsilon_\lambda$ be the super-adiabatic projection associated to $H_\lambda$ with eigenvalue $e_\lambda$. Further, assume $f \in \mathcal{A}$, $k > 2n+1$ and $R \in S^k(\varepsilon, \mathcal{B}_{\mathrm{sa}}(\mathcal{H}_\mathrm{f}))$ a classical symbol. Then,*

$$\begin{aligned}
&\mathrm{tr}_{\mathcal{H}}\left(f(\hat{H}^\varepsilon_\lambda)\,\hat{R}^\varepsilon\,\hat{\Pi}^\varepsilon_\lambda\right) \\
&\quad = (2\pi\varepsilon)^{-n}\int_{\Lambda_\lambda}\Big(f(h(q,p)) + \varepsilon^2\,Q_{\mathrm{BO}}(q,p)\Big)\,r^{(2)}(q,p)\,\nu^\varepsilon(q)\,\mathrm{d}q\,\mathrm{d}p \\
&\qquad + (2\pi\varepsilon)^{-n}\Big(\int_{\mathbb{R}^{2n}\setminus\Lambda_\lambda} f^\varepsilon(h_\lambda,\pi_\lambda)\,r^{(2)}_\lambda(q,p)\,\nu^\varepsilon_\lambda(q,p)\,\mathrm{d}q\,\mathrm{d}p \\
&\qquad\qquad + \varepsilon^2\int_{\mathbb{R}^{2n}\setminus\Lambda_\lambda} Q(h_{\lambda,0},\mathbf{g}_0)(q,p)\,r^{(2)}_\lambda(q,p)\,\mathrm{d}q\,\mathrm{d}p\Big) \\
&\qquad + \mathcal{O}\Big(\varepsilon^{3-n}\sum_{i=0}^{m}\|R_i\|_{L^1}\Big)
\end{aligned} \tag{7.8}$$

*with classical Hamiltonian*

$$h(q,p) := \tfrac{1}{2}\,|p - \varepsilon\,A(q)|^2 + e_v(q) + \tfrac{1}{2}\,\varepsilon^2\,\|p - \varepsilon\,A(q)\|^2_{W(q)}\,,$$

*Liouville measure*

$$\nu^\varepsilon(q) = 1 + \varepsilon^2\,\mathrm{Tr}_n(W)(q)$$

*and quantum correction to the equilibrium state*

$$\begin{aligned} Q_{\mathrm{BO}}(q,p) &= \tfrac{1}{2}\, f'(e(q,p))\,\mathrm{Tr}_n(g_0(q)) + \tfrac{1}{4}\, f''(e(q,p))\,\|p-\varepsilon\, A(q)\|^2_{g_0(q)} \\ &\quad - \tfrac{1}{8}\, f''(e(q,p))\,\Delta e_v(q) \\ &\quad - \tfrac{1}{24}\, f'''(e(q,p))\left(\|p-\varepsilon\, A(q)\|^2_{\nabla^2 e_v(q)} + |\nabla e_v(q)|^2\right) \end{aligned}$$

*where in the first summand of the r.h.s. of (7.8) we restrict the integration over phase space to* $\Lambda_\lambda := \{(q,p) \in \mathbb{R}^{2n} : |p-\varepsilon\, A(q)|^2 \leq \lambda\}$. *The effective symbol* $r^{(2)}$ *is the effective symbol of* $R(q,p)$ *defined by (3.26) with the* $\pi_i$*s associated to* $H(q,p) = \frac{1}{2}\,|p-\varepsilon\, A(q)|^2 + V(q)$ *and eigenvalue* $e(q,p) = \frac{1}{2}\,|p-\varepsilon\, A(q)|^2 + e_v(q)$.

*The effective equilibrium distribution* $f^\varepsilon(h_\lambda, \pi_\lambda)$ *is given by (4.28) with classical Hamiltonian* $h_\lambda$ *given by (7.3) and* $\pi_\lambda$ *the symbol of* $\hat{\pi}^\varepsilon_\lambda = \hat{\Pi}^\varepsilon_\lambda + \mathcal{O}(\varepsilon^\infty)$. *The quantum correction* $Q(h_{\lambda,0}, \mathrm{g}_0)$ *is defined by (4.30) with Fubini-Study metric* $\mathrm{g}_0$ *given by (7.7). The Liouville density* $\nu^\varepsilon_\lambda(q,p)$ *is given by* (7.6). *The effective symbol* $r_\lambda \in S^k(\varepsilon, \mathbb{R})$ *is the effective symbol of* $R(q,p)$ *associated to* $\hat{\Pi}^\varepsilon_\lambda$.

REMARK 7.4 The expression of interest in (7.8) is the expression one gets when formally considering the original Hamiltonian (7.2), i.e. the phase space integral over $\Lambda_\lambda$. In the following we will argue why one can actually neglect the additional phase space integral at least in the case of special assumptions on $f$. Every summand in (7.8) has a $j$-th derivative of $f$ evaluated at $h_0(q,p)$ as prefactor and $e_v$ is bounded. Hence, it is obvious that in the case where $f$ is compactly supported, the terms with $|p-\varepsilon\, A|^2$ larger than $\lambda$ vanish independent of $\varepsilon$ by choosing $\lambda$ sufficiently large. If $f$ is rapidly decreasing the behavior of the error terms is not so clear at this point. On the one hand, one can choose $\lambda$ depending on $\varepsilon$ in a way that the derivatives of $f$ are sufficiently small, i.e. some order in $\varepsilon$. The problem here is that by increasing $\lambda$ one will also increase every term of this extra error that includes a factor $p-\varepsilon\, A(q)$. Clearly, for the terms in the expansion this can be handled since their norm can be estimated by some polynomial of $|p-\varepsilon\, A(q)|$ and thus can be controlled by $f$. The big uncertainty here are the estimates for the approximation error $\mathcal{O}(\varepsilon^{3-n})$. By increasing $\lambda$ the constants in this estimate will get larger and they may even grow exponentially with $\lambda$. On the other hand the $p-\varepsilon\, A(q)$ factors stem from derivatives of $H_\lambda$ and $e_\lambda$. Since all the estimates leading to this error are related to the estimate of the Moyal remainders (2.3) we expect that one can control the error terms by some expression of the form $\|e_\lambda\|_{0,\tilde{r}_2}\,\|H_\lambda\|_{0,r_1}$. Assuming this to be true, one can control the growth of the error with respect to $\lambda$ by some polynomial of $|p-\varepsilon\, A(q)|$ which is exactly what we are looking for. Moreover, this leads to full control over the errors depending on $\lambda$ so that one can even let $\lambda$ tend to infinity.

PROOF Fix $\lambda > 0$. Clearly, $\hat{H}^\varepsilon_\lambda$, $f$ and $\hat{R}^\varepsilon$ satisfy the assumptions of Theorem 4.4. Hence, (4.29) yields

$$\begin{aligned}
&\operatorname{tr}_{\mathcal{H}}\Big(f(\hat{H}^\varepsilon_\lambda)\,\hat{R}^\varepsilon\,\hat{\Pi}^\varepsilon\Big)\\
&\quad= (2\pi\varepsilon)^{-n}\bigg(\int_{\mathbb{R}^{2n}} f^\varepsilon(h_\lambda,\pi_\lambda)(z)\, r^{(2)}_\lambda(z)\,\nu^\varepsilon_\lambda(z)\,\mathrm{d}z\\
&\qquad+\varepsilon^2\int_{\mathbb{R}^{2n}} Q(h_{\lambda,0},g_0)(z)\, r^{(2)}_\lambda(z)\,\mathrm{d}z\bigg)\\
&\qquad+\mathcal{O}\bigg(\varepsilon^{3-n}\Big(\|R\|^\varepsilon_{L^1}+\sum_{i=0}^{2}\Big(\|R_i\|_{L^1}+\|\varepsilon^{-(i+1)}(R-R^{(i)})\|^\varepsilon_{L^1}\Big)\Big)\bigg).
\end{aligned}$$

In addition, by definition of $\chi_\lambda$ we have for every $(q,p)\in\Lambda_\lambda$ that

$$\chi_\lambda\Big(|p-A(q)|^2\Big) = |p-A(q)|^2, \qquad \chi'_\lambda\Big(|p-A(q)|^2\Big) = 1$$

and

$$\chi^{(j)}_\lambda\Big(|p-A(q)|^2\Big) = 0 \quad \text{for} \quad j>1\,.$$

It follows directly that

$$\begin{aligned}
&\int_{\Lambda_\lambda} f^\varepsilon(h_\lambda,\pi_\lambda)\, r^{(2)}_\lambda(q,p)\,\nu^\varepsilon_\lambda(q,p)\,\mathrm{d}q\,\mathrm{d}p + \varepsilon^2\int_{\Lambda_\lambda} Q(h_{\lambda,0},\mathbf{g}_0)(q,p)\, r^{(2)}_\lambda(q,p)\,\mathrm{d}q\,\mathrm{d}p\\
&\qquad= \int_{\Lambda_\lambda} f^\varepsilon(h,\pi)(q,p)\, r^{(2)}(q,p)\,\nu^\varepsilon(q)\,\mathrm{d}q\,\mathrm{d}p\\
&\qquad\qquad+\varepsilon^2\int_{\Lambda_\lambda} Q(h_0,\mathbf{g}_0)(q,p)\, r^{(2)}(q,p)\,\mathrm{d}q\,\mathrm{d}p\,.
\end{aligned}$$

Clearly,

$$\nabla h_0(q,p) = \begin{pmatrix}\nabla e_v(q)\\ p-\varepsilon\,A(q)\end{pmatrix} + \mathcal{O}(\varepsilon)$$

and

$$\nabla^2 h_0(q,p) = \begin{pmatrix}\nabla^2 e_v(q) & 0\\ 0 & \mathbf{1}_n\end{pmatrix} + \mathcal{O}(\varepsilon)\,.$$

Then, a straight forward computation shows

$$\begin{aligned}
Q(h_0,\mathbf{g}_0)(q,p) &= \tfrac{1}{2}\operatorname{Tr}_{2n}(\omega^0\,\nabla(f'(h_0(q,p))\,\mathbf{g}_0(q)\,\omega^0\,\nabla h_0(q,p)))\\
&= \tfrac{1}{2}\,f''(e(q,p))\,\|p-\varepsilon\,A(q)\|^2_{g_0(q)}\\
&\quad+\tfrac{1}{2}\,f'(e(q,p))\,\operatorname{Tr}_n(g_0(q)) + \mathcal{O}(\varepsilon)
\end{aligned}$$

as well as

$$
\begin{aligned}
f^{\mathrm{sc}}(h)(q,p) &= -\tfrac{1}{24}\, f'''(h_0(q,p))\, \langle\, \omega^0\, \nabla h_0(q,p)\,,\; \nabla^2 h_0(q,p)\, \omega^0\, \nabla h_0(q,p)\,\rangle \\
&\quad + \tfrac{1}{16}\, f''(h_0(q,p))\, \mathrm{Tr}_{2n}(\omega^0\, \nabla^2 h_0(q,p)\, \omega^0\, \nabla^2 h_0(q,p)) \\
&= -\tfrac{1}{24}\, f'''(e(q,p))\, \Big( \|p - \varepsilon\, A(q)\|^2_{\nabla^2 e_v(q)} + |\nabla e_v(q)|^2 \Big) \\
&\quad - \tfrac{1}{8}\, f''(e(q,p))\, \Delta e_v(q) + \mathcal{O}(\varepsilon)
\end{aligned}
$$

and

$$
\begin{aligned}
f^{\mathrm{adi}}(h,\pi) &= -\tfrac{1}{4}\, f''(h_0(q,p))\, \|\omega^0\, \nabla h_0(q,p)\|^2_{\mathbf{g}_0(q)} \\
&= -\tfrac{1}{4}\, f''(e(q,p))\, \|p - \varepsilon\, A(q)\|^2_{g_0(q)}\,.
\end{aligned}
$$

To finish the proof we combine the above results with (3.57) and (2.13). □

## 7.3 An Egorov Type Theorem

In addition to the approximation of expectation values in thermodynamic equilibrium we also want to approximate the quantum evolution of an observable in the adiabatic subspace $\hat{\Pi}^{\varepsilon}_{\lambda}$. Clearly, one can directly apply Theorem 5.2 to the quantum evolution generated by $\hat{H}^{\varepsilon}_{\lambda}$ to obtain a semiclassical approximation dependent of the Hamiltonian system $(h^{\lambda}, \omega^{\varepsilon}_{\lambda})$ and the quantum correction associated to $H_{\lambda}$ and $e_{\lambda}$. However, our goal here is to derive an approximation that relates to $H(q,p)$, at least for $\lambda$ large enough. To achieve this we introduce an operator $\zeta_{\mu}(\hat{H}^{\varepsilon}_{\lambda})$ that cuts off large energies. This then leads to the following result.

**Proposition 7.5** *Let $\varepsilon$ small enough, $R$ a classical symbol in $S^0(\mathcal{B}_{\mathrm{sa}}(\mathcal{H}_{\mathrm{f}}))$ and $\zeta_{\mu} : \mathbb{R} \to \mathbb{R}$, $\mu > 0$ a smooth cutoff function satisfying $\zeta_{\mu}(x) = 1$ for $x \leq \mu$ and $\zeta_{\mu}(x) = 0$ for $x \geq \mu + 1$. Then, there exist $\lambda_{\mu} > \tilde{\lambda}_{\mu} > 0$ and a $T_{\mu,\lambda_{\mu}} > 0$ such that for $\hat{\Pi}^{\varepsilon}_{\lambda_{\mu}}$ the super-adiabatic projection associated to $H_{\lambda_{\mu}}$ with eigenvalue $e_{\lambda_{\mu}}$ and $0 \leq t < T_{\mu,\lambda_{\mu}}$ we have*

$$
\begin{aligned}
&\Big\|\, \hat{\Pi}^{\varepsilon}_{\lambda_{\mu}} \Big( \mathrm{e}^{\mathrm{i}\, \hat{H}^{\varepsilon}_{\lambda_{\mu}}\, t/\varepsilon}\, \hat{R}^{\varepsilon}\, \mathrm{e}^{-\mathrm{i}\, \hat{H}^{\varepsilon}_{\lambda_{\mu}}\, t/\varepsilon} - \mathrm{op}_{\varepsilon}\Big( \Big( r^{(2)}(\Phi^t_{\varepsilon}) + \varepsilon^2\, \mathfrak{A}(t) \Big)\, \xi_{\tilde{\lambda}_{\mu},\lambda_{\mu}} \Big) \Big)\, \hat{\Pi}^{\varepsilon}_{\lambda_{\mu}}\, \zeta_{\mu}(\hat{H}^{\varepsilon}_{\lambda_{\mu}})\, \Big\| \\
&\qquad = \mathcal{O}(\varepsilon^3)\,.
\end{aligned}
\tag{7.9}
$$

*Here, $\xi_{\tilde{\lambda}_{\mu},\lambda_{\mu}}$ is a smooth cutoff function with $\xi_{\tilde{\lambda}_{\mu},\lambda_{\mu}}(q,p) = 1$ for $(q,p) \in \Lambda_{\tilde{\lambda}_{\mu}}$ and $\xi_{\tilde{\lambda}_{\mu},\lambda_{\mu}}(q,p) = 0$ for $(q,p) \in \mathbb{R} \setminus \Lambda_{(\tilde{\lambda}_{\mu}+\lambda_{\mu})/2}$ where $\Lambda_{\lambda} := \{(q,p) \in \mathbb{R}^{2n} : |p - \varepsilon\, A(q)|^2 \leq \lambda\}$. The effective symbol $r^{(2)}$ of $R(q,p)$ is defined by (3.26) with the $\pi_i$s associated to $H(q,p) = \frac{1}{2}\,|p - \varepsilon\, A(q)|^2 + V(q)$ and eigenvalue*

*$e(q,p) = \frac{1}{2}\,|p - \varepsilon\, A(q)|^2 + e_v(q)$. The Hamiltonian flow $\Phi^t_\varepsilon$ is the flow of the Hamiltonian system $(h, \omega^\varepsilon)$ with classical Hamiltonian*

$$h(q,p) = \tfrac{1}{2}\,|p - \varepsilon\, A(q)|^2 + e_v(q) + \tfrac{1}{2}\,\varepsilon^2\ \|p - \varepsilon\, A(q)\|^2_{W(q)}$$

*and symplectic form*

$$\omega^\varepsilon(q,p) = \omega^0 + \varepsilon\, \mathbf{\Omega}_0(q) + \varepsilon^2\, \mathbf{\Omega}_1(q,p)$$

*where $\mathbf{\Omega}_0(q)$ and $\mathbf{\Omega}_1(q,p)$ are defined by (7.4) and (7.5), respectively. The resulting Hamiltonian equations are given by*

$$\dot{q} \ = \ p - \varepsilon\, A(q) + \mathcal{O}(\varepsilon^3)$$

*and*

$$\begin{aligned}\dot{p}_i \ = \ & -\partial_i e_v(q) + \varepsilon\ \langle \partial_i A(q)\,,\, p - \varepsilon\, A(q)\rangle - \varepsilon\, \Omega^{ij}(q,p)\,(p - \varepsilon\, A(q))_j \\ & - \tfrac{1}{2}\,\varepsilon^2\ \langle p - \varepsilon\, A(q)\,,\, \partial_i W(q)\,(p - \varepsilon\, A(q))\rangle \\ & + \varepsilon^2\, W_{ij}(q)\,\partial_j e_v(q) + \mathcal{O}(\varepsilon^3)\,.\end{aligned}$$

*The quantum correction $\mathfrak{A}(t)$ is given by*

$$\mathfrak{A}(t) = \int_0^t \mathfrak{A}^c_h(r_0(\Phi^\tau_\varepsilon)) \circ \Phi^{t-\tau}_\varepsilon\, \mathrm{d}\tau$$

*with*

$$\begin{aligned}\mathfrak{A}^c_h(r_0)(q,p) = & -\tfrac{1}{2}\,\mathrm{Tr}_n\Big(\partial^2_{pq} r_0(q,p)\, g_0(q)\Big) - \tfrac{1}{4}\,\langle \partial_p r_0(q,p)\,,\, \nabla\, \mathrm{Tr}_n(g_0(q))\rangle \\ & + \tfrac{1}{4}\,\partial^2_{p_j p_l} r_0(q,p)\,(p - \varepsilon\, A(q))_i\, \partial_i g_0^{jl}(q) \\ & + \tfrac{1}{24}\,\partial^3_{p_i p_j p_l} r_0(q,p)\,\partial^3_{ijl} e_v(q,p) + \mathcal{O}(\varepsilon)\,.\end{aligned}$$

REMARK 7.6 In Remark 7.1 we stated that instead of our classical Hamiltonian $h(q,p)$ we can also use the symbol of the effective Hamiltonian from [PST07]

$$\widetilde{h}(q,p) = \tfrac{1}{2}\,|p - \varepsilon\, A(q)|^2 + e_v(q) + \tfrac{1}{4}\,\varepsilon^2\,\mathrm{Tr}_n(g_0)(q) - \tfrac{1}{2}\,\varepsilon^2\ \|p - \varepsilon\, A(q)\|^2_{W(q)}$$

to semiclassically approximate the quantum evolution up to errors of order $\varepsilon^3$. Note, in addition to including the Born-Huang potential $\mathrm{Tr}_n(g_0)(q)$ also the sign of the last summand changed here. Clearly, we have to adjust the coefficients of the symplectic form $\omega^\varepsilon$ as well as the quantum correction $\mathfrak{A}^c_h$

in order to get similar result to Proposition 7.5. We change the coefficients of the symplectic to

$$\widetilde{\omega}^{\varepsilon}(q,p) = \omega^0 + \varepsilon\, \boldsymbol{\Omega}_0(q) + \varepsilon^2\, \widetilde{\boldsymbol{\Omega}}_1(q,p)$$

where

$$\widetilde{\boldsymbol{\Omega}}_1(q,p) := \begin{pmatrix} \widetilde{\Omega}_1(q, p - \varepsilon\, A(q)) & W(q) \\ W(q) & 0 \end{pmatrix}$$

with

$$\Omega_1^{ij}(q,\kappa) := \partial_j W_{il}(q)\, \kappa_l\,.$$

In this case $\widetilde{\omega}^{\varepsilon}(q,p)$ is not skew-symmetric and therefore does not define a symplectic form. For the quantum correction we use

$$\begin{aligned}\mathfrak{A}_h^c(r_0(q,p),q,p) = &-\tfrac{1}{2}\,\mathrm{Tr}_n\Big(\nabla^2_{pq} r_0(q,p)\, g_0(q)\Big)\\ &+\tfrac{1}{4}\,\partial^2_{p_j p_l} r_0(q,p)\,(p-\varepsilon\, A(q))_i\,\partial_i g_0^{jl}(q)\\ &+\tfrac{1}{24}\,\partial^3_{p_i p_j p_l} r_0(q,p)\,\partial^3_{ijl} e_v(q) + \mathcal{O}(\varepsilon)\,.\end{aligned} \tag{7.10}$$

Then, (7.9) holds with $\Phi_\varepsilon^t$ being the flow of the system of ordinary differential equations

$$\dot{z} = -\widetilde{\omega}^{\varepsilon}(z)^{-1}\, \nabla \widetilde{h}(z)\,.$$

Note here that the change of the sign in the last term of the scalar Hamiltonian causes the change in the symplectic form. Hence, by solely including the Born-Huang potential $\mathrm{Tr}_n(g)$ one can approximate the quantum evolution up to errors of order $\varepsilon^3$ using the simpler quantum correction resulting from (7.10).

PROOF For now, choose an arbitrary momentum cutoff $\mu > 0$, energy cutoff $\lambda > 0$ and time $t \geq 0$. We will make a specific choice for $\tilde{\lambda}_\mu$, $\lambda_\mu$ and $T_{\mu,\lambda_\mu}$ later in the proof. Since $\hat{H}_\lambda^\varepsilon$ is self-adjoint on $\mathcal{H}$ and $\zeta_\mu \in \mathcal{A}$ the Helffer-Sjöstrand formula (4.1) together with the fact that $\hat{\Pi}_\lambda^\varepsilon$ almost commutes with the Hamiltonian $\hat{H}_\lambda^\varepsilon$ yields

$$\hat{\Pi}_\lambda^\varepsilon\, \zeta_\mu(\hat{H}_\lambda^\varepsilon) = \hat{\Pi}_\lambda^\varepsilon\, \zeta_\mu(\hat{H}_\lambda^\varepsilon)\, \hat{\Pi}_\lambda^\varepsilon + \mathcal{O}(\varepsilon^\infty)\,.$$

By Proposition 4.3

$$\hat{\Pi}_\lambda^\varepsilon\, \zeta_\mu(\hat{H}_\lambda^\varepsilon)\, \hat{\Pi}_\lambda^\varepsilon = \hat{\Pi}_\lambda^\varepsilon\, \mathrm{op}_\varepsilon\Big(\zeta_\mu^\varepsilon(h_\lambda,\pi_\lambda)\Big)\, \hat{\Pi}_\lambda^\varepsilon + \mathcal{O}(\varepsilon^3)$$

where

$$\zeta_\mu^\varepsilon(h_\lambda,\pi_\lambda) = \zeta_\mu(h_\lambda) + \varepsilon^2\, \zeta_\mu^{\mathrm{sc}}(h_\lambda) + \varepsilon^2\, \zeta_\mu^{\mathrm{adi}}(h_\lambda,\pi_\lambda)$$

with $\zeta_\mu^{\rm sc}(h_\lambda)$ and $\zeta_\mu^{\rm adi}(h_\lambda,\pi_\lambda)$ given by (4.12) and (4.13), respectively. In addition, by Theorem 5.2 the Hamiltonian flow $\Phi^t_{\varepsilon,\lambda}$ of $(h_\lambda,\omega^\varepsilon_\lambda)$ exists globally and

$$\hat\Pi^\varepsilon_\lambda\, \mathrm{e}^{\mathrm{i}\,\hat H^\varepsilon_\lambda\, t/\varepsilon}\, \hat R^\varepsilon\, \mathrm{e}^{-\mathrm{i}\,\hat H^\varepsilon_\lambda\, t/\varepsilon}\, \hat\Pi^\varepsilon_\lambda = \hat\Pi^\varepsilon_\lambda\, \mathrm{op}_\varepsilon\Big(r^{(2)}_\lambda(\Phi^t_{\varepsilon,\lambda}) + \varepsilon^2\, \mathfrak{A}_\lambda(t)\Big)\, \hat\Pi^\varepsilon_\lambda + \mathcal{O}(\varepsilon^3)$$

where $r_\lambda \in S^0(\varepsilon,\mathbb{R})$ is the symbol of the effective Operator of $\hat R^\varepsilon$ restricted to the adiabatic subspace $\hat\Pi^\varepsilon_\lambda\,\mathcal{H}$ and $\mathfrak{A}_\lambda(t)\in S^0(\varepsilon,\mathbb{R})$ is

$$\mathfrak{A}_\lambda(t) = \int_0^t \mathfrak{A}^c_{h^\lambda}(r_{\lambda,0}(\Phi^\tau_{\varepsilon,\lambda}))\circ \Phi^{t-\tau}_{\varepsilon,\lambda}\,\mathrm{d}\tau$$

with

$$\begin{aligned}\mathfrak{A}^c_{h^\lambda}(r_{\lambda,0})(q,p) &= 2\,\mathrm{i}\,\{h^\lambda_0\,,r_{\lambda,0}\,\}_3(q,p) - \tfrac12\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big(\{\{h^\lambda_0\,,P_0\,\}\,,\{r_{\lambda,0}\,,P_0\}\,\}\Big)(q,p)\\ &\quad + \mathcal{O}(\varepsilon)\,.\end{aligned}$$

Combining the above results we conclude

$$\begin{aligned}&\hat\Pi^\varepsilon_\lambda\, \mathrm{e}^{\mathrm{i}\,\hat H^\varepsilon_\lambda\, t/\varepsilon}\, \hat R^\varepsilon\, \mathrm{e}^{-\mathrm{i}\,\hat H^\varepsilon_\lambda\, t/\varepsilon}\, \hat\Pi^\varepsilon_\lambda\,\zeta_\mu(\hat H^\varepsilon_\lambda)\\ &\quad= \hat\Pi^\varepsilon_\lambda\, \mathrm{op}_\varepsilon\Big(r^{(2)}_\lambda(\Phi^t_{\varepsilon,\lambda}) + \varepsilon^2\, \mathfrak{A}_\lambda(t)\Big)\, \hat\Pi^\varepsilon_\lambda\, \mathrm{op}_\varepsilon\Big(\zeta^\varepsilon_\mu(h_\lambda,\pi_\lambda)\Big)\, \hat\Pi^\varepsilon_\lambda + \mathcal{O}(\varepsilon^3)\\ &\quad= \hat\Pi^\varepsilon_\lambda\, \mathrm{op}_\varepsilon\Big((r^{(2)}_\lambda(\Phi^t_{\varepsilon,\lambda}) + \varepsilon^2\, \mathfrak{A}_\lambda(t))\,\#\,\pi_\lambda\,\#\,\zeta^\varepsilon_\mu(h_\lambda,\pi_\lambda)\Big)\, \hat\Pi^\varepsilon_\lambda + \mathcal{O}(\varepsilon^3)\,.\end{aligned} \tag{7.11}$$

By definition, $\zeta_\mu(x)$ is zero for every $x > \mu+1$. In addition, $e_v$ is assumed to be bounded. Hence, there exists a $\tilde\lambda_\mu > 0$ such that for every $\lambda \geq \tilde\lambda_\mu$ it holds that

$$\zeta^{(j)}_\mu(h^\lambda_0(q,p)) = 0 \qquad \text{for all} \quad j\in\mathbb{N}_0 \quad\text{and}\quad (q,p)\in\mathbb{R}^{2n}\setminus\Lambda_{\tilde\lambda_\mu}\,.$$

Here, $\zeta^{(j)}_\mu(x)$ denotes the $j$-th derivative with respect to $x$ of $\zeta_\mu(x)$. As a consequence we have for every $\lambda\geq\tilde\lambda_\mu$ that

$$\zeta^\varepsilon_\mu(h^\lambda,\pi_\lambda) = 0 \qquad \text{for all} \quad (q,p)\in\mathbb{R}^{2n}\setminus\Lambda_{\tilde\lambda_\mu}\,. \tag{7.12}$$

It follows for every $\lambda\geq\tilde\lambda_\mu$ and every $(q,p)\in\mathbb{R}^{2n}\setminus\Lambda_{\tilde\lambda_\mu}$ that

$$\Big((r^{(2)}_\lambda(\Phi^t_{\varepsilon,\lambda}) + \varepsilon^2\,\mathfrak{A}_\lambda(t))\,\#\,\pi_\lambda\,\#\,\zeta^\varepsilon_\mu(h^\lambda,\pi_\lambda)\Big)(q,p) = 0\,. \tag{7.13}$$

Now, choose $\lambda_\mu > \tilde{\lambda}_\mu$ and $\delta = \frac{\lambda_\mu - \tilde{\lambda}_\mu}{2}$. Clearly, for every $(q,p) \in \Lambda_{\lambda_\mu}$ it holds

$$\pi^{(2)}_{\lambda_\mu}(q,p) = \pi^{(2)}(q,p), \quad h^{\lambda_\mu}(q,p) = h(q,p), \quad \text{and} \quad r^{(2)}_{\lambda_\mu}(q,p) = r^{(2)}(q,p)\,. \tag{7.14}$$

Since the Hamiltonian flow $\Phi^t_{\varepsilon,\lambda_\mu}$ depends smoothly on $t$ and $\Lambda_{\tilde{\lambda}_\mu+\delta} \subset \Lambda_{\lambda_\mu}$ there exists a $T_{\mu,\lambda_\mu} > 0$ such that

$$\Phi^t_{\varepsilon,\lambda_\mu}(q,p) \in \Lambda_{\lambda_\mu} \qquad \text{for every} \quad (q,p) \in \Lambda_{\tilde{\lambda}_\mu+\delta} \quad \text{and} \quad t \in [0, T_{\mu,\lambda_\mu})\,. \tag{7.15}$$

Combining (7.14) and (7.15) it holds for every $(q,p) \in \Lambda_{\tilde{\lambda}_\mu+\delta}$ and $t \in [0, T_{\mu,\lambda_\mu})$ that $\Phi^t_\varepsilon(q,p)$ exists and $\Phi^t_{\varepsilon,\lambda_\mu}(q,p) = \Phi^t_\varepsilon(q,p)$. Furthermore, a straight forward computation shows for $(q,p) \in \Lambda_{\lambda_\mu}$ that

$$\begin{aligned}
\mathfrak{A}^c_{h^{\lambda_\mu}}(r_{\lambda_\mu,0})(q,p) &= 2\,\mathrm{i}\,\{h_0\,, r_0\,\}_3(q,p) - \tfrac{1}{2}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big(\{\{h_0\,, P_0\}\,, \{r_0\,, P_0\}\,\}\Big)(q,p) \\
&= -\,\tfrac{1}{2}\,\mathrm{Tr}_n\Big(\nabla^2_{pq} r_0(q,p)\, g_0(q)\Big) - \tfrac{1}{4}\,\langle \nabla_p r_0(q,p)\,,\, \nabla\, \mathrm{Tr}_n(g_0(q))\rangle \\
&\quad + \tfrac{1}{4}\,\partial^2_{p_j p_l} r_0(q,p)\,(p - \varepsilon\, A(q))_i\, \partial_i g_0^{jl}(q) \\
&\quad + \tfrac{1}{24}\,\partial^3_{p_i p_j p_l} r_0(q,p)\, \partial^3_{ijl} e_v(q,p) \\
&= \mathfrak{A}^c_h(r_0)(q,p)
\end{aligned}$$

which shows $\mathfrak{A}_{\lambda_\mu}(t)(q,p) = \mathfrak{A}(t)(q,p)$ for every $(q,p) \in \Lambda_{\tilde{\lambda}_\mu}$ and $t \in [0, T_{\mu,\lambda_\mu})$. We conclude that

$$\begin{aligned}
&\Big((r^{(2)}_{\lambda_\mu}(\Phi^t_{\varepsilon,\lambda_\mu}) + \varepsilon^2\, \mathfrak{A}_{\lambda_\mu}(t))\,\#\,\pi_{\lambda_\mu}\,\#\,\zeta^\varepsilon_\mu(h_{\lambda_\mu}, \pi_{\lambda_\mu})\Big)(q,p) \\
&\qquad = \Big((r^{(2)}(\Phi^t_\varepsilon) + \varepsilon^2\, \mathfrak{A}(t))\,\#\,\pi_{\lambda_\mu}\,\#\,\zeta^\varepsilon_\mu(h_{\lambda_\mu}, \pi_{\lambda_\mu})\Big)(q,p)
\end{aligned} \tag{7.16}$$

for every $t \in [0, T_{\mu,\lambda_\mu})$ and every $(q,p) \in \Lambda_{\tilde{\lambda}_\mu+\delta}$. Moreover, (7.12) implies that for every $(q,p) \in \mathbb{R} \setminus \Lambda_{\tilde{\lambda}_\mu} \supset \mathbb{R} \setminus \Lambda_{\lambda_\mu}$ and $t \in [0, T_{\mu,\lambda_\mu})$ we have

$$\begin{aligned}
0 &= \Big((r^{(2)}(\Phi^t_\varepsilon) + \varepsilon^2\, \mathfrak{A}(t))\,\#\,\pi_{\lambda_\mu}\,\#\,\zeta^\varepsilon_\mu(h_{\lambda_\mu}, \pi_{\lambda_\mu})\Big)(q,p) \\
&= \Big((r^{(2)}(\Phi^t_\varepsilon) + \varepsilon^2\, \mathfrak{A}(t))\, \xi_{\tilde{\lambda}_\mu,\lambda_\mu}\,\#\,\pi_{\lambda_\mu}\,\#\,\zeta^\varepsilon_\mu(h_{\lambda_\mu}, \pi_{\lambda_\mu})\Big)(q,p)
\end{aligned} \tag{7.17}$$

where $\xi_{\tilde{\lambda}_\mu,\lambda_\mu}$ is a smooth cutoff function with $\xi_{\tilde{\lambda}_\mu,\lambda_\mu}(q,p) = 1$ for $(q,p) \in \Lambda_{\tilde{\lambda}_\mu}$ and $\xi_{\tilde{\lambda}_\mu,\lambda_\mu}(q,p) = 0$ for $(q,p) \in \mathbb{R} \setminus \Lambda_{\tilde{\lambda}_\mu+\delta}$. By combining (7.16) with (7.13) and (7.17) we obtain for every $(q,p) \in \mathbb{R}^{2n}$ and every $t \in [0, T_{\mu,\lambda_\mu})$

$$\begin{aligned}
&\Big((r^{(2)}_\lambda(\Phi^t_{\varepsilon,\lambda_\mu}) + \varepsilon^2\, \mathfrak{A}_{\lambda_\mu}(t))\,\#\,\pi_{\lambda_\mu}\,\#\,\zeta^\varepsilon_\mu(h_{\lambda_\mu}, \pi_{\lambda_\mu})\Big)(q,p) \\
&\qquad = \Big((r^{(2)}(\Phi^t_\varepsilon) + \varepsilon^2\, \mathfrak{A}(t))\,\#\,\pi_{\lambda_\mu}\,\#\,\zeta^\varepsilon_\mu(h_{\lambda_\mu}, \pi_{\lambda_\mu})\Big)(q,p) \\
&\qquad = \Big((r^{(2)}(\Phi^t_\varepsilon) + \varepsilon^2\, \mathfrak{A}(t))\, \xi_{\tilde{\lambda}_\mu,\lambda_\mu}\,\#\,\pi_{\lambda_\mu}\,\#\,\zeta^\varepsilon_\mu(h_{\lambda_\mu}, \pi_{\lambda_\mu})\Big)(q,p)\,.
\end{aligned}$$

Note here, the reason why we introduced $\xi_{\tilde\lambda_\mu,\lambda_\mu}$ is that the Weyl quantization of $r^{(2)}(\Phi^t_\varepsilon) + \varepsilon^2\,\mathfrak{A}(t))$ may not make sense for all $t \in [0, T_{\mu,\lambda_\mu})$ since the Hamiltonian flow $\Phi^t_\varepsilon$ may not exist for arbitrary $(q,p) \in \mathbb{R}^{2n}$ and $t \in [0, T_{\mu,\lambda_\mu})$. Including the cut off, the expression $r^{(2)}(\Phi^t_\varepsilon) + \varepsilon^2\,\mathfrak{A}(t))\,\xi_{\tilde\lambda_\mu,\lambda_\mu}$ is smooth and bounded with all its derivatives for any $t \in [0, T_{\mu,\lambda_\mu})$. Then, similar to (7.11) we get

$$
\begin{aligned}
&\mathrm{op}_\varepsilon\Big((r^{(2)}(\Phi^t_\varepsilon) + \varepsilon^2\,\mathfrak{A}(t))\,\xi_{\tilde\lambda_\mu,\lambda_\mu} \,\#\, \pi_{\lambda_\mu} \,\#\, \zeta^\varepsilon_\mu(h_{\lambda_\mu}, \pi_{\lambda_\mu})\Big) \\
&\qquad = \mathrm{op}_\varepsilon\Big((r^{(2)}(\Phi^t_\varepsilon) + \varepsilon^2\,\mathfrak{A}(t))\,\xi_{\tilde\lambda_\mu,\lambda_\mu}\Big)\,\hat\Pi^\varepsilon_{\lambda_\mu}\,\zeta_\mu(\hat H^\varepsilon_{\lambda_\mu}) + \mathcal{O}(\varepsilon^3).
\end{aligned}
$$

Then, combining the two results above and (7.11) finishes the proof. □

## 7.4 Numerical Experiments

In this section we apply the numerical scheme described in Section 5.2 to a simple example of Born-Oppenheimer type where we will restrict to approximations to errors of order $\varepsilon^3$. Our main goal is to show that the algorithm suggested in Section 5.2 can reach the accuracy of order $\varepsilon^3$, does so in a efficient way and is therefore feasible also in a moderately high dimensional setting. On the contrary, we will also discuss a situation where the algorithm fails to reach the expected accuracy.

We consider the Hamiltonian

$$
\hat H^\varepsilon = -\tfrac{\varepsilon^2}{2}\Delta_x + V(x)
$$

acting on the Hilbert space $\mathcal{H} = L^2(\mathbb{R}) \otimes \mathbb{C}^2$ with matrix valued potential

$$
V(x) = \begin{pmatrix} \tanh(x) & \delta \\ \delta & -\tanh(x) \end{pmatrix}, \qquad \delta > 0\,.
$$

The eigenvalue bands of $V(x)$ are

$$
e^{(0)}(x) = -\sqrt{\tanh^2(x) + \delta^2} \qquad \text{and} \qquad e^{(1)}(x) = -e^{(0)}(x)
$$

with associated eigenprojections $P_i(x) = |\varphi_i(x)\rangle\langle\varphi_i(x)|$ where $\varphi_i(x) = \tilde\varphi_i/|\tilde\varphi_i|$,

$$
\tilde\varphi_i = \begin{pmatrix} \frac{1}{\delta}(e^{(i)} + \tanh(x)) \\ 1 \end{pmatrix} \qquad \text{for} \quad i = 0, 1\,.
$$

See Figure 7.1 for a plot of the eigenvalues for $\delta = 0.1$.

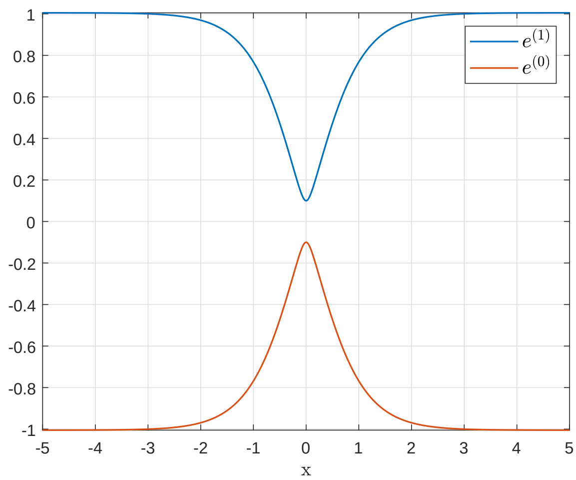



**Figure 7.1.** Eigenvalues $e^{(0)}(x)$ and $e^{(1)}(x)$ of the matrix valued potential $V(x)$ for $\delta = 0.1$.

As initial wave function $\psi_0(x)$ we consider a gaussian wave packet centered at $(q_0, p_0) \in \mathbb{R}^2$ that is a section of the eigenbundle $P_0(x)\,\mathbb{C}^2$, i.e.

$$\psi_0(x) = (\pi\,\varepsilon)^{-1/4}\,\exp\Big(-\tfrac{1}{2\,\varepsilon}\,|x-q_0|^2 + \tfrac{\mathrm{i}}{\varepsilon}\,p_0\cdot(x-q_0)\Big)\,\langle\varphi_0(x)|\,.$$

Then, the initial wave function is in the almost-invariant subspace $\hat{\Pi}^\varepsilon\mathcal{H}$ associated to $e^{(0)}$. The scalar Wigner function $w^{\psi_0}(z) := \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(W^{\psi_0})(z)$ of $\psi_0$ can be computed analytically and satisfies

$$w^{\psi_0}(z) = (\pi\,\varepsilon)^{-1}\,\exp\Big(-\tfrac{1}{\varepsilon}\,|z-(q_0,p_0)|^2\Big)\,,$$

see e.g. [LR10, §3].

We consider an observable $\hat{A}^\varepsilon$ with symbol $A$ taking value in the hermitian matrices over $\mathbb{C}^2$. By (5.32) the quantum mechanical expectation value at time $t > 0$ with respect to the observable $\hat{A}^\varepsilon$ and initial state $\hat{\rho}^{\psi_0} = |\psi_0\rangle\langle\psi_0|$ is approximated by

$$\begin{aligned}\mathrm{tr}_{\mathcal{H}}(\hat{\rho}^{\psi_t}\,\hat{A}^\varepsilon) &= \int_{\mathbb{R}^{2n}} w^{\psi_0}(z)\,\Big(a(\Phi^t_\varepsilon) + \varepsilon^2\,\mathfrak{A}^2(t)\Big)(z)\,\mathrm{d}z + \mathcal{O}(\varepsilon^3)\\ &\approx I^{N_0}(a(\Phi^t_0)) + \varepsilon^2\,I^{N_1}(\widetilde{\mathfrak{A}}^2_2(t))\,.\end{aligned} \tag{7.18}$$

Here, we use quasi-Monte Carlo quadrature, i.e. quadrature nodes $\{z_j\}_{j=1}^M \subset \mathbb{R}^2$ of low star discrepancy with respect to the multivariate normal distribution. Then, for an appropriate $f : \mathbb{R} \times \mathbb{R}^2 \to \mathbb{R}$ the Koksma-Hlawka inequality yields a constant $C = C(f(t)) > 0$ such that

$$\Big| \int_{\mathbb{R}^{2n}} w^{\psi_0}(z)\, f(t,z)\, \mathrm{d}z - \frac{1}{M} \sum_{j=1}^{M} f(t,z_j) \Big| \leq C\, (log(M))^{c_d}\, M^{-1} \qquad (7.19)$$

where $c_d \geq 2$, see e.g. [LR10, §3.2].

Note, in (7.18) we use the approximation scheme that results from the reformulation of Theorem 5.2 derived in Remark 5.5. When applying the numerical scheme to systems with Born-Oppenheimer type Hamiltonian without external Magnetic field then this reformulation has a big impact on the efficiency of the algorithm. The main reason hereto is the following. The simple structure of the canonical Hamiltonian equations of motion $\binom{\dot q}{\dot p} = \binom{p}{-\nabla e^{(0)}(q)}$ allows the use of very effective symplectic integrators. Roughly speaking, this is due to the fact that the r.h.s. of the differential equations for $q(t)$ and $p(t)$ are independent of $q(t)$ or $p(t)$, respectively. Hence, when treating the differential equations for $q(t)$ and $p(t)$ independently then they attain the trivial solutions $q(t) = t\, p_0$ and $p(t) = -t\, \nabla e^{(0)}(q_0)$. This property allows the use of high order splitting schemes. Here, we will use a eighth-order splitting scheme with time-step size $\tau_0$. For details see e.g. [GL14, Section 3.3].

Of course the use of the canonical Hamiltonian equations for the Hamiltonian flow results in additional correction terms. Due to the $\varepsilon^2$ prefactor of all corrections those terms can be approximated rather coarsely to achieve the same overall accuracy. Clearly, this effect is more prominent for smaller $\varepsilon$. Nonetheless, we see in Table 7.2 that even for a relatively large $\varepsilon$ of $0.1$ the run-time for the approximation of the classical Hamiltonian flow $\Phi_0^t$ already excels the run-time to approximate the second order corrections for a given overall accuracy.

Following the procedure in Section 5.2 the corrections $\widetilde{\mathfrak{A}}_2^2(t)$ can be reformulated to

$$\widetilde{\mathfrak{A}}_2^2(t,z) = \sum_{k=0}^{l} \Gamma_k(t,z, D^{m_k} a \circ \Phi_\varepsilon^t(z))$$

where

$$\Gamma_k(t,z) : \mathbb{R}^{\overbrace{2 \times \cdots \times 2}^{m_k-\text{times}}} \to \mathbb{R}$$

are explicitly defined linear mappings from the space of $m_k$-tensors to the real numbers that are independent of $a$. Then, for fixed $z \in \mathbb{R}^2$ the vectorized tensor $\left(\Gamma^k(t,z)\right)_{0\le k\le l}$ denoted by $\vec{\Gamma}(t,z)$ solves a system of initial value problems

$$\frac{\partial}{\partial t}\vec{\Gamma}(t,z) = N(\Phi_0^t(z))\,\vec{\Gamma}(t,z) + b(\Phi_0^t(z)), \qquad \vec{\Gamma}(0,z) = 0$$

where $\vec{\Gamma} : \mathbb{R}\times\mathbb{R}^2 \to \mathbb{R}^{N_\Gamma}, N_\Gamma = \sum_{k=0}^{l} 2^{m_k}$. The components of the Matrix $N : \mathbb{R}^2 \to \mathbb{R}^{N_\Gamma\times N_\Gamma}$ and the vector $b : \mathbb{R}^2 \to \mathbb{R}^{N_\Gamma}$ are given explicitly in terms of the eigenvalues $e^{(i)}$, the eigenfunctions $\varphi_i(x)$, $i = 0,1$ as well as their derivatives. In this work will not state the explicit expressions for $N(z)$ and $b(z)$. An interested reader may follow the procedure of Section 5.2 to determine the expressions. For the expression of the IVP that is associated to the quantum correction

$$2\,\mathrm{i}\int_0^t \{h_0\,, a_0(\Phi_\varepsilon^\tau)\}_3 \circ \Phi_\varepsilon^{t-\tau}\,\mathrm{d}\tau,$$

see [GL14, Section 2.2].

Similar to [GL14], we resort $\vec{\Gamma}(t,z)$ and split it into two parts $\tilde{\Xi}^1(t,z)$, $\Xi^2(t,z) : \mathbb{R}\times\mathbb{R}^2 \to \mathbb{R}^{N_\Gamma/2}$ to transform the system of IVPs into a similar structure as the canonical Hamiltonian equations. This then allows the direct use of higher order splitting schemes. In particular, there exists a $\sigma \in S^{N_\Gamma}$ such that

$$\begin{aligned}\frac{\partial}{\partial t}\begin{pmatrix}\tilde{\Xi}^1(t,z)\\ \Xi^2(t,z)\end{pmatrix} &:= \frac{\partial}{\partial t}\vec{\Gamma}_\sigma(t,z) = N_\sigma(\Phi_0^t(z))\,\vec{\Gamma}_\sigma(t,z) + b_\sigma(\Phi_0^t(z))\\ &=: \begin{pmatrix}\mathbf{0} & \tilde{A}_1(\Phi_q^t(z))\\ \tilde{A}_2(\Phi_q^t(z)) & \mathbf{0}\end{pmatrix}\begin{pmatrix}\tilde{\Xi}^1(t,z)\\ \Xi^2(t,z)\end{pmatrix} + \begin{pmatrix}\tilde{b}^1(\Phi_q^t(z))\\ b^2(\Phi_0^t(z))\end{pmatrix}\end{aligned}$$

where $\vec{\Gamma}_\sigma = \left(\vec{\Gamma}_{\sigma(i)}\right)_{\{1\le i\le N_\Gamma\}}$, $N_\sigma = \left(N_{\sigma(i),j}\right)_{\{1\le i,j\le N_\Gamma\}}$, $b_\sigma = \left(b_{\sigma(i)}\right)_{\{1\le i\le N_\Gamma\}}$, $\tilde{A}_1,\tilde{A}_2 : \mathbb{R}\to\mathbb{R}^{N_\Gamma/2\times N_\Gamma/2}$, $\tilde{b}_1 : \mathbb{R}\to\mathbb{R}^{N_\Gamma/2}$, $b_2 : \mathbb{R}^2\to\mathbb{R}^{N_\Gamma/2}$ and $\Phi_0^t(z) = \left(\Phi_q^t(z),\,\Phi_p^t(z)\right)^T$.

Additionally including the canonical Hamiltonian equations, we get

$$\frac{\partial}{\partial t}\begin{pmatrix}\Xi^0\\ \Xi^1\\ \Xi^2\end{pmatrix} = \begin{pmatrix}0 & A_0 & \mathbf{0}\\ 0 & \mathbf{0} & A_1(\Xi^0)\\ 0 & A_2(\Xi^0) & \mathbf{0}\end{pmatrix}\begin{pmatrix}\Xi^0\\ \Xi^1\\ \Xi^2\end{pmatrix} + \begin{pmatrix}0\\ b^1(\Xi^0)\\ b^2(\Xi^0,\Xi_0^1)\end{pmatrix} \tag{7.20}$$

where $\Xi^0(t,z) = \Phi_q^t(z)$, $\tilde{\Xi}^1(t,z) := \begin{pmatrix} \Phi_p^t(z) \\ \Xi^1(t,z) \end{pmatrix}$, $b^1(q) = \begin{pmatrix} -\nabla e^{(0)}(q) \\ \tilde{b}^1(q) \end{pmatrix}$, $A_0 = (1, \overbrace{0, \dots, 0}^{N_\gamma-\text{times}})$, $A_1(q) = \begin{pmatrix} \mathbf{0} \\ \tilde{A}_1(q) \end{pmatrix}$ and $A_2(q) = (\mathbf{0},\ \tilde{A}_2(q))$.

Note, the above system of IVPs has exactly the same structure as the one in [GL14]. Most importantly we again have that e.g. the r.h.s. of the differential equations for $\Xi^1$ is independent of $\Xi^1$. It follows that we can construct a fourth order splitting scheme in the same way as done in [GL14]. We will skip the details for this step here. To conclude, we obtain an approximation scheme

$$\begin{aligned} \operatorname{tr}_{\mathcal{H}}(\hat{\rho}^{\psi_t}\, \hat{A}^{\varepsilon}) = & \frac{1}{N_0} \sum_{j=1}^{N_0} a(\phi^{\tau_0}(t, z_j^0))) + \frac{\varepsilon^2}{N_1} \sum_{k=0}^{l} \sum_{j=1}^{N_1} \Gamma_k^{\tau_1}(t, z_j^1, D^{m_k} a \circ \phi^{\tau_1}(t, z_j^1)) \\ & + \mathcal{O}\Big((log(N_0))^{c_d}\, N_0^{-1} + \tau_0^9 + \varepsilon^2\, (log(N_1))^{c_d}\, N_1^{-1} + \varepsilon^2\, \tau_1^5 + \varepsilon^3\Big)\,. \end{aligned} \tag{7.21}$$

where $\phi^{\tau_0}(t)$ is the approximation of the Hamiltonian flow using an eighth order splitting scheme with time-step $\tau_0$ and $\Gamma_k^{\tau_1}(t,z,\cdot)$ results from the approximation of the above system of IVPs using a fourth-order splitting scheme with time-step $\tau_1$.

Regarding the quasi-Monte Carlo points $(z_j^0)_{1\le j\le N_0}, (z_j^1)_{1\le j\le N_1} \subset \mathbb{R}^2$: We use the cumulative distribution function of the normal distribution to map Halton points to low star discrepancy points with respect to the normal distribution.

Note, for every quantum system with Born-Oppenheimer type Hamiltonian and without external magnetic field the associated IVP can be brought into the structure (7.20) which allows a numerical treatment with the procedure above. Whenever a magnetic field is present the zero pattern in (7.20) does not hold up. Hence, a direct application of high order splitting schemes is not feasible in this case. Clearly, any other feasible numerical integrator as e.g. a classical Runge-Kuta method may be used. This of course has an impact in the run-time of the algorithm. Nevertheless, we still expect the leading order to be the limiting factor regarding run-time at least for moderately small dimensions and $\varepsilon$.

In what follows we will validate the approach developed above for different observables, namely the position $a(q,p) = q$, second $a(q,p) = q^2$ and third moment $a(q,p) = q^3$. In the validation we will focus mainly on the second order contributions.

As reference we use grid-based solutions computed by a Strang splitting scheme with Fourier collocation (see [LR10, Appendix]). The parameters we used for computing the reference solution are given in Table 7.1. Except for the experiments where we examine a situation where the numerics fails, we use the time interval $[0, 7]$ in all our experiments.

**Table 7.1.** The parameters for the grid-based reference solutions computed by a Strang splitting scheme with Fourier collocation.

| $\varepsilon$ | # time-steps | domain | # grid points |
|---|---|---|---|
| $0.1$ | $1.2 * 10^5$ | $[-5, 20]$ | $4096$ |
| $0.05$ | $3.6 * 10^5$ | $[-5, 20]$ | $4096$ |
| $0.02$ | $3.6 * 10^5$ | $[-5, 20]$ | $4096$ |
| $0.01$ | $1.2 * 10^6$ | $[-5, 20]$ | $4096$ |

In what follows we will present the result of several numerical experiments. We begin with the time-evolution of the quantum mechanical expectation value $\mathrm{tr}_{\mathcal{H}}(\hat{\rho}^{\psi_t}\,\hat{A}^{\varepsilon})$. Figure 7.2 shows the absolute error of the Egorov approximation

$$\mathrm{tr}_{\mathcal{H}}(\hat{\rho}^{\psi_t}\,\hat{A}^{\varepsilon}) \approx \frac{1}{N_0}\sum_{j=1}^{N_0} a(\phi^{\tau_0}(t, z_j^0)) \tag{7.22}$$

and the full approximation (7.21) compared to the position expectation computed from the reference solution for both $\varepsilon = 0.1$ and $\varepsilon = 0.01$. In addition, it is shown how the error evolves when we exclude certain parts form the full approximation. Namely, the corrections resulting from the second order corrections that are incorporated in the $\varepsilon$-dependent classical Hamiltonian system 'no classical', second-order the quantum correction in the semiclassical approximation of Hamiltonians with scalar symbol 'no scalar Q-corr' and the quantum corrections that result from the adiabatic perturbation "no adiabatic Q-corr". We see in both cases $\varepsilon = 0.1$ and $\varepsilon = 0.01$ that the error of the full approximation is almost two orders in $\varepsilon$ smaller than the error of the Egorov approximation this although only an increase in accuracy of order $\varepsilon$ is expected. Also, it seems like the 'scalar' quantum correction has the least influence on the error while the corrections to the Hamiltonian system have the largest. Of course this may just be true for this particular Hamiltonian. The values for the number of sampling points and the time-step sizes are given in Table 7.2. In addition, the run-times for the Egorov algorithm (7.21) and the approximation for the second order correction

$$\mathrm{tr}_{\mathcal{H}}(\hat{\rho}^{\psi_0}\,\mathrm{op}_\varepsilon\left(\mathfrak{A}^2(t)\right)) \approx \frac{1}{N_1}\sum_{k=0}^{l}\sum_{j=1}^{N_1}\Gamma_k^{\tau_1}(t, z_j^1, D^{m_k}a\circ\phi^{\tau_1}(t,z_j^1)) \tag{7.23}$$

are shown. We observe that even for large $\varepsilon = 0.1$ the run-time for the Egorov approximation excels the computing-time for the second order correction. As the dimension of the system of initial value problems to approximate the second-order corrections grows with order three in the dimension $N$ of the configuration space while the dimension of the classical Hamiltonian grows linearly with $N$, the computing time for the quantum corrections excels the computing time of the Egorov algorithm for large $N$ and $\varepsilon$. Nevertheless, for small enough $\varepsilon$ the computing-time of the algorithm to be feasible even for moderately high dimension $N$.

**Table 7.2.** Number of quasi-Monte Carlo points $N_0$ and $N_1$, time-steps $\tau_0$ and $\tau_1$ as well as the run-times $t_0^{\mathrm{elapsed}}$ and $t_1^{\mathrm{elapsed}}$ for the approximation of the leading order (7.22) as well as the second order contributions (7.21) for each value of $\varepsilon$ used in Figure 7.2, Figure 7.3 and Figure 7.4.

| $\varepsilon$ | $N_0$ | $\tau_0$ | $t_0^{\mathrm{elapsed}}$ | $N_1$ | $\tau_1$ | $t_1^{\mathrm{elapsed}}$ |
|---|---|---|---|---|---|---|
| 0.1 | $10^5$ | $7/30/2^1$ | 10.25 sec | 500 | $7/30/2^0$ | 1.51 sec |
| 0.05 | $10^6$ | $7/30/2^1$ | 120.70 sec | $10^3$ | $7/30/2^1$ | 3.96 sec |
| 0.02 | $2\cdot 10^7$ | $7/30/2^1$ | 45.08 min | $10^4$ | $7/30/2^2$ | 52.41 sec |
| 0.01 | $10^8$ | $7/30/2^2$ | 345, 72 min | $5\cdot 10^4$ | $7/30/2^2$ | 203.77 sec |

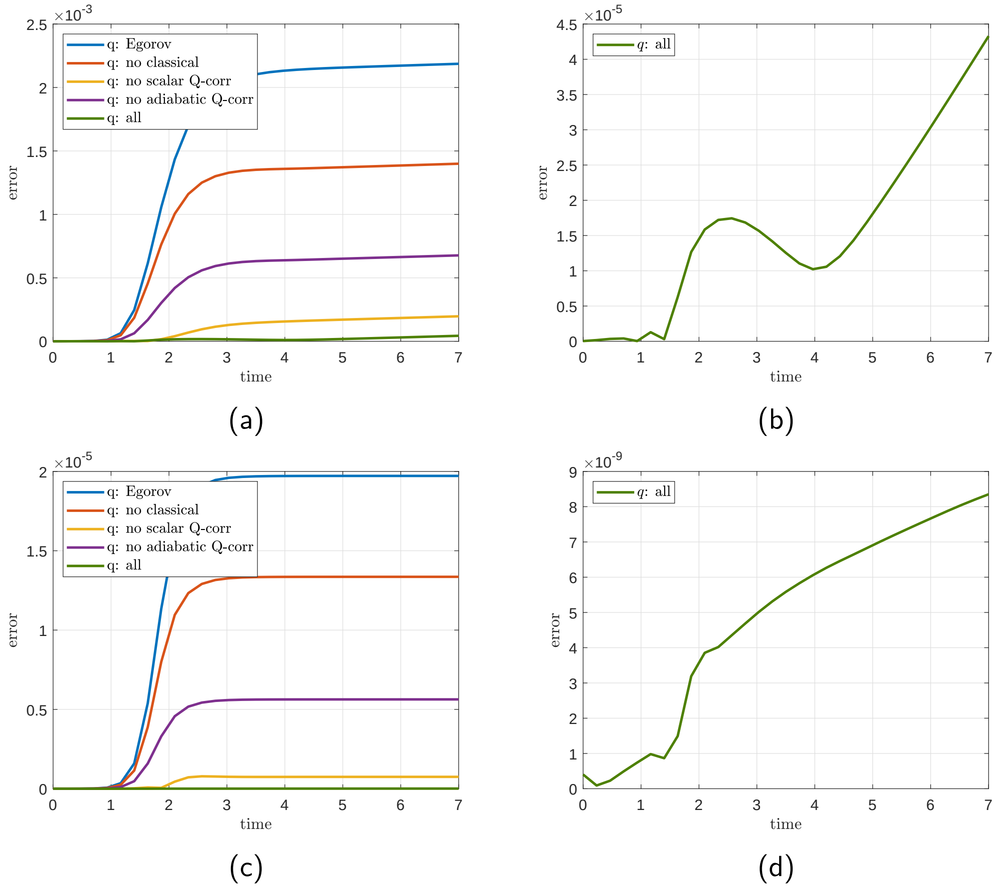
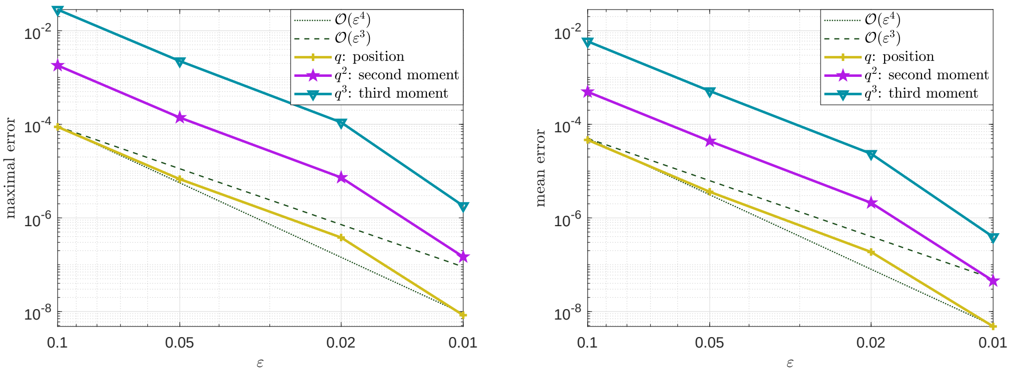



**Figure 7.2.** The error of the expectation values of position for $\varepsilon = 0.1$ (top) and $\varepsilon = 0.01$ (bottom). The figures (b) and (d) show the error for the full approximation (7.21). The figures on the (a) and (c) show the error for the Egorov approximation (7.22), when excluding the correction to the classical Hamiltonian system, when excluding the 'scalar' quantum correction, when excluding the adiabatic quantum correction as well as the full approximation (7.21). For the used values for the number of sampling points and the time-step sizes see Table 7.2. The gap parameter $\delta = 1$.

To verify the asymptotic accuracy, namely that the algorithm (7.21) is of order $\varepsilon^3$, we determine the mean and maximal error over time of the position, second and third moment expectations for $\varepsilon = 0.1, 0.05, 0.02, 0.01$, see Figure 7.3.

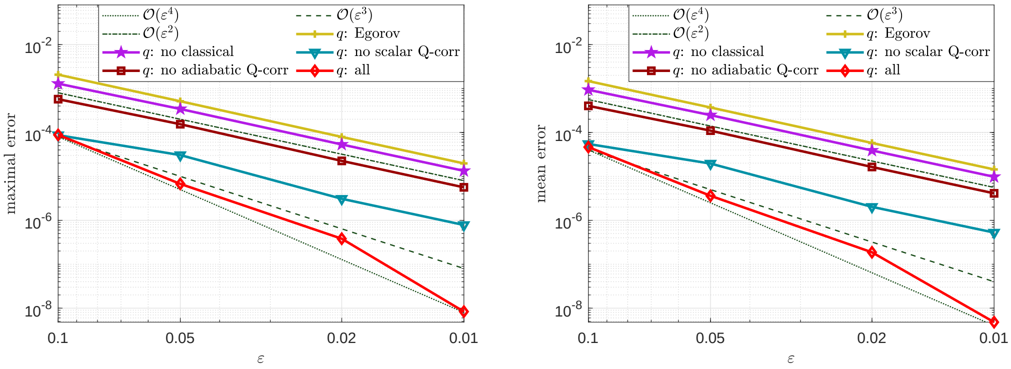



(a) (b)

**Figure 7.3.** The mean (a) and maximal (b) error over time of the expectation value of position, second and third moment as function of $\varepsilon$. The used number of sampling points and step sizes are given in Table 7.2. The gap parameter $\delta = 1$.

Moreover, Figure 7.4 compares the mean and maximal errors over time of the position expectation for $\varepsilon = 0.1, 0.05, 0.02, 0.01$ from the approximation by the Egorov algorithm (7.22), the complete second-order algorithm and the second-order algorithm when omitting corrections to the classical Hamiltonian system, the semi-classical correction for scalar symboled Hamiltonians and the correction from the adiabatic approximation. We observe that only the complete algorithm reaches an asymptotic accuracy of order $\varepsilon^3$, all other algorithms reach only $\varepsilon^2$.

Next, we examine the discretization errors in the approximation of the second order contributions (7.23). Hereto, we present the mean and maximal error over time of the expectation value of position, second and third moment for $\varepsilon = 0.01$ as function of the number of sampling points $N_1$ Figure 7.5 and the time-step size $\tau_1$ Figure 7.6. While we use a time-step size of $\tau_1 = 7/30/2^2$ in the analysis of the $N_1$-dependence, we chose the number of sampling points $N_1$ in the examination of the $\tau_1$-dependence as $N_1 = 5 * 10^4$. For the approximation of the leading order we use $N_0 = 10^8$ sampling points and a time-step size $\tau_0 = 7/30/2^2$. We observe that the mean and also the maximum error decrease with an order of $1/N_1$ in the number of sampling points until they reach a lower bond of order $\varepsilon^3$. Regarding the time-step



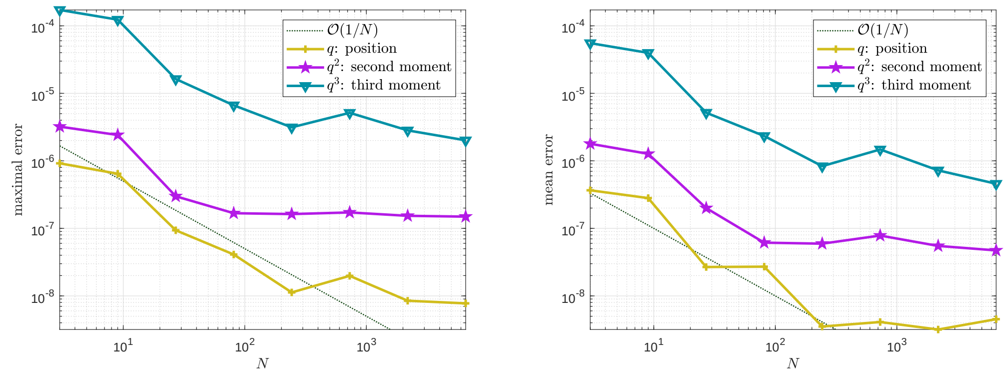

(a) (b)

**Figure 7.4.** The mean (a) and maximal (b) error over time of the expectation value of position as function of $\varepsilon$ for only leading order contribution (7.22), without second order contributions for the $\varepsilon$-dependent classical Hamiltonian system, without semiclassic quantum correction, without adiabatic quantum correction as well as the full approximation (7.21). The discretization parameters are presented in Table 7.2. The gap parameter $\delta = 1$.

size, we see that the degression of the mean as well as maximal error does not quite reach an order of $\tau_1^5$ but is slightly better than order $\tau_1^4$.

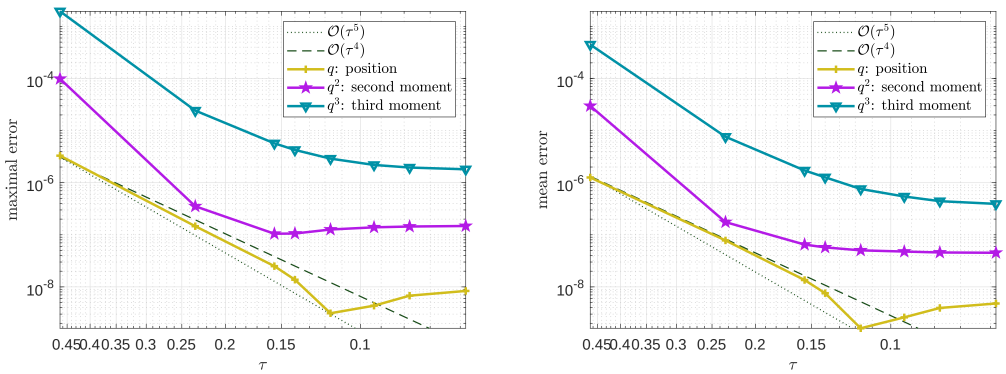
In Figure 7.7 we compare the maximal error over time of the expectation value of position as function of $\varepsilon$ for both, $\delta = 0.5$ and $\delta = 1$. We observe that due to poor adiabatic decoupling for small gap $\delta$ and large large $\varepsilon$ we do not reach an order $\varepsilon^3$ error. In this case, the second order corrections show no improvement over the leading order approximation. We even see that for $\varepsilon = 0.1$ and $\delta = 0.5$ the error of the Egorov algorithm (7.22) shows a slightly smaller maximal error compared to the error of the full second-order approximation (7.21). Nevertheless, as one expects the error decreases rapidly as $\varepsilon$ gets smaller and is of order $\varepsilon^3$ once $\varepsilon$ is smaller than $0.02$.

In Figure 7.8 we see a situation where the numerics of the algorithm fails. Here, we consider a Gaussian wave-packet centered at $(q_0, p_0) = (-3, 0.91)$ where the total energy $h_0(q_0, p_0) = \frac{p_0^2}{2} + e^{(0)}(q_0)$ satisfies $h_0(q_0, p_0) \approx -1 = h_0(0, 0) = -\delta$. So, roughly speaking the average particle just reaches the maximum of the potential $e^{(0)}$ and the wave-packet splits into two parts after reaching the maximimum of the potential $e^{(0)}$, one moving to the 'left' and the other to the 'right' of the maximum. We see in Figure 7.8a that the error resulting from the full second-order algorithm (7.21) rises to order $10^6$ while the error of the leading order approximation is of order $10^{-3}$. Removing the 'scalar' quantum correction from the approximation reduces the error significantly (see Figure 7.8b) but also the 'adiabatic' quantum



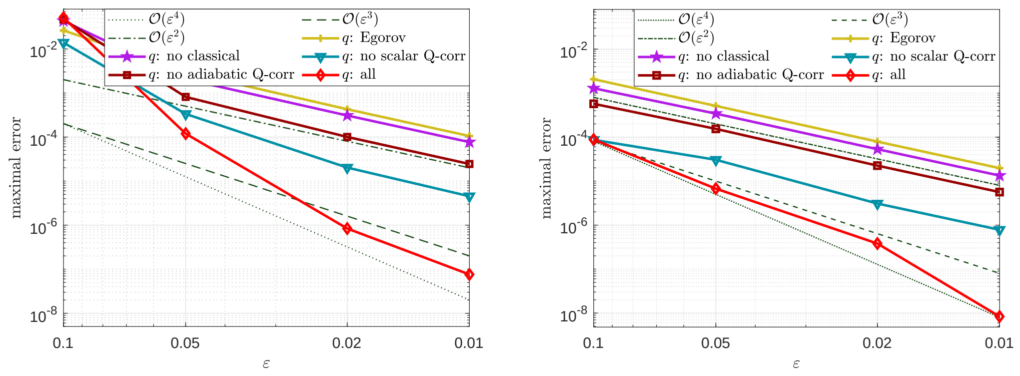

(a) (b)

**Figure 7.5.** The mean (a) and maximal (b) error over time of the expectation value of position, second and third moment as function of the number of sampling points $N_1$. The semiclassical parameter is chosen as $\varepsilon = 0.01$, the gap size $\delta = 1$ and the time-step size $\tau_1 = 7/30/2^2$. For the leading order approximation $N_0 = 10^8$ sampling points and a step size of $\tau_0 = 7/30/2^2$ are used. In both plots the error decreases with order $N_1^{-1}$ until the lower bound of order $\varepsilon^3$ is reached.




(a) (b)

**Figure 7.6.** The mean (a) and maximal (b) error over time of the expectation value of position, second and third moment as function of the time-step size $\tau_1$. The semiclassical parameter is chosen as $\varepsilon = 0.01$, the gap size $\delta = 1$ and the number of sampling points $N_1 = 5 * 10^4$. In both plots the error decreases with order slightly worse than $\tau_1^5$ until the lower bound of order $\varepsilon^3$ is reached.




(a) (b)

**Figure 7.7.** The maximal error over time of the expectation value of position as function of $\varepsilon$ with gap (a) $\delta = 0.5$ and (b) $\delta = 1$ for only leading order contribution (7.22), without second order contributions for the $\varepsilon$-dependent classical Hamiltonian system, without semiclassic quantum correction, without adiabatic quantum correction as well as the full approximation (7.21). For large $\varepsilon$ and small gap $\delta = 0.5$ the error is relatively large as the two adiabatic subspaces associated to the eigenvalues $e^{(0)}$ and $e^{(1)}$ are not well decoupled. The used number of sampling points and step sizes are given in Table 7.2.

correction contributes to a relatively large error when comparing to the Egorov algorithm (7.22).

So, where does the numerics fail in such a situation? Recall that in the approximation of the second-order corrections we approximate the phase space integral

$$\begin{aligned} \operatorname{tr}_{\mathcal{H}}(\hat{\rho}^{\psi_0} \operatorname{op}_\varepsilon \big(\mathfrak{A}^2(t)\big)) &= \int_{\mathbb{R}^{2n}} w^{\psi_0}(z)\, \mathfrak{A}^2(t,z)\, \mathrm{d}z \\ &= \sum_{k=0}^{l} \int_{\mathbb{R}^{2n}} w^{\psi_0}(z)\, \Gamma_k(t,z,D^{m_k} a \circ \Phi_\varepsilon^t(z))\, \mathrm{d}z \end{aligned}$$

using a quasi-Monte Carlo method. Here, it is important to know that the constant $C = C(f(t))$ in the Koksma-Hlawka inequality (7.19) depends on the variation of the integrand $f(t)$. This means that the quasi-Monte Carlo method looses accuracy with large variation of the integrand which of course makes sense considering the nature of Monte Carlo type methods. The occurrence of such large variations in the integrand $w^{\psi_0}(z)\, \Gamma_k(t,z,D^{m_k} a \circ \Phi_\varepsilon^t(z))$ is exactly the issue here. To exemplify the issue in place we select a particular $\Gamma_i(t,z,D^{m_i} a \circ \Phi_\varepsilon^t(z))$ that stems from the second-order quantum

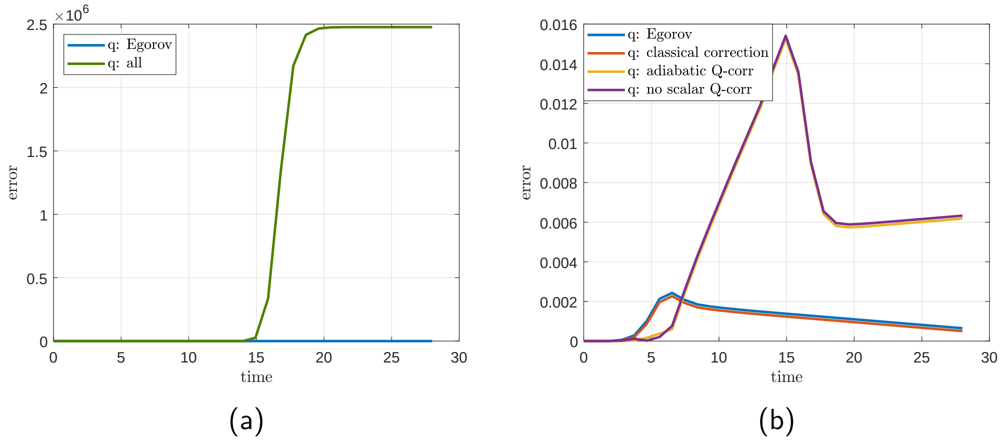



**Figure 7.8.** The error of the expectation values of position for $\varepsilon = 0.05$ and $\delta = 1$. The initial wave-function $\psi_0$ is a Gaussian wave-packet centered at $(q_0, p_0) = (-3, 0.91)$. Figure (a) compares the error of the leading order approximation (7.22) with the error of the full second-order algorithm (7.21). Figure (b) shows the errors of the leading order approximation (7.22), the approximation with only the second-order correction to the classical Hamiltonian system, the approximation with only the adiabatic quantum correction and the approximation with classical and adiabatic quantum correction. For semiclassical approximation $N_0 = 10^6$ and $N_1 = 10^4$ particles and time-step sizes $\tau_0 = 7/30/2^3$ and $\tau_1 = 7/30/2^2$ are used.

correction in the semiclassical approximation for Hamiltonians with scalar symbol. So, there is a $0 \leq i \leq l$ such that

$$\Gamma_i(t, z, D^{m_i} a \circ \Phi^t_\varepsilon(z)) \\ = -\frac{1}{24}\left(Da \circ \Phi^t\right)_i \int_0^t \left[\left(D^3\Phi^\tau\right)_{ijkl}\left(JD^3 h_0\right)_{lkj}\right] \circ \Phi(t-\tau, z)d\tau \,,$$

see [GL14, Theorem 2.1]. Note, all $\Gamma_i(t, z, D^{m_i} a \circ \Phi^t_\varepsilon(z))$ are quite of this form and in particular include an expression of the form $D^m_{q,p}\Phi^\tau$ where the 'scalar' correction is the only expressions that includes a third order derivative of the Hamiltonian flow with respect to the initial configuration. Now, choose a particle with initial configuration $(q_0, p_0)$ where the total energy $h_0(q_0, p_0)$ satisfies $h_0(q_0, p_0) = \frac{p_0^2}{2} + e^{(0)}(q_0) = h(0, 0) = -\delta$. Then the particle reaches exactly and stays at the unstable maximum of the potential $e^{(0)}$, i.e. $\Phi^t(q_0, p_0) = \Phi^{t_0}(q_0, p_0) = (0, 0)$ for $t \geq t_0$. However, an arbitrary small perturbation to the initial configuration lets the particle 'fall' from the maximum left or right, see Figure 7.9. Therefore, the derivative $D_{q,p}\Phi^t(q_0, p_0)$ increases rapidly in time $t$ once the particle gets close to $\Phi^t(q, p) \approx (0, 0)$. On the other hand, most particles never reach the configuration $\Phi^t(q, p) \approx (0, 0)$ as their total energy $h_0(q_0, p_0)$ is either larger or smaller than $-\delta$ and therefore the derivative $D_{q,p}\Phi^t(q_0, p_0)$ stays relatively small for such particles. Clearly, this effect increases with the order of derivatives acting on the Hamiltonian flow $\Phi^t(q_0, p_0)$. To conclude, there is a neighborhood of the set $M = \{(q_0, p_0) \in \mathbb{R}^2 : h_0(q_0, p_0) = -\delta, \operatorname{sgn}(q_0 * p_0) = -1\}$ where the derivatives $D^m_{q,p}\Phi^\tau$ and thus also $\Gamma_i(t, z, D^{m_i} a \circ \Phi^t_\varepsilon(z))$ get very large for some time $t > 0$ while outside this neighborhood the magnitude of these functions is relatively small. The quasi-Monte Carlo method can not cope with these large variations at least not with a reasonable number of particles.

To support the above explanation, in Figure 7.10, we show the error when excluding all particles with total energy $|h_0(q_0, p_0) + \delta| < 0.1$ from the Monte Carlo integration. We see that this exclusion of particles leads to significant reduction of the error. Clearly, we will not reach an order $\varepsilon^3$ accuracy by simply excluding 'critical' particles. As the modified classical Hamiltonian system $(h, \omega^\varepsilon)$ has it's maximum of the total energy at a slightly different place in phase space, it is worth considering the algorithm (5.26) resulting from our original Egorov theorem for these 'critical' particles. Nevertheless, as the correction of the total energy is only of order $\varepsilon^2$ it is not clear whether this approach leads to a significant improvement. So, at this point it is not clear how to solve this issue and we have no aspiration to so within this work.

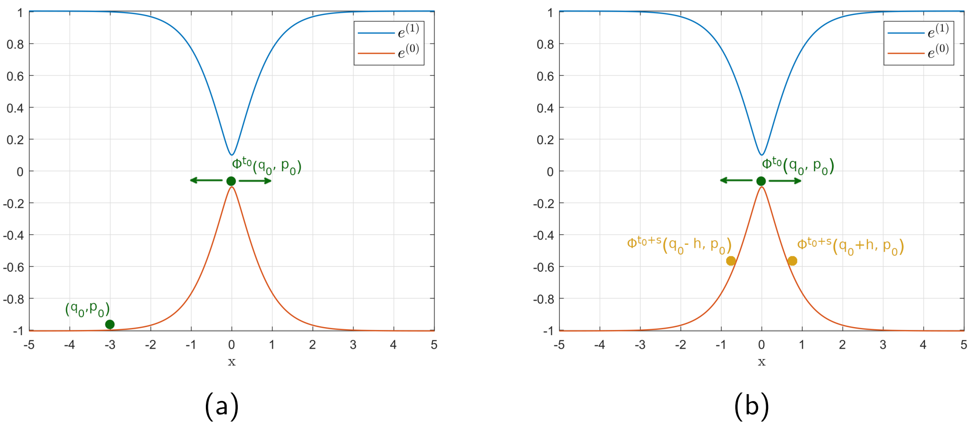



**Figure 7.9.** Sketch of the classical evolution $\Phi^t(q_0, p_0)$ of a particle with (a) initial configuration $(q_0, p_0)$ and (b) perturbed initial configuration $(q_0 \pm h, p_0)$, $h > 0$ where the total energy $h_0(q_0, p_0)$ satisfies $h_0(q_0, p_0) = \frac{p_0^2}{2} + e^{(0)}(q_0) = h(0, 0) = -\delta$ for gap parameter $\delta = 0.1$. For initial configuration $(q_0, p_0)$ the particle stays at the unstable maximum of the potential $e^{(0)}$, i.e. $\Phi^t(q_0, p_0) = \Phi^{t_0}(q_0, p_0) = (0, 0)$ for $t \geq t_0$. On the contrary, for an arbitrary small perturbation $h$ of the initial configuration $(q_0, p_0)$ the particle will 'drop' left or right of the maximum for $t > t_0$.

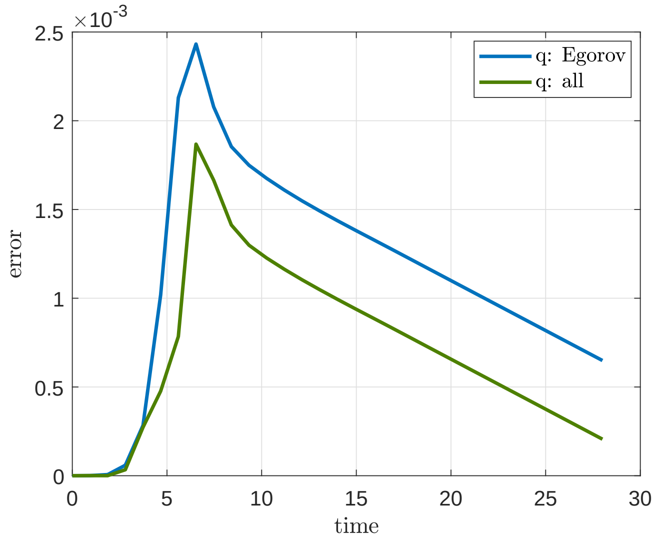



**Figure 7.10.** The error of the expectation values of position for $\varepsilon = 0.05$ and $\delta = 1$. The initial wave-function $\psi_0$ is Gaussian wave-packet centered at $(q_0, p_0) = (-3, 0.91)$. In the approximation of the quantum corrections all particles satisfying $|h_0(q_0, p_0) + \delta| < 0.1$ were excluded. We compare the error of the leading order approximation (7.22) with the error of the full second-order algorithm (7.21). For the semiclassical approximation $N_0 = 10^6$ and $N_1 = 10^4$ particles are used where through the exclusion of particle only $4832$ particles affect the approximation of the quantum corrections. The time-step sizes are $\tau_0 = 7/30/2^3$ and $\tau_1 = 7/30/2^2$.

# Technical Lemmata

# A

This chapter consists of a collection of technical lemmata used in the general Chapters 2-5. Lemmata A.1 and A.7 are used in the derivation of trace formulae for the Lebesgue density of Liouville measures, Section 2.2. Lemma A.1 applied in the derivation of effective operators. The results of Lemmata A.8 - A.10 are needed for the error estimates of the approximation by effective operators. Lemma A.11 is used in the error estimate of the semiclassical approximation of equilibrium states.

**Lemma A.1** *Let $k \in \mathbb{N}$ and $m_1, \ldots, m_k \in \{1, \ldots, 2n\}$. In addition, we assume $B^1, \ldots, B^k \in \mathbb{R}^{2n\times 2n}$ to be skew-symmetric matrices. Then, the matrix $\Lambda^k_{m_1,\ldots,m_{k-1}}(B^1, \ldots, B^k)$ as defined by (2.25) is skew-symmetric.*

PROOF We proof the skew-symmetry of $\Lambda^k$ by induction over $k$. So let $B^1 \in \mathbb{R}^{2n\times 2n}$ be skew-symmetric then $\Lambda^1_{i,j}(B^1) := B^1_{i\,j}$ is skew-symmetric. For $k = 2$, let $B^1, B^2 \in \mathbb{R}^{2n\times 2n}$ be skew-symmetric matrices and $m_1 \in \{1, \ldots .2n\}$. By the skew-symmetry of $B^1, B^2$ as well as $\omega^0$

$$\begin{aligned}
\Lambda^2_{m_1;j,i}(B^1, B^2) &= B^2_{j\,m_1}\, \omega^0_{m_1\,\lfloor m_1+n\rfloor_{2n}}\, B^1_{\lfloor m_1+n\rfloor_{2n}\, i} \\
&\quad + B^1_{j\,\lfloor m_1+n\rfloor_{2n}}\, \omega^0_{\lfloor m_1+n\rfloor_{2n}\, m_1}\, B^2_{m_1\, i} \\
&= -\, B^1_{i\,\lfloor m_1+n\rfloor_{2n}}\, \omega^0_{\lfloor m_1+n\rfloor_{2n}\, m_1}\, B^2_{m_1\, j} \\
&\quad -\, B^2_{i\,m_1}\, \omega^0_{m_1\,\lfloor m_1+n\rfloor_{2n}}\, B^1_{\lfloor m_1+n\rfloor_{2n}\, j} \\
&= -\, \Lambda^2_{m_1;i,j}(B^1, B^2)\,.
\end{aligned}$$

Now, assume $\Lambda^r_{m_1,\ldots,m_{r-i};i,j}(B^1, \ldots, B^r)$ to be skew-symmetric for $r < k$ we prove it for $k$. By definition

$$\Lambda^k_{m_1,\ldots,m_{k-1}}(B^1, \ldots, B^k) = \sum_{l=1}^{k-1} \Lambda^{k-1}_{m_1,\ldots,m_{k-2}}(B^1, \ldots, \Lambda^2_{m_{k-1}}(B^l, B^k), \ldots, B^{k-1})\,.$$

By induction assumption $\Lambda^2_{m_{k-1}}(B^l, B^k)$ is skew-symmetric for every $1 \le l \le k-1$. Then, also

$$\Lambda^{k-1}_{m_1,\ldots,m_{k-2}}(B^1, \ldots, \Lambda^2_{m_{k-1}}(B^l, B^k), \ldots, B^{k-1}) \quad \text{for} \quad 1 \le l \le k-1$$

is skew-symmetric by assumption. We conclude that $\Lambda^k_{m_1,\dots,m_{k-1}}(B^1,\dots,B^k)$ is skew-symmetric as a sum of skew-symmetric matrices.

Let $B^1,\dots,B^k \in \mathbb{R}^{2n\times 2n}$ and for $k \le n$, $\sigma \in S_k$ a permutation of $\{1,\dots,k\}$ and $L = \{I+n\}$, $I \subset \{1,\dots,n\}$, $|I| = k$. $\square$

**Lemma A.2** *Let $\Omega \in \mathbb{R}^{2n\times 2n}$ skew-symmetric and $m_1,\dots,m_k \in \{1,\dots,2n\}$. In addition, let $r \in \mathbb{N}$, $l_1,\dots,l_r \in \{1,\dots,k\}$ and $\alpha \in \{\uparrow,\downarrow\}^r$. We will show some important properties of the short notation introduced in (2.50)-(2.51).*

*We have*

$$l_1^{\alpha_1}\, l_1^{\overline{\alpha_1}} = 0 \tag{A.1}$$

*as well as*

$$\mathrm{Tr}_{l_1^{\alpha_1}}\left(l_2^{\alpha_2}\, l_3^{\alpha_3}\cdots l_r^{\alpha_r}\, l_1^{\overline{\alpha_1}}\right) = 0\,. \tag{A.2}$$

*The trace is cyclic in the sense that*

$$\mathrm{Tr}_{l_1^{\alpha_1}}\left(l_2^{\alpha_2}\, l_3^{\alpha_3}\cdots l_r^{\alpha_r}\right) = \mathrm{Tr}_{l_r^{\alpha_r}}\left(l_1^{\alpha_1}\, l_2^{\alpha_2}\cdots l_{r-1}^{\alpha_{r-1}}\right). \tag{A.3}$$

*The trace is symmetric in the sense that*

$$\mathrm{Tr}_{l_1^{\alpha_1}}\left(l_2^{\alpha_2}\, l_3^{\alpha_3}\cdots l_r^{\alpha_r}\right) = \mathrm{Tr}_{l_r^{\overline{\alpha_r}}}\left(l_{r-1}^{\overline{\alpha_{r-1}}}\, l_{r-2}^{\overline{\alpha_{r-2}}}\cdots l_2^{\overline{\alpha_2}}\, l_1^{\overline{\alpha_1}}\right). \tag{A.4}$$

*In case there are two equal symbols contained in a trace then the trace can be split into two traces, i.e.*

$$\mathrm{Tr}_{l_1^{\alpha_1}}\left(l_2^{\alpha_2}\cdots l_{s-1}^{\alpha_{s-1}}\, l_1^{\alpha_1}\, l_{s+1}^{\alpha_{s+1}}\cdots l_r^{\alpha_r}\right) = \mathrm{Tr}_{l_1^{\alpha_1}}\left(l_2^{\alpha_2}\cdots l_{s-1}^{\alpha_{s-1}}\right)\mathrm{Tr}_{l_1^{\alpha_1}}\left(l_{s+1}^{\alpha_{s+1}}\cdots l_r^{\alpha_r}\right) \tag{A.5}$$

*for any let $1 < s <= r$. The part in between two symbols with equal index and inverted direction is skew-symmetric in the sense that for $1 < s <= r$*

$$\begin{aligned}
&\mathrm{Tr}_{l_1^{\alpha_1}}\left(l_2^{\alpha_2}\cdots l_{s-1}^{\alpha_{s-1}}\, l_1^{\overline{\alpha_1}}\, l_{s+1}^{\alpha_{s+1}}\cdots l_r^{\alpha_r}\right)\\
&\quad= -\mathrm{Tr}_{l_1^{\alpha_1}}\left(l_{s-1}^{\overline{\alpha_{s-1}}}\, l_{s-2}^{\overline{\alpha_{s-2}}}\cdots l_2^{\overline{\alpha_2}}\, l_1^{\overline{\alpha_1}}\, l_{s+1}^{\alpha_{s+1}}\cdots l_r^{\alpha_r}\right)\\
&\quad= -\mathrm{Tr}_{l_1^{\alpha_1}}\left(l_2^{\alpha_2}\cdots l_{s-1}^{\alpha_{s-1}}\, l_1^{\overline{\alpha_1}}\, l_r^{\overline{\alpha_r}}\, l_{r-1}^{\overline{\alpha_{r-1}}}\cdots l_{s+1}^{\overline{\alpha_{s+1}}}\right)\\
&\quad= \mathrm{Tr}_{l_1^{\alpha_1}}\left(l_{s-1}^{\overline{\alpha_{s-1}}}\, l_{s-2}^{\overline{\alpha_{s-2}}}\cdots l_2^{\overline{\alpha_2}}\, l_1^{\overline{\alpha_1}}\, l_r^{\overline{\alpha_r}}\, l_{r-1}^{\overline{\alpha_{r-1}}}\cdots l_{s+1}^{\overline{\alpha_{s+1}}}\right).
\end{aligned} \tag{A.6}$$

PROOF Let $\Omega \in \mathbb{R}^{2n\times 2n}$ skew-symmetric and $m_1, \ldots, m_k \in \{1, \ldots, 2n\}$. To show (A.1) assume $l_1 \in \{1, \ldots, k\}$ and $\alpha_1 =\downarrow$. Then,

$$(l_1^{\alpha_1}\, l_1^{\overline{\alpha_1}})_{ji} = \Omega_{j\, m_1}\, \omega^0_{m_1\, \lfloor m_1+n\rfloor_{2n}}\, \Omega_{\lfloor m_1+n\rfloor_{2n}\, \lfloor m_1+n\rfloor_{2n}}\, \omega^0_{\lfloor m_1+n\rfloor_{2n}\, m_1}\, \Omega_{m_1\, i} = 0$$

by the skew-symmetry of $\Omega$. It's easy to see that the same result holds for the case where $\alpha_1 =\uparrow$. Note that in the following we will use the symbol $(\cdot)$ as placeholder for indices that are not important for the argument. Let $r \in \mathbb{N}$, $l_1, \ldots, l_r \in \{1, \ldots, k\}$ and $\alpha \in \{\uparrow, \downarrow\}^r$ with $\alpha_1 =\downarrow$

$$\begin{aligned}
&\mathrm{Tr}_{l_1^{\alpha_1}}\left(l_2^{\alpha_2}\, l_3^{\alpha_3} \cdots l_r^{\alpha_r}\, l_1^{\overline{\alpha_1}}\right) \\
&\quad = \omega^0_{m_1\, \lfloor m_1+n\rfloor_{2n}}\, \Omega_{\lfloor m_1+n\rfloor_{2n}\, (\cdot)} \cdots \Omega_{(\cdot)\, \lfloor m_1+n\rfloor_{2n}}\, \omega^0_{\lfloor m_1+n\rfloor_{2n}\, m_1}\, \Omega_{m_1\, m_1} \\
&\quad = 0
\end{aligned}$$

where we again used the skew-symmetry of $\Omega$. Obviously, the analogous holds for the case where $\alpha_1 =\uparrow$ which proves (A.2).

Regarding (A.3), let $r \in \mathbb{N}$, $l_1, \ldots, l_r \in \{1, \ldots, k\}$ and $\alpha \in \{\uparrow, \downarrow\}^r$ with $\alpha_1 = \alpha_2 = \alpha_r =\downarrow$ then

$$\begin{aligned}
&\mathrm{Tr}_{l_1^{\alpha_1}}\left(l_2^{\alpha_2}\, l_3^{\alpha_3} \cdots l_r^{\alpha_r}\right) \\
&\quad = \omega^0_{m_1\, \lfloor m_1+n\rfloor_{2n}}\, \Omega_{\lfloor m_1+n\rfloor_{2n}\, m_2}\, \omega^0_{m_2\, \lfloor m_2+n\rfloor_{2n}}\, \Omega_{\lfloor m_2+n\rfloor_{2n}\, (\cdot)} \cdots \\
&\qquad \Omega_{(\cdot)\, m_r}\, \omega^0_{m_r\, \lfloor m_r+n\rfloor_{2n}}\, \Omega_{\lfloor m_r+n\rfloor_{2n}\, m_1} \\
&\quad = \omega^0_{m_2\, \lfloor m_2+n\rfloor_{2n}}\, \Omega_{\lfloor m_2+n\rfloor_{2n}\, (\cdot)} \cdots \\
&\qquad \Omega_{(\cdot)\, m_r}\, \omega^0_{m_r\, \lfloor m_r+n\rfloor_{2n}}\, \Omega_{\lfloor m_r+n\rfloor_{2n}\, m_1}\, \omega^0_{m_1\, \lfloor m_1+n\rfloor_{2n}}\, \Omega_{\lfloor m_1+n\rfloor_{2n}\, m_2} \\
&\quad = \mathrm{Tr}_{l_2^{\alpha_2}}\left(l_3^{\alpha_3} \cdots l_r^{\alpha_r}\, l_1^{\alpha_1}\right).
\end{aligned}$$

Clearly, the analogous holds for arbitrary $\alpha_1, \alpha_2, \alpha_r \in \{\uparrow, \downarrow\}$.

Now, let $r \in \mathbb{N}$, $l_1, \ldots, l_r \in \{1, \ldots, k\}$ and $\alpha \in \{\uparrow, \downarrow\}^r$ with $\alpha_1 = \alpha_r =\downarrow$ then

$$\begin{aligned}
\mathrm{Tr}_{l_1^{\alpha_1}}\left(l_2^{\alpha_2}\, l_3^{\alpha_3} \cdots l_r^{\alpha_r}\right) &= \omega^0_{m_1\, \lfloor m_1+n\rfloor_{2n}}\, \Omega_{\lfloor m_1+n\rfloor_{2n}\, (\cdot)} \cdots \\
&\qquad \Omega_{(\cdot)\, m_r}\, \omega^0_{m_r\, \lfloor m_r+n\rfloor_{2n}}\, \Omega_{\lfloor m_r+n\rfloor_{2n}\, m_1}.
\end{aligned}$$

All the $2r$ matrices occurring in the above equation are skew-symmetric. Thus, reversing the order of the matrices and transposing each matrix leads to

$$\begin{aligned}
&\omega^0_{m_1\, \lfloor m_1+n\rfloor_{2n}}\, \Omega_{\lfloor m_1+n\rfloor_{2n}\, (\cdot)} \cdots \Omega_{(\cdot)\, m_r}\, \omega^0_{m_r\, \lfloor m_r+n\rfloor_{2n}}\, \Omega_{\lfloor m_r+n\rfloor_{2n}\, m_1} \\
&\quad = \Omega_{m_1\, \lfloor m_r+n\rfloor_{2n}}\, \omega^0_{\lfloor m_r+n\rfloor_{2n}\, m_r}\, \Omega_{m_r\, (\cdot)} \cdots \Omega_{(\cdot)\, \lfloor m_1+n\rfloor_{2n}}\, \omega^0_{\lfloor m_1+n\rfloor_{2n}\, m_1}.
\end{aligned}$$

Finally, moving $\Omega_{m_1\,\lfloor m_r+n\rfloor_{2n}}$ from the first to the last position in the result above yields

$$\begin{aligned}
&\Omega_{m_1\,\lfloor m_r+n\rfloor_{2n}}\,\omega^0_{\lfloor m_r+n\rfloor_{2n}\,m_r}\,\Omega_{m_r\,(\cdot)}\,\cdots\,\Omega_{(\cdot)\,\lfloor m_1+n\rfloor_{2n}}\,\omega^0_{\lfloor m_1+n\rfloor_{2n}\,m_1}\\
&\qquad=\omega^0_{\lfloor m_r+n\rfloor_{2n}\,m_r}\,\Omega_{m_r\,(\cdot)}\,\cdots\,\Omega_{(\cdot)\,\lfloor m_1+n\rfloor_{2n}}\,\omega^0_{\lfloor m_1+n\rfloor_{2n}\,m_1}\,\Omega_{m_1\,\lfloor m_r+n\rfloor_{2n}}\\
&\qquad=\mathrm{Tr}_{l_r^{\overline{\alpha_r}}}\left(l_{r-1}^{\overline{\alpha_{r-1}}}\,l_{r-2}^{\overline{\alpha_{r-2}}}\cdots l_2^{\overline{\alpha_2}}\,l_1^{\overline{\alpha_1}}\right)
\end{aligned}$$

Combining the three results above shows (A.4) for the special case where $\alpha_1=\alpha_r=\downarrow$. As before, the result clearly holds for any $\alpha_1,\alpha_r\in\{\downarrow,\uparrow\}$.

Regarding (A.5), let $r\in\mathbb{N}$, $1<s<=r$, $l_1,\ldots,l_r\in\{1,\ldots,k\}$ and $\alpha\in\{\uparrow,\downarrow\}^r$ with $\alpha_1=\alpha_{s-1}=\alpha_r=\downarrow$. Then,

$$\begin{aligned}
&\mathrm{Tr}_{l_1^{\alpha_1}}\left(l_2^{\alpha_2}\cdots l_{s-1}^{\alpha_{s-1}}\,l_1^{\alpha_1}\,l_{s+1}^{\alpha_{s+1}}\cdots l_r^{\alpha_r}\right)\\
&\qquad=\omega^0_{m_1\,\lfloor m_1+n\rfloor_{2n}}\,\Omega_{\lfloor m_1+n\rfloor_{2n}\,(\cdot)}\,\cdots\,\Omega_{(\cdot)\,m_{s-1}}\,\omega^0_{m_{s-1}\,\lfloor m_{s-1}+n\rfloor_{2n}}\,\Omega_{\lfloor m_{s-1}+n\rfloor_{2n}\,m_1}\\
&\qquad\quad\omega^0_{m_1\,\lfloor m_1+n\rfloor_{2n}}\,\Omega_{\lfloor m_1+n\rfloor_{2n}\,(\cdot)}\,\cdots\,\Omega_{(\cdot)\,m_r}\,\omega^0_{m_r\,\lfloor m_r+n\rfloor_{2n}}\,\Omega_{\lfloor m_r+n\rfloor_{2n}\,m_1}\\
&\qquad=\mathrm{Tr}_{l_1^{\alpha_1}}\left(l_2^{\alpha_2}\cdots l_{s-1}^{\alpha_{s-1}}\right)\mathrm{Tr}_{l_1^{\alpha_1}}\left(l_{s+1}^{\alpha_{s+1}}\cdots l_r^{\alpha_r}\right)
\end{aligned}$$

which is true for any $\alpha_1,\alpha_{s-1},\alpha_r\in\{\downarrow,\uparrow\}$. Note that in the special case where $s=r$ we get

$$\mathrm{Tr}_{l_1^{\alpha_1}}\left(l_2^{\alpha_2}\cdots l_{r-1}^{\alpha_{r-1}}\,l_1^{\alpha_1}\right)=\mathrm{Tr}_{l_1^{\alpha_1}}\left(l_2^{\alpha_2}\cdots l_{r-1}^{\alpha_{r-1}}\right)\mathrm{Tr}_{l_1^{\alpha_1}}\left(\right)$$

which is consistent with our notation.

What is left is to show (A.6). Let $r\in\mathbb{N}$, $1<s<=r$, $l_1,\ldots,l_r\in\{1,\ldots,k\}$ and $\alpha\in\{\uparrow,\downarrow\}^r$ with $\alpha_1=\alpha_2=\alpha_{s-1}=\alpha_r=\downarrow$.

$$\begin{aligned}
&\mathrm{Tr}_{l_1^{\alpha_1}}\left(l_2^{\alpha_2}\cdots l_{s-1}^{\alpha_{s-1}}\,l_1^{\overline{\alpha_1}}\,l_{s+1}^{\alpha_{s+1}}\cdots l_r^{\alpha_r}\right)\\
&\qquad=\omega^0_{m_1\,\lfloor m_1+n\rfloor_{2n}}\,\Omega_{\lfloor m_1+n\rfloor_{2n}\,m_2}\,\omega^0_{m_2\,\lfloor m_2+n\rfloor_{2n}}\,\Omega_{\lfloor m_2+n\rfloor_{2n}\,(\cdot)}\,\cdots\\
&\qquad\quad\Omega_{(\cdot)\,m_{s-1}}\,\omega^0_{m_{s-1}\,\lfloor m_{s-1}+n\rfloor_{2n}}\,\Omega_{\lfloor m_{s-1}+n\rfloor_{2n}\,\lfloor m_1+n\rfloor_{2n}}\\
&\qquad\quad\omega^0_{\lfloor m_1+n\rfloor_{2n}\,m_1}\,\Omega_{m_1\,(\cdot)}\,\cdots\,\Omega_{(\cdot)\,m_r}\,\omega^0_{m_r\,\lfloor m_r+n\rfloor_{2n}}\,\Omega_{\lfloor m_r+n\rfloor_{2n}\,m_1}\,.
\end{aligned}$$

By the skew-symmetry of $\Omega$ and $\omega^0$ we have

$$\begin{aligned}
&\Omega_{\lfloor m_1+n\rfloor_{2n}\,m_2}\,\omega^0_{m_2\,\lfloor m_2+n\rfloor_{2n}}\,\Omega_{\lfloor m_2+n\rfloor_{2n}\,(\cdot)}\,\cdots\\
&\quad\Omega_{(\cdot)\,m_{s-1}}\,\omega^0_{m_{s-1}\,\lfloor m_{s-1}+n\rfloor_{2n}}\,\Omega_{\lfloor m_{s-1}+n\rfloor_{2n}\,\lfloor m_1+n\rfloor_{2n}}\\
&\qquad=-\Omega_{\lfloor m_1+n\rfloor_{2n}\,\lfloor m_{s-1}+n\rfloor_{2n}}\,\omega^0_{\lfloor m_{s-1}+n\rfloor_{2n}\,m_{s-1}}\,\Omega_{m_{s-1}\,(\cdot)}\,\cdots\\
&\qquad\quad\Omega_{(\cdot)\,\lfloor m_2+n\rfloor_{2n}}\,\omega^0_{\lfloor m_2+n\rfloor_{2n}\,m_2}\,\Omega_{m_2\,\lfloor m_1+n\rfloor_{2n}}\,.
\end{aligned}$$

Combining the two above results we get

$$\begin{aligned}
&\mathrm{Tr}_{l_1^{\alpha_1}}\left(l_2^{\alpha_2}\cdots l_{s-1}^{\alpha_{s-1}}\, l_1^{\overline{\alpha_1}}\, l_{s+1}^{\alpha_{s+1}}\cdots l_r^{\alpha_r}\right)\\
&\quad= -\omega^0_{m_1\,\lfloor m_1+n\rfloor_{2n}}\,\Omega_{\lfloor m_1+n\rfloor_{2n}\,\lfloor m_{s-1}+n\rfloor_{2n}}\,\omega^0_{\lfloor m_{s-1}+n\rfloor_{2n}\,m_{s-1}}\,\Omega_{m_{s-1}\,(\cdot)}\cdots\\
&\qquad \Omega_{(\cdot)\,\lfloor m_2+n\rfloor_{2n}}\,\omega^0_{\lfloor m_2+n\rfloor_{2n}\,m_2}\,\Omega_{m_2\,\lfloor m_1+n\rfloor_{2n}}\\
&\qquad \omega^0_{\lfloor m_1+n\rfloor_{2n}\,m_1}\,\Omega_{m_1\,(\cdot)}\cdots\Omega_{(\cdot)\,m_r}\,\omega^0_{m_r\,\lfloor m_r+n\rfloor_{2n}}\,\Omega_{\lfloor m_r+n\rfloor_{2n}\,m_1}\\
&\quad= -\mathrm{Tr}_{l_1^{\alpha_1}}\left(l_{s-1}^{\overline{\alpha_{s-1}}}\, l_{s-2}^{\overline{\alpha_{s-2}}}\cdots l_2^{\overline{\alpha_2}}\, l_1^{\overline{\alpha_1}}\, l_{s+1}^{\alpha_{s+1}}\cdots l_r^{\alpha_r}\right).
\end{aligned}$$

The other two claims in (A.6) follow by additionally using the cyclicity (A.3). Again, the above result obviously holds for any $\alpha_1, \alpha_2, \alpha_{s-1}, \alpha_r \in \{\downarrow, \uparrow\}$ which shows (A.6) and with this finishes the proof. □

**Lemma A.3** *Let* $k \in \mathbb{N}$*,* $k \geq 2$*,* $m \in \{1, \ldots, n\}^k$ *and* $R = \{R_1, \ldots, R_{|R|}\} \subset \{1, \ldots, k\}$*. Then, for* $i, j \in \{1, \ldots |R|\}$

$$\begin{aligned}
&\sum_{\alpha\in\{\uparrow,\downarrow\}^k}\ \sum_{\sigma\in\mathrm{Sym}(R\setminus\{R_i\})} \mathrm{Tr}_{R_i^{\alpha_k}}(\sigma_1^{\alpha_1}\cdots\sigma_{k-1}^{\alpha_{k-1}})\\
&\qquad= \sum_{\alpha\in\{\uparrow,\downarrow\}^k}\ \sum_{\sigma\in\mathrm{Sym}(R\setminus\{R_j\})} \mathrm{Tr}_{R_j^{\alpha_k}}(\sigma_1^{\alpha_1}\cdots\sigma_{k-1}^{\alpha_{k-1}})\,.
\end{aligned}$$

Proof Let $k \in \mathbb{N}$, $k \geq 2$, $I \subset (1, \ldots, n)$, $m \in I^k$, $R = \{R_1, \ldots, R_{|R|}\} \subset \{1, \ldots, k\}$ and $i, j \in \{1, \ldots |R|\}$, $i \neq j$. Then,

$$\begin{aligned}
&\sum_{\alpha\in\{\uparrow,\downarrow\}^k}\ \sum_{\sigma\in\mathrm{Sym}(R\setminus\{R_i\})} \mathrm{Tr}_{R_i^{\alpha_k}}(\sigma_1^{\alpha_1}\cdots\sigma_{k-1}^{\alpha_{k-1}})\\
&\quad= \sum_{\alpha\in\{\uparrow,\downarrow\}^k}\ \sum_{r=1}^{k-1}\ \sum_{\substack{\sigma\in\mathrm{Sym}(R\setminus\{R_i\}),\\ \sigma(r)=R_j}} \mathrm{Tr}_{R_i^{\alpha_k}}(\sigma_1^{\alpha_1}\cdots\sigma_{r-1}^{\alpha_{r-1}}\, R_j^{\alpha_r}\, \sigma_{r+1}^{\alpha_{r+1}}\cdots\sigma_{k-1}^{\alpha_{k-1}})
\end{aligned}$$

By the cyclicity of the trace (A.3) we get

$$\begin{aligned}
&\sum_{\alpha\in\{\uparrow,\downarrow\}^k}\ \sum_{r=1}^{k-1}\ \sum_{\substack{\sigma\in\mathrm{Sym}(R\setminus\{R_i\}),\\ \sigma(r)=R_j}} \mathrm{Tr}_{R_i^{\alpha_k}}(\sigma_1^{\alpha_1}\cdots\sigma_{r-1}^{\alpha_{r-1}}\, R_j^{\alpha_r}\, \sigma_{r+1}^{\alpha_{r+1}}\cdots\sigma_{k-1}^{\alpha_{k-1}})\\
&\quad= \sum_{\alpha\in\{\uparrow,\downarrow\}^k}\ \sum_{r=1}^{k-1}\ \sum_{\substack{\sigma\in\mathrm{Sym}(R\setminus\{R_i\}),\\ \sigma(r)=R_j}} \mathrm{Tr}_{R_j^{\alpha_r}}(\sigma_{r+1}^{\alpha_{r+1}}\cdots\sigma_{k-1}^{\alpha_{k-1}}\, R_i^{\alpha_k}\, \sigma_1^{\alpha_1}\cdots\sigma_{r-1}^{\alpha_{r-1}})\,.
\end{aligned}$$

By renaming the $\alpha$s and $\sigma$s we get

$$\begin{aligned}
&\sum_{\alpha\in\{\uparrow,\downarrow\}^k} \sum_{r=1}^{k-1} \sum_{\substack{\sigma\in\mathrm{Sym}(R\setminus\{R_i\}),\\ \sigma(r)=R_j}} \mathrm{Tr}_{R_j^{\alpha_r}}\big(\sigma_{r+1}^{\alpha_{r+1}}\cdots\sigma_{k-1}^{\alpha_{k-1}}\, R_i^{\alpha_k}\, \sigma_1^{\alpha_1}\cdots\sigma_{r-1}^{\alpha_{r-1}}\big)\\
&\quad= \sum_{\alpha\in\{\uparrow,\downarrow\}^k} \sum_{r=1}^{k-1} \sum_{\substack{\sigma\in\mathrm{Sym}(R\setminus\{R_i\}),\\ \sigma(k-r)=R_j}} \mathrm{Tr}_{R_j^{\alpha_k}}\big(\sigma_1^{\alpha_1}\cdots\sigma_{k-r-1}^{\alpha_{k-r-1}}\, R_i^{\alpha_{k-r}}\, \sigma_{k-r+1}^{\alpha_{k-r+1}}\cdots\sigma_{k-1}^{\alpha_{k-1}}\big)\,.
\end{aligned}$$

Substituting $k-r$ by $\tilde{r}$ yields

$$\begin{aligned}
&\sum_{\alpha\in\{\uparrow,\downarrow\}^k} \sum_{r=1}^{k-1} \sum_{\substack{\sigma\in\mathrm{Sym}(R\setminus\{R_i\}),\\ \sigma(k-r)=R_j}} \mathrm{Tr}_{R_j^{\alpha_k}}\big(\sigma_1^{\alpha_1}\cdots\sigma_{k-r-1}^{\alpha_{k-r-1}}\, R_i^{\alpha_{k-r}}\, \sigma_{k-r+1}^{\alpha_{k-r+1}}\cdots\sigma_{k-1}^{\alpha_{k-1}}\big)\\
&\quad= \sum_{\alpha\in\{\uparrow,\downarrow\}^k} \sum_{\tilde{r}=1}^{k-1} \sum_{\substack{\sigma\in\mathrm{Sym}(R\setminus\{R_i\}),\\ \sigma(\tilde{r})=R_j}} \mathrm{Tr}_{R_j^{\alpha_k}}\big(\sigma_1^{\alpha_1}\cdots\sigma_{\tilde{r}-1}^{\alpha_{\tilde{r}-1}}\, R_i^{\alpha_{\tilde{r}}}\, \sigma_{\tilde{r}+1}^{\alpha_{\tilde{r}+1}}\cdots\sigma_{k-1}^{\alpha_{k-1}}\big)\,.\cdots
\end{aligned}$$

As last step note that

$$\begin{aligned}
&\sum_{\alpha\in\{\uparrow,\downarrow\}^k} \sum_{\tilde{r}=1}^{k-1} \sum_{\substack{\sigma\in\mathrm{Sym}(R\setminus\{R_i\}),\\ \sigma(\tilde{r})=R_j}} \mathrm{Tr}_{R_j^{\alpha_k}}\big(\sigma_1^{\alpha_1}\cdots\sigma_{\tilde{r}-1}^{\alpha_{\tilde{r}-1}}\, R_i^{\alpha_{\tilde{r}}}\, \sigma_{\tilde{r}+1}^{\alpha_{\tilde{r}+1}}\cdots\sigma_{k-1}^{\alpha_{k-1}}\big)\\
&\quad= \sum_{\alpha\in\{\uparrow,\downarrow\}^k} \sum_{\tilde{r}=1}^{k-1} \sum_{\substack{\sigma\in\mathrm{Sym}(R\setminus\{R_j\}),\\ \sigma(\tilde{r})=R_i}} \mathrm{Tr}_{R_j^{\alpha_k}}\big(\sigma_1^{\alpha_1}\cdots\sigma_{\tilde{r}-1}^{\alpha_{\tilde{r}-1}}\, R_i^{\alpha_{\tilde{r}}}\, \sigma_{\tilde{r}+1}^{\alpha_{\tilde{r}+1}}\cdots\sigma_{k-1}^{\alpha_{k-1}}\big)\\
&\quad= \sum_{\alpha\in\{\uparrow,\downarrow\}^k} \sum_{\sigma\in\mathrm{Sym}(R\setminus\{R_j\})} \mathrm{Tr}_{R_j^{\alpha_k}}\big(\sigma_1^{\alpha_1}\cdots\sigma_{k-1}^{\alpha_{k-1}}\big)\,.
\end{aligned}$$

Then, combining the above results finishes the proof. □

**Lemma A.4** *Let $k \in \mathbb{N}$, $k \geq 2$ and $m \in \{1, \ldots, n\}^k$. In addition, assume $i \in \{1, \ldots, k\}$ and $R = \{R_1, \ldots, R_{|R|}\} \subset \{1, \ldots, k\} \setminus \{i\}$. Then, for every $1 \leq r \leq |R| + 1$ it holds that*

$$\sum_{\alpha \in \{\uparrow,\downarrow\}^{|R|+2}} \sum_{\sigma \in \mathrm{Sym}(R)} \mathrm{Tr}_{i^{\alpha_{|R|+1}}} \Big( \sigma_1^{\alpha_1} \cdots \sigma_{r-1}^{\alpha_{r-1}} \, i^{\alpha_{|R|+2}} \, \sigma_r^{\alpha_r} \cdots \sigma_{|R|}^{\alpha_{|R|}} \Big)$$
$$= \frac{1}{2} \sum_{\substack{A \dot\cup B = R, \\ |A| = r-1}} \Bigg( \Big( \sum_{\alpha \in \{\uparrow,\downarrow\}^{|A|+1}} \sum_{\sigma \in \mathrm{Sym}(A)} \mathrm{Tr}_{i^{\alpha_{|A|+1}}} \Big( \sigma_1^{\alpha_1} \cdots \sigma_{|A|}^{\alpha_{|A|}} \Big) \Big)$$
$$\Big( \sum_{\beta \in \{\uparrow,\downarrow\}^{|B|+1}} \sum_{\tau \in \mathrm{Sym}(B)} \mathrm{Tr}_{i^{\beta_{|B|+1}}} \Big( \tau_r^{\beta_1} \cdots \tau_{|B|}^{\beta_{|B|}} \Big) \Big) \Bigg) .$$

PROOF Let $k \in \mathbb{N}$, $k \geq 2$, $m \in \{1, \ldots, n\}^k$, $i \in \{1, \ldots, k\}$ and $R \subset \{1, \ldots, k\} \setminus \{i\}$. We start with the following observation. Combining (A.2) and (A.3) we have for any $\alpha \in \{\uparrow, \downarrow\}^{|R|+1}$ and $\sigma \in \mathrm{Sym}(R)$ that

$$\mathrm{Tr}_{i^{|R|+1}} \Big( i^{\overline{|R|+1}} \, \sigma_1^{\alpha_1} \cdots \sigma_{|R|}^{\alpha_{|R|}} \Big) = \mathrm{Tr}_{i^{|R|+1}} \Big( \sigma_1^{\alpha_1} \cdots \sigma_{|R|}^{\alpha_{|R|}} \, i^{\overline{|R|+1}} \Big) = 0 \, .$$

Moreover, by (A.6) we have for $2 \leq r \leq |R|$, $\alpha \in \{\uparrow, \downarrow\}^{|R|+1}$ and $\sigma \in \mathrm{Sym}(R)$ that

$$\begin{aligned} 0 = &\ \mathrm{Tr}_{i^{|B|+1}} \Big( \sigma_1^{\alpha_1} \cdots \sigma_{r-1}^{\alpha_{r-1}} \, i^{\overline{|B|+1}} \, \sigma_r^{\alpha_r} \cdots \sigma_{|R|}^{\alpha_{|R|}} \Big) \\ &+ \mathrm{Tr}_{i^{|B|+1}} \Big( \sigma_{r-1}^{\overline{\alpha_{r-1}}} \cdots \sigma_1^{\overline{\alpha_1}} \, i^{\overline{|B|+1}} \, \sigma_r^{\alpha_r} \cdots \sigma_{|R|}^{\alpha_{|R|}} \Big) \\ &+ \mathrm{Tr}_{i^{|B|+1}} \Big( \sigma_1^{\alpha_1} \cdots \sigma_{r-1}^{\alpha_{r-1}} \, i^{\overline{|B|+1}} \, \sigma_{|R|}^{\overline{\alpha_{|R|}}} \cdots \sigma_r^{\overline{\alpha_r}} \Big) \\ &+ \mathrm{Tr}_{i^{|B|+1}} \Big( \sigma_{r-1}^{\overline{\alpha_{r-1}}} \cdots \sigma_1^{\overline{\alpha_1}} \, i^{\overline{|B|+1}} \, \sigma_{|R|}^{\overline{\alpha_{|R|}}} \cdots \sigma_r^{\overline{\alpha_r}} \Big) \end{aligned}$$

From now on, let $1 \leq r \leq |R| + 1$. Combining the two results above shows

$$\sum_{\alpha \in \{\uparrow,\downarrow\}^{|R|+1}} \sum_{\sigma \in \mathrm{Sym}(R)} \mathrm{Tr}_{i^{|B|+1}} \Big( \sigma_1^{\alpha_1} \cdots \sigma_{r-1}^{\alpha_{r-1}} \, i^{\overline{|B|+1}} \, \sigma_r^{\alpha_r} \cdots \sigma_{|R|}^{\alpha_{|R|}} \Big) = 0 \, . \tag{A.7}$$

By (A.5)

$$\sum_{\alpha \in \{\uparrow,\downarrow\}^{|R|+1}} \sum_{\sigma \in \mathrm{Sym}(R)} \mathrm{Tr}_{i^{|B|+1}} \Big( \sigma_1^{\alpha_1} \cdots \sigma_{r-1}^{\alpha_{r-1}} \, i^{|B|+1} \, \sigma_r^{\alpha_r} \cdots \sigma_{|R|}^{\alpha_{|R|}} \Big)$$
$$= \sum_{\alpha \in \{\uparrow,\downarrow\}^{|R|}} \sum_{\sigma \in \mathrm{Sym}(R)} \Big( \mathrm{Tr}_{i^{|B|+1}} \Big( \sigma_1^{\alpha_1} \cdots \sigma_{r-1}^{\alpha_{r-1}} \Big) \mathrm{Tr}_{i^{|B|+1}} \Big( \sigma_r^{\alpha_r} \cdots \sigma_{|L|}^{\alpha_{|R|}} \Big) \Big) .$$

Combining (A.3) and (A.4) we get for every $l \subset \{1, \ldots, k\}$, $\alpha \in \{\uparrow, \downarrow\}^{|l|+1}$ that

$$\begin{aligned}
2 &\left( \mathrm{Tr}_{i^{\alpha_{|l|+1}}} \left( l_1^{\alpha_1} \cdots l_{|l|}^{\alpha_{|l|}} \right) + \mathrm{Tr}_{i^{\alpha_{|l|+1}}} \left( l_{|l|}^{\overline{\alpha_{|l|}}} \cdots l_1^{\overline{\alpha_1}} \right) \right) \\
&= \mathrm{Tr}_{i^{\alpha_{|l|+1}}} \left( l_1^{\alpha_1} \cdots l_{|l|}^{\alpha_{|l|}} \right) + \mathrm{Tr}_{i^{\overline{\alpha_{|l|+1}}}} \left( l_{|l|}^{\overline{\alpha_{|l|}}} \cdots l_1^{\overline{\alpha_1}} \right) \\
&\quad + \mathrm{Tr}_{i^{\alpha_{|l|+1}}} \left( l_{|l|}^{\overline{\alpha_{|l|}}} \cdots l_1^{\overline{\alpha_1}} \right) + \mathrm{Tr}_{i^{\overline{\alpha_{|l|+1}}}} \left( l_1^{\alpha_1} \cdots l_{|l|}^{\alpha_{|l|}} \right) \\
&= \sum_{\beta \in \{\uparrow \downarrow\}} \left( \mathrm{Tr}_{i^\beta} \left( l_1^{\alpha_1} \cdots l_{|l|}^{\alpha_{|l|}} \right) + \mathrm{Tr}_{i^\beta} \left( l_{|l|}^{\overline{\alpha_{|l|}}} \cdots l_1^{\overline{\alpha_1}} \right) \right).
\end{aligned}$$

We conclude from the result above that

$$\begin{aligned}
&2 \sum_{\alpha \in \{\uparrow,\downarrow\}^{|R|+1}} \sum_{\sigma \in \mathrm{Sym}(R)} \left( \mathrm{Tr}_{i^{\alpha_{|R|+1}}} \left( \sigma_1^{\alpha_1} \cdots \sigma_{r-1}^{\alpha_{r-1}} \right) \mathrm{Tr}_{i^{\alpha_{|R|+1}}} \left( \sigma_r^{\alpha_r} \cdots \sigma_{|R|}^{\alpha_{|R|}} \right) \right) \\
&\quad = \sum_{\alpha \in \{\uparrow,\downarrow\}^{|R|+2}} \sum_{\sigma \in \mathrm{Sym}(R)} \left( \mathrm{Tr}_{i^{\alpha_{|R|+1}}} \left( \sigma_1^{\alpha_1} \cdots \sigma_{r-1}^{\alpha_{r-1}} \right) \mathrm{Tr}_{i^{\alpha_{|R|+2}}} \left( \sigma_r^{\alpha_r} \cdots \sigma_{|L|}^{\alpha_{|R|}} \right) \right)
\end{aligned} \tag{A.8}$$

In the next step we sort the sum over the partitions of $R$ by splitting $R$ into two disjoint sets $A$ and $B$ which leads to

$$\begin{aligned}
&\sum_{\alpha \in \{\uparrow,\downarrow\}^{|R|+2}} \sum_{\sigma \in \mathrm{Sym}(R)} \left( \mathrm{Tr}_{i^{\alpha_{|R|+1}}} \left( \sigma_1^{\alpha_1} \cdots \sigma_{r-1}^{\alpha_{r-1}} \right) \mathrm{Tr}_{i^{\alpha_{|R|+2}}} \left( \sigma_r^{\alpha_r} \cdots \sigma_{|R|}^{\alpha_{|R|}} \right) \right) \\
&\quad = \sum_{\substack{A \dot\cup B = R, \\ |A| = r-1}} \left( \left( \sum_{\alpha \in \{\uparrow,\downarrow\}^{|A|+1}} \sum_{\sigma \in \mathrm{Sym}(A)} \mathrm{Tr}_{i^{\alpha_{|A|+1}}} \left( \sigma_1^{\alpha_1} \cdots \sigma_{|A|}^{\alpha_{|A|}} \right) \right) \right. \\
&\qquad \left. \left( \sum_{\beta \in \{\uparrow,\downarrow\}^{|B|+1}} \sum_{\tau \in \mathrm{Sym}(B)} \mathrm{Tr}_{i^{\beta_{|B|+1}}} \left( \tau_r^{\beta_1} \cdots \tau_{|B|}^{\beta_{|B|}} \right) \right) \right).
\end{aligned} \tag{A.9}$$

Then, combining (A.7)-(A.9) finishes the proof. □

**Lemma A.5** *Let $k \in \mathbb{N}$, $k \geq 2$, $I \subset (1, \ldots, n)$ and $m \in I^k$ satisfying that there are $i, l \in \{1, \ldots, k\}$, $i \neq l$ such that $m_i = m_l$. In addition, assume $R \subset \{1, \ldots, k\}$ with $i, l \in R$. Then,*

$$\sum_{\alpha \in \{\uparrow,\downarrow\}^{|R|}} \sum_{\sigma \in \mathrm{Sym}(\{R_1,\ldots,R_{(|R|-1)}\})} \mathrm{Tr}_{R_{|R|}^{\alpha_{|R|}}} (\sigma_1^{\alpha_1} \cdots \sigma_{|R|-1}^{\alpha_{|R|-1}})$$
$$= \frac{1}{2} \sum_{A \dot\cup B = R \setminus \{i,l\}} \Bigg( \Bigg( \sum_{\alpha \in \{\uparrow,\downarrow\}^{|A|+1}} \sum_{\sigma \in \mathrm{Sym}(A)} \mathrm{Tr}_{i^{\alpha_{|A|+1}}} \Big( \sigma_1^{\alpha_1} \cdots \sigma_{|A|}^{\alpha_{|A|}} \Big) \Bigg)$$
$$\Bigg( \sum_{\beta \in \{\uparrow,\downarrow\}^{|B|+1}} \sum_{\tau \in \mathrm{Sym}(B)} \mathrm{Tr}_{i^{\beta_{|B|+1}}} \Big( \tau_r^{\beta_1} \cdots \tau_{|B|}^{\beta_{|B|}} \Big) \Bigg) \Bigg).$$

PROOF We start our proof by considering the case where $R_{|R|} = i$. Then,

$$\begin{aligned} &\sum_{\alpha \in \{\uparrow,\downarrow\}^{|R|}} \sum_{\sigma \in \mathrm{Sym}(\{R_1,\ldots,R_{(|R|-1)}\})} \mathrm{Tr}_{R_{|R|}^{\alpha_{|R|}}} (\sigma_1^{\alpha_1} \cdots \sigma_{|R|-1}^{\alpha_{|R|-1}}) \\ &= \sum_{\alpha \in \{\uparrow,\downarrow\}^{|R|}} \sum_{r_1 \in \{1,\ldots,|R|-1\}} \sum_{\substack{\sigma \in \mathrm{Sym}(\{R_1,\ldots,R_{(|R|-1)}\}), \\ \sigma_{r_1} = l}} \\ &\qquad \mathrm{Tr}_{i^{\alpha_{|R|}}} (\sigma_1^{\alpha_1} \cdots l^{\alpha_{r_1}} \cdots \sigma_{|R|-1}^{\alpha_{|R|-1}}) \\ &= \sum_{\alpha \in \{\uparrow,\downarrow\}^{|R|}} \sum_{r_1 \in \{1,\ldots,|R|-1\}} \sum_{\substack{\sigma \in \mathrm{Sym}(\{R_1,\ldots,R_{(|R|-1)}\}), \\ \sigma_{r_1} = l}} \\ &\qquad \mathrm{Tr}_{i^{\alpha_{|R|}}} (\sigma_1^{\alpha_1} \cdots i^{\alpha_{r_1}} \cdots \sigma_{|R|-1}^{\alpha_{|R|-1}}) \end{aligned} \tag{A.10}$$

Clearly, in the case where $R_{|R|} = l$ we get the same result, i.e.

$$\begin{aligned} &\sum_{\alpha \in \{\uparrow,\downarrow\}^{|R|}} \sum_{\sigma \in \mathrm{Sym}(\{R_1,\ldots,R_{(|R|-1)}\})} \mathrm{Tr}_{R_{|R|}^{\alpha_{|R|}}} (\sigma_1^{\alpha_1} \cdots \sigma_{|R|-1}^{\alpha_{|R|-1}}) \\ &= \sum_{\alpha \in \{\uparrow,\downarrow\}^{|R|}} \sum_{r_1 \in \{1,\ldots,|R|-1\}} \sum_{\substack{\sigma \in \mathrm{Sym}(\{R_1,\ldots,R_{(|R|-1)}\}), \\ \sigma_{r_1} = l}} \\ &\qquad \mathrm{Tr}_{i^{\alpha_{|R|}}} (\sigma_1^{\alpha_1} \cdots i^{\alpha_{r_1}} \cdots \sigma_{|R|-1}^{\alpha_{|R|-1}}) \end{aligned} \tag{A.11}$$

Now, we examine the case $R_{|R|} \neq i, l$. By the cyclicity of the trace (A.3) and the assumption that $m_i = m_l$

$$\begin{aligned} &\sum_{\alpha \in \{\uparrow,\downarrow\}^{|R|}} \sum_{\substack{\sigma \in \mathrm{Sym}(\{R_1,\ldots,R_{(|R|-1)}\}), \\ \sigma_{r_1} = i, \sigma_{r_2} = l}} \mathrm{Tr}_{R_{|R|}^{\alpha_{|R|}}} (\sigma_1^{\alpha_1} \cdots i^{\alpha_{r_1}} \cdots l^{\alpha_{r_2}} \cdots \sigma_{|R|-1}^{\alpha_{|R|-1}}) \\ &= \sum_{\alpha \in \{\uparrow,\downarrow\}^{|R|}} \sum_{\substack{\sigma \in \mathrm{Sym}(\{R_1,\ldots,R_{(|R|-1)}\}), \\ \sigma_{r_1} = i, \sigma_{r_2} = l}} \\ &\qquad \mathrm{Tr}_{i^{\alpha_{r_1}}} (\sigma_{r_1+1}^{\alpha_{r_1+1}} \cdots i^{\alpha_{r_2}} \cdots \sigma_{|R|-1}^{\alpha_{|R|-1}} \, R_{|R|}^{\alpha_{|R|}} \, \sigma_1^{\alpha_1} \cdots \sigma_{r_1-1}^{\alpha_{r_1-1}}) \end{aligned} \tag{A.12}$$

for any $r_1, r_2 \in \{1, \ldots, |R|-1\}, r_1 < r_2$. By symmetry of the symmetric group $\mathrm{Sym}(\{R_1, \ldots, R_{(|R|-1)}$ we obtain for any $r_2 \in \{1, \ldots, |R|-1\}$ that

$$\begin{aligned}
&\sum_{\substack{r_1\in\{1,\ldots,|R|-1\},\\ r_1<r_2}} \sum_{\alpha\in\{\uparrow,\downarrow\}^{|R|}} \sum_{\substack{\sigma\in\mathrm{Sym}(\{R_1,\ldots,R_{(|R|-1)}\}),\\ \sigma_{r_1}=i,\,\sigma_{r_2}=l}} \\
&\qquad \mathrm{Tr}_{i^{\alpha_{r_1}}}\big(\sigma_{r_1+1}^{\alpha_{r_1+1}} \cdots i^{\alpha_{r_2}} \cdots \sigma_{|R|-1}^{\alpha_{|R|-1}}\, R_{|R|}^{\alpha_{|R|}}\, \sigma_1^{\alpha_1} \cdots \sigma_{r_1-1}^{\alpha_{r_1-1}}\big) \\
&\quad = \sum_{\alpha\in\{\uparrow,\downarrow\}^{|R|}} \sum_{\substack{r_1\in\{1,\ldots,|R|-1\},\\ r_1<r_2}} \sum_{\substack{\sigma\in\mathrm{Sym}(R\setminus\{i\}),\\ \sigma_{|R|-r_1}=R_{|R|},\,\sigma_{r_2-r_1}=l}} \\
&\qquad\qquad \mathrm{Tr}_{i^{\alpha_{|R|}}}\big(\sigma_1^{\alpha_1} \cdots i^{\alpha_{r_2-r_1}} \cdots R_{|R|}^{\alpha_{|R|-r_1}} \cdots \sigma_{|R|-1}^{\alpha_{|R|-1}}\big)\,.
\end{aligned} \tag{A.13}$$

Substituting $r_1$ by $|R| - \tilde{r}$ we get

$$\begin{aligned}
&\sum_{\alpha\in\{\uparrow,\downarrow\}^{|R|}} \sum_{\substack{r_1\in\{1,\ldots,|R|-1\},\\ r_1<r_2}} \sum_{\substack{\sigma\in\mathrm{Sym}(R\setminus\{i\}),\\ \sigma_{|R|-r_1}=R_{|R|},\,\sigma_{r_2-r_1}=l}} \\
&\qquad \mathrm{Tr}_{i^{\alpha_{|R|}}}\big(\sigma_1^{\alpha_1} \cdots i^{\alpha_{r_2-r_1}} \cdots R_{|R|}^{\alpha_{|R|-r_1}} \cdots \sigma_{|R|-1}^{\alpha_{|R|-1}}\big) \\
&\quad = \sum_{\alpha\in\{\uparrow,\downarrow\}^{|R|}} \sum_{\substack{\tilde{r}\in\{1,\ldots,|R|-1\},\\ |R|-\tilde{r}<r_2}} \sum_{\substack{\sigma\in\mathrm{Sym}(R\setminus\{i\}),\\ \sigma_{\tilde{r}}=R_{|R|},\,\sigma_{r_2+\tilde{r}-|R|}=l}} \\
&\qquad\qquad \mathrm{Tr}_{i^{\alpha_{|R|}}}\big(\sigma_1^{\alpha_1} \cdots i^{\alpha_{r_2+\tilde{r}-|R|}} \cdots R_{|R|}^{\alpha_{\tilde{r}}} \cdots \sigma_{|R|-1}^{\alpha_{|R|-1}}\big)
\end{aligned} \tag{A.14}$$

for any $r_2 \in \{1, \ldots, |R|-1\}$. Combining (A.12) - (A.14) and summation over $r_2$ yields

$$\begin{aligned}
&\sum_{\substack{r_1,r_2\in\{1,\ldots,|R|-1\},\\ r_1<r_2}} \sum_{\alpha\in\{\uparrow,\downarrow\}^{|R|}} \sum_{\substack{\sigma\in\mathrm{Sym}(\{R_1,\ldots,R_{(|R|-1)}\}),\\ \sigma_{r_1}=i,\,\sigma_{r_2}=l}} \\
&\qquad \mathrm{Tr}_{R_{|R|}^{\alpha_{|R|}}}\big(\sigma_1^{\alpha_1} \cdots i^{\alpha_{r_1}} \cdots l^{\alpha_{r_2}} \cdots \sigma_{|R|-1}^{\alpha_{|R|-1}}\big) \\
&\quad = \sum_{\alpha\in\{\uparrow,\downarrow\}^{|R|}} \sum_{\substack{\tilde{r},r_2\in\{1,\ldots,|R|-1\},\\ |R|-\tilde{r}<r_2}} \sum_{\substack{\sigma\in\mathrm{Sym}(R\setminus\{i\}),\\ \sigma_{\tilde{r}}=R_{|R|},\,\sigma_{r_2+\tilde{r}-|R|}=l}} \\
&\qquad\qquad \mathrm{Tr}_{i^{\alpha_{|R|}}}\big(\sigma_1^{\alpha_1} \cdots i^{\alpha_{r_2+\tilde{r}-|R|}} \cdots R_{|R|}^{\alpha_{\tilde{r}}} \cdots \sigma_{|R|-1}^{\alpha_{|R|-1}}\big)\,.
\end{aligned} \tag{A.15}$$

Analogously, we get

$$\sum_{\substack{r_1,r_2\in\{1,\dots,|R|-1\},\\ r_1>r_2}} \sum_{\alpha\in\{\uparrow,\downarrow\}^{|R|}} \sum_{\substack{\sigma\in\mathrm{Sym}(\{R_1,\dots,R_{(|R|-1)}\}),\\ \sigma_{r_1}=i,\,\sigma_{r_2}=l}} \mathrm{Tr}_{R_{|R|}^{\alpha_{|R|}}}\big(\sigma_1^{\alpha_1}\cdots i^{\alpha_{r_1}}\cdots l^{\alpha_{r_2}}\cdots\sigma_{|R|-1}^{\alpha_{|R|-1}}\big)$$
$$= \sum_{\alpha\in\{\uparrow,\downarrow\}^{|R|}} \sum_{\substack{\tilde r,r_2\in\{1,\dots,|R|-1\},\\ |R|-\tilde r>r_2}} \sum_{\substack{\sigma\in\mathrm{Sym}(R\setminus\{i\}),\\ \sigma_{\tilde r}=R_{|R|},\,\sigma_{r_2+\tilde r-|R|}=l}} \mathrm{Tr}_{i^{\alpha_{|R|}}}\big(\sigma_1^{\alpha_1}\cdots R_{|R|}^{\alpha_{\tilde r}}\cdots i^{\alpha_{r_2+\tilde r}}\cdots\sigma_{|R|-1}^{\alpha_{|R|-1}}\big)\,. \tag{A.16}$$

Then, by (A.15) and (A.16) we obtain

$$\sum_{\substack{r_1,r_2\in\{1,\dots,|R|-1\},\\ r_1\neq r_2}} \sum_{\alpha\in\{\uparrow,\downarrow\}^{|R|}} \sum_{\substack{\sigma\in\mathrm{Sym}(\{R_1,\dots,R_{(|R|-1)}\}),\\ \sigma_{r_1}=i,\,\sigma_{r_2}=l}} \mathrm{Tr}_{R_{|R|}^{\alpha_{|R|}}}\big(\sigma_1^{\alpha_1}\cdots i^{\alpha_{r_1}}\cdots l^{\alpha_{r_2}}\cdots\sigma_{|R|-1}^{\alpha_{|R|-1}}\big)$$
$$= \sum_{\alpha\in\{\uparrow,\downarrow\}^{|R|}} \sum_{\substack{\tilde r,r_2\in\{1,\dots,|R|-1\},\\ \tilde r\neq r_2}} \sum_{\substack{\sigma\in\mathrm{Sym}(R\setminus\{i\}),\\ \sigma_{\tilde r}=R_{|R|},\,\sigma_{r_2}=l}} \mathrm{Tr}_{i^{\alpha_{|R|}}}\big(\sigma_1^{\alpha_1}\cdots R_{|R|}^{\alpha_{\tilde r}}\cdots i^{\alpha_{r_2}}\cdots\sigma_{|R|-1}^{\alpha_{|R|-1}}\big)$$
$$= \sum_{\alpha\in\{\uparrow,\downarrow\}^{|R|}} \sum_{r_2\in\{1,\dots,|R|-1\}} \sum_{\substack{\sigma\in\mathrm{Sym}(R\setminus\{i\}),\\ \sigma_{r_2}=l}} \mathrm{Tr}_{i^{\alpha_{|R|}}}\big(\sigma_1^{\alpha_1}\cdots i^{\alpha_{r_2}}\cdots\sigma_{|R|-1}^{\alpha_{|R|-1}}\big)\,. \tag{A.17}$$

As is easy to see, the result of (A.17) can be reformulated leading to

$$\sum_{\alpha\in\{\uparrow,\downarrow\}^{|R|}} \sum_{r\in\{1,\dots,|R|-1\}} \sum_{\substack{\sigma\in\mathrm{Sym}(R\setminus\{i\}),\\ \sigma_r=l}} \mathrm{Tr}_{i^{\alpha_{|R|}}}\big(\sigma_1^{\alpha_1}\cdots i^{\alpha_r}\cdots\sigma_{|R|-1}^{\alpha_{|R|-1}}\big)$$
$$= \sum_{\alpha\in\{\uparrow,\downarrow\}^{|R|}} \sum_{r\in\{1,\dots,|R|-1\}} \sum_{\sigma\in\mathrm{Sym}(R\setminus\{i,l\})} \mathrm{Tr}_{i^{\alpha_{|R|-1}}}\big(\sigma_1^{\alpha_1}\cdots\sigma_{r-1}^{\alpha_{r-1}}\, i^{\alpha_{|R|}}\,\sigma_r^{\alpha_r}\cdots\sigma_{|R|-2}^{\alpha_{|R|-2}}\big)\,. \tag{A.18}$$

Combining (A.10), (A.11), (A.17) and (A.18) we get

$$\sum_{\alpha\in\{\uparrow,\downarrow\}^{|R|}} \sum_{\sigma\in\mathrm{Sym}(\{R_1,\dots,R_{(|R|-1)}\})} \mathrm{Tr}_{R_{|R|}^{\alpha_{|R|}}}\big(\sigma_1^{\alpha_1}\cdots\sigma_{|R|-1}^{\alpha_{|R|-1}}\big)$$
$$= \sum_{\alpha\in\{\uparrow,\downarrow\}^{|R|}} \sum_{r\in\{1,\dots,|R|-1\}} \sum_{\sigma\in\mathrm{Sym}(R\setminus\{i,l\})} \mathrm{Tr}_{i^{\alpha_{|R|-1}}}\big(\sigma_1^{\alpha_1}\cdots\sigma_{r-1}^{\alpha_{r-1}}\, i^{\alpha_{|R|}}\,\sigma_r^{\alpha_r}\cdots\sigma_{|R|-2}^{\alpha_{|R|-2}}\big)\,.$$

Then, applying Lemma A.4 with $\tilde{R} = R \setminus \{i, l\}$ shows

$$\begin{aligned}
&\sum_{\alpha\in\{\uparrow,\downarrow\}^{|R|}} \sum_{\sigma\in\mathrm{Sym}(\{R_1,\dots,R_{(|R|-1)}\})} \mathrm{Tr}_{R_{|R|}^{\alpha_{|R|}}}(\sigma_1^{\alpha_1}\cdots\sigma_{|R|-1}^{\alpha_{|R|-1}}) \\
&\quad = \frac{1}{2} \sum_{r\in\{1,\dots,|R|-1\}} \sum_{\substack{A\dot{\cup}B=R\setminus\{i,l\},\\ |A|=r-1}} \\
&\qquad\qquad \Bigg(\bigg(\sum_{\alpha\in\{\uparrow,\downarrow\}^r} \sum_{\sigma\in\mathrm{Sym}(A)} \mathrm{Tr}_{i^{\alpha_r}}\Big(\sigma_1^{\alpha_1}\cdots\sigma_{r-1}^{\alpha_{r-1}}\Big)\bigg) \\
&\qquad\qquad \bigg(\sum_{\beta\in\{\uparrow,\downarrow\}^{|B|+1}} \sum_{\tau\in\mathrm{Sym}(B)} \mathrm{Tr}_{i^{\beta_{|B|+1}}}\Big(\tau_r^{\beta_1}\cdots\tau_{|B|}^{\beta_{|B|}}\Big)\bigg)\Bigg)
\end{aligned}$$

which finishes the proof. □

**Lemma A.6** *Let $k \in \mathbb{N}$ and $m \in \{1, \dots, n\}^k$. In addition, assume $R \subset \{1, \dots, k\}$ and $i \in \{1, \dots, k\}$ with $i \in R$. Then,*

$$\begin{aligned}
&\sum_{\alpha\in\{\uparrow,\downarrow\}^{|R|}} \sum_{\sigma\in\mathrm{Sym}(\{R_1,\dots,R_{(|R|-1)}\})} \mathrm{Tr}_{R_{|R|}^{\alpha_{|R|}}}(\sigma_1^{\alpha_1}\cdots\sigma_{|R|-1}^{\alpha_{|R|-1}}) \\
&\quad = \sum_{\alpha\in\{\uparrow,\downarrow\}^{|R|}} \sum_{\sigma\in\mathrm{Sym}(R\setminus\{i\})} \mathrm{Tr}_{i^{\alpha_{|R|}}}(\sigma_1^{\alpha_1}\cdots\sigma_{|R|-1}^{\alpha_{|R|-1}}) \,.
\end{aligned}$$

PROOF Clearly, the assertion holds in the case where $i = R_{|R|}$. So, from now on we assume $i \neq R_{|R|}$. By the cyclicity of the trace (A.3) we obtain

$$\begin{aligned}
&\sum_{\alpha\in\{\uparrow,\downarrow\}^{|R|}} \sum_{\sigma\in\mathrm{Sym}(\{R_1,\dots,R_{(|R|-1)}\})} \mathrm{Tr}_{R_{|R|}^{\alpha_{|R|}}}(\sigma_1^{\alpha_1}\cdots\sigma_{|R|-1}^{\alpha_{|R|-1}}) \\
&\quad = \sum_{\alpha\in\{\uparrow,\downarrow\}^{|R|}} \sum_{r\in\{1,\dots,|R|-1\}} \sum_{\substack{\sigma\in\mathrm{Sym}(\{R_1,\dots,R_{(|R|-1)}\}),\\ \sigma_r=i}} \\
&\qquad\qquad \mathrm{Tr}_{R_{|R|}^{\alpha_{|R|}}}(\sigma_1^{\alpha_1}\cdots i^{\alpha_r}\cdots\sigma_{|R|-1}^{\alpha_{|R|-1}}) \qquad\qquad (A.19) \\
&\quad = \sum_{\alpha\in\{\uparrow,\downarrow\}^{|R|}} \sum_{r\in\{1,\dots,|R|-1\}} \sum_{\substack{\sigma\in\mathrm{Sym}(\{R_1,\dots,R_{(|R|-1)}\}),\\ \sigma_r=i}} \\
&\qquad\qquad \mathrm{Tr}_{i^{\alpha_r}}(\sigma_{r+1}^{\alpha_{r+1}}\cdots\sigma_{|R|-1}^{\alpha_{|R|-1}}\, R_{|R|}^{\alpha_{|R|}}\, \sigma_1^{\alpha_1}\cdots\sigma_{r-1}^{\alpha_{r-1}})
\end{aligned}$$

By the symmetry of the symmetric group $\mathrm{Sym}(\{R_1, \dots, R_{(|R|-1)}\})$ and renaming of the $\alpha_j$s we have

$$\begin{aligned}
&\sum_{\alpha\in\{\uparrow,\downarrow\}^{|R|}} \sum_{r\in\{1,\dots,|R|-1\}} \sum_{\substack{\sigma\in\mathrm{Sym}(\{R_1,\dots,R_{(|R|-1)}\}),\\ \sigma_r=i}} \\
&\qquad \mathrm{Tr}_{i^{\alpha_r}}\left(\sigma_{r+1}^{\alpha_{r+1}} \cdots \sigma_{|R|-1}^{\alpha_{|R|-1}} \, R_{|R|}^{\alpha_{|R|}} \, \sigma_1^{\alpha_1} \cdots \sigma_{r-1}^{\alpha_{r-1}}\right) \\
&= \sum_{\alpha\in\{\uparrow,\downarrow\}^{|R|}} \sum_{r\in\{1,\dots,|R|-1\}} \sum_{\substack{\sigma\in\mathrm{Sym}(R\setminus\{i\}),\\ \sigma_{|R|-r}=R_{|R|}}} \\
&\qquad \mathrm{Tr}_{i^{\alpha_{|R|}}}\left(\sigma_1^{\alpha_1} \cdots R_{|R|}^{\alpha_{|R|-r}} \cdots \sigma_{|R|-1}^{\alpha_{|R|-1}}\right).
\end{aligned} \tag{A.20}$$

Substituting $|R| - r$ by $\tilde{r}$ be get

$$\begin{aligned}
&\sum_{\alpha\in\{\uparrow,\downarrow\}^{|R|}} \sum_{r\in\{1,\dots,|R|-1\}} \sum_{\substack{\sigma\in\mathrm{Sym}(R\setminus\{i\}),\\ \sigma_{|R|-r}=R_{|R|}}} \\
&\qquad \mathrm{Tr}_{i^{\alpha_{|R|}}}\left(\sigma_1^{\alpha_1} \cdots R_{|R|-r}^{\alpha_{|R|-r}} \cdots \sigma_{|R|-1}^{\alpha_{|R|-1}}\right) \\
&= \sum_{\alpha\in\{\uparrow,\downarrow\}^{|R|}} \sum_{\tilde{r}\in\{1,\dots,|R|-1\}} \sum_{\substack{\sigma\in\mathrm{Sym}(R\setminus\{i\}),\\ \sigma_{\tilde{r}}=R_{|R|}}} \\
&\qquad \mathrm{Tr}_{i^{\alpha_{|R|}}}\left(\sigma_1^{\alpha_1} \cdots R_{\tilde{r}}^{\alpha_{\tilde{r}}} \cdots \sigma_{|R|-1}^{\alpha_{|R|-1}}\right) \\
&= \sum_{\alpha\in\{\uparrow,\downarrow\}^{|R|}} \sum_{\sigma\in\mathrm{Sym}(R\setminus\{i\})} \\
&\qquad \mathrm{Tr}_{i^{\alpha_{|R|}}}\left(\sigma_1^{\alpha_1} \cdots \sigma_{|R|-1}^{\alpha_{|R|-1}}\right).
\end{aligned} \tag{A.21}$$

To finish the proof we combine (A.19)- (A.21) □

**Lemma A.7** *Let $k \in \mathbb{N}$ and $m \in \{1, \dots, n\}^k$ satisfying that there are $i, l \in \{1, \dots, k\}$, $i \neq l$ such that $m_i = m_l$. In addition, let $p \in P(k)$ a partition of $\{1, \dots, k\}$ satisfying that there is a $\mu \in \{1, \dots, |p|\}$ such that $i, l \in p_\mu$. Also, let $K^{p_\mu}$ be the set of all partitions of $p_\mu$ into two sets $\rho_1, \rho_2$ with $i \in \rho_1$ and $l \in \rho_2$, i.e. $K^{p_\mu} := \{\{\rho_1, \rho_2\} : \rho_1 \dot{\cup} \rho_2 = p_\mu, i \in \rho_1, l \in \rho_2\}$. Then, $T^\rho = p \setminus \{p_\mu\} \cup \rho \in P(k)$ for all $\rho \in K^{p_\mu}$ and*

$$\begin{aligned}
0 = (-1)^{|p|} \, 2^{k-|p|} &\prod_{j\in\{1,\dots,|p|\}} \\
&\left(\sum_{\alpha\in\{\uparrow,\downarrow\}^{|p_j|}} \sum_{\sigma\in\mathrm{Sym}(\{(p_j)_1,\dots,(p_j)_{(|p_j|-1)}\})} \mathrm{Tr}_{{(p_j)_{|p_j|}}^{\alpha_{|p_j|}}}\left(\sigma_1^{\alpha_1} \cdots \sigma_{|p_j|-1}^{\alpha_{|p_j|-1}}\right)\right) \\
+ \sum_{\rho\in K^{p_\mu}} (-1)^{|T^\rho|} \, 2^{k-|T^\rho|} &\prod_{j\in\{1,\dots,|T^\rho|\}} \\
&\left(\sum_{\alpha\in\{\uparrow,\downarrow\}^{|T_j^\rho|-1}} \sum_{\sigma\in\mathrm{Sym}(\{(T^\rho{}_j)_1,\dots,(T_j^\rho)_{(|T_j^\rho|-1)}\})} \mathrm{Tr}_{{(T_j^\rho)_{|T_j^\rho|}}^{\alpha_{|p_j|}}}\left(\sigma_1^{\alpha_1} \cdots \sigma_{|T_j^\rho|-1}^{\alpha_{|T_j^\rho|-1}}\right)\right).
\end{aligned}$$

PROOF Let $k \in \mathbb{N}$ and $m \in \{1,\dots,n\}^k$ satisfying that there are $i,l \in \{1,\dots,k\}$, $i \neq l$ such that $m_i = m_l$. In addition, choose $p \in P(k)$ a partition of $\{1,\dots,k\}$ satisfying that there is a $\mu \in \{1,\dots,|p|\}$ such that $i,l \in p_\mu$. We start with the following observation. By definition

$$\begin{aligned}
&\sum_{\rho\in K^{p_\mu}} (-1)^{|T^\rho|}\, 2^{k-|T^\rho|} \prod_{j\in\{1,\dots,|T^\rho|\}} \\
&\quad \Bigg( \sum_{\alpha\in\{\uparrow,\downarrow\}^{|T_j^\rho|-1}} \sum_{\sigma\in\mathrm{Sym}(\{(T^\rho{}_j)_1,\dots,(T_j^\rho)_{(|T_j^\rho|-1)}\})} \mathrm{Tr}_{(T_j^\rho)_{|T_j^\rho|}^{\alpha_{|p_j|}}}\big(\sigma_1^{\alpha_1}\cdots\sigma_{|T_j^\rho|-1}^{\alpha_{|T_j^\rho|-1}}\big)\Bigg) \\
&= \sum_{\rho\in K^{p_\mu}} (-1)^{|p|+1}\, 2^{k-|p|-1} \Bigg[ \\
&\quad \Bigg( \sum_{\alpha\in\{\uparrow,\downarrow\}^{|\rho_1|-1}} \sum_{\sigma\in\mathrm{Sym}(\{(\rho_1)_1,\dots,(\rho_1)_{(|\rho_1|-1)}\})} \mathrm{Tr}_{(\rho_1)_{|\rho_1|}^{\alpha_{|\rho_1|}}}\big(\sigma_1^{\alpha_1}\cdots\sigma_{|\rho_1|-1}^{\alpha_{|\rho_1|-1}}\big)\Bigg) \\
&\quad \Bigg( \sum_{\alpha\in\{\uparrow,\downarrow\}^{|\rho_2|-1}} \sum_{\sigma\in\mathrm{Sym}(\{(\rho_2)_1,\dots,(\rho_2)_{(|\rho_2|-1)}\})} \mathrm{Tr}_{(\rho_2)_{|\rho_2|}^{\alpha_{|\rho_2|}}}\big(\sigma_1^{\alpha_1}\cdots\sigma_{|\rho_2|-1}^{\alpha_{|\rho_2|-1}}\big)\Bigg) \\
&\quad \prod_{\substack{j\in\{1,\dots,|p|\},\\ j\neq\mu}} \Bigg( \sum_{\alpha\in\{\uparrow,\downarrow\}^{|p_j|-1}} \sum_{\sigma\in\mathrm{Sym}(\{(p_j)_1,\dots,(p_j)_{(|p_j|-1)}\})} \mathrm{Tr}_{(p_j)_{|p_j|}^{\alpha_{|p_j|}}}\big(\sigma_1^{\alpha_1}\cdots\sigma_{|p_j|-1}^{\alpha_{|p_j|-1}}\big)\Bigg)\Bigg].
\end{aligned} \tag{A.22}$$

By Lemma A.6 we have

$$\begin{aligned}
&\sum_{\rho\in K^{p_\mu}} \Bigg[\Bigg( \sum_{\alpha\in\{\uparrow,\downarrow\}^{|\rho_1|}} \sum_{\sigma\in\mathrm{Sym}(\{(\rho_1)_1,\dots,(\rho_1)_{(|\rho_1|-1)}\})} \mathrm{Tr}_{(\rho_1)_{|\rho_1|}^{\alpha_{|\rho_1|}}}\big(\sigma_1^{\alpha_1}\cdots\sigma_{|\rho_1|-1}^{\alpha_{|\rho_1|-1}}\big)\Bigg) \\
&\quad \Bigg( \sum_{\alpha\in\{\uparrow,\downarrow\}^{|\rho_2|}} \sum_{\sigma\in\mathrm{Sym}(\{(\rho_2)_1,\dots,(\rho_2)_{(|\rho_2|-1)}\})} \mathrm{Tr}_{(\rho_2)_{|\rho_2|}^{\alpha_{|\rho_2|}}}\big(\sigma_1^{\alpha_1}\cdots\sigma_{|\rho_2|-1}^{\alpha_{|\rho_2|-1}}\big)\Bigg)\Bigg] \\
&= \sum_{\rho\in K^{p_\mu}} \Bigg[\Bigg( \sum_{\alpha\in\{\uparrow,\downarrow\}^{|\rho_1|}} \sum_{\sigma\in\mathrm{Sym}(\{(\rho_1)_1,\dots,(\rho_1)_{(|\rho_1|)}\}\setminus\{i\})} \mathrm{Tr}_{i^{\alpha_{|\rho_1|}}}\big(\sigma_1^{\alpha_1}\cdots\sigma_{|\rho_1|-1}^{\alpha_{|\rho_1|-1}}\big)\Bigg) \\
&\quad \Bigg( \sum_{\alpha\in\{\uparrow,\downarrow\}^{|\rho_2|}} \sum_{\sigma\in\mathrm{Sym}(\{(\rho_2)_1,\dots,(\rho_2)_{(|\rho_2|-1)}\}\setminus\{l\})} \mathrm{Tr}_{i^{\alpha_{|\rho_2|}}}\big(\sigma_1^{\alpha_1}\cdots\sigma_{|\rho_2|-1}^{\alpha_{|\rho_2|-1}}\big)\Bigg)\Bigg] \\
&= \sum_{A\dot\cup B=p_\mu\setminus\{i,l\}} \Bigg[\Bigg( \sum_{\alpha\in\{\uparrow,\downarrow\}^{|A|+1}} \sum_{\sigma\in\mathrm{Sym}(\{A\})} \mathrm{Tr}_{i^{\alpha_{|A|+1}}}\big(\sigma_1^{\alpha_1}\cdots\sigma_{|A|}^{\alpha_{|A|}}\big)\Bigg) \\
&\quad \Bigg( \sum_{\alpha\in\{\uparrow,\downarrow\}^{|B|+1}} \sum_{\sigma\in\mathrm{Sym}(\{B\})} \mathrm{Tr}_{i^{\alpha_{|B|+1}}}\big(\sigma_1^{\alpha_1}\cdots\sigma_{|B|}^{\alpha_{|B|}}\big)\Bigg)\Bigg].
\end{aligned} \tag{A.23}$$

Combining (A.22) and (A.23) we get

$$\begin{aligned}
&\sum_{\rho\in K^{p_\mu}} (-1)^{|T^\rho|}\, 2^{k-|T^\rho|} \prod_{j\in\{1,\dots,|T^\rho|\}} \\
&\quad\Bigg( \sum_{\alpha\in\{\uparrow,\downarrow\}^{|T^\rho_j|-1}} \sum_{\sigma\in\mathrm{Sym}(\{(T^\rho{}_j)_1,\dots,(T^\rho_j)_{(|T^\rho_j|-1)}\})} \mathrm{Tr}_{(T^\rho_j)^{\alpha_{|p_j|}}_{|T^\rho_j|}} \big(\sigma_1^{\alpha_1}\cdots\sigma_{|T^\rho_j|-1}^{\alpha_{|T^\rho_j|-1}}\big)\Bigg) \\
&\quad= -\frac{1}{2}\,(-1)^{|p|}\, 2^{k-|p|} \qquad\qquad (\text{A.24}) \\
&\qquad \sum_{A\dot\cup B=p_\mu\setminus\{i,l\}} \Bigg[\Bigg( \sum_{\alpha\in\{\uparrow,\downarrow\}^{|A|+1}} \sum_{\sigma\in\mathrm{Sym}(\{A\})} \mathrm{Tr}_{i^{\alpha_{|A|+1}}} \big(\sigma_1^{\alpha_1}\cdots\sigma_{|A|}^{\alpha_{|A|}}\big)\Bigg) \\
&\qquad\qquad \Bigg( \sum_{\alpha\in\{\uparrow,\downarrow\}^{|B|+1}} \sum_{\sigma\in\mathrm{Sym}(\{B\})} \mathrm{Tr}_{i^{\alpha_{|B|+1}}} \big(\sigma_1^{\alpha_1}\cdots\sigma_{|B|}^{\alpha_{|B|}}\big)\Bigg)\Bigg] \\
&\qquad \prod_{\substack{j\in\{1,\dots,|p|\},\\ j\neq\mu}} \Bigg[ \sum_{\alpha\in\{\uparrow,\downarrow\}^{|p_j|-1}} \sum_{\sigma\in\mathrm{Sym}(\{(p_j)_1,\dots,(p_j)_{(|p_j|-1)}\})} \mathrm{Tr}_{(p_j)^{\alpha_{|p_j|}}_{|p_j|}} \big(\sigma_1^{\alpha_1}\cdots\sigma_{|p_j|-1}^{\alpha_{|p_j|-1}}\big)\Bigg].
\end{aligned}$$

On the other hand, an application of Lemma A.5 with $L = p_\mu$ yields

$$\begin{aligned}
&\sum_{\alpha\in\{\uparrow,\downarrow\}^{|p_\mu|}} \sum_{\sigma\in\mathrm{Sym}(\{(p_\mu)_1,\dots,(p_\mu)_{(|p_\mu|-1)}\})} \mathrm{Tr}_{(p_\mu)^{\alpha_{|p_\mu|}}_{|p_\mu|}} \big(\sigma_1^{\alpha_1}\cdots\sigma_{|p_\mu|-1}^{\alpha_{|p_\mu|-1}}\big) \\
&\quad= \frac{1}{2} \sum_{A\dot\cup B=p_\mu\setminus\{i,l\}} \Bigg(\Bigg( \sum_{\alpha\in\{\uparrow,\downarrow\}^{|A|+1}} \sum_{\sigma\in\mathrm{Sym}(A)} \mathrm{Tr}_{i^{\alpha_{|A|+1}}} \Big(\sigma_1^{\alpha_1}\cdots\sigma_{|A|}^{\alpha_{|A|}}\Big)\Bigg) \\
&\qquad\qquad \Bigg( \sum_{\beta\in\{\uparrow,\downarrow\}^{|B|+1}} \sum_{\tau\in\mathrm{Sym}(B)} \mathrm{Tr}_{i^{\beta_{|B|+1}}} \Big(\tau_r^{\beta_1}\cdots\tau_{|B|}^{\beta_{|B|}}\Big)\Bigg)\Bigg).
\end{aligned}$$

Therefore,

$$\begin{aligned}
&(-1)^{|p|}\, 2^{k-|p|} \prod_{j\in\{1,\dots,|p|\}} \\
&\quad\Bigg( \sum_{\alpha\in\{\uparrow,\downarrow\}^{|p_j|}} \sum_{\sigma\in\mathrm{Sym}(\{(p_j)_1,\dots,(p_j)_{(|p_j|-1)}\})} \mathrm{Tr}_{(p_j)^{\alpha_{|p_j|}}_{|p_j|}} \big(\sigma_1^{\alpha_1}\cdots\sigma_{|p_j|-1}^{\alpha_{|p_j|-1}}\big)\Bigg) \\
&\quad= \frac{1}{2}\,(-1)^{|p|}\, 2^{k-|p|} \qquad\qquad (\text{A.25}) \\
&\qquad \sum_{A\dot\cup B=p_\mu\setminus\{i,l\}} \Bigg(\Bigg( \sum_{\alpha\in\{\uparrow,\downarrow\}^{|A|+1}} \sum_{\sigma\in\mathrm{Sym}(A)} \mathrm{Tr}_{i^{\alpha_{|A|+1}}} \Big(\sigma_1^{\alpha_1}\cdots\sigma_{|A|}^{\alpha_{|A|}}\Big)\Bigg) \\
&\qquad\qquad \Bigg( \sum_{\beta\in\{\uparrow,\downarrow\}^{|B|+1}} \sum_{\tau\in\mathrm{Sym}(B)} \mathrm{Tr}_{i^{\beta_{|B|+1}}} \Big(\tau_r^{\beta_1}\cdots\tau_{|B|}^{\beta_{|B|}}\Big)\Bigg)\Bigg) \\
&\qquad \prod_{\substack{j\in\{1,\dots,|p|\},\\ j\neq\mu}} \Bigg( \sum_{\alpha\in\{\uparrow,\downarrow\}^{|p_j|}} \sum_{\sigma\in\mathrm{Sym}(\{(p_j)_1,\dots,(p_j)_{(|p_j|-1)}\})} \mathrm{Tr}_{(p_j)^{\alpha_{|p_j|}}_{|p_j|}} \big(\sigma_1^{\alpha_1}\cdots\sigma_{|p_j|-1}^{\alpha_{|p_j|-1}}\big)\Bigg).
\end{aligned}$$

Adding (A.24) to (A.25) finishes the proof. □

**Lemma A.8** *Let $N \in \mathbb{N}_0$, $B$ a symbol in $S^k \in (\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f}))$, $k \geq 0$ and $\mathcal{B}_\alpha \in S^k(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f}))$ for $\alpha \in \mathbb{N}_0$ defined by*

$$\mathcal{B}_\alpha(\varepsilon) := \Big\{ \{\pi_{\alpha_1}, B(\varepsilon)\}_{\alpha_2}, \pi_{\alpha_3} \Big\}_{\alpha_4} .$$

*Then*

$$\sum_{\alpha \in \mathbb{N}_0^4, |\alpha| = N} \mathcal{B}_\alpha(\varepsilon) = \sum_{\alpha, \beta \in \mathbb{N}_0^4, |\alpha| + |\beta| = N} \Big\{ \{\pi_{\beta_1}, \mathcal{B}_\alpha(\varepsilon)\}_{\beta_2}, \pi_{\beta_3} \Big\}_{\beta_4} .$$

PROOF To simplify the notation we assume that $B$ is independent of $\varepsilon$, i.e. $B \in S^k(\mathcal{B}(\mathcal{H}_\mathrm{f}))$. By the asymptotic expansion of the Moyal product for classical symbols (2.9) we have

$$\pi \# B \# \pi \asymp \sum_{i=0}^{\infty} \varepsilon^i \, (\pi \# B \# \pi)_i = \sum_{i=0}^{\infty} \varepsilon^i \sum_{\alpha \in \mathbb{N}_0^4, |\alpha| = i} \mathcal{B}_\alpha$$

and

$$\begin{aligned} \pi \# \pi \# B \# \pi \# \pi &\asymp \sum_{i=0}^{\infty} \varepsilon^i \, (\pi \# \pi \# B \# \pi \# \pi)_i \\ &= \sum_{i=0}^{\infty} \varepsilon^i \sum_{\alpha, \beta \in \mathbb{N}_0^4, |\alpha| + |\beta| = i} \Big\{ \{\pi_{\beta_1}, \mathcal{B}_\alpha\}_{\beta_2}, \pi_{\beta_3} \Big\}_{\beta_4} . \end{aligned}$$

On the other hand, $\pi$ is a Moyal projection, i.e. $\pi = \pi \# \pi + \mathcal{O}(\varepsilon^\infty)$. Thus

$$(\pi \# B \# \pi)_N = (\pi \# \pi \# B \# \pi \# \pi)_N \quad \text{for any } N \in \mathbb{N}_0$$

which proves our claim for symbols that are independent of $\varepsilon$. Note that besides the notation, we never actually used that $B$ is independent of $\varepsilon$. Therefore the proof is complete. □

**Lemma A.9** *Let $N \in \mathbb{N}_0$ and $B$ be a symbol in $S^k(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f}))$, $k \in \mathbb{N}_0$ with $b \in S^k(\varepsilon, \mathbb{C})$ the associated effective symbol as defined in Section 3.2. Then there exist $Q_\alpha^{N,r} \in S^0(\mathcal{J}(\mathcal{H}_\mathrm{f}))$, $0 \leq r \leq N$, $\alpha \in \{1, \ldots, 2n\}^r$ such that*

$$b_N(\varepsilon) = \sum_{r=0}^{N} \sum_{\alpha \in \{1,\ldots,2n\}^r} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(Q_\alpha^{N,r} \, \nabla_\alpha^r B(\varepsilon)) . \qquad \text{(A.26)}$$

PROOF We start with the following observation. Assume $R \in S^k(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f}))$, $k \in \mathbb{N}_0$ and $l \in \mathbb{N}_0$. By the definition of the generalized Poisson bracket (2.5) the expression

$$\sum_{\substack{\alpha\in\mathbb{N}_0,\\|\alpha|=l}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big(P_0 \left\{\{\pi_{\alpha_1}, R(\varepsilon)\}_{\alpha_2}, \pi_{\alpha_3}\right\}_{\alpha_4}\Big)$$

can be expressed as sum where each summand is of the form

$$\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\partial_\beta \pi_{\alpha_1}\, \partial_\gamma R(\varepsilon)\, \partial_\delta \pi_{\alpha_3}\, P_0)$$

where $\beta, \gamma, \delta \in \mathbb{N}_0^{2d}$ are multiindices with $|\beta|, |\gamma|, |\delta| \leq l$. By the cyclicity of the trace we find that for each $l \in \mathbb{N}_0$ there exist $\widetilde{Q}^{l,\tilde{r}}_{\beta_1,\dots,\beta_{\tilde{r}}} \in S^0(\mathcal{J}(\mathcal{H}_\mathrm{f}))$, $\beta \in \{1, \dots, 2n\}^{\tilde{r}}$, $0 \leq \tilde{r} \leq l$ such that

$$\sum_{\substack{\alpha\in\mathbb{N}_0,\\|\alpha|=l}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big(P_0 \left\{\{\pi_{\alpha_1}, R(\varepsilon)\}_{\alpha_2}, \pi_{\alpha_3}\right\}_{\alpha_4}\Big) = \sum_{\tilde{r}=0}^{l} \sum_{\beta\in\{1,\dots,2n\}^{\tilde{r}}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\widetilde{Q}^{l,\tilde{r}}_\beta\, \nabla^{\tilde{r}}_\beta R(\varepsilon))\,. \tag{A.27}$$

We want to show inductively that the $b_j$s can be represented in a similar manner. Defining $P_0 := Q^{0,0}$ we have $b_0(\varepsilon) = \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(Q^{0,0}\, B(\varepsilon))$. Assuming (A.26) to hold for all $j \leq N$, we will prove it for $N+1$. By definition

$$\begin{aligned} b_{N+1}(\varepsilon) = &\sum_{\substack{\alpha\in\mathbb{N}_0^4,\\|\alpha|=N+1}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}\left(P_0 \left\{\{\pi_{\alpha_1}, B(\varepsilon)\}_{\alpha_2}, \pi_{\alpha_3}\right\}_{\alpha_4}\right) \\ &- \sum_{i=0}^{N} \sum_{\substack{\alpha\in\mathbb{N}_0^4,\\|\alpha|=N+1-i}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}\left(\left\{\{\pi_{\alpha_1}, b_i(\varepsilon)\}_{\alpha_2}, \pi_{\alpha_3}\right\}_{\alpha_4}\right)\,. \end{aligned}$$

Applying (A.27) yields

$$\begin{aligned} b_{N+1}(\varepsilon) = &\sum_{\tilde{r}=0}^{N+1} \sum_{\beta\in\{1,\dots,2n\}^{\tilde{r}}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\widetilde{Q}^{N+1,\tilde{r}}_\beta\, \nabla^{\tilde{r}}_\beta B(\varepsilon)) \\ &- \sum_{i=0}^{N} \sum_{\tilde{r}=0}^{N+1-i} \sum_{\beta\in\{1,\dots,2n\}^{\tilde{r}}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\widetilde{Q}^{N+1-i,\tilde{r}}_\beta\, \nabla^{\tilde{r}}_\beta b_i(\varepsilon))\,. \end{aligned}$$

Finally, applying the induction hypothesis yields

$$\begin{aligned}
b_{N+1}(\varepsilon) &= \sum_{\tilde{r}=0}^{N+1} \sum_{\beta\in\{1,\dots,2n\}^{\tilde{r}}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\widetilde{Q}_\beta^{N+1,\tilde{r}}\,\nabla_\beta^{\tilde{r}} B(\varepsilon)) \\
&\quad - \sum_{i=0}^{N} \sum_{\tilde{r}=0}^{N+1-i} \sum_{\beta\in\{1,\dots,2n\}^{\tilde{r}}} \sum_{r=0}^{i} \sum_{\alpha\in\{1,\dots,2n\}^{r}} \\
&\qquad\qquad \mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big(\widetilde{Q}_\beta^{N+1-i,\tilde{r}}\,\nabla_\beta^{\tilde{r}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(Q_\alpha^{i,r}\,\nabla_\alpha^r B(\varepsilon))\Big) \\
&= \sum_{\tilde{r}=0}^{N+1} \sum_{\beta\in\{1,\dots,2n\}^{\tilde{r}}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\widetilde{Q}_\beta^{N+1,\tilde{r}}\,\nabla_\beta^{\tilde{r}} B(\varepsilon)) \\
&\quad - \sum_{i=0}^{N} \sum_{\tilde{r}=0}^{N+1-i} \sum_{\beta\in\{1,\dots,2n\}^{\tilde{r}}} \sum_{r=0}^{i} \sum_{\alpha\in\{1,\dots,2n\}^{r}} \\
&\qquad\qquad \mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big(\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\widetilde{Q}_\beta^{N+1-i,\tilde{r}})\,\nabla_\beta^{\tilde{r}} (Q_\alpha^{i,r}\,\nabla_\alpha^r B(\varepsilon))\Big)\,.
\end{aligned}$$

A simple verification using the product rule and regrouping the resulting terms shows that $b_{N+1}$ is of the desired form, finishing the proof. □

**Proposition A.10** *Let $\varepsilon \geq 0$ small enough, $\alpha \in \mathbb{N}_0^{2n}$, $R, S \in S^0(\varepsilon, \mathcal{J}(\mathcal{H}_\mathrm{f}))$ be classical symbols, $Q \in S^0(\mathcal{J}(\mathcal{H}_\mathrm{f}))$ and $B \in S^k(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f}))$, $k > 2n+1$. Then there exist constants $C_N > 0$ and $\tilde{C}_N > 0$ for every $N \in \mathbb{Z}$, $N \geq -1$ such that*

$$\begin{aligned}
&\bigg| \int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big( R(\varepsilon) \# B(\varepsilon) \# S(\varepsilon) \\
&\qquad - \sum_{j=0}^{N} \varepsilon^j \sum_{\substack{\alpha\in\mathbb{N}_0^4,\\ |\alpha|=j}} \Big\{ \{R_{\alpha_1}, B(\varepsilon)\}_{\alpha_2}, S_{\alpha_3} \Big\}_{\alpha_4} \Big)(\varepsilon, z)\,\mathrm{d}z \bigg| \\
&\qquad \leq \varepsilon^{N+1} C_N \, \|B(\varepsilon)\|_{L^1}^{\varepsilon}\,.
\end{aligned} \tag{A.28}$$

*and*

$$\begin{aligned}
&\bigg| \int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big( R(\varepsilon) \# \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(Q\,\partial^\alpha B(\varepsilon))\mathbf{1}_{\mathcal{H}_\mathrm{f}} \# S(\varepsilon) \\
&\qquad - \sum_{j=0}^{N} \varepsilon^j \sum_{\substack{\alpha\in\mathbb{N}_0^4,\\ |\alpha|=j}} \Big\{ \{R_{\alpha_1}, \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(Q\,\partial^\alpha B(\varepsilon))\mathbf{1}_{\mathcal{H}_\mathrm{f}}\}_{\alpha_2}, S_{\alpha_3} \Big\}_{\alpha_4} \Big)(\varepsilon, z)\,\mathrm{d}z \bigg| \\
&\qquad \leq \varepsilon^{N+1} \tilde{C}_N \, \|B(\varepsilon)\|_{L^1}^{\varepsilon}\,.
\end{aligned} \tag{A.29}$$

PROOF Before we start with the actual proof we will introduce the basic idea, state some known results and introduce the notation. For now, let $B$ be a symbol in $S^k(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f}))$, $k > 2n$ and $R, S$ be symbols independent of $\varepsilon$

taking value in the trace class operator acting on $\mathcal{H}_{\mathrm{f}}$, i.e. $R, S \in S^0(\mathcal{J}(\mathcal{H}_{\mathrm{f}}))$. By the continuity of the Moyal remainder we have for any $N \in \mathbb{Z}$, $N \geq -1$

$$\varepsilon^{-(N+1)}\Big(R \# B \# S - \sum_{j=0}^{N} \varepsilon^j \sum_{i=0}^{j} \{\{R\,, B(\varepsilon)\}_i\ , S\}_{j-i}\Big) \in S^k(\varepsilon, \mathcal{J}(\mathcal{H}_{\mathrm{f}}))\,.$$

Therefore, it holds for any $N \in \mathbb{N}_0$ that

$$\begin{aligned}\int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_{\mathrm{f}}}\Big(R \# B \# S - \sum_{j=0}^{N} \varepsilon^j \sum_{i=0}^{j} \{\{R\,, B(\varepsilon)\}_i\ , S\}_{j-i}\Big)(\varepsilon, z)\,\mathrm{d}z \\ = \mathcal{O}(\varepsilon^{N+1})\,.\end{aligned} \tag{A.30}$$

So, $\int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_{\mathrm{f}}}(R \# B \# S)(\varepsilon, z)\,\mathrm{d}z$ has an asymptotic expansion given by

$$\begin{aligned}&\int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_{\mathrm{f}}}(R \# B \# S)(\varepsilon, z)\,\mathrm{d}z \\ &\quad\asymp \sum_{j=0}^{\infty} \varepsilon^j \int_{\mathbb{R}^{2n}} \sum_{i=0}^{j} \mathrm{tr}_{\mathcal{H}_{\mathrm{f}}}\Big(\ \{\{R\,, B(\varepsilon)\}_i\ , S\}_{j-i}\Big)(\varepsilon, z)\,\mathrm{d}z\,.\end{aligned}$$

By integration by parts there exist constants $C_j > 0$ for each $j \in \mathbb{N}_0$ such that

$$\begin{aligned}&\Big|\int_{\mathbb{R}^{2n}} \sum_{i=0}^{j} \mathrm{tr}_{\mathcal{H}_{\mathrm{f}}}(\{\{R\,, B(\varepsilon)\}_i\ , S\}_{j-i})(\varepsilon, z)\,\mathrm{d}z\Big| \\ &\quad\leq C_j \int_{\mathbb{R}^{2n}} \sup_{\varepsilon \in [0,\varepsilon_0)} \|B(\varepsilon, z)\|\,\|R\|_{0,3j,1}\,\|S\|_{0,3j}\,\mathrm{d}z \\ &\quad= C_j\,\|B\|^{\varepsilon}_{L^1}\,\|R\|_{0,3j,1}\,\|S\|_{0,3j}\,.\end{aligned} \tag{A.31}$$

Combining (A.30) and (A.31)

$$\begin{aligned}&\Big|\int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_{\mathrm{f}}}\Big(R \# B \# S - \sum_{j=0}^{N} \varepsilon^j \sum_{i=0}^{j} \{\{R\,, B(\varepsilon)\}_i\ , S\}_{j-i}\Big)(\varepsilon, z)\,\mathrm{d}z\Big| \\ &\quad\leq \Big|\int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_{\mathrm{f}}}\Big(R \# B(\varepsilon) \# S - \sum_{j=0}^{\tilde{N}} \varepsilon^j \sum_{i=0}^{j} \{\{R\,, B(\varepsilon)\}_i\ , S\}_{j-i}\Big)(\varepsilon, z)\,\mathrm{d}z\Big| \\ &\qquad+ \Big|\sum_{j=N+1}^{\tilde{N}} \varepsilon^j \sum_{i=0}^{j} \int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_{\mathrm{f}}}\Big(\ \{\{R\,, B(\varepsilon)\}_i\ , S\}_{j-i}\Big)(\varepsilon, z)\,\mathrm{d}z\Big| \\ &\quad= \mathcal{O}(\varepsilon^{N+1}\|B\|^{\varepsilon}_{L^1}) + \mathcal{O}(\varepsilon^{N+\tilde{N}+1})\end{aligned}$$

for every $N, \tilde{N} \in \mathbb{N}_0$, $\tilde{N} \geq N$.

The difficulty to obtain (A.28) is to get access to the error terms in the expansion of the Moyal product. Therefore the idea is to reproduce the proof of the Moyal expansion and further estimate the resulting terms to make integration by parts applicable. The proof reproduced here is the proof of [Zwo12, Theorem 4.17]. In [Zwo12] all the symbols are scalar valued and independent of $\varepsilon$ but it is straightforward to generalize the results to symbols in $S^k(\varepsilon, \mathcal{B}(\mathcal{H}_{\mathrm{f}}))$ using the same proofs. Throughout this proof we will denote $(x_1, \ldots, x_l) := (x_1^T, \ldots, x_l^T)^T$ for $x_1, \ldots, x_l \in \mathbb{R}^{2n}$, $l \in \mathbb{N}$. If $R, S, B \in \mathscr{S}(\varepsilon, \mathcal{B}(\mathcal{H}_{\mathrm{f}}))$ the Moyal product can be represented as

$$
\begin{aligned}
&(R \# B \# S)(\varepsilon, z) \\
&\quad := \mathrm{e}^{\mathrm{i}\frac{\varepsilon}{2}\sigma(\mathfrak{D}_x, \mathfrak{D}_y)} \mathrm{e}^{\mathrm{i}\frac{\varepsilon}{2}\sigma(\mathfrak{D}_z, \mathfrak{D}_w)} R(\varepsilon, z+x)\, B(\varepsilon, w+x)\, S(\varepsilon, y)\Big|_{w=y=z,\, x=0} \\
&\quad = \left(\frac{1}{\pi\varepsilon}\right)^{4n} \int_{\mathbb{R}^{8n}} \mathrm{e}^{-\frac{2\mathrm{i}}{\varepsilon}\sigma(x,y)} \mathrm{e}^{-\frac{2\mathrm{i}}{\varepsilon}\sigma(u,w)} \\
&\qquad\qquad R(\varepsilon, z+u+x)\, B(\varepsilon, z+w+x)\, S(\varepsilon, z+y)\, \mathrm{d}u\, \mathrm{d}w\, \mathrm{d}y\, \mathrm{d}x
\end{aligned}
$$

(see for instance [Zwo12, Theorem 4.11]). For $R, S \in S^0(\varepsilon, \mathcal{J}(\mathcal{H}_{\mathrm{f}}))$, $B \in S^k(\varepsilon, \mathcal{B}(\mathcal{H}_{\mathrm{f}}))$ the integral

$$
\begin{aligned}
&(R \# B \# S)(\varepsilon, z) \\
&\quad := (\pi\varepsilon)^{-4n} \int_{\mathbb{R}^{8n}} \mathrm{e}^{-\frac{2\mathrm{i}}{\varepsilon}\sigma(x,y)} \mathrm{e}^{-\frac{2\mathrm{i}}{\varepsilon}\sigma(u,w)} \\
&\qquad\qquad R(\varepsilon, z+u+x)\, B(\varepsilon, z+w+x)\, S(\varepsilon, z+y) \\
&\qquad \mathrm{d}u\, \mathrm{d}w\, \mathrm{d}x\, \mathrm{d}x
\end{aligned}
\tag{A.32}
$$

uniquely defines an element of $\mathscr{S}'(\varepsilon, \mathcal{J}(\mathcal{H}_{\mathrm{f}}))$ by [Zwo12, Theorem 3.18], extending $R \# B \# S$. Additionally, by examining the proof of [Zwo12, Theorem 4.11] one can find that for $R, B \in \mathcal{C}_0^\infty(\varepsilon, \mathcal{B}(\mathcal{H}_{\mathrm{f}}))$, $N \in \mathbb{Z}$, $N \geq -1$

$$
\begin{aligned}
&\left(\frac{1}{\pi\varepsilon}\right)^{2n} \int_{\mathbb{R}^{4n}} \mathrm{e}^{-\frac{2\mathrm{i}}{\varepsilon}\sigma(u,w)} R(\varepsilon, z+u)\, B(\varepsilon, z+w)\, \mathrm{d}u\, \mathrm{d}w \\
&\quad = \sum_{m=0}^{N} \frac{(\mathrm{i}\varepsilon)^m}{2^m m!} \Big[\sigma(\mathfrak{D}_u, \mathfrak{D}_w)^m R(\varepsilon, z+u)\, B(\varepsilon, z+w)\Big]\Big|_{w=u=0} \\
&\qquad + \frac{(\mathrm{i}\varepsilon)^{N+1}}{2^{N+1} N!} \int_0^1 (1-t_1)^N \Big[\mathrm{e}^{\frac{\mathrm{i}\varepsilon t}{2}\sigma(\mathfrak{D}_u, \mathfrak{D}_w)} \sigma(\mathfrak{D}_u, \mathfrak{D}_w)^{N+1} \\
&\qquad\qquad R(\varepsilon, z+u)\, B(\varepsilon, z+w)\Big]\Big|_{w=u=0} \mathrm{d}t\,.
\end{aligned}
\tag{A.33}
$$

The operator $\mathrm{e}^{\frac{\mathrm{i}\varepsilon t}{2}\sigma(\mathfrak{D}_u, \mathfrak{D}_w)} \sigma(\mathfrak{D}_u, \mathfrak{D}_w)^{N+1}$ is defined as a Fourier multiplier $\mathcal{F}_{(u,w)}^{-1} \mathrm{e}^{\frac{\mathrm{i}\varepsilon t}{2}\sigma(\xi_1, \xi_2)} \sigma(\xi_1, \xi_2)^{N+1} \mathcal{F}_{(u,w)}$ with $\mathcal{F}_{(u,w)}$ the Fourier transform and $\xi_1, \xi_2 \in \mathbb{R}^{2n}$.

From now on, let $R, S \in S^0(\varepsilon, \mathcal{J}(\mathcal{H}_{\mathrm{f}}))$ be classical symbols, $B$ a symbol in $S^k(\varepsilon, \mathcal{B}(\mathcal{H}_{\mathrm{f}}))$, $k > 2n$ and $N \in \mathbb{Z}$, $N \geq -1$. In addition, let $\chi : \mathbb{R}^{8n} \to \mathbb{R}$ be a smooth function with $\chi(z,w,x,y)=1$ in $B_0(1) := \{\xi \in \mathbb{R}^{8n} : |\xi| < 1\}$ and $\operatorname{supp}(\chi) = \overline{B_2(0)}$. By (A.32)

$$(R \# B \# S)(\varepsilon, z) = M_1(\varepsilon, z) + M_2(\varepsilon, z)$$

where

$$\begin{aligned} M_1(\varepsilon,z) = \left(\frac{1}{\pi\varepsilon}\right)^{4n} \int_{\mathbb{R}^{8n}} & \mathrm{e}^{-\frac{2\mathrm{i}}{\varepsilon}\sigma(x,y)} \mathrm{e}^{-\frac{2\mathrm{i}}{\varepsilon}\sigma(u,w)} \\ & R(\varepsilon, z+u+x)\, B(\varepsilon, z+w+x)\, S(\varepsilon, z+y)\, (1-\chi(u,w,x,y)) \\ & \mathrm{d}u\, \mathrm{d}w\, \mathrm{d}x\, \mathrm{d}y \end{aligned}$$

and

$$\begin{aligned} M_2(\varepsilon,z) = \left(\frac{1}{\pi\varepsilon}\right)^{4n} \int_{\mathbb{R}^{8n}} & \mathrm{e}^{-\frac{2\mathrm{i}}{\varepsilon}\sigma(x,y)} \mathrm{e}^{-\frac{2\mathrm{i}}{\varepsilon}\sigma(u,w)} \\ & R(\varepsilon, z+u+x)\, B(\varepsilon, z+w+x)\, S(\varepsilon, z+y)\, \chi(u,w,x,y) \\ & \mathrm{d}u\, \mathrm{d}w\, \mathrm{d}x\, \mathrm{d}y \end{aligned}$$

We split the proof into two parts. In the first part we estimate $M_1$. In the second part we handle $M_2$ where we make use of the fact that $R(\varepsilon, z+u+x)\, B(\varepsilon, z+w+x)\, S(\varepsilon, z+y)\, \chi(u,w,x,y)$ has compact support. Therefore, the basic idea is to apply (A.33) to $M_2$ and estimate the resulting terms.

**1. Estimates for $M_1$**

Define $L_{(x,y)} := \frac{\left\langle \nabla_{(x,y)}\sigma(x,y)\,,\, -\frac{\varepsilon}{2}\mathfrak{D}_{(x,y)} \right\rangle}{|\nabla_{(x,y)}\sigma(x,y)|^2}$. Since

$$\nabla_{(x,y)}\sigma(x,y) = (-y_2, y_1, x_2, -x_1) \tag{A.34}$$

for $x=(x_1,x_2)$, $y=(y_1,y_2)$, $x_1,x_2,y_1,y_2 \in \mathbb{R}^n$ we have

$$L_{(x,y)} = \frac{\left\langle \nabla_{(x,y)}\sigma(x,y)\,,\, -\frac{\varepsilon}{2}\mathfrak{D}_{(x,y)} \right\rangle}{|(x,y)|^2}\,.$$

Then $L_{(x,y)}\,\mathrm{e}^{-\frac{2\mathrm{i}}{\varepsilon}\sigma(x,y)} = \mathrm{e}^{-\frac{2\mathrm{i}}{\varepsilon}\sigma(x,y)}$ such that for $\tilde{N} \in \mathbb{N}, \tilde{N} > 2n+1+N$

$$
\begin{aligned}
M_1(\varepsilon,z) = (\pi\varepsilon)^{-4n} \int_{\mathbb{R}^{8n}} & \Big((L_{(x,y)})^{\tilde{N}} \mathrm{e}^{-\frac{2\mathrm{i}}{\varepsilon}\sigma(x,y)}\Big)\Big((L_{(u,w)})^{\tilde{N}} \mathrm{e}^{-\frac{2\mathrm{i}}{\varepsilon}\sigma(u,w)}\Big) \\
& R(\varepsilon, z+u+x)\, B(\varepsilon, z+w+x)\, S(\varepsilon, z+y) \\
& (1-\chi(u,w,x,y))\,\mathrm{d}u\,\mathrm{d}w\,\mathrm{d}x\,\mathrm{d}y \\
= (\pi\varepsilon)^{-4n} \int_{\mathbb{R}^{8n}} & \mathrm{e}^{-\frac{2\mathrm{i}}{\varepsilon}\sigma(x,y)} \mathrm{e}^{-\frac{2\mathrm{i}}{\varepsilon}\sigma(u,w)} \\
& (L^*_{x,y})^{\tilde{N}} (L^*_{u,w})^{\tilde{N}} R(\varepsilon, z+u+x)\, B(\varepsilon, z+w+x)\, S(\varepsilon, z+y) \\
& (1-\chi(u,w,x,y))\,\mathrm{d}u\,\mathrm{d}w\,\mathrm{d}x\,\mathrm{d}y
\end{aligned}
$$

where $L^*_{(x,y)} = \frac{\varepsilon}{2}\left\langle \mathfrak{D}_{(x,y)}\,,\, \frac{\nabla_{(x,y)}\sigma(x,y)}{|(x,y)|^2}\right\rangle$ denotes the adjoint of $L_{(x,y)}$. Then, there exists a constant $C_1 > 0$ such that for all $x, y, u, w \in \mathbb{R}^{2n}$ and $l_1, l_2, j_1, j_2 \in \mathbb{N}, l_1 \geq j_1, l_2 \geq j_2$:

$$
\left| \frac{1}{|(u,w)|^{l_1}} \frac{1}{|(x,y)|^{l_2}} (1-\chi(u,w,x,y)) \right| \leq C_1 \frac{1}{\langle (u,w)\rangle^{j_1} \langle (x,y)\rangle^{j_2}}\,.
$$

By (A.34)

$$
\partial_l \frac{\partial_k \sigma(x,y)}{|(x,y)|^2} = \begin{cases} \frac{|(x,y)|^2 - (x,y)_l^2}{|(x,y)|^4}, & \text{for } (x,y)_l = (-y_2, y_1, x_2, -x_1)_k \\ \frac{(-y_2,y_1,x_2,-x_1)_k\,(-2(x,y)_l)}{|(x,y)|^4}, & \text{otherwise} \end{cases} \tag{A.35}
$$

Therefore, there exists a constant $C > 0$ such that

$$
\begin{aligned}
\mathrm{tr}_{\mathcal{H}_\mathrm{f}} \Big| & (L^*_{x,y})^{\tilde{N}} (L^*_{u,w})^{\tilde{N}} R(\varepsilon, z+u+x) \\
& B(\varepsilon, z+w+x)\, S(\varepsilon, z+y)\, (1-\chi(u,w,x,y)) \Big| \\
& \leq C \langle (u,w)\rangle^{-\tilde{N}} \langle (x,y)\rangle^{-\tilde{N}} \langle z\rangle^{-k} \|R\|^{\varepsilon}_{0,2\tilde{N},1}\, \|B\|^{\varepsilon}_{k,2\tilde{N}}\, \|S\|^{\varepsilon}_{0,\tilde{N}}
\end{aligned} \tag{A.36}
$$

where we used the fact that $\left\| \frac{\langle z\rangle^k}{\langle z\rangle^k} \partial_z^\alpha B(\varepsilon, z+w+x) \right\| \leq \frac{1}{\langle z\rangle^k} \|B\|^{\varepsilon}_{k,2\tilde{N}}$ for any $\alpha \in \mathbb{N}_0^{2n}$, $|\alpha| \leq 2\tilde{N}$. It follows that

$$
\begin{aligned}
\mathrm{e}^{-\frac{2\mathrm{i}}{\varepsilon}\sigma(x,y)} \mathrm{e}^{-\frac{2\mathrm{i}}{\varepsilon}\sigma(u,w)} & (L^*_{x,y})^{\tilde{N}} (L^*_{u,w})^{\tilde{N}} R(\varepsilon, z+u+x)\, B(\varepsilon, z+w+x) \\
& S(\varepsilon, z+y)\, (1-\chi(u,w,x,y))
\end{aligned}
$$

is Bochner-integrable as map from $\mathbb{R}^{8n}$ to $\mathcal{J}(\mathcal{H}_\mathrm{f})$. Since $\mathrm{tr}_{\mathcal{H}_\mathrm{f}} : \mathcal{J}(\mathcal{H}_\mathrm{f}) \to \mathbb{C}$ is a continuous linear operator we have that

$$\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(M_1(\varepsilon, z)) = (\pi\varepsilon)^{-4n} \int_{\mathbb{R}^{8n}} \mathrm{e}^{-\frac{2\mathrm{i}}{\varepsilon}\sigma(x,y)} \mathrm{e}^{-\frac{2\mathrm{i}}{\varepsilon}\sigma(u,w)} \, (L^*_{(x,y)})^{\tilde{N}} (L^*_{(u,w)})^{\tilde{N}} \\ \mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big( R(\varepsilon, z+u+x) \, B(\varepsilon, z+w+x) \, S(\varepsilon, z+y) \\ (1-\chi(u,w,x,y))\Big) \, \mathrm{d}u \, \mathrm{d}w \, \mathrm{d}x \, \mathrm{d}y.$$

By (A.36) exists a constant $C > 0$ such that

$$\int_{\mathbb{R}^{2n}} |\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(M_1(\varepsilon, z))| \, \mathrm{d}z \leq C \int_{\mathbb{R}^{2n}} \frac{1}{\langle z \rangle^k} \mathrm{d}z < \infty$$

and thus

$$\Big| \int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(M_1(\varepsilon, z)) \, \mathrm{d}z \Big| = (\tfrac{\varepsilon}{2})^{2\tilde{N}} \, (\pi\varepsilon)^{-4n} \Big| \int_{\mathbb{R}^{10n}} \mathrm{e}^{-\frac{2\mathrm{i}}{\varepsilon}\sigma(x,y)} \mathrm{e}^{-\frac{2\mathrm{i}}{\varepsilon}\sigma(u,w)} \\ \Big\langle \mathfrak{D}_{(x,y)} \, , \, \frac{\nabla_{(x,y)}\sigma(x,y)}{|(x,y)|^2} \Big\rangle^{\tilde{N}} \Big\langle \mathfrak{D}_{(u,w)} \, , \, \frac{\nabla_{(u,w)}\sigma(x,y)}{|(u,w)|^2} \Big\rangle^{\tilde{N}} \\ \mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big( R(\varepsilon, z+u+x) \, B(\varepsilon, z+w+x) \\ S(\varepsilon, z+y) \, (1-\chi(u,w,x,y))\Big) \, \mathrm{d}z \, \mathrm{d}u \, \mathrm{d}w \, \mathrm{d}x \, \mathrm{d}y \Big| . \tag{A.37}$$

In the next step we apply an integration by parts with respect to $z$ to the right hand side of (A.37) and make use of the cyclicity of the trace. Then there exists a differential operator $\tilde{\nabla}_{z,x,y,z}$ of order $3\tilde{N}$ such that

$$\Big| \int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(M_1(\varepsilon, z)) \, \mathrm{d}z \Big| = (\tfrac{\varepsilon}{2})^{2\tilde{N}} \, (\pi\varepsilon)^{-4n} \Big| \int_{\mathbb{R}^{10n}} \mathrm{e}^{-\frac{2\mathrm{i}}{\varepsilon}\sigma(x,y)} \mathrm{e}^{-\frac{2\mathrm{i}}{\varepsilon}\sigma(u,w)} \\ \mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big( \widetilde{\nabla}_{u,x,y,z} \, \big( S(\varepsilon, z+y) \, R(\varepsilon, z+u+x) \\ (1-\chi(u,w,x,y))\big) \, B(\varepsilon, z+w+x) \Big) \\ \mathrm{d}z \, \mathrm{d}u \, \mathrm{d}w \, \mathrm{d}x \, \mathrm{d}y \Big| .$$

With similar arguments as in the estimate (A.36) there exists a constant $C > 0$ such that

$$\Big| \mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big( B(\varepsilon, z+w+x) \, \tilde{\nabla}_{u,w,x,y}\Big( S(\varepsilon, z+y) \, R(\varepsilon, z+u+x)(1-\chi(u,w,x,y))\Big)\Big) \Big| \\ \leq C \, \langle (u,w) \rangle^{-\tilde{N}} \langle (x,y) \rangle^{-\tilde{N}} \, \| B(\varepsilon, z+u+x) \| \, \| R \|^{\varepsilon}_{0,3\tilde{N},1} \, \| S \|^{\varepsilon}_{0,3\tilde{N}} \, .$$

Consequently there is a $C_{N,1} > 0$ such that

$$\Big| \int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(M_1(\varepsilon, z))\, \mathrm{d}z \Big| \leq C_{N,1}\, \varepsilon^{2\tilde{N}-4n} \, \|B\|_{L_1} \leq C_{N,1}\, \varepsilon^{2N+2} \, \|B\|_{L_1}$$
$$\leq C_{N,1}\, \varepsilon^{N+1} \, \|B\|_{L_1} \, .$$

**2. Estimates for $M_2$**

Recall $M_2(\varepsilon, z)$ is given by

$$M_2(\varepsilon, z) = \Big(\frac{1}{\pi\varepsilon}\Big)^{4n} \int_{\mathbb{R}^{8n}} \mathrm{e}^{-\frac{2\mathrm{i}}{\varepsilon}\sigma(x,y)} \mathrm{e}^{-\frac{2\mathrm{i}}{\varepsilon}\sigma(u,w)}$$
$$R(\varepsilon, z+u+x)\, B(\varepsilon, z+w+x)\, S(\varepsilon, z+y)\, \chi(u,w,x,y)$$
$$\mathrm{d}u\, \mathrm{d}w\, \mathrm{d}x\, \mathrm{d}y \, .$$

Note that $R(\varepsilon, z+u+x)\, B(\varepsilon, z+w+x)\, S(\varepsilon, z+y)\chi(u,w,x,y)$ has compact support. Applying (A.33) twice yields

$$M_2(\varepsilon, z) = K_1(\varepsilon, z) + K_2(\varepsilon, z) + K_3(\varepsilon, z) + K_4(\varepsilon, z)$$

where

$$K_1(\varepsilon, z) = \sum_{m_2=0}^{N} \sum_{m_1=0}^{N} \frac{(\mathrm{i}\varepsilon)^{m_2+m_1}}{2^{m_2+m_1} m_2!\, m_1!} \sigma(\mathfrak{D}_x, \mathfrak{D}_y)^{m_2} \sigma(\mathfrak{D}_u, \mathfrak{D}_w)^{m_1}\, R(\varepsilon, z+u+x)$$
$$B(\varepsilon, z+w+x)\, S(\varepsilon, z+y)\, \chi(u,w,x,y)\Big|_{w=u=x=y=0} ,$$

$$K_2(\varepsilon, z) = \sum_{m_2=0}^{N} \frac{(\mathrm{i}\varepsilon)^{m_2+N+1}}{2^{m_2+N+1} m_2!\, N!} \int_0^1 (1-t_1)^N \sigma(\mathfrak{D}_x, \mathfrak{D}_y)^{m_2}$$
$$\mathrm{e}^{\frac{\mathrm{i}\varepsilon t_1}{2}\sigma(\mathfrak{D}_u, \mathfrak{D}_w)} \sigma(\mathfrak{D}_u, \mathfrak{D}_w)^{N+1} R(\varepsilon, z+u+x)\, B(\varepsilon, z+w+x)$$
$$S(\varepsilon, z+y)\, \chi(u,w,x,y)\Big|_{w=u=x=y=0} \mathrm{d}t_1 \, ,$$

$$K_3(\varepsilon, z) = \sum_{m_1=0}^{N} \frac{(\mathrm{i}\varepsilon)^{m_1+N+1}}{2^{m_1+N+1} m_1!\, N!} \int_0^1 (1-t_2)^N \mathrm{e}^{\frac{\mathrm{i}\varepsilon t_2}{2}\sigma(\mathfrak{D}_x, \mathfrak{D}_y)} \sigma(\mathfrak{D}_x, \mathfrak{D}_y)^{N+1}$$
$$\sigma(\mathfrak{D}_u, \mathfrak{D}_w)^{m_1} R(\varepsilon, z+u+x)\, B(\varepsilon, z+w+x)$$
$$S(\varepsilon, z+y)\, \chi(u,w,x,y)\Big|_{w=u=x=y=0} \mathrm{d}t_2$$

and

$$
\begin{aligned}
K_4(\varepsilon, z) =& \frac{(\mathrm{i}\varepsilon)^{2N+2}}{2^{2N+2}(N!)^2} \int_0^1 (1-t_2)^N \int_0^1 (1-t_1)^N \\
& \mathrm{e}^{\frac{\mathrm{i}\varepsilon t_2}{2}\sigma(\mathfrak{D}_x,\mathfrak{D}_y)} \sigma(\mathfrak{D}_x, \mathfrak{D}_y)^{N+1} \, \mathrm{e}^{\frac{\mathrm{i}\varepsilon t_1}{2}\sigma(\mathfrak{D}_u,\mathfrak{D}_w)} \sigma(\mathfrak{D}_u, \mathfrak{D}_w)^{N+1} \\
& R(\varepsilon, z+u+x) \, B(\varepsilon, z+w+x) \, S(\varepsilon, z+y) \\
& \chi(u,w,x,y) \Big|_{w=u=x=y=0} \mathrm{d}t_1 \; \mathrm{d}t_2 \,.
\end{aligned}
$$

We will focus on $K_4(\varepsilon, z)$ first. By definition of the Fourier multipliers we have

$$
\begin{aligned}
& \mathrm{e}^{\frac{\mathrm{i}\varepsilon t_2}{2}\sigma(\mathfrak{D}_x,\mathfrak{D}_y)} \sigma(\mathfrak{D}_x, \mathfrak{D}_y)^{N+1} \, \mathrm{e}^{\frac{\mathrm{i}\varepsilon t_1}{2}\sigma(\mathfrak{D}_u,\mathfrak{D}_w)} \sigma(\mathfrak{D}_u, \mathfrak{D}_w)^{N+1} \\
& \qquad R(\varepsilon, z+u+x) \, B(\varepsilon, z+w+x) \, S(\varepsilon, z+y) \chi(u,w,x,y) \Big|_{w=u=x=y=0} \\
& \quad = (2\pi)^{-8n} \int_{\mathbb{R}^{16n}} \mathrm{e}^{\mathrm{i}\langle \xi_1 \, , \, \tilde{u}-u\rangle} \mathrm{e}^{\mathrm{i}\langle \xi_2 \, , \, \tilde{w}-w\rangle} \mathrm{e}^{\mathrm{i}\langle \xi_3 \, , \, \tilde{x}-x\rangle} \mathrm{e}^{\mathrm{i}\langle \xi_4 \, , \, \tilde{y}-y\rangle} \\
& \qquad\quad \mathrm{e}^{\frac{\mathrm{i}\varepsilon t_2}{2}\sigma(\xi_3,\xi_4)} \sigma(\xi_3, \xi_4)^{N+1} \, \mathrm{e}^{\frac{\mathrm{i}\varepsilon t_1}{2}\sigma(\xi_1,\xi_2)} \sigma(\xi_1, \xi_2)^{N+1} \\
& \qquad\quad R(\varepsilon, z+u+x) \, B(\varepsilon, z+w+x) \, S(\varepsilon, z+y) \, \chi(u,w,x,y) \\
& \qquad \mathrm{d}u \, \mathrm{d}w \, \mathrm{d}\xi_1 \, \mathrm{d}\xi_2 \, \mathrm{d}x \, \mathrm{d}y \, \mathrm{d}\xi_3 \, \mathrm{d}\xi_4 \Big|_{\tilde{u}=\tilde{w}=\tilde{x}=\tilde{y}=0} \\
& \quad = (2\pi)^{-8n} \int_{\mathbb{R}^{16n}} \mathrm{e}^{-\mathrm{i}\langle \xi_1 \, , \, u\rangle} \mathrm{e}^{-\mathrm{i}\langle \xi_2 \, , \, w\rangle} \mathrm{e}^{-\mathrm{i}\langle \xi_3 \, , \, x\rangle} \mathrm{e}^{-\mathrm{i}\langle \xi_4 \, , \, y\rangle} \\
& \qquad\quad \mathrm{e}^{\frac{\mathrm{i}\varepsilon t_2}{2}\sigma(\xi_3,\xi_4)} \sigma(\xi_3, \xi_4)^{N+1} \, \mathrm{e}^{\frac{\mathrm{i}\varepsilon t_1}{2}\sigma(\xi_1,\xi_2)} \sigma(\xi_1, \xi_2)^{N+1} \\
& \qquad\quad R(\varepsilon, z+u+x) \, B(\varepsilon, z+w+x) \, S(\varepsilon, z+y) \, \chi(u,w,x,y) \\
& \qquad \mathrm{d}u \, \mathrm{d}w \, \mathrm{d}\xi_1 \, \mathrm{d}\xi_2 \, \mathrm{d}x \, \mathrm{d}y \, \mathrm{d}\xi_3 \, \mathrm{d}\xi_4
\end{aligned}
$$

Define $L_{\xi,z} := \frac{1-\langle \xi \, , \, \mathfrak{D}_z\rangle}{\langle \xi \rangle^2}$ so that $L_{\xi,z}\mathrm{e}^{-\mathrm{i}\langle \xi \, , \, z\rangle} = \mathrm{e}^{-\mathrm{i}\langle \xi \, , \, z\rangle}$. For $\tilde{N} > 2n + N + 2$ we obtain

$$
\begin{aligned}
& \int_{\mathbb{R}^{16n}} L^{\tilde{N}}_{\xi_1,u} \mathrm{e}^{-\mathrm{i}\langle \xi_1 \, , \, u\rangle} \, L^{\tilde{N}}_{\xi_2,w} \mathrm{e}^{-\mathrm{i}\langle \xi_2 \, , \, w\rangle} \, L^{\tilde{N}}_{\xi_3,x} \mathrm{e}^{-\mathrm{i}\langle \xi_3 \, , \, x\rangle} \, L^{\tilde{N}}_{\xi_4,y} \mathrm{e}^{-\mathrm{i}\langle \xi_4 \, , \, y\rangle} \\
& \qquad\quad \mathrm{e}^{\frac{\mathrm{i}\varepsilon t_2}{2}\sigma(\xi_3,\xi_4)} \sigma(\xi_3, \xi_4)^{N+1} \, \mathrm{e}^{\frac{\mathrm{i}\varepsilon t_1}{2}\sigma(\xi_1,\xi_2)} \sigma(\xi_1, \xi_2)^{N+1} \\
& \qquad\quad R(\varepsilon, z+u+x) \, B(\varepsilon, z+w+x) \, S(\varepsilon, z+y) \, \chi(u,w,x,y) \\
& \qquad \mathrm{d}u \, \mathrm{d}w \, \mathrm{d}\xi_1 \, \mathrm{d}\xi_2 \, \mathrm{d}x \, \mathrm{d}y \, \mathrm{d}\xi_3 \, \mathrm{d}\xi_4 \\
& \quad = \int_{\mathbb{R}^{16n}} \mathrm{e}^{-\mathrm{i}\langle \xi_1 \, , \, u\rangle} \, \mathrm{e}^{-\mathrm{i}\langle \xi_2 \, , \, w\rangle} \, \mathrm{e}^{-\mathrm{i}\langle \xi_3 \, , \, x\rangle} \, \mathrm{e}^{-\mathrm{i}\langle \xi_4 \, , \, y\rangle} \\
& \qquad\quad \mathrm{e}^{\frac{\mathrm{i}\varepsilon t_2}{2}\sigma(\xi_3,\xi_4)} \sigma(\xi_3, \xi_4)^{N+1} \, \mathrm{e}^{\frac{\mathrm{i}\varepsilon t_1}{2}\sigma(\xi_1,\xi_2)} \sigma(\xi_1, \xi_2)^{N+1} \\
& \qquad\quad (L^*_{\xi_1,u})^{\tilde{N}} \, (L^*_{\xi_2,w})^{\tilde{N}} \, (L^*_{\xi_3,x})^{\tilde{N}} \, (L^*_{\xi_4,y})^{\tilde{N}} R(\varepsilon, z+u+x) \, B(\varepsilon, z+w+x) \\
& \qquad\quad S(\varepsilon, z+y) \, \chi(u,w,x,y) \, \mathrm{d}u \, \mathrm{d}w \, \mathrm{d}\xi_1 \, \mathrm{d}\xi_2 \, \mathrm{d}x \, \mathrm{d}y \, \mathrm{d}\xi_3 \, \mathrm{d}\xi_4
\end{aligned}
$$

where $L^*_{\xi,z} = \frac{1+\langle \xi \,,\, \mathfrak{D}_z \rangle}{\langle \xi \rangle^2}$. Thus there exists a constant $C > 0$ such that

$$\begin{aligned} &\mathrm{tr}_{\mathcal{H}_\mathrm{f}} \Big| \sigma(\xi_3, \xi_4)^{N+1} \, \sigma(\xi_1, \xi_2)^{N+1} (L^*_{\xi_1,u})^{\tilde{N}} \, (L^*_{\xi_2,w})^{\tilde{N}} \, (L^*_{\xi_3,x})^{\tilde{N}} \, (L^*_{\xi_4,y})^{\tilde{N}} \\ &\qquad R(\varepsilon, z+u+x) \, B(\varepsilon, z+w+x) \, S(\varepsilon, z+y) \Big| \\ &\quad \leq C \langle \xi_1 \rangle^{-\tilde{N}+N+1} \, \langle \xi_2 \rangle^{-\tilde{N}+N+1} \, \langle \xi_3 \rangle^{-\tilde{N}+N+1} \, \langle \xi_4 \rangle^{\tilde{N}+N+1} \, \langle z \rangle^{-k} \\ &\qquad \| R(\varepsilon) \|_{0,2\tilde{N},1} \, \| B(\varepsilon) \|_{k,2\tilde{N}} \, \| S(\varepsilon) \|_{0,\tilde{N}} \, \chi(u, w, x, y). \end{aligned} \tag{A.38}$$

As a consequence

$$\begin{aligned} &\mathrm{e}^{-\mathrm{i}\langle \xi_1 \,,\, u \rangle} \, \mathrm{e}^{-\mathrm{i}\langle \xi_2 \,,\, w \rangle} \, \mathrm{e}^{-\mathrm{i}\langle \xi_3 \,,\, x \rangle} \, \mathrm{e}^{-\mathrm{i}\langle \xi_4 \,,\, y \rangle} \mathrm{e}^{\frac{\mathrm{i}\varepsilon t_2}{2} \sigma(\xi_3,\xi_4)} \sigma(\xi_3, \xi_4)^{N+1} \, \mathrm{e}^{\frac{\mathrm{i}\varepsilon t_1}{2} \sigma(\xi_1,\xi_2)} \sigma(\xi_1, \xi_2)^{N+1} \\ &(L^*_{\xi_1,u})^{\tilde{N}} \, (L^*_{\xi_2,w})^{\tilde{N}} \, (L^*_{\xi_3,x})^{\tilde{N}} \, (L^*_{\xi_4,y})^{\tilde{N}} R(\varepsilon, z+u+x) \, B(\varepsilon, z+w+x) S(\varepsilon, z+y) \end{aligned}$$

is Bochner-integrable as operator from $\mathbb{R}^{16n}$ to $\mathcal{J}(\mathcal{H}_\mathrm{f})$ and since $\mathrm{tr}_{\mathcal{H}_\mathrm{f}} : \mathcal{J}(\mathcal{H}_\mathrm{f}) \to \mathbb{C}$ is a continuous linear operator

$$\begin{aligned} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(K_4(\varepsilon, z)) = &\frac{(\mathrm{i}\varepsilon)^{2N+2}}{2^{(2N+2)} (N!)^2 \, (2\pi)^{8n}} \int_0^1 (1-t_2)^N \int_0^1 (1-t_1)^N \\ &\int_{\mathbb{R}^{16n}} \mathrm{e}^{-\mathrm{i}\langle \xi_1 \,,\, u \rangle} \mathrm{e}^{-\mathrm{i}\langle \xi_2 \,,\, w \rangle} \mathrm{e}^{-\mathrm{i}\langle \xi_3 \,,\, x \rangle} \mathrm{e}^{-\mathrm{i}\langle \xi_4 \,,\, y \rangle} \\ &\quad \mathrm{e}^{\frac{\mathrm{i}\varepsilon t_2}{2} \sigma(\xi_3,\xi_4)} \sigma(\xi_3, \xi_4)^{N+1} \, \mathrm{e}^{\frac{\mathrm{i}\varepsilon t_1}{2} \sigma(\xi_1,\xi_2)} \sigma(\xi_1, \xi_2)^{N+1} \\ &\quad (L^*_{\xi_1,u})^{\tilde{N}} \, (L^*_{\xi_2,w})^{\tilde{N}} \, (L^*_{\xi_3,x})^{\tilde{N}} \, (L^*_{\xi_4,y})^{\tilde{N}} \\ &\quad \mathrm{tr}\Big( R(\varepsilon, z+u+x) \, B(\varepsilon, z+w+x) \, S(\varepsilon, z+y) \Big) \\ &\quad \chi(u, w, x, y) \, \mathrm{d}u \, \mathrm{d}w \, \mathrm{d}\xi_1 \, \mathrm{d}\xi_2 \, \mathrm{d}x \, \mathrm{d}y \, \mathrm{d}\xi_3 \, \mathrm{d}\xi_4 \, \mathrm{d}t_1 \, \mathrm{d}t_2. \end{aligned}$$

Furthermore, by (A.38) there exists a constant $C > 0$ such that

$$\int_{\mathbb{R}^{2n}} |\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(K_4)(\varepsilon, z)| \mathrm{d}z \leq C \int_{\mathbb{R}^{2n}} \frac{1}{\langle z \rangle^k} \mathrm{d}z < \infty.$$

Thus

$$
\begin{aligned}
&\Big| \int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_{\mathrm{f}}}(K_4(\varepsilon, z))\, \mathrm{d}z \Big| \\
&\quad = \ \Big| \frac{(\mathrm{i}\varepsilon)^{(2N+2)}}{2^{2N+2}(N!)^2\,(2\pi)^{8n}} \int_0^1 (1-t_2)^N \int_0^1 (1-t_1)^N \\
&\qquad \int_{\mathbb{R}^{16n}} \mathrm{e}^{-\mathrm{i}\langle \xi_1\,,\,u\rangle} \mathrm{e}^{-\mathrm{i}\langle \xi_2\,,\,w\rangle} \mathrm{e}^{-\mathrm{i}\langle \xi_3\,,\,x\rangle} \mathrm{e}^{-\mathrm{i}\langle \xi_4\,,\,y\rangle} \\
&\qquad\quad \mathrm{e}^{\frac{\mathrm{i}\varepsilon t_2}{2}\sigma(\xi_3,\xi_4)} \sigma(\xi_3,\xi_4)^{N+1}\, \mathrm{e}^{\frac{\mathrm{i}\varepsilon t_1}{2}\sigma(\xi_1,\xi_2)} \sigma(\xi_1,\xi_2)^{N+1} \\
&\qquad\quad \int_{\mathbb{R}^{2n}} (L^*_{\xi_1,u})^{\tilde N}\, (L^*_{\xi_2,w})^{\tilde N}\, (L^*_{\xi_3,x})^{\tilde N}\, (L^*_{\xi_4,y})^{\tilde N} \\
&\qquad\qquad \mathrm{tr}_{\mathcal{H}_{\mathrm{f}}}\Big( R(\varepsilon, z+u+x)\, B(\varepsilon, z+w+x)\, S(\varepsilon, z+y)\Big)\, \mathrm{d}z \\
&\qquad\quad \chi(u,w,x,y)\, \mathrm{d}u\, \mathrm{d}w\, \mathrm{d}\xi_1\, \mathrm{d}\xi_2\, \mathrm{d}x\, \mathrm{d}y\, \mathrm{d}\xi_3\, \mathrm{d}\xi_4\, \mathrm{d}t_1\, \mathrm{d}t_2 \Big|
\end{aligned}
$$

This again takes us to the point where we apply an integration by parts with respect to $z$ to remove all derivatives acting on $B(\varepsilon, z+w+x)$ and make use of the cyclicity of the trace. Then, there exists a differential operator $\tilde\nabla^{\xi_1,\xi_2,\xi_3,\xi_4}_{u,x,y,z}$ of order $3\tilde N$ such that

$$
\begin{aligned}
&\Big| \int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_{\mathrm{f}}}(K_4(\varepsilon, z))\, \mathrm{d}z \Big| \\
&\quad = \Big| \frac{(\mathrm{i}\varepsilon)^{2N+2}}{2^{(2N+2)}(N!)^2\,(2\pi)^{8n}} \int_0^1 (1-t_2)^N \int_0^1 (1-t_1)^N \\
&\qquad \int_{\mathbb{R}^{16n}} \mathrm{e}^{-\mathrm{i}\langle \xi_1\,,\,u\rangle} \mathrm{e}^{-\mathrm{i}\langle \xi_2\,,\,w\rangle} \mathrm{e}^{-\mathrm{i}\langle \xi_3\,,\,x\rangle} \mathrm{e}^{-\mathrm{i}\langle \xi_4\,,\,y\rangle} \\
&\qquad\quad \mathrm{e}^{\frac{\mathrm{i}\varepsilon t_2}{2}\sigma(\xi_3,\xi_4)} \sigma(\xi_3,\xi_4)^{N+1}\, \mathrm{e}^{\frac{\mathrm{i}\varepsilon t_1}{2}\sigma(\xi_1,\xi_2)} \sigma(\xi_1,\xi_2)^{N+1} \\
&\qquad\quad \int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_{\mathrm{f}}}\Big( B(\varepsilon, z+w+x) \\
&\qquad\quad \tilde\nabla^{\xi_1,\xi_2,\xi_3,\xi_4}_{u,x,y,z}\Big( S(\varepsilon, z+y)\, R(\varepsilon, z+u+x)\, \chi(u,w,x,y)\Big)\Big) \\
&\qquad\quad \mathrm{d}z\, \mathrm{d}u\, \mathrm{d}w\, \mathrm{d}\xi_1\, \mathrm{d}\xi_2\, \mathrm{d}x\, \mathrm{d}y\, \mathrm{d}\xi_3\, \mathrm{d}\xi_4\, \mathrm{d}t_1\, \mathrm{d}t_2 \Big| .
\end{aligned}
$$

With similar arguments as in estimate (A.38) there is a constant $C > 0$ such that

$$\begin{aligned}
&\Big|\frac{(\mathrm{i}\varepsilon)^{2N+2}}{2^{(2N+2)}(N!)^2\,(2\pi)^{8n}}\int_0^1 (1-t_2)^N \int_0^1 (1-t_1)^N \mathrm{e}^{-\mathrm{i}\langle \xi_1\,,\,u\rangle}\mathrm{e}^{-\mathrm{i}\langle \xi_2\,,\,w\rangle}\mathrm{e}^{-\mathrm{i}\langle \xi_3\,,\,x\rangle}\mathrm{e}^{-\mathrm{i}\langle \xi_4\,,\,y\rangle} \\
&\qquad \mathrm{e}^{\frac{\mathrm{i}\varepsilon t_2}{2}\sigma(\xi_3,\xi_4)}\sigma(\xi_3,\xi_4)^{N+1}\,\mathrm{e}^{\frac{\mathrm{i}\varepsilon t_1}{2}\sigma(\xi_1,\xi_2)}\sigma(\xi_1,\xi_2)^{N+1}\mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big(B(\varepsilon,z+w+x) \\
&\qquad \tilde{\nabla}^{\xi_1,\xi_2,\xi_3,\xi_4}_{u,x,y}\Big(S(\varepsilon,z+y)\,R(\varepsilon,z+u+x)\,\chi(u,w,x,y)\Big)\Big)\mathrm{d}t_1\,\mathrm{d}t_2\Big| \\
&\quad \le C\,\varepsilon^{2N+2}\langle\xi_1\rangle^{-\tilde{N}+N+1}\,\langle\xi_2\rangle^{-\tilde{N}+N+1}\,\langle\xi_3\rangle^{-\tilde{N}+N+1}\,\langle\xi_4\rangle^{\tilde{N}+N+1} \\
&\qquad \|B(\varepsilon)\|\,\|R\|^{\varepsilon}_{0,3\tilde{N},1}\,\|S\|^{\varepsilon}_{0,3\tilde{N}}\,\chi(u,w,x,y).
\end{aligned} \tag{A.39}$$

Consequently, there is a constant $C_{N,4} > 0$ such that

$$\Big|\int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(K_4(\varepsilon,z))\,\mathrm{d}z\Big| \le C_{N,4}\,\varepsilon^{2N+2}\,\|B\|^{\varepsilon}_{L^1} \le C_{N,4}\,\varepsilon^{N+1}\,\|B\|^{\varepsilon}_{L^1}$$

The estimation of $K_2$ and $K_3$ is analogous to $K_4$ and leads to the following estimates. There are constants $C_{N,3} > 0$ and $C_{N,4} > 0$ such that

$$\Big|\int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(K_2(\varepsilon,z))\,\mathrm{d}z\Big| \le C_{N,3}\,\varepsilon^{N+1}\,\|B\|^{\varepsilon}_{L^1}$$

and

$$\Big|\int_{\mathbb{R}^{2n}} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(K_3(\varepsilon,z))\,\mathrm{d}z\Big| \le C_{N,4}\,\varepsilon^{N+1}\,\|B\|^{\varepsilon}_{L^1}\,.$$

Regarding $K_1$, note that by (2.4) and the fact that $\chi(u,w,x,y)$ is constant on $\mathrm{B}_1(0)$

$$\begin{aligned}
\int_{\mathbb{R}^{2n}} \operatorname{tr}_{\mathcal{H}_\mathrm{f}}(K_1(\varepsilon,z))\,\mathrm{d}z = &\sum_{\beta\in\{0,\dots,N\}^2} \frac{(\mathrm{i}\,\varepsilon)^{|\beta|}}{2^{|\beta|}\,\beta!} \int_{\mathbb{R}^{2n}} \sigma(\mathfrak{D}_x,\mathfrak{D}_y)^{\beta_2}\sigma(\mathfrak{D}_u,\mathfrak{D}_w)^{\beta_1} \\
&\operatorname{tr}_{\mathcal{H}_\mathrm{f}}\Big(R(\varepsilon,z+u+x)\,B(\varepsilon,z+w+x) \\
&S(\varepsilon,z+y)\,\chi(u,w,x,y)\Big)\Big|_{w=u=x=y=0}\,\mathrm{d}z \\
=&\sum_{j=0}^{N}\varepsilon^j \sum_{\substack{\alpha\in\mathbb{N}_0^4,\\ |\alpha|=j}} \int_{\mathbb{R}^{2n}} \operatorname{tr}_{\mathcal{H}_\mathrm{f}}\Big(\Big\{\{R_{\alpha_1}, B(\varepsilon)\}_{\alpha_2}, S_{\alpha_3}\Big\}_{\alpha_4}\Big)(z)\,\mathrm{d}z \\
&+\sum_{\substack{\beta\in\{0,\dots,N\}^4\\ |\beta|>N}} \frac{(\mathrm{i}\,\varepsilon)^{|\beta|}}{2^{|\beta|}\,\beta!} \int_{\mathbb{R}^{2n}} \sigma(\mathfrak{D}_x,\mathfrak{D}_y)^{\beta_2}\sigma(\mathfrak{D}_u,\mathfrak{D}_w)^{\beta_1} \\
&\operatorname{tr}_{\mathcal{H}_\mathrm{f}}\Big(R_{\beta_3}(z+u+x)\,B(\varepsilon,z+w+x) \\
&S_{\beta_4}(z+y)\,\chi(u,w,x,y)\Big)\Big|_{w=u=x=y=0}\,\mathrm{d}z \\
&+\sum_{\beta\in\{0,\dots,N\}^2} \frac{(\mathrm{i}\,\varepsilon)^{|\beta|}}{2^{|\beta|}\,\beta!} \int_{\mathbb{R}^{2n}} \sigma(\mathfrak{D}_x,\mathfrak{D}_y)^{\beta_2}\sigma(\mathfrak{D}_u,\mathfrak{D}_w)^{\beta_1} \\
&\operatorname{tr}_{\mathcal{H}_\mathrm{f}}\Big((R-R^{(N)})(\varepsilon,z+u+x)\,B(\varepsilon,z+w+x) \\
&(S-S^{(N)})(\varepsilon,z+y)\,\chi(u,w,x,y)\Big)\Big|_{w=u=x=y=0}\,\mathrm{d}z \\
=:&\sum_{j=0}^{N}\varepsilon^j \sum_{\substack{\alpha\in\mathbb{N}_0^4,\\ |\alpha|=j}} \int_{\mathbb{R}^{2n}} \operatorname{tr}_{\mathcal{H}_\mathrm{f}}\Big(\Big\{\{R_{\alpha_1}, B(\varepsilon)\}_{\alpha_2}, S_{\alpha_3}\Big\}_{\alpha_4}\Big)(z)\,\mathrm{d}z \\
&+\tilde{k}_1(\varepsilon)+\tilde{k}_2(\varepsilon)\,.
\end{aligned}$$

Since $S$ and $R$ are classical symbols, an estimate similar to (A.39) yields

$$\Big|\tilde{k}_1(\varepsilon)\Big| \le C_{N,5}\,\varepsilon^{N+1}\,\|B\|^\varepsilon_{L^1} \qquad \text{and} \qquad \Big|\tilde{k}_2(\varepsilon)\Big| \le C_{N,6}\,\varepsilon^{N+1}\,\|B\|^\varepsilon_{L^1}\,.$$

for some $C_{N,5}>0$ and $C_{N,6}>0$. Finally, assembling the above results we obtain

$$\begin{aligned}
&\Big|\int_{\mathbb{R}^{2n}} \operatorname{tr}_{\mathcal{H}_\mathrm{f}}\Big(R\,\#\,B\,\#\,S - \sum_{j=0}^{N}\varepsilon^j \sum_{\substack{\alpha\in\mathbb{N}_0^4,\\ |\alpha|=j}} \Big\{\{R_{\alpha_1}, B(\varepsilon)\}_{\alpha_2}, S_{\alpha_3}\Big\}_{\alpha_4}\Big)(z)\,\mathrm{d}z\Big| \\
&\quad\le \sum_{i=1}^{6} C_{N,i}\,\varepsilon^{N+1}\,\|B\|^\varepsilon_{L^1} =: C_n\,\varepsilon^{N+1}\,\|B\|^\varepsilon_{L^1}
\end{aligned}$$

This finishes the proof, since $\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(Q\,\partial^\alpha B)\mathbf{1}_{\mathcal{H}_\mathrm{f}} \in S^0(\mathcal{B}(\mathcal{H}_\mathrm{f}))$. Therefore (A.29) follows with almost the same proof, replacing $B$ by $\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(Q\,\partial^\alpha B)\mathbf{1}_{\mathcal{H}_\mathrm{f}} \in S^0(\mathcal{B}(\mathcal{H}_\mathrm{f}))$ and removing $\partial_z^\alpha$ form $B$ whenever applying an integration by parts. □

**Lemma A.11** *Let* $a \in S^k(\varepsilon, \mathbb{C})$*,* $k > 2n$*,* $b, c \in S^0(\varepsilon, \mathbb{C})$*. Then*

$$\int_{\mathbb{R}^{2n}} c(z)\, \{a(z)\,, b(z)\}_l \,\mathrm{d}z = \int_{\mathbb{R}^{2n}} \{c(z)\,, a(z)\}_l\, b(z)\,\mathrm{d}z$$

*and*

$$\int_{\mathbb{R}^{2n}} \{a(z)\,, b(z)\}_l \,\mathrm{d}z = 0$$

*for any* $l \in \mathbb{N}$*.*

PROOF Let $l \in \mathbb{N}$. By the skew-symmetry of $\omega^0$ and integration by parts

$$\begin{aligned}
&\int_{\mathbb{R}^{2n}} c(z)\,\omega^0_{ij}\,\partial_j a(z)\,\partial_i b(z)\,\mathrm{d}z \\
&\qquad = -\int_{\mathbb{R}^{2n}} c(z)\,\omega^0_{ij}\,\partial^2_{ji} a(z)\,b(z)\,\mathrm{d}z - \int_{\mathbb{R}^{2n}} \partial_i c(z)\,\omega^0_{ij}\,\partial_j a(z)\,b(z)\,\mathrm{d}z \\
&\qquad = \int_{\mathbb{R}^{2n}} \omega^0_{ji}\,\partial_i c(z)\,\partial_j a(z)\,b(z)\,\mathrm{d}z.
\end{aligned}$$

This and the definition of the generalized Poisson bracket implies

$$\begin{aligned}
&\int_{\mathbb{R}^{2n}} c(z)\,\{a(z)\,, b(z)\}_l\,\mathrm{d}z \\
&\qquad = \tfrac{1}{(2\,\mathrm{i})^l\, l!}\int_{\mathbb{R}^{2n}} c(z)\,\omega^0_{i_1 j_1}\cdots\omega^0_{i_l j_l}\,\partial^l_{j_1\ldots j_l} a(z)\,\partial^l_{i_1\ldots i_l} b(z)\,\mathrm{d}z \\
&\qquad = \tfrac{1}{(2\,\mathrm{i})^l\, l!}\int_{\mathbb{R}^{2n}} \Big(\omega^0_{i_1 j_1}\,\omega^0_{i_2 j_2}\cdots\omega^0_{i_l j_l}\,\partial_{j_1} c(z)\,\partial^l_{i_1 j_2\ldots j_l} a(z)\,\partial^{l-1}_{i_2\ldots i_l} b(z)\,\mathrm{d}z \\
&\qquad\ \vdots \\
&\qquad = \tfrac{1}{(2\,\mathrm{i})^l\, l!}\int_{\mathbb{R}^{2n}} \Big(\omega^0_{i_1 j_1}\,\omega^0_{i_2 j_2}\cdots\omega^0_{i_l j_l}\,\partial^l_{j_1\ldots j_l} c(z)\,\partial^l_{i_1\ldots i_l} a(z)\,b(z)\,\mathrm{d}z \\
&\qquad = \int_{\mathbb{R}^{2n}} \{c(z)\,, a(z)\}_l\,b(z)\,\mathrm{d}z.
\end{aligned}$$

Finally, by choosing $c(z) = 1$

$$\int_{\mathbb{R}^{2n}} \{a(z)\,, b(z)\}_l \,\mathrm{d}z = 0$$

□

# Computations

# B

This chapter consists of a collection of computations used to derive explicit expressions of semiclassical approximations to errors of order $\varepsilon^3$. Lemmata B.1 and B.2 are applied in the derivation of the asymptotic expansion to second order of the space-adiabatic projection's symbol $\pi$. Lemmata B.3 and B.4 are used in the proof of the Egorov Theorem to errors of order $\varepsilon^3$. The results of Lemmata B.5 and B.6 are used in the derivation of the explicit expressions of the classical Hamoltonian system for Born-Oppenheimer type Hamiltonians. Finally, Lemmata B.7 - B.10 give the larger part of the derivation of the second order semiclassical expressions for Hamiltonians with periodic potentials.

**Lemma B.1** *Let* $\mathrm{P} \in S^0(\varepsilon, \mathcal{J}(\mathcal{H}_\mathrm{f}))$ *be a pointwise rank-one projection and* $B \in S^0(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f}))$. *If* $B$ *is diagonal with respect to* $\mathrm{P}$ *then*

$$\begin{aligned} \mathrm{P}\,[\,\partial_j\mathrm{P}\,,\partial_i B\,]\,\mathrm{P} =& \mathrm{P}\,\partial_j\mathrm{P}\,\partial_i\mathrm{P}\,B\,\mathrm{P} - P_0\,B\,\partial_i\mathrm{P}\,\partial_j\mathrm{P}\,\mathrm{P} \\ &- \mathrm{P}\,[\,\partial_j\mathrm{P}\,|B\,|\,\partial_i\mathrm{P}\,]\,\mathrm{P} \\ \mathrm{P}^\perp\,[\,\partial_j\mathrm{P}\,,\partial_i B\,]\,\mathrm{P}^\perp =& - \mathrm{P}^\perp\,\partial_j\mathrm{P}\,\partial_i\mathrm{P}\,B\,\mathrm{P}^\perp + \mathrm{P}^\perp\,B\,\partial_i\mathrm{P}\,\partial_j\mathrm{P}\,\mathrm{P}^\perp \\ &+ \mathrm{P}^\perp\,[\,\partial_j\mathrm{P}\,|B\,|\,\partial_i\mathrm{P}\,]\,\mathrm{P}^\perp\,. \end{aligned} \tag{B.1}$$

PROOF By the product rule

$$\begin{aligned} \partial_i(\mathrm{P}\,B\,\mathrm{P}) =& \mathrm{P}\,\partial_i(B\,\mathrm{P}) + \partial_i\mathrm{P}\,B\,\mathrm{P} = \partial_i(\mathrm{P}\,B)\,\mathrm{P} + \mathrm{P}\,B\,\partial_i\mathrm{P} \\ \partial_i(\mathrm{P}^\perp\,B\,\mathrm{P}^\perp) =& \mathrm{P}^\perp\,\partial_i(B\,\mathrm{P}^\perp) - \partial_i\mathrm{P}\,B\,\mathrm{P}^\perp = \partial_i(\mathrm{P}^\perp\,B)\,\mathrm{P}^\perp - \mathrm{P}^\perp\,B\,\partial_i\mathrm{P}\,. \end{aligned}$$

Since $\partial_j\mathrm{P}$ is off diagonal with respect to $\mathrm{P}$

$$\begin{aligned} \mathrm{P}\,\partial_j\mathrm{P}\,\partial_i B\,\mathrm{P} &= \mathrm{P}\,\partial_j\mathrm{P}\,\partial_i\mathrm{P}\,B\,\mathrm{P} - \mathrm{P}\,\partial_j\mathrm{P}\,B\,\partial_i\mathrm{P}\,\mathrm{P}\,, \\ \mathrm{P}\,\partial_i B\,\partial_j\mathrm{P}\,\mathrm{P} &= \mathrm{P}\,B\,\partial_i\mathrm{P}\,\partial_j\mathrm{P}\,\mathrm{P} - \mathrm{P}\,\partial_i\mathrm{P}\,B\,\partial_j\mathrm{P}\,\mathrm{P}\,, \\ \mathrm{P}^\perp\,\partial_j\mathrm{P}\,\partial_i B\,\mathrm{P}^\perp &= \mathrm{P}^\perp\,\partial_j\mathrm{P}\,B\,\partial_i\mathrm{P}\,\mathrm{P}^\perp - \mathrm{P}^\perp\,\partial_j\mathrm{P}\,\partial_i\mathrm{P}\,B\,\mathrm{P}^\perp\,, \end{aligned}$$

and

$$\mathrm{P}^\perp\,\partial_i B\,\partial_j\mathrm{P}\,\mathrm{P}^\perp = \mathrm{P}^\perp\,\partial_i\mathrm{P}\,B\,\partial_j\mathrm{P}\,\mathrm{P}^\perp - \mathrm{P}^\perp\,B\,\partial_i\mathrm{P}\,\partial_j\mathrm{P}\,\mathrm{P}^\perp\,,$$

which directly implies (B.1). □

**Lemma B.2** *Let Assumption 2.10 and 2.11 hold. Then for* $(H_0-e_0)^{-1}$ *denoting the reduced resolvent, i.e.* $(H_0-e_0)^{-1}=P_0^{\perp}\,(H_0-e_0)^{-1}\,P_0^{\perp}$ *and*

$$\begin{aligned}F_1 =&H_0\,\tilde{\pi}_0-\tilde{\pi}_0\,H_0+H_0^1\,P_0-P_0\,H_0^1\\&-\tfrac{\mathrm{i}}{2}\,\{H_0+\xi\cdot z\,,P_0\}+\tfrac{\mathrm{i}}{2}\,\{P_0\,,H_0+\xi\cdot z\}\end{aligned}$$

*with*

$$\tilde{\pi}_0=-\tfrac{1}{4}\,P_0\,\mathrm{Tr}_{2n}(\omega^0\,\Omega_0^{op})\,P_0+\tfrac{1}{4}\,P_0^{\perp}\,\mathrm{Tr}_{2n}(\omega^0\,\Omega_0^{op})\,P_0^{\perp}$$

*we have*

$$\begin{aligned}P_0\,F_1\,(H_0-e_0)^{-1}\,P_0^{\perp}=&\tfrac{\mathrm{i}}{2}\,P_0\left\langle\omega^0\,\nabla P_0\,,\,\nabla(H_0+e_0)+2\,\xi\right\rangle(H_0-e_0)^{-1}\\&-P_0\,H_0^1\,(H_0-e_0)^{-1}\end{aligned}\tag{B.2}$$

*as well as*

$$\begin{aligned}P_0^{\perp}\,(H_0-e_0)^{-1}\,F_1\,P_0=&\tfrac{\mathrm{i}}{2}\,(H_0-e_0)^{-1}\left\langle\nabla(H_0+e_0)+2\,\xi\,,\,\omega^0\,\nabla P_0\right\rangle P_0\\&+(H_0-e_0)^{-1}\,H_0^1\,P_0\,.\end{aligned}\tag{B.3}$$

*In addition for*

$$\begin{aligned}G_2=&\tilde{\pi}_0\,P_1+P_1\,\tilde{\pi}_0+\tilde{\pi}_0\,\tilde{\pi}_0-\tfrac{\mathrm{i}}{2}\,\omega_{ij}^0\,\partial_jP_0\,\partial_iP_1-\tfrac{\mathrm{i}}{2}\,\omega_{ij}^0\,\partial_jP_1\,\partial_iP_0\\&-\tfrac{\mathrm{i}}{2}\,\omega_{ij}^0\,\partial_jP_0\,\partial_i\tilde{\pi}_0-\tfrac{\mathrm{i}}{2}\,\omega_{ij}^0\,\partial_j\tilde{\pi}_0\,\partial_iP_0-\tfrac{1}{8}\,\omega_{ij}^0\,\omega_{lm}^0\,\partial_{jm}^2P_0\;\partial_{il}^2P_0\end{aligned}$$

*where*

$$\begin{aligned}P_1=&\tfrac{\mathrm{i}}{2}\,P_0\left\langle\omega^0\,\nabla P_0\,,\,\nabla(H_0+e_0)+2\,\xi\right\rangle(H_0-e_0)^{-1}-P_0\,H_0^1\,(H_0-e_0)^{-1}\\&-\tfrac{\mathrm{i}}{2}\,(H_0-e_0)^{-1}\left\langle\nabla(H_0+e_0)+2\,\xi\,,\,\omega^0\,\nabla P_0\right\rangle P_0-(H_0-e_0)^{-1}\,H_0^1\,P_0\end{aligned}$$

*we have*

$$\begin{aligned}P_0\,G_2\,P_0=&\tfrac{1}{4}\,P_0\,\mathrm{Tr}_{2n}(\omega^0\,\Omega_1^{op})\,P_0-\tfrac{1}{16}\,P_0\,\mathrm{Tr}_{2n}(\omega^0\,\Omega_0^{op})\,\mathrm{Tr}_{2n}(\omega^0\,\Omega_0^{op})\,P_0\\&+\tfrac{1}{8}\,P_0\,\mathrm{Tr}_{2n}(\omega^0\,\Omega_0^{op}\,\omega^0\,\Omega_0^{op})\,P_0\\&+\tfrac{1}{8}\,P_0\,\mathrm{Tr}_{2n}(\omega^0\,\nabla^2P_0\,P_0^{\perp}\,\omega^0\,\nabla^2P_0)\,P_0\,,\end{aligned}\tag{B.4}$$

$$\begin{aligned}P_0^{\perp}\,G_2\,P_0^{\perp}=&\tfrac{1}{4}\,P_0^{\perp}\,\mathrm{Tr}_{2n}(\omega^0\,\Omega_1^{op})\,P_0^{\perp}+\tfrac{1}{8}\,P_0^{\perp}\,\mathrm{Tr}_{2n}(\omega^0\,\Omega_0^{op}\,\omega^0\,\Omega_0^{op})\,P_0^{\perp}\\&-\tfrac{1}{16}\,P_0^{\perp}\,\mathrm{Tr}_{2n}(\omega^0\,\Omega_0^{op})\,\mathrm{Tr}_{2n}(\omega^0\,\Omega_0^{op})\,P_0^{\perp}\\&+\tfrac{1}{8}\,P_0^{\perp}\,\mathrm{Tr}_{2n}(\omega^0\,\nabla^2P_0\,P_0\,\omega^0\,\nabla^2P_0)\,P_0^{\perp}\end{aligned}\tag{B.5}$$

*and*

$$
\begin{aligned}
\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0^\perp\, G_2\, P_0^\perp) = &-\tfrac{1}{4}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\,\mathrm{Tr}_{2n}(\omega^0\,\Omega_1^{op})) - \tfrac{1}{8}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\,\mathrm{Tr}_{2n}(\omega^0\,\Omega_0^{op}\,\omega^0\,\Omega_0^{op}))\\
&+ \tfrac{1}{16}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\,\mathrm{Tr}_{2n}(\omega^0\,\Omega_0^{op})\,\mathrm{Tr}_{2n}(\omega^0\,\Omega_0^{op}))\\
&+ \tfrac{1}{8}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\;\mathrm{Tr}_{2n}(\omega^0\,\nabla^2 P_0\,P_0^\perp\,\omega^0\,\nabla^2 P_0))\,.
\end{aligned}
\tag{B.6}
$$

PROOF As $P_0$ is the eigenprojection of $H_0$ to the eigenvalue $e_0$ and $\tilde{\pi}$ is diagonal with respect to $P_0$ we have

$$
H_0\,\tilde{\pi}_0 = e_0\,P_0\,\tilde{\pi}_0\,P_0 + H_0\,P_0^\perp\,\tilde{\pi}_0\,P_0^\perp = P_0\,\tilde{\pi}_0\,P_0\,H_0 + H_0\,P_0^\perp\,\tilde{\pi}_0\,P_0^\perp
$$

leading to

$$
\begin{aligned}
F_1 =&\tfrac{1}{4}\,H_0\,P_0^\perp\,\mathrm{Tr}_{2n}(\omega^0\,\Omega_0^{op})\,P_0^\perp - \tfrac{1}{4}\,P_0^\perp\,\mathrm{Tr}_{2n}(\omega^0\,\Omega_0^{op})\,P_0^\perp\,H_0\\
&+ H_0^1\,P_0 - P_0\,H_0^1 + \mathrm{i}\,\omega_{ij}^0\,\partial_j P_0\,\xi_i\\
&+ \tfrac{\mathrm{i}}{2}\,\omega_{ij}^0 \partial_j P_0\,\partial_i H_0 - \tfrac{\mathrm{i}}{2}\,\omega_{ij}^0\,\partial_j H_0\,\partial_i P_0
\end{aligned}
$$

where we also used that $\xi_j$ is a real value and thus commutes with any operator acting on $\mathcal{H}_\mathrm{f}$. Therefore

$$
\begin{aligned}
&P_0\,F_1\,(H_0 - e_0)^{-1}\,P_0^\perp\\
&\quad= \tfrac{1}{4}\,P_0\,H_0\,(H_0 - e_0)^{-1}\,P_0^\perp\,\mathrm{Tr}_{2n}(\omega^0\,\Omega_0^{op})\,P_0^\perp\\
&\qquad - P_0\,H_0^1\,(H_0 - e_0)^{-1} + \mathrm{i}\,\omega_{ij}^0\,P_0\,\partial_j P_0\,\xi_i\,(H_0 - e_0)^{-1}\\
&\qquad + \tfrac{\mathrm{i}}{2}\,\omega_{ij}^0 P_0\,\partial_j P_0\,\partial_i H_0\,(H_0 - e_0)^{-1} - \tfrac{\mathrm{i}}{2}\,\omega_{ij}^0\,P_0\,\partial_j H_0\,\partial_i P_0\,(H_0 - e_0)^{-1}\,.
\end{aligned}
$$

Using that $e_0$ is a scalar function, $\partial_j P_0$ is off diagonal with respect to $P_0$ and

$$
0 = \partial_j(P_0\,(e_0 - H_0)) = \partial_j P_0\,(e_0 - H_0) + P_0\,\partial_j(e_0 - H_0)
$$

yields

$$
\begin{aligned}
&\tfrac{\mathrm{i}}{2}\,\omega^0_{ij}\,P_0\,\partial_j P_0\,\partial_i(H_0+e_0)\,(H_0-e_0)^{-1}\\
&\quad= \tfrac{\mathrm{i}}{2}\,\omega^0_{ij}\,P_0\,\partial_j P_0\,\partial_i H_0\,(H_0-e_0)^{-1} + \tfrac{\mathrm{i}}{2}\,\omega^0_{ij}\,P_0\,\partial_j P_0\,\partial_i e_0\,(H_0-e_0)^{-1}\\
&\quad= \tfrac{\mathrm{i}}{2}\,\omega^0_{ij}\,P_0\,\partial_j P_0\,\partial_i H_0\,(H_0-e_0)^{-1} - \tfrac{\mathrm{i}}{2}\,\omega^0_{ij}\,P_0\,\partial_j e_0\,\partial_i P_0\,(H_0-e_0)^{-1}\\
&\quad= \tfrac{\mathrm{i}}{2}\,\omega^0_{ij}\,P_0\,\partial_j P_0\,\partial_i H_0\,(H_0-e_0)^{-1} - \tfrac{\mathrm{i}}{2}\,\omega^0_{ij}\,P_0\,\partial_j H_0\,\partial_i P_0\,(H_0-e_0)^{-1}\\
&\qquad - \tfrac{\mathrm{i}}{2}\,\omega^0_{ij}\,P_0\,\partial_j (e_0-H_0)\,\partial_i P_0\,(H_0-e_0)^{-1}\\
&\quad= \tfrac{\mathrm{i}}{2}\,\omega^0_{ij}\,P_0\,\partial_j P_0\,\partial_i H_0\,(H_0-e_0)^{-1} - \tfrac{\mathrm{i}}{2}\,\omega^0_{ij}\,P_0\,\partial_j H_0\,\partial_i P_0\,(H_0-e_0)^{-1}\\
&\qquad + \tfrac{\mathrm{i}}{2}\,\omega^0_{ij}\,\partial_j P_0\,(e_0-H_0)\,\partial_i P_0\,(H_0-e_0)^{-1}\\
&\quad= \tfrac{\mathrm{i}}{2}\,\omega^0_{ij}\,P_0\,\partial_j P_0\,\partial_i H_0\,(H_0-e_0)^{-1} - \tfrac{\mathrm{i}}{2}\,\omega^0_{ij}\,P_0\,\partial_j H_0\,\partial_i P_0\,(H_0-e_0)^{-1}\,.
\end{aligned}
$$

This and the fact that $H_0$ and $P_0$ commute finally shows

$$
\begin{aligned}
&P_0\,F_1\,(H_0-e_0)^{-1}\\
&\quad= -P_0\,H^1_0\,(H_0-e_0)^{-1} + \mathrm{i}\,\omega^0_{ij}\,\xi_i\,P_0\,\partial_j P_0\,(H_0-e_0)^{-1}\\
&\qquad + \tfrac{\mathrm{i}}{2}\,P_0\,\omega^0_{ij}\,\partial_j P_0\,\partial_i(H_0+e_0)\,(H_0-e_0)^{-1}\\
&\quad= \tfrac{\mathrm{i}}{2}\,P_0\,\Big\langle \omega^0\,\nabla P_0\,,\,\nabla(H_0+e_0)+2\,\xi\Big\rangle\,(H_0-e_0)^{-1} - P_0\,H^1_0\,(H_0-e_0)^{-1}
\end{aligned}
$$

and analogously

$$
\begin{aligned}
(H_0-e_0)^{-1}\,F_1\,P_0 = {} & \tfrac{\mathrm{i}}{2}\,(H_0-e_0)^{-1}\,\Big\langle \nabla(H_0+e_0)+2\,\xi\,,\,\omega^0\,\nabla P_0\Big\rangle\,P_0\\
&+ (H_0-e_0)^{-1}\,H^1_0\,P_0\,.
\end{aligned}
$$

To show (B.4), first note that

$$
\begin{aligned}
P_0\,G_2\,P_0 = {} & P_0\,\tilde\pi_0\,\tilde\pi_0\,P_0 - \tfrac{\mathrm{i}}{2}\,\omega^0_{ij}\,P_0\,\partial_j P_0\,\partial_i P_1\,P_0 - \tfrac{\mathrm{i}}{2}\,\omega^0_{ij}\,P_0\,\partial_j P_1\,\partial_i P_0\,P_0\\
&- \tfrac{\mathrm{i}}{2}\,\omega^0_{ij}\,P_0\,\partial_j P_0\,\partial_i\tilde\pi_0\,P_0 - \tfrac{\mathrm{i}}{2}\,\omega^0_{ij}\,P_0\,\partial_j\tilde\pi_0\,\partial_i P_0\,P_0\\
&- \tfrac{1}{8}\,\omega^0_{ij}\,\omega^0_{lm}\,P_0\,\partial^2_{jm}P_0\;\partial^2_{il}P_0\,P_0
\end{aligned}
\tag{B.7}
$$

By the skew-symmetry of $\omega^0$

$$
\begin{aligned}
\mathrm{Tr}_{2n}(\omega^0\,g^{op}_0\,\omega^0\,\Omega^{op}_0) &= \mathrm{Tr}_{2n}(g^{op}_0\,\omega^0\,\Omega^{op}_0\,\omega^0)\\
&= g^{op}_{0,ij}\,\omega^0_{jl}\,\Omega^{op}_{0,lm}\,\omega^0_{mi} = g^{op}_{0,ij}\,\omega^0_{mi}\,\Omega^{op}_{0,lm}\,\omega^0_{jl}\\
&= -g^{op}_{0,ij}\,\omega^0_{im}\,\Omega^{op}_{0,ml}\,\omega^0_{lj} = -g^{op}_{0,ji}\,\omega^0_{im}\,\Omega^{op}_{0,ml}\,\omega^0_{lj}\\
&= -\mathrm{Tr}_{2n}(\omega^0\,g^{op}_0\,\omega^0\,\Omega^{op}_0)
\end{aligned}
$$

and similarly

$$\mathrm{Tr}_{2n}(\omega^0\,\Omega_0^{op}\,\omega^0\,g_0^{op}) = -\mathrm{Tr}_{2n}(\omega^0\,\Omega_0^{op}\,\omega^0\,g_0^{op})$$

which yields

$$\mathrm{Tr}_{2n}(\omega^0\,g_0^{op}\,\omega^0\,\Omega_0^{op}) = \mathrm{Tr}_{2n}(\omega^0\,\Omega_0^{op}\,\omega^0\,g_0^{op}) = 0\,.$$

By definition of $\tilde{\pi}_0$, $\mathcal{T}^{op}$, $g^{op}$, $\Omega^{op}$ and the equation above

$$\begin{aligned}
&\mathrm{i}\,\omega_{ij}^0\,P_0\,\partial_j P_0\,\tilde{\pi}_0\,\partial_i P_0\,P_0\\
&\qquad= \tfrac{1}{2}\,\omega_{ij}^0\,\omega_{lm}^0\,P_0\,\partial_j P_0\,\partial_m P_0\,\partial_l P_0\,\partial_i P_0\,P_0\\
&\qquad= \tfrac{1}{2}\,\omega_{ij}^0\,\omega_{lm}^0\,P_0\,\mathcal{T}_{0,jm}^{op}\,\mathcal{T}_{0,li}^{op}\,P_0\\
&\qquad= \tfrac{1}{8}\,\omega_{ij}^0\,\omega_{lm}^0\,P_0\,g_{0,jm}^{op}\,g_{0,li}^{op}\,P_0 + \tfrac{\mathrm{i}}{8}\,\omega_{ij}^0\,\omega_{lm}^0\,P_0\,\Omega_{0,jm}^{op}\,g_{0,li}^{op}\,P_0\\
&\qquad\quad+ \tfrac{\mathrm{i}}{8}\,\omega_{ij}^0\,\omega_{lm}^0\,P_0\,g_{0,jm}^{op}\,\Omega_{0,li}^{op}\,P_0 - \tfrac{1}{8}\,\omega_{ij}^0\,\omega_{lm}^0\,P_0\,\Omega_{0,jm}^{op}\,\Omega_{0,li}^{op}\,P_0\\
&\qquad= -\tfrac{1}{8}\,P_0\,\mathrm{Tr}_{2n}(\omega^0\,g_0^{op}\,\omega^0\,g_0^{op})\,P_0 + \tfrac{1}{8}\,P_0\,\mathrm{Tr}_{2n}(\omega^0\,\Omega_0^{op}\,\omega^0\,\Omega_0^{op})\,P_0
\end{aligned} \tag{B.8}$$

In addition, by (2.15)

$$-\tfrac{\mathrm{i}}{2}\,\omega_{ij}^0\,P_0\,\partial_j P_0\,\partial_i P_0\,\tilde{\pi}_0\,P_0 = -\tfrac{\mathrm{i}}{2}\,\omega_{ij}^0\,P_0\,\tilde{\pi}_0\,\partial_j P_0\,\partial_i P_0\,P_0\,.$$

Therefore, Lemma B.1 and (B.8) leads to

$$\begin{aligned}
&-\tfrac{\mathrm{i}}{2}\,\omega_{ij}^0\,P_0\,[\,\partial_j P_0\,,\partial_i\tilde{\pi}_0\,]\,P_0\\
&\qquad= -\tfrac{\mathrm{i}}{2}\,\omega_{ij}^0\,P_0\,[\,\partial_j P_0\,,\partial_i P_0\,]\,\tilde{\pi}_0\,P_0 + \tfrac{\mathrm{i}}{2}\,\omega_{ij}^0\,P_0\,\tilde{\pi}_0\,[\,\partial_j P_0\,,\partial_i P_0\,]\,P_0\\
&\qquad\quad+ \tfrac{\mathrm{i}}{2}\,\omega_{ij}^0\,P_0\,[\,\partial_j P_0\,|\tilde{\pi}_0\,|\,\partial_i P_0\,]\,P_0\\
&\qquad= -\tfrac{\mathrm{i}}{2}\,\omega_{ij}^0\,P_0\,[\,\partial_j P_0\,,\partial_i P_0\,]\,\tilde{\pi}_0\,P_0\\
&\qquad\quad+ \mathrm{i}\,\omega_{ij}^0\,P_0\,\partial_j P_0\tilde{\pi}_0\partial_i P_0\,P_0\\
&\qquad= -\tfrac{1}{8}\,\mathrm{Tr}_{2n}(\omega^0\,\Omega_0^{op})\,\mathrm{Tr}_{2n}(\omega^0\,\Omega_0^{op})\,P_0\\
&\qquad\quad- \tfrac{1}{8}\,P_0\,\mathrm{Tr}_{2n}(\omega^0\,g_0^{op}\,\omega^0\,g_0^{op})\,P_0 + \tfrac{1}{8}\,P_0\,\mathrm{Tr}_{2n}(\omega^0\,\Omega_0^{op}\,\omega^0\,\Omega_0^{op})\,P_0.
\end{aligned} \tag{B.9}$$

In addition, by (2.16)

$$\begin{aligned}
&-\tfrac{1}{8}\,\omega_{ij}^0\,\omega_{lm}^0\,P_0\,\partial_{jm}^2 P_0\;\partial_{il}^2 P_0\,P_0\\
&\qquad= -\tfrac{1}{8}\,\omega_{ij}^0\,\omega_{lm}^0\,P_0\,\partial_{jm}^2 P_0\,P_0^{\perp}\,\partial_{il}^2 P_0\,P_0\\
&\qquad\quad- \tfrac{1}{8}\,\omega_{ij}^0\,\omega_{lm}^0\,P_0\,[\,\partial_j P_0\,,\partial_m P_0\,]_+\,[\,\partial_i P_0\,,\partial_l P_0\,]\,P_0\\
&\qquad= -\tfrac{1}{8}\,\omega_{ij}^0\,\omega_{lm}^0\,P_0\,\partial_{jm}^2 P_0\,P_0^{\perp}\,\partial_{il}^2 P_0\,P_0 + \tfrac{1}{8}\,P_0\,\mathrm{Tr}_{2n}(\omega^0\,g_0^{op}\,\omega^0\,g_0^{op})\,P_0
\end{aligned} \tag{B.10}$$

We now use that $P_1$ is off-diagonal and $\tilde{\pi}_0$ diagonal with respect to $P_0$ such that

$$0 = P_0\,\tilde{\pi}_0\,P_1\,P_0 = P_0\,P_1\,\tilde{\pi}_0\,P_0\,.$$

Then combining (B.7) with the equation above, (B.9) and (B.10) finally yields

$$\begin{aligned}
P_0\,G_2\,P_0 =& P_0\,\tilde{\pi}_0\,\tilde{\pi}_0\,P_0 \\
& - \tfrac{\mathrm{i}}{2}\,\omega^0_{ij}\,P_0\,\partial_j P_0\,\partial_i P_1\,P_0 - \tfrac{\mathrm{i}}{2}\,\omega^0_{ij}\,P_0\,\partial_j P_1\,\partial_i P_0\,P_0 \\
& - \tfrac{\mathrm{i}}{2}\,\omega^0_{ij}\,P_0\,\partial_j P_0\,\partial_i \tilde{\pi}_0\,P_0 - \tfrac{\mathrm{i}}{2}\,\omega^0_{ij}\,P_0\,\partial_j \tilde{\pi}_0\,\partial_i P_0\,P_0 \\
& - \tfrac{1}{8}\,\omega^0_{ij}\,\omega^0_{lm}\,P_0\,\partial^2_{jm}P_0\;\partial^2_{il}P_0\,P_0 \\
=& \tfrac{1}{16}\,P_0\,\mathrm{Tr}_{2n}(\omega^0\,\Omega^{op}_0)\,\mathrm{Tr}_{2n}(\omega^0\,\Omega^{op}_0)\,P_0 \\
& - \tfrac{\mathrm{i}}{4}\,\omega^0_{ij}\,P_0\,[\,\partial_j P_0\,,\partial_i P_1\,]\,P_0 - \tfrac{\mathrm{i}}{4}\,\omega^0_{ij}\,P_0\,[\,\partial_j P_1\,,\partial_i P_0\,]\,P_0 \\
& - \tfrac{\mathrm{i}}{2}\,\omega^0_{ij}\,P_0\,[\,\partial_j P_0\,,\partial_i \tilde{\pi}_0\,]\,P_0 \\
& - \tfrac{1}{8}\,\omega^0_{ij}\,\omega^0_{lm}\,P_0\,\partial^2_{jm}P_0\;\partial^2_{il}P_0\,P_0 \\
=& \tfrac{1}{4}\,P_0\,\mathrm{Tr}_{2n}(\omega^0\,\Omega^{op}_1)\,P_0 - \tfrac{1}{16}\,P_0\,\mathrm{Tr}_{2n}(\omega^0\,\Omega^{op}_0)\,\mathrm{Tr}_{2n}(\omega^0\,\Omega^{op}_0)\,P_0 \\
& + \tfrac{1}{8}\;P_0\,\mathrm{Tr}_{2n}(\omega^0\,\Omega^{op}_0\,\omega^0\,\Omega^{op}_0)\,P_0 - \tfrac{1}{8}\,\omega^0_{ij}\,\omega^0_{lm}\,P_0\,\partial^2_{jm}P_0\,P_0^\perp\,\partial^2_{il}P_0\,P_0
\end{aligned}$$

Analogously it follows that

$$\begin{aligned}
P_0^\perp\,G_2\,P_0^\perp =& \tfrac{1}{4}\,P_0^\perp\,\mathrm{Tr}_{2n}(\omega^0\,\Omega^{op}_1)\,P_0^\perp - \tfrac{1}{16}\,P_0^\perp\,\mathrm{Tr}_{2n}(\omega^0\,\Omega^{op}_0)\,\mathrm{Tr}_{2n}(\omega^0\,\Omega^{op}_0)\,P_0^\perp \\
& + \tfrac{1}{8}\,P_0^\perp\,\mathrm{Tr}_{2n}(\omega^0\,\Omega^{op}_0\,\omega^0\,\Omega^{op}_0)\,P_0^\perp \\
& + \tfrac{1}{8}\,P_0^\perp\,\mathrm{Tr}_{2n}(\omega^0\,\nabla^2 P_0\,P_0\,\omega^0\,\nabla^2 P_0)\,P_0^\perp\,.
\end{aligned}$$

What is left is to show (B.6). By the cyclicity of the trace

$$\begin{aligned}
& - \tfrac{1}{16}\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0^\perp\,\mathrm{Tr}_{2n}(\omega^0\,\Omega^{op}_0)\,\mathrm{Tr}_{2n}(\omega^0\,\Omega^{op}_0)) \\
& \quad = \tfrac{1}{16}\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0^\perp\,\omega^0_{ij}\,[\,\partial_j P_0\,,\partial_i P_0\,]\,\omega^0_{lm}\,[\,\partial_m P_0\,,\partial_l P_0\,]) \\
& \quad = \tfrac{1}{4}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0^\perp\,\omega^0_{ij}\,\omega^0_{lm}\,\partial_j P_0\,\partial_i P_0\,\partial_m P_0\,\partial_l P_0) \\
& \quad = \tfrac{1}{4}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\,\omega^0_{ij}\,\omega^0_{lm}\,\partial_l P_0\,\partial_j P_0\,\partial_i P_0\,\partial_m P_0)\,.
\end{aligned}$$

This and a computation similar to (B.8) shows

$$\begin{aligned}
& - \tfrac{1}{16}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0^\perp\,\mathrm{Tr}_{2n}(\omega^0\,\Omega^{op}_0)\,\mathrm{Tr}_{2n}(\omega^0\,\Omega^{op}_0)) \\
& \quad = \tfrac{1}{16}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\,\mathrm{Tr}_{2n}(\omega^0\,g^{op}_0\,\omega^0\,g^{op}_0)) - \tfrac{1}{16}\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\,\mathrm{Tr}_{2n}(\omega^0\,\Omega^{op}_0\,\omega^0\,\Omega^{op}_0))
\end{aligned} \tag{B.11}$$

and analogously

$$
\begin{aligned}
&\tfrac{1}{8}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0^\perp\,\mathrm{Tr}_{2n}(\omega^0\,\Omega_0^{op}\,\omega^0\,\Omega_0^{op}))\\
&\qquad=\tfrac{1}{16}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\,\mathrm{Tr}_{2n}(\omega^0\,\Omega_0^{op})\,\mathrm{Tr}_{2n}(\omega^0\,\Omega_0^{op}))\\
&\qquad\quad-\tfrac{1}{16}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\,\mathrm{Tr}_{2n}(\omega^0\,g_0^{op}\,\omega^0\,g_0^{op}))-\tfrac{1}{16}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\,\mathrm{Tr}_{2n}(\omega^0\,\Omega_0^{op}\,\omega^0\,\Omega_0^{op}))\,.
\end{aligned}
\tag{B.12}
$$

In addition,

$$
\begin{aligned}
&\tfrac{1}{4}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0^\perp\,\omega_{ij}^0\,\Omega_{1,ji}^{op}\,P_0^\perp)\\
&\qquad=-\tfrac{\mathrm{i}}{4}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0^\perp\,\omega_{ij}^0\,[\,\partial_jP_0\,,\partial_iP_1\,]\,P_0^\perp)-\tfrac{\mathrm{i}}{4}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0^\perp\,\omega_{ij}^0\,[\,\partial_jP_1\,,\partial_iP_0\,]\,P_0^\perp)\\
&\qquad=-\tfrac{\mathrm{i}}{4}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\,\omega_{ij}^0\,[\,\partial_iP_1\,,\partial_jP_0\,]\,P_0)-\tfrac{\mathrm{i}}{4}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\,\omega_{ij}^0\,[\,\partial_iP_0\,,\partial_jP_1\,]\,P_0)\\
&\qquad=-\tfrac{1}{4}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\,\omega_{ij}^0\,\Omega_{1,ji}^{op}\,P_0)
\end{aligned}
\tag{B.13}
$$

and

$$
\begin{aligned}
&-\tfrac{1}{8}\,\omega_{ij}^0\,\omega_{lm}^0\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0^\perp\,\partial_{jm}^2P_0\,P_0\,\partial_{il}^2P_0\,P_0^\perp)\\
&\qquad=-\tfrac{1}{8}\,\omega_{ij}^0\,\omega_{lm}^0\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\,\partial_{il}^2P_0\,P_0^\perp\,\partial_{jm}^2P_0)\\
&\qquad=\tfrac{1}{8}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\,\mathrm{Tr}_{2n}(\omega^0\,\nabla^2P_0\,P_0^\perp\,\omega^0\,\nabla^2P_0))
\end{aligned}
\tag{B.14}
$$

Combining (B.11)-(B.14) yields

$$
\begin{aligned}
&\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0^\perp\,G_2\,P_0^\perp)\\
&\qquad=\mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big(\tfrac{1}{4}\,P_0^\perp\,\mathrm{Tr}_{2n}(\omega^0\,\Omega_1^{op})\,P_0^\perp-\tfrac{1}{16}\,P_0^\perp\,\mathrm{Tr}_{2n}(\omega^0\,\Omega_0^{op})\,\mathrm{Tr}_{2n}(\omega^0\,\Omega_0^{op})\,P_0^\perp\\
&\qquad\quad+\tfrac{1}{8}\,P_0^\perp\,\mathrm{Tr}_{2n}(\omega^0\,\Omega_0^{op}\,\omega^0\,\Omega_0^{op})\,P_0^\perp-\tfrac{1}{8}\,\omega_{ij}^0\,\omega_{lm}^0\,P_0^\perp\,\partial_{jm}^2P_0\,P_0\,\partial_{il}^2P_0\,P_0^\perp\Big)\\
&\qquad=-\tfrac{1}{4}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\,\mathrm{Tr}_{2n}(\omega^0\,\Omega_1^{op}))-\tfrac{1}{8}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\,\mathrm{Tr}_{2n}(\omega^0\,\Omega_0^{op}\,\omega^0\,\Omega_0^{op}))\\
&\qquad\quad+\tfrac{1}{16}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\,\mathrm{Tr}_{2n}(\omega^0\,\Omega_0^{op})\,\mathrm{Tr}_{2n}(\omega^0\,\Omega_0^{op}))\\
&\qquad\quad+\tfrac{1}{8}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\,\mathrm{Tr}_{2n}(\omega^0\,\nabla^2P_0\,P_0^\perp\,\omega^0\,\nabla^2P_0))
\end{aligned}
$$

finishing the proof. □

**Lemma B.3** *Let the assumptions of Lemma 5.1 hold and the operator-valued symbol $B \in S^0(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f}))$ be given by*

$$B(\varepsilon, z) := \Big[ \, \{h(\varepsilon, z)\, , \pi(\varepsilon, z)\} \, , \{a(\varepsilon, z)\, , \pi(\varepsilon, z)\} \, \Big]$$

*Then, the effective symbol $b \in S_0(\varepsilon, \mathbb{C})$ of $B(\varepsilon, z)$ has an asymptotic expansion starting with*

$$\begin{aligned} b \asymp \, & \mathrm{i} \Big\langle \omega^0 \, \Omega^\varepsilon \, \omega^0 \, \nabla h \, , \, \nabla a \Big\rangle - \tfrac{\mathrm{i}}{4} \, \varepsilon \, \mathrm{Tr}_{2n}(\omega^0 \, \Omega^\varepsilon) \Big\langle \omega^0 \, \Omega^\varepsilon \, \omega^0 \, \nabla h \, , \, \nabla a \Big\rangle \\ & + \tfrac{3\mathrm{i}}{4} \, \varepsilon \, \Big\langle \omega^0 \, (\Omega^\varepsilon \, \omega^0)^2 \, \nabla h \, , \, \nabla a \Big\rangle - \tfrac{3\mathrm{i}}{4} \, \varepsilon \, \Big\langle \omega^0 \, (g^\varepsilon \, \omega^0)^2 \, \nabla h \, , \, \nabla a \Big\rangle \\ & + \mathcal{O}(\varepsilon^2) \, . \end{aligned}$$

*Moreover, there exists a constant $C > 0$ and a $\tilde{r} \in \mathbb{N}_0$ for every $r \in \mathbb{N}_0$ such that*

$$\begin{aligned} & \Big\| \, \pi \, \# \Big[ \, \{h \, , \pi\} \, , \{a \, , \pi\} \, \Big] \, \# \, \pi \\ & \quad - \pi \, \# \Big( \mathrm{i} \Big\langle \omega^0 \, \Omega^\varepsilon \, \omega^0 \, \nabla h \, , \, \nabla a \Big\rangle - \tfrac{\mathrm{i}}{4} \, \varepsilon \, \mathrm{Tr}_{2n}(\omega^0 \, \Omega^\varepsilon) \Big\langle \omega^0 \, \Omega^\varepsilon \, \omega^0 \, \nabla h \, , \, \nabla a \Big\rangle \\ & \qquad + \tfrac{3\mathrm{i}}{4} \, \varepsilon \Big\langle \omega^0 \, (\Omega^\varepsilon \, \omega^0)^2 \, \nabla h \, , \, \nabla a \Big\rangle - \tfrac{3\mathrm{i}}{4} \, \varepsilon \Big\langle \omega^0 \, (g \, \omega^0)^2 \, \nabla h \, , \, \nabla a \Big\rangle \Big) \, \# \, \pi \, \Big\|_{0,r} \\ & \quad \leq C \, \varepsilon^2 \, \|a\|^\varepsilon_{0,\tilde{r}} \, . \end{aligned}$$

PROOF We start our proof by reformulating $\mathcal{K} := [\{h \, , \pi\} \, , \{a \, , \pi\}]$. We have

$$\begin{aligned} \mathcal{K} &= \partial_k h \, \partial_l a \, \Big[ \omega^0_{ik} \partial_i \pi \, , \omega^0_{jl} \partial_j \pi \Big] = \omega^0_{lj} \, [\, \partial_j \pi \, , \partial_i \pi \,] \, \omega^0_{ik} \, \partial_k h \, \partial_l a \\ &=: \omega^0_{lj} \, K_{ji} \, \omega^0_{ik} \, \partial_k h \, \partial_l a = \langle \, \omega^0 \, K \, \omega^0 \, \nabla h \, , \, \nabla a \, \rangle \, . \end{aligned}$$

Defining

$$k^0_{ij} := \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(K_{ij} \, P_0) = \mathrm{tr}_{\mathcal{H}_\mathrm{f}}([\, \partial_i \pi \, , \partial_j \pi \,] \; P_0)$$

we have

$$\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\mathcal{K} \, P_0) = \langle \, \omega^0 \, k^0 \, \omega^0 \, \nabla h \, , \, \nabla a \, \rangle =: \kappa_0 \, .$$

By the definition of $\pi$ (see Proposition 3.2)

$$k^0_{ij} = \mathrm{tr}_{\mathcal{H}_\mathrm{f}}([\, \partial_i (P + \varepsilon \tilde{\pi}) \, , \partial_j (P + \varepsilon \tilde{\pi}) \,] \; P_0) \, .$$

In addition, $\tilde{\pi}$ is diagonal with respect to $P_0$. Therefore, applying Lemma B.1 results in

$$\begin{aligned} k^0_{ij} &= \mathrm{tr}_{\mathcal{H}_\mathrm{f}}([\,\partial_i P\,,\partial_j P\,]\;P_0) + \varepsilon\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\,\tilde{\pi}\,P_0\;[\,\partial_i P\,,\partial_j P_0\,]) \\ &\quad - \varepsilon\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\Big[\,\partial_i P\,\Big|P_0^\perp\,\tilde{\pi}\,P_0^\perp\,\Big|\,\partial_j P_0\,\Big]\;P_0) + \varepsilon\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\,\tilde{\pi}\,P_0\;[\,\partial_i P_0\,,\partial_j P\,]) \\ &\quad - \varepsilon\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\Big[\,\partial_i P_0\,\Big|P_0^\perp\,\tilde{\pi}\,P_0^\perp\,\Big|\,\partial_j P\,\Big]\;P_0) + \mathcal{O}(\varepsilon^2)\,. \end{aligned}$$

Recall that $\partial_i P_0$ is off-diagonal with respect to $P_0$ and $P_1^D = 0$. Hence,

$$\begin{aligned} k^0_{ij} &= \mathrm{tr}_{\mathcal{H}_\mathrm{f}}([\,\partial_i P\,,\partial_j P\,]\;P) + 2\,\varepsilon\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\,\tilde{\pi}\,P_0\;[\,\partial_i P\,,\partial_j P_0\,]) \\ &\quad + 2\,\varepsilon\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0^\perp\,\tilde{\pi}\,P_0^\perp\;[\,\partial_i P\,,\partial_j P_0\,]) + \mathcal{O}(\varepsilon^2)\,. \end{aligned}$$

Replacing $\tilde{\pi}$ by its expansion (3.19) in the previous equation leads to

$$\begin{aligned} k^0_{ij} &= \mathrm{tr}_{\mathcal{H}_\mathrm{f}}([\,\partial_i P\,,\partial_j P\,]\;P) - \tfrac{1}{2}\,\varepsilon\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\,\mathrm{Tr}_{2n}(\omega^0\,\Omega_0^{op}))\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\;[\,\partial_i P\,,\partial_j P_0\,]) \\ &\quad + \tfrac{1}{2}\,\varepsilon\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0^\perp\,\mathrm{Tr}_{2n}(\omega^0\,\Omega_0^{op})\,P_0^\perp\;[\,\partial_i P\,,\partial_j P_0\,]) + \mathcal{O}(\varepsilon^2)\,. \end{aligned} \tag{B.15}$$

By (3.9) $\mathcal{P}^\varepsilon = P + \mathcal{O}(\varepsilon^\infty) = P_0 + \mathcal{O}(\varepsilon)$. Hence,

$$\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\;[\,\partial_i P\,,\partial_j P_0\,]) = \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\mathcal{P}^\varepsilon\;[\,\partial_i \mathcal{P}^\varepsilon\,,\partial_j \mathcal{P}^\varepsilon\,]) + \mathcal{O}(\varepsilon) = \mathrm{i}\,\Omega^\varepsilon_{ij} \tag{B.16}$$

and

$$\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\,\mathrm{Tr}_{2n}(\omega^0\,\Omega_0^{op})) = -\mathrm{i}\,\omega^0_{ji}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\;[\,\partial_i P_0\,,\partial_j P_0\,]) = \mathrm{Tr}_{2n}(\omega^0\,\Omega^\varepsilon) + \mathcal{O}(\varepsilon)\,. \tag{B.17}$$

By (3.9), the cyclicity of trace and the skew-symmetry of $\omega^0$

$$\begin{aligned} &\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0^\perp\,\mathrm{Tr}_{2n}(\omega^0\,\Omega_0^{op})\,P_0^\perp\;[\,\partial_i P\,,\partial_j P_0\,]) \\ &\qquad = -2\,\mathrm{i}\,\omega^0_{lk}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\mathcal{P}^\varepsilon\,\partial_l \mathcal{P}^\varepsilon\,\partial_i \mathcal{P}^\varepsilon\,\partial_j \mathcal{P}^\varepsilon\,\partial_k \mathcal{P}^\varepsilon) \\ &\qquad\quad + 2\,\mathrm{i}\,\omega^0_{lk}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\mathcal{P}^\varepsilon\,\partial_i \mathcal{P}^\varepsilon\,\partial_k \mathcal{P}^\varepsilon\,\partial_l \mathcal{P}^\varepsilon\,\partial_j \mathcal{P}^\varepsilon) + \mathcal{O}(\varepsilon) \end{aligned} \tag{B.18}$$

Plugging in the definition of $\mathcal{T}^\varepsilon$ (3.73) and using the symmetry of the Fubini-Study metric $g^\varepsilon$ as well as the skew-symmetry of the symplectic forms $\Omega^\varepsilon$ and $\omega^0$ we get

$$\begin{aligned} &\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0^\perp\,\mathrm{Tr}_{2n}(\omega^0\,\Omega_0^{op})\,P_0^\perp\;[\,\partial_i P\,,\partial_j P_0\,]) \\ &\quad = -2\,\mathrm{i}\,\omega^0_{lk}\,\mathcal{T}^\varepsilon_{li}\,\mathcal{T}^\varepsilon_{jk} + 2\,\mathrm{i}\,\omega^0_{lk}\,\mathcal{T}^\varepsilon_{ik}\,\mathcal{T}^\varepsilon_{lj} \\ &\quad = -\tfrac{1}{2}\,\mathrm{i}\,\omega^0_{lk}\,g^\varepsilon_{li}\,g^\varepsilon_{jk} + \tfrac{1}{2}\,\mathrm{i}\,\omega^0_{lk}\,\Omega^\varepsilon_{li}\,\Omega^\varepsilon_{jk} + \tfrac{1}{2}\,\mathrm{i}\,\omega^0_{lk}\,g^\varepsilon_{ik}\,g^\varepsilon_{lj} - \tfrac{1}{2}\,\mathrm{i}\,\omega^0_{lk}\,\Omega^\varepsilon_{ik}\,\Omega^\varepsilon_{lj} \\ &\quad = -\mathrm{i}\,g^\varepsilon_{ik}\,\omega^0_{kl}\,g^\varepsilon_{lj} + \mathrm{i}\,\Omega^\varepsilon_{ik}\,\omega^0_{kl}\,\Omega^\varepsilon_{lj}\,. \end{aligned} \tag{B.19}$$

Combining (B.15)- (B.19) shows

$$\begin{aligned} k^0_{ij} =& \,\mathrm{i}\, \Omega^\varepsilon_{ij} - \varepsilon \tfrac{\mathrm{i}}{2} \operatorname{Tr}_{2n}(\omega^0 \, \Omega^\varepsilon) \, \Omega^\varepsilon_{ij} - \varepsilon \tfrac{\mathrm{i}}{2} \, (g^\varepsilon \, \omega^0 \, g^\varepsilon)_{ij} \\ &+ \varepsilon \tfrac{\mathrm{i}}{2} \, (\Omega^\varepsilon \, \omega^0 \, \Omega^\varepsilon)_{ij} + \mathcal{O}(\varepsilon^2) \, . \end{aligned} \tag{B.20}$$

Next we want to compute the first order terms in the effective symbol of $\mathcal{K}$. Since $[\, K_{ij} \, , P_0 \,] = \mathcal{O}(\varepsilon)$ we have

$$\begin{aligned} (\mathcal{K} - \kappa_0) \, P_0 =& \langle \, \omega^0 \, (P_0 \, K \, P_0 - k^0 \, P_0) \, \omega^0 \, \nabla h \, , \, \nabla a \, \rangle + \mathcal{O}(\varepsilon) \\ =& \langle \, \omega^0 \, (\operatorname{tr}_{\mathcal{H}_\mathrm{f}}(P_0 \, K) \, P_0 - k^0 \, P_0) \, \omega^0 \, \nabla h \, , \, \nabla a \, \rangle + \mathcal{O}(\varepsilon) \\ =& \, \mathcal{O}(\varepsilon) \end{aligned}$$

which implies

$$\partial_i (\mathcal{K} - \kappa_0) \, P_0 = -(\mathcal{K} - \kappa_0) \, \partial_i P_0 + \mathcal{O}(\varepsilon) \, .$$

Then

$$\begin{aligned} \varepsilon^{-1} \, \pi \# (\mathcal{K} - \kappa) \# \pi =& \, \pi_1 \, (\mathcal{K} - \kappa_0) \, P_0 + P_0 \, (\mathcal{K} - \kappa_0) \, \pi_1 + \{ P_0 \, , \mathcal{K} - \kappa_0 \, \}_1 \, P_0 \\ &+ P_0 \, \{ \mathcal{K} - \kappa_0 \, , P_0 \, \}_1 + \{ P_0 \, | \, \mathcal{K} - \kappa_0 \, | \, P_0 \, \}_1 + \mathcal{O}(\varepsilon) \\ =& - \{ P_0 \, | \, \mathcal{K} - \kappa_0 \, | \, P_0 \, \}_1 + \mathcal{O}(\varepsilon) \\ =& \, \tfrac{\mathrm{i}}{2} \, \langle \, \omega^0 \, \{ P_0 \, | \, K - k^0 \, | \, P_0 \, \} \, \omega^0 \, \nabla h \, , \, \nabla a \, \rangle + \mathcal{O}(\varepsilon) \end{aligned}$$

which suggests defining $k^1$ by

$$k^1_{ij} = \tfrac{\mathrm{i}}{2} \operatorname{tr}_{\mathcal{H}_\mathrm{f}}(\{ P_0 \, | \, K_{ij} - k^0_{ij} \, | \, P_0 \, \} \, P_0).$$

such that

$$\kappa_1 := \tfrac{\mathrm{i}}{2} \operatorname{tr}_{\mathcal{H}_\mathrm{f}}(\langle \, \omega^0 \, \{ P_0 \, | \, K - k^0 \, | \, P_0 \, \} \, \omega^0 \, \nabla h \, , \, \nabla a \, \rangle \, P_0) = \langle \, \omega^0 \, k^1 \, \omega^0 \, \nabla h \, , \, \nabla a \, \rangle \, .$$

Plugging in the definition of $K$ and $k^0$ and using the cyclicity of the trace yields

$$\begin{aligned} k^1_{ij} =& - \tfrac{\mathrm{i}}{2} \operatorname{tr}_{\mathcal{H}_\mathrm{f}}(P_0^\perp \, \{ P_0 \, , P_0 \} \, [\, \partial_i P_0 \, , \partial_j P_0 \,]) \\ &- \tfrac{\mathrm{i}}{2} \operatorname{tr}_{\mathcal{H}_\mathrm{f}}(\{ P_0 , P_0 \} \operatorname{tr}_{\mathcal{H}_\mathrm{f}}([\, \partial_i P_0 \, , \partial_j P_0 \,]) \, P_0) + \mathcal{O}(\varepsilon). \end{aligned}$$

A similar computation as the one leading to (B.20) shows

$$k^1_{ij} = -\tfrac{\mathrm{i}}{4} (g^\varepsilon \, \omega^0 \, g^\varepsilon)_{ij} + \tfrac{\mathrm{i}}{4} (\Omega^\varepsilon \, \omega^0 \, \Omega^\varepsilon)_{ij} + \tfrac{\mathrm{i}}{4} \operatorname{Tr}_{2n}(\omega^0 \, \Omega^\varepsilon) \, \Omega^\varepsilon_{ij} + \mathcal{O}(\varepsilon).$$

Fix $r \in \mathbb{N}_0$. By definition of the effective symbol (3.26) of $[\,\{h\,,\pi\}\,,\{a\,,\pi\}\,]$ and Theorem 3.6 there exists a constant $C_1 > 0$ and a $\tilde{r}_1 \in \mathbb{N}_0$ such that

$$\Big\| \pi \,\#\, \Big[\ \{h\,,\pi\}\ ,\{a\,,\pi\}\ \Big] \,\#\, \pi \\ - \pi \,\#\, \Big( \mathrm{i}\ \Big\langle \omega^0\, \Omega^\varepsilon\, \omega^0\, \nabla h\,,\ \nabla a \Big\rangle - \tfrac{\mathrm{i}}{4}\, \varepsilon\, \mathrm{Tr}_{2n}(\omega^0\, \Omega^\varepsilon)\ \Big\langle \omega^0\, \Omega^\varepsilon\, \omega^0\, \nabla h\,,\ \nabla a \Big\rangle \\ + \tfrac{3\mathrm{i}}{4}\, \varepsilon\ \Big\langle \omega^0\, (\Omega^\varepsilon\, \omega^0)^2\, \nabla h\,,\ \nabla a \Big\rangle - \tfrac{3\mathrm{i}}{4}\, \varepsilon\ \Big\langle \omega^0\, (g^\varepsilon\, \omega^0)^2\, \nabla h\,,\ \nabla a \Big\rangle \Big) \,\#\, \pi\ \Big\|_{0,r} \\ \leq C_1\, \varepsilon^2\, \|\, [\,\{h\,,\pi\}\ ,\{a\,,\pi\}\,]\, \|^\varepsilon_{0,\tilde{r}_1}$$

Finally, choosing $C = C_1\, \max_{1 \leq i \leq 2n} \|\partial_i h\|^\varepsilon_{0,\tilde{r}_1+1}\, (\|\pi\|^\varepsilon_{0,\tilde{r}_1+1})^2$ and $\tilde{r} = \tilde{r}_1 + 1$ finishes the proof. □

**Lemma B.4** *Let the assumptions of Lemma 5.1 hold and the operator-valued symbol $B \in S^0(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f}))$ be given by*

$$B(\varepsilon) := \Big\{\ \{h(\varepsilon)\,,\pi(\varepsilon)\}\ ,\{a(\varepsilon)\,,\pi(\varepsilon)\}\ \Big\}_1 - \Big\{\ \{a(\varepsilon)\,,\pi(\varepsilon)\}\ ,\{h(\varepsilon)\,,\pi(\varepsilon)\}\ \Big\}_1$$

*Then, the effective symbol $b \in S_0(\varepsilon, \mathbb{C})$ of $B(\varepsilon, z)$ has an asymptotic expansion starting with*

$$b \asymp -\tfrac{\mathrm{i}}{2}\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\{\{h\,,P_0\}\ ,\{a\,,P_0\}\}) + \tfrac{3\mathrm{i}}{4}\ \Big\langle \omega^0\, (g^\varepsilon\, \omega^0)^2\, \nabla h\,,\ \nabla a \Big\rangle \\ + \tfrac{\mathrm{i}}{4}\ \Big\langle \omega^0\, (\Omega^\varepsilon\, \omega^0)^2\, \nabla h\,,\ \nabla a \Big\rangle + \tfrac{\mathrm{i}}{4}\ \mathrm{Tr}_{2n}(\omega^0\, \Omega^\varepsilon)\ \Big\langle \omega^0\, \Omega^\varepsilon\, \omega^0\, \nabla h\,,\ \nabla a \Big\rangle + \mathcal{O}(\varepsilon)\,.$$

*Moreover, there exists a constant $C > 0$ and a $\tilde{r} \in \mathbb{N}_0$ for every $r \in \mathbb{N}_0$ such that*

$$\Big\| \pi \,\#\, \Big( \Big\{\ \{h\,,\pi\}\ ,\{a\,,\pi\}\ \Big\}_1 - \Big\{\ \{a\,,\pi\}\ ,\{h\,,\pi\}\ \Big\}_1 \Big) \,\#\, \pi \\ - \pi \,\#\, \Big( -\tfrac{\mathrm{i}}{2}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\{\{h\,,P_0\}\ ,\{a\,,P_0\}\}) + \tfrac{3\mathrm{i}}{4}\ \Big\langle \omega^0\, (g^\varepsilon\, \omega^0)^2\, \nabla h\,,\ \nabla a \Big\rangle \\ + \tfrac{\mathrm{i}}{4}\ \Big\langle \omega^0\, (\Omega^\varepsilon\, \omega^0)^2\, \nabla h\,,\ \nabla a \Big\rangle + \tfrac{\mathrm{i}}{4}\ \mathrm{Tr}_{2n}(\omega^0\, \Omega^\varepsilon)\ \Big\langle \omega^0\, \Omega^\varepsilon\, \omega^0\, \nabla h\,,\ \nabla a \Big\rangle \Big) \,\#\, \pi\ \Big\|_{0,r} \\ \leq C\, \varepsilon\, \|a\|^\varepsilon_{0,\tilde{r}}\,.$$

PROOF We start with the observation that by (2.16) and the fact that $\mathcal{P}^\varepsilon = P + \mathcal{O}(\varepsilon^\infty) = P_0 + \mathcal{O}(\varepsilon)$ (3.9)

$$P_0\, \partial^2_{ij} P_0\, P_0 = -\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\ [\,\partial_i P_0\,, \partial_j P_0\,]_+\ P_0)\, P_0 = g^\varepsilon_{ij}\, P_0 + \mathcal{O}(\varepsilon)\,.$$

Therefore,

$$\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\{\partial_i P_0\, |P_0\, |\, \partial_j P_0\}\ P_0) = \omega^0_{kl} \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\partial^2_{il} P_0\, P_0\, \partial^2_{jk} P_0\, P_0) \\ = \omega^0_{kl}\, g^\varepsilon_{il}\, g^\varepsilon_{jk} + \mathcal{O}(\varepsilon) = -(g^\varepsilon\, \omega^0\, g^\varepsilon)_{ij} + \mathcal{O}(\varepsilon). \tag{B.21}$$

By the cyclicity of the trace as well as that $\partial_i P_0$ is off diagonal with respect to $P_0$ we obtain

$$\begin{aligned}
&\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\Big\{\partial_i P_0 \,\Big|P_0^\perp\,\Big|\,\partial_j P_0\Big\}\;P_0^\perp) = \omega^0_{kl}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\partial^2_{il}P_0\,P_0^\perp\,\partial^2_{jk}P_0\,P_0^\perp)\\
&\quad = \omega^0_{kl}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\partial_k P_0\,\partial_i P_0\,\partial_l P_0\,\partial_j P_0\,P_0) + \omega^0_{kl}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\partial_k P_0\,\partial_l P_0\,\partial_i P_0\,\partial_j P_0\,P_0)\\
&\qquad + \omega^0_{kl}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\partial_l P_0\,\partial_k P_0\,\partial_j P_0\,\partial_i P_0\,P_0) + \omega^0_{kl}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\partial_i P_0\,\partial_k P_0\,\partial_j P_0\,\partial_l P_0\,P_0).
\end{aligned}$$

Now, by (3.9) and the definition of $\mathcal{T}^\varepsilon$ (3.73)

$$\begin{aligned}
&\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\Big\{\partial_i P_0 \,\Big|P_0^\perp\,\Big|\,\partial_j P_0\Big\}\;P_0^\perp)\\
&\quad = \omega^0_{kl}\mathcal{T}^\varepsilon_{ki}\mathcal{T}^\varepsilon_{lj} + \omega^0_{kl}\mathcal{T}^\varepsilon_{ik}\mathcal{T}^\varepsilon_{jl} + \omega^0_{kl}\mathcal{T}^\varepsilon_{kl}\mathcal{T}^\varepsilon_{ij} + \omega^0_{kl}\mathcal{T}^\varepsilon_{lk}\mathcal{T}^\varepsilon_{ji} + \mathcal{O}(\varepsilon)\\
&\quad = \tfrac{1}{2}\,\omega^0_{kl}\,g^\varepsilon_{ki}\,g^\varepsilon_{lj} - \tfrac{1}{2}\,\omega^0_{kl}\,\Omega^\varepsilon_{ki}\,\Omega^\varepsilon_{lj} + \tfrac{1}{2}\,\omega^0_{kl}\,g^\varepsilon_{kl}\,g^\varepsilon_{ij} - \tfrac{1}{2}\,\omega^0_{kl}\,\Omega^\varepsilon_{kl}\,\Omega^\varepsilon_{ij} + \mathcal{O}(\varepsilon)\\
&\quad = \tfrac{1}{2}\,(g^\varepsilon\,\omega^0\,g^\varepsilon)_{ij} + \tfrac{1}{2}\,(\Omega^\varepsilon\,\omega^0\,\Omega^\varepsilon)_{ij} + \tfrac{1}{2}\,\mathrm{Tr}_{2n}(\omega^0\,\Omega^\varepsilon)\,\Omega^\varepsilon_{ij} + \mathcal{O}(\varepsilon)\,.
\end{aligned} \tag{B.22}$$

By the cyclicity of the trace we get

$$\begin{aligned}
&-\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\{\partial_i P_0\,,\partial_j P_0\}\;P_0) + \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\{\partial_j P_0\,,\partial_i P_0\}\;P_0)\\
&\quad = -\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\{\partial_i P_0\,|P_0\,|\,\partial_j P_0\}\;P_0) - \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\Big\{\partial_i P_0 \,\Big|P_0^\perp\,\Big|\,\partial_j P_0\Big\}\;P_0)\\
&\qquad - \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\{\partial_i P_0\,|P_0\,|\,\partial_j P_0\}\;P_0) - \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\{\partial_i P_0\,|P_0\,|\,\partial_j P_0\}\;P_0^\perp)\\
&\qquad - \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\Big\{\partial_i P_0 \,\Big|P_0^\perp\,\Big|\,\partial_j P_0\Big\}\;P_0^\perp) + \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\Big\{\partial_i P_0 \,\Big|P_0^\perp\,\Big|\,\partial_j P_0\Big\}\;P_0^\perp)\\
&\quad = -\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\{\partial_i P_0\,,\partial_j P_0\})\\
&\qquad - \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\{\partial_i P_0\,|P_0\,|\,\partial_j P_0\}\;P_0) + \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\Big\{\partial_i P_0 \,\Big|P_0^\perp\,\Big|\,\partial_j P_0\Big\}\;P_0^\perp)\,.
\end{aligned}$$

Then, plugging in the results from (B.21) and (B.22) into the above equation yields

$$\begin{aligned}
&-\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\{\partial_i P_0\,,\partial_j P_0\}\;P_0) + \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\{\partial_j P_0\,,\partial_i P_0\}\;P_0)\\
&\quad = -\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\{\partial_i P_0\,,\partial_j P_0\})\\
&\qquad + \tfrac{3}{2}\,(g^\varepsilon\,\omega^0\,g^\varepsilon)_{ij} + \tfrac{1}{2}\,(\Omega^\varepsilon\,\omega^0\,\Omega^\varepsilon)_{ij} + \tfrac{1}{2}\,\mathrm{Tr}_{2n}(\omega^0\,\Omega^\varepsilon)\,\Omega^\varepsilon_{ij} + \mathcal{O}(\varepsilon)\,.
\end{aligned} \tag{B.23}$$

In addition, we have

$$\begin{aligned}
&-\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\,\partial_k P_0\;\{\partial_i h\,,\partial_l P_0\}) + \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\;\{\partial_l P_0\,,\partial_i h\}\;\partial_k P_0)\\
&\quad = -\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\,\partial_k P_0\;\{\partial_i h\,,\partial_l P_0\}) - \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0^\perp\,\partial_k P_0\;\{\partial_i h\,,\partial_l P_0\})\\
&\quad = -\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\partial_k P_0\;\{\partial_i h\,,\partial_l P_0\})
\end{aligned}$$

and similarly

$$
\begin{aligned}
&- \operatorname{tr}_{\mathcal{H}_\mathrm{f}}(P_0 \,\{\partial_k P_0 \,, \partial_j a\}\, \partial_l P_0) + \operatorname{tr}_{\mathcal{H}_\mathrm{f}}(P_0\, \partial_l \pi \,\{\partial_j a \,, \partial_k P_0\}) \\
&\qquad = -\operatorname{tr}_{\mathcal{H}_\mathrm{f}}(\{\partial_k P_0 \,, \partial_j a\}\, \partial_l P_0)
\end{aligned}
$$

as well as

$$
\begin{aligned}
&- \{\partial_i h \,, \partial_j a\}\, \operatorname{tr}_{\mathcal{H}_\mathrm{f}}(P_0\, \partial_k P_0\, \partial_l P_0) + \{\partial_j a \,, \partial_i h\}\, \operatorname{tr}_{\mathcal{H}_\mathrm{f}}(P_0\, \partial_l P_0\, \partial_k P_0) \\
&\qquad = - \{\partial_i h \,, \partial_j a\}\, \operatorname{tr}_{\mathcal{H}_\mathrm{f}}(\partial_k P_0\, \partial_l P_0)\,.
\end{aligned} \tag{B.24}
$$

Finally, the product rule followed by an application of (B.23)-(B.24) gives

$$
\begin{aligned}
&\operatorname{tr}_{\mathcal{H}_\mathrm{f}}\Big((-\tfrac{\mathrm{i}}{2}\,\{\{h\,,\pi\}\ ,\{a\,,\pi\}\} + \tfrac{\mathrm{i}}{2}\,\{\{a\,,\pi\}\ ,\{h\,,\pi\}\})\,P\Big) \\
&\quad = \tfrac{\mathrm{i}}{2}\,\omega^0_{ki}\,\omega^0_{lj}\Big( - \operatorname{tr}_{\mathcal{H}_\mathrm{f}}(P_0\, \{\partial_i h\, \partial_k P_0 \,, \partial_j a\, \partial_l P_0\}) \\
&\qquad + \operatorname{tr}_{\mathcal{H}_\mathrm{f}}(P_0\, \{\partial_j a\, \partial_l P_0 \,, \partial_i h\, \partial_k P_0\})\Big) + \mathcal{O}(\varepsilon) \\
&\quad = \tfrac{\mathrm{i}}{2}\,\omega^0_{ki}\,\omega^0_{lj}\Big( - \operatorname{tr}_{\mathcal{H}_\mathrm{f}}(\{\partial_i h\, \partial_k P_0 \,, \partial_j a\, \partial_l P_0\}) \\
&\qquad + \tfrac{3}{2}\,(g^\varepsilon\,\omega^0\,g^\varepsilon)_{ij} + \tfrac{1}{2}\,(\Omega^\varepsilon\,\omega^0\,\Omega^\varepsilon)_{ij} + \tfrac{1}{2}\,\mathrm{Tr}_{2n}(\omega^0\,\Omega^\varepsilon)\,\Omega^\varepsilon_{ij}\Big) + \mathcal{O}(\varepsilon) \\
&\quad = -\tfrac{\mathrm{i}}{2}\operatorname{tr}_{\mathcal{H}_\mathrm{f}}(\{\{h\,,P_0\}\ ,\{a\,,P_0\}\}) + \tfrac{3\mathrm{i}}{4}\,\Big\langle\omega^0\,(g^\varepsilon\,\omega^0)^2\,\nabla h\,,\ \nabla^T a\Big\rangle \\
&\qquad + \tfrac{\mathrm{i}}{4}\,\Big\langle\omega^0\,(\Omega^\varepsilon\,\omega^0)^2\,\nabla h\,,\ \nabla a\Big\rangle + \tfrac{\mathrm{i}}{4}\,\mathrm{Tr}_{2n}(\omega^0\,\Omega^\varepsilon)\,\Big\langle\omega^0\,\Omega^\varepsilon\,\omega^0\,\nabla h\,,\ \nabla a\Big\rangle \\
&\qquad + \mathcal{O}(\varepsilon)\,.
\end{aligned}
$$

By definition of the effective symbol (3.26) of the operator valued symbol $\{\{h\,,\pi\}\ ,\{a\,,\pi\}\}_1 - \{\{a\,,\pi\}\ ,\{h\,,\pi\}\}_1$ and Theorem 3.6 there exists a constant $C_1 > 0$ and a $\tilde r_1 \in \mathbb{N}_0$ such that

$$
\begin{aligned}
&\Big\|\,\pi \,\#\, \Big(\Big\{\,\{h\,,\pi\}\ ,\{a\,,\pi\}\,\Big\}_1 - \Big\{\,\{a\,,\pi\}\ ,\{h\,,\pi\}\,\Big\}_1\Big) \,\#\, \pi \\
&\quad - \pi \,\#\, \Big( - \tfrac{\mathrm{i}}{2}\operatorname{tr}_{\mathcal{H}_\mathrm{f}}(\{\{h\,,P_0\}\ ,\{a\,,P_0\}\}) + \tfrac{3\mathrm{i}}{4}\,\Big\langle\omega^0\,(g^\varepsilon\,\omega^0)^2\,\nabla h\,,\ \nabla a\Big\rangle \\
&\qquad + \tfrac{\mathrm{i}}{4}\,\Big\langle\omega^0\,(\Omega^\varepsilon\,\omega^0)^2\,\nabla h\,,\ \nabla a\Big\rangle + \tfrac{\mathrm{i}}{4}\,\mathrm{Tr}_{2n}(\omega^0\,\Omega^\varepsilon)\,\Big\langle\omega^0\,\Omega^\varepsilon\,\omega^0\,\nabla h\,,\ \nabla a\Big\rangle\Big) \,\#\, \pi\,\Big\|_{0,r} \\
&\quad \le C_1\,\varepsilon\,\|\{\{h\,,\pi\}\ ,\{a\,,\pi\}\}_1 - \{\{a\,,\pi\}\ ,\{h\,,\pi\}\}_1\|^\varepsilon_{0,\tilde r_1}\,.
\end{aligned}
$$

Which finishes the proof choosing $C = C_1\,\max_{1\le i\le 2n}\|\partial_i h\|^\varepsilon_{0,\tilde r_1+1}\,(\|\pi\|^\varepsilon_{0,\tilde r_1+2})^2$ and $\tilde r = \tilde r_1 + 2$. □

**Lemma B.5** *Let* $H : \mathbb{R}^{2n} \to \mathcal{B}_{\mathrm{sa}}(\mathcal{H}_{\mathrm{f}}) : (q,p) \mapsto \frac{1}{2}\chi(|p - \varepsilon A(q)|^2) + V(q)$ *where* $V : \mathbb{R}^n \to \mathcal{B}_{\mathrm{sa}}(\mathcal{H}_{\mathrm{f}})$ *and* $\chi : \mathbb{R} \to \mathbb{R}$ *are smooth and bounded with all their derivatives. In addition, assume* $e_v : \mathbb{R}^n \to \mathbb{R}$ *to be an eigenband of* $V$ *with associated eigenprojection* $P_0(q)$ *satisfying the gap condition (7.1). Then,* $e_0(q,p) := \frac{1}{2}\chi(|p - \varepsilon A(q)|^2) + e_v(q)$ *is an eigenband of* $H$ *with eigenprojection* $P_0(q)$ *satisfying Assumption 2.11 and the associated classical Hamiltonian is given by*

$$\begin{aligned} h(q,p) = \tfrac{1}{2}\,\chi(|p - \varepsilon A(q)|^2) + e_v(q) \\ + \tfrac{1}{2}\,\varepsilon^2\,\chi'(|p - \varepsilon A(q)|^2)^2\,\langle\, p - \varepsilon A(q)\,,\, W(q)\,(p - \varepsilon A(q))\,\rangle \\ + \mathcal{O}(\varepsilon^3) \end{aligned} \tag{B.25}$$

*where*

$$W_{ij}(q) := \mathrm{tr}_{\mathcal{H}_{\mathrm{f}}}([\,\partial_i P_0 \,|\, (V - e_v)^{-1} \,|\, \partial_j P_0\,]_+)(q)\,.$$

*The symplectic form is*

$$\begin{aligned} \omega^\varepsilon(q,p) = \omega^0 + \varepsilon\,\boldsymbol{\Omega}_0(q) + \varepsilon^2\,\chi'(|p - \varepsilon A(q)|^2)\,\boldsymbol{\Omega}_1(q,p) \\ + \varepsilon^2\,\chi''(|p - \varepsilon A(q)|^2)\,\boldsymbol{\Omega}_{\mathrm{cut}}(q,p) + \mathcal{O}(\varepsilon^3) \end{aligned} \tag{B.26}$$

*where*

$$\boldsymbol{\Omega}_0(q) = \begin{pmatrix} \Omega_0(q) & 0 \\ 0 & 0 \end{pmatrix} \quad \textit{with} \quad \Omega_0(q) = -\mathrm{i}\,\mathrm{tr}_{\mathcal{H}_{\mathrm{f}}}([\,\partial_i P_0\,,\partial_j P_0\,]\,P_0)(q)$$

*and*

$$\boldsymbol{\Omega}_1(q,p) = \begin{pmatrix} \Omega_1(q, p - \varepsilon A(q)) & W(q) \\ -W(q) & 0 \end{pmatrix}$$

*with*

$$\Omega_1^{ij}(q,\kappa) = -(\partial_i W_{jl}(q) - \partial_j W_{il}(q))\,\kappa_l\,.$$

*The matrix* $\boldsymbol{\Omega}_{\mathrm{cut}}(q,p)$ *is defined by*

$$\boldsymbol{\Omega}_{\mathrm{cut}}(q,p) = \begin{pmatrix} 0 & \Omega_{\mathrm{cut}}^T(q,p) \\ -\Omega_{\mathrm{cut}}(q,p) & 0 \end{pmatrix}$$

*where* $\Omega_{\mathrm{cut}}(q,p) = \big(p - \varepsilon A(q)\big) \otimes \big(W(q)\,(p - \varepsilon A(q))\big)$.

*The associated Liouville measure satisfies* $\lambda^\varepsilon = \nu^\varepsilon(q,p)\,\mathrm{d}q_1\wedge\cdots\wedge\mathrm{d}p_n$ *with*

$$\begin{aligned}\nu^\varepsilon(q,p) =& 1+\varepsilon^2\,\chi'(|p-\varepsilon\,A(q)|^2)\,\mathrm{Tr}_n(W)(q)\\ &+\varepsilon^2\,\chi''(|p-\varepsilon\,A(q)|^2)\,\langle p-\varepsilon\,A(q)\,,\,W(q)\,(p-\varepsilon\,A(q))\rangle+\mathcal{O}(\varepsilon^3)\,.\end{aligned} \tag{B.27}$$

PROOF Clearly, $e_0(q,p) := \frac{1}{2}\chi(|p-\varepsilon\,A(q)|^2)+e_v(q)$ is an eigenband of $H(q,p)$ with eigenprojection $P_0(q)$ that satisfies the gap condition. Regarding the classical Hamiltonian. By (3.65)

$$\begin{aligned}h =& e_0+\varepsilon\Big(\mathrm{Tr}_{2n}(\omega^0\,M)\Big)\Big(1-\tfrac{1}{4}\,\varepsilon\,\mathrm{Tr}_{2n}(\omega^0\,\Omega_0)\Big)\\ &+\varepsilon^2\Big[\tfrac{1}{2}\,\langle\,\omega^0\,(\nabla e_0)\,,\,W\,\omega^0\,(\nabla e_0)\,\rangle\\ &-\mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big((\,\mathrm{Tr}_{2n}(\omega^0\,M^{op})\,)\,(V-e_v)^{-1}\,(\,\mathrm{Tr}_{2n}((\omega^0\,M^{op})^*\,)\,)\,P_0\Big)\\ &-\tfrac{\mathrm{i}}{2}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big(\langle\,\omega^0\,\nabla\mathrm{Tr}_{2n}(\omega^0\,M^{op})\,,\,\nabla P_0\,\rangle\,P_0\Big)\\ &+\tfrac{1}{8}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big(\mathrm{Tr}_{2n}(\,\omega^0\,\nabla^2 P_0\,\omega^0\,\nabla^2(V-e_v)\,)\,P_0\Big)\Big]\end{aligned}$$

By the fact that $P_0$ and $V-e_v$ are independent of $p$ we have

$$\mathbf{\Omega}_0^{ij}(q,p) = \begin{pmatrix}-\mathrm{i}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(P_0\,[\partial_i P_0,\partial_j P_0])(q) & 0\\ 0 & 0\end{pmatrix}\,,$$

$$\mathbf{W}_{ij}(q,p) = \begin{pmatrix}\mathrm{tr}_{\mathcal{H}_\mathrm{f}}([\,\partial_i P_0\,|\,(V-e_v)^{-1}\,|\,\partial_j P_0\,]_+)(q) & 0\\ 0 & 0\end{pmatrix}\,,$$

$$\mathbf{M}_{ij} = \begin{pmatrix}\frac{\mathrm{i}}{2}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\partial_i P_0\,(V-e_v)\,\partial_j P_0)(q) & 0\\ 0 & 0\end{pmatrix}$$

and

$$\mathbf{M}_{ij}^{op} = \begin{pmatrix}-\frac{\mathrm{i}}{2}\,\partial_i P_0(q)\,\partial_j(V-e_v)(q) & 0\\ 0 & 0\end{pmatrix}\,,$$

It follows that

$$\begin{aligned}0 &= \mathrm{Tr}_{2n}(\omega^0\,\mathbf{M}) = \mathrm{Tr}_{2n}(\omega^0\,\mathbf{\Omega}_0) = \mathrm{Tr}_{2n}(\omega^0\,\mathbf{M}^{op})\\ &= \mathrm{Tr}_{2n}(\,\omega^0\,\nabla^2 P_0\,\omega^0\,\nabla^2(V-e_v)\,)\,.\end{aligned} \tag{B.28}$$

In addition, we have

$$\nabla e_0(q,p) = \begin{pmatrix}-\varepsilon\,\chi'(|p-\varepsilon\,A(q)|^2)\,\nabla A(q)\,(p-\varepsilon\,A(q))+\nabla e_V(q)\\ \chi'(|p-\varepsilon\,A(q)|^2)\,(p-\varepsilon\,A(q))\end{pmatrix}\,. \tag{B.29}$$

Hence, the classical Hamiltonian $h(q,p)$ simplifies to (B.25). By (3.70) the symplectic form $\omega^\varepsilon$ up to second order is

$$\omega^\varepsilon_{ij} = \omega^0_{ij} + \varepsilon\, \mathbf{\Omega}_0^{ij} + \varepsilon^2\, \widetilde{\mathbf{\Omega}}_1^{ij}$$

where by (3.71)

$$\widetilde{\mathbf{\Omega}}_1^{ij} = \partial_i \widetilde{\mathbf{S}}_j(q,p) - \partial_j \widetilde{\mathbf{S}}_i(q,p) \tag{B.30}$$

with

$$\widetilde{\mathbf{S}}(q,p) = \begin{pmatrix} -\mathrm{i}\, \mathrm{tr}_{\mathcal{H}_\mathrm{f}}([\, P_1(q,p)\,, \nabla P_0(q)\,]\, P_0(q)) \\ 0 \end{pmatrix}$$

and by (3.12)

$$\begin{aligned} P_1(q,p) = &- P_0(q)\,(\, \mathrm{Tr}_{2n}(\omega^0\, \mathbf{M}^{op})\,)(q)(V-e_v)^{-1}(q) \\ &+ \mathrm{i}\, P_0(q)\, \langle\, \omega^0\, \nabla_{(q,p)} P_0(q)\,,\, \nabla e_0(q,p)\,\rangle\, (V-e_v)^{-1}(q) \\ &- (V-e_v)^{-1}(q)\,(\, \mathrm{Tr}_{2n}((\omega^0\, \mathbf{M}^{op})^*)\,)(q)\, P_0(q) \\ &- \mathrm{i}\,(V-e_v)^{-1}(q)\langle\, \nabla e_0(q,p)\,,\, \omega^0\, \nabla_{(q,p)} P_0(q)\,\rangle\, P_0(q)\,. \end{aligned}$$

Substituting (B.28) and (B.29) into the above equation for $P_1$ we obtain

$$\begin{aligned} P_1(q,p) = &- \mathrm{i}\, \chi'(|p-\varepsilon\, A(q)|^2)\, P_0(q)\, \langle\, \nabla P_0(q)\,,\, p-\varepsilon\, A(q)\,\rangle\, (V-e_v)^{-1}(q) \\ &+ \mathrm{i}\, \chi'(|p-\varepsilon\, A(q)|^2)\, (V-e_v)^{-1}(q)\, \langle\, p-\varepsilon\, A(q)\,,\, \nabla P_0(q)\,\rangle\, P_0(q)\,. \end{aligned}$$

Hence,

$$\begin{aligned} \widetilde{\mathbf{S}}_{q_i}(q,p) &= - \mathrm{i}\, \mathrm{tr}_{\mathcal{H}_\mathrm{f}}([\, P_1(q,p)\,, \partial_i P_0(q)\,]\, P_0(q)) \\ &= - \chi'(|p-\varepsilon\, A(q)|^2) \\ &\qquad \Big( \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\partial_j P_0(q)\, (V-e_v)^{-1}(q)\, \partial_i P_0(q)\, P_0(q))\, (p-\varepsilon\, A(q))_j \\ &\qquad + \mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\partial_i P_0(q)\, (V-e_v)^{-1}(q)\, \partial_j P_0(q)\, P_0(q))\, (p-\varepsilon\, A(q))_j \Big) \\ &= - \chi'(|p-\varepsilon\, A(q)|^2)\, W_{ij}(q)\, (p-\varepsilon\, A(q))_j\,. \end{aligned}$$

We conclude that

$$\widetilde{\mathbf{S}}(q,p) = \begin{pmatrix} -\chi'(|p-\varepsilon\, A(q)|^2)\, W(q)\, (p-\varepsilon\, A(q)) \\ 0 \end{pmatrix}\,.$$

Then, a staight forward computation using the above result and (B.30) yields

$$\widetilde{\mathbf{\Omega}}_1^{ij}(q,p) = \chi'(|p-\varepsilon\,A(q)|^2)\begin{pmatrix}\Omega_1(q,p-\varepsilon\,A(q)) & W(q)\\ -W(q) & 0\end{pmatrix}$$
$$+\,\chi''(|p-\varepsilon\,A(q)|^2)\,\mathbf{\Omega}_{\mathrm{cut}}(q,p) + \mathcal{O}(\varepsilon)$$

what finishes the proof for (B.26). By (3.75) the density of the associated Liouville measure is

$$\nu^\varepsilon = 1 - \tfrac{1}{2}\,\varepsilon\,\mathrm{Tr}_{2n}(\omega^0\,\mathbf{\Omega}_0) - \tfrac{1}{2}\,\varepsilon^2\,\mathrm{Tr}_{2n}(\omega^0\,\widetilde{\mathbf{\Omega}}_1)$$
$$+\,\tfrac{1}{8}\,\varepsilon^2\,\mathrm{Tr}_{2n}(\omega^0\,\mathbf{\Omega}_0)^2 - \tfrac{1}{4}\,\varepsilon^2\,\mathrm{Tr}_{2n}(\omega^0\,\mathbf{\Omega}_0\,\omega^0\,\mathbf{\Omega}_0) + \mathcal{O}(\varepsilon^3)\,.$$

We have

$$\mathrm{Tr}_{2n}(\omega^0\,\mathbf{\Omega}_1(q,p)) = \mathrm{Tr}_n(\mathbf{\Omega}_1^{pq}(q,p) - \mathbf{\Omega}_1^{qp}(q,p)) = \mathrm{Tr}_n(-W(q) - W(q))$$

and

$$\mathrm{Tr}_{2n}(\omega^0\,\mathbf{\Omega}_{\mathrm{cut}}(q,p)) = -\mathrm{Tr}_n\Big(\Omega_{\mathrm{cut}}(q,p)\Big) - \mathrm{Tr}_n\Big(\Omega_{\mathrm{cut}}^T(q,p)\Big)$$
$$= -2\,\langle p-\varepsilon\,A(q)\,,\,W(q)\,(p-\varepsilon\,A(q))\rangle\ .$$

Therefore, additionally using (B.28) as well as the fact that

$$\mathrm{Tr}_{2n}(\omega^0\,\mathbf{\Omega}_0\,\omega^0\,\mathbf{\Omega}_0) = 0$$

finishes the proof of (B.27). □

**Lemma B.6** *Let the assumptions of Lemma B.5 hold and $(h,\omega^\varepsilon)$ be the Hamiltonian system with classical Hamiltonian $h$ given by (B.25) and symplectic form $\omega^\varepsilon$ given by (B.26). Then, the inverse of the symplectic form's coefficient matrix has an expansion starting with*

$$(\omega^\varepsilon)^{-1}(q,p) = \begin{pmatrix}0 & -\mathbf{1}_n\\ \mathbf{1}_n & \varepsilon\,\Omega(q,p)\end{pmatrix} + \varepsilon^2\,\chi'(|p-\varepsilon\,A(q)|^2)\begin{pmatrix}0 & W(q)\\ -W(q) & 0\end{pmatrix}$$
$$+\,\varepsilon^2\,\chi''(|p-\varepsilon\,A(q)|^2)\begin{pmatrix}0 & \Omega_{\mathrm{cut}}(q,p)\\ -\Omega_{\mathrm{cut}}^T(q,p) & 0\end{pmatrix} + \mathcal{O}(\varepsilon^3) \tag{B.31}$$

*where $\Omega(q,p) := \Omega_0(q) + \varepsilon\,\chi'(|p-\varepsilon\,A(q)|^2)\,\Omega_1(q,p-\varepsilon\,A(q))$.*

*Moreover, the Hamiltonian equations are*

$$\dot{q} = \chi'(|p - \varepsilon\, A(q)|^2)\ (p - \varepsilon\, A(q)) + \mathcal{O}(\varepsilon^3)$$

*and*

$$\begin{aligned}\dot{p}_i =& - \partial_i e_v(q) + \varepsilon\, \chi'(|p - \varepsilon\, A(q)|^2)\ \langle \partial_i A(q)\, ,\, p - \varepsilon\, A(q)\rangle \\ & - \varepsilon\, \chi'(|p - \varepsilon\, A(q)|^2)\ \Omega^{ij}(q,p)\,(p - \varepsilon\, A(q))_j \\ & - \tfrac{1}{2}\,\varepsilon^2\, \chi'(|p - \varepsilon\, A(q)|^2)^2\ \langle p - \varepsilon\, A(q)\, ,\, \partial_i W(q)\,(p - \varepsilon\, A(q))\rangle \\ & + \varepsilon^2\, \chi'(|p - \varepsilon\, A(q)|^2)\ W_{ij}(q)\,\partial_j e_v(q) \\ & + \varepsilon^2\, \chi''(|p - \varepsilon\, A(q)|^2)\ \langle p - \varepsilon\, A(q)\, ,\, \nabla e_v(q)\rangle\ W(q)\,(p - \varepsilon\, A(q))_i \\ & + \mathcal{O}(\varepsilon^3)\, .\end{aligned}$$

PROOF By the Neumann series for $(\omega^\varepsilon)^{-1}$ (5.4) we have

$$(\omega^\varepsilon)^{-1} = -\omega^0 - \varepsilon\,\omega^0\,\mathbf{\Omega}\,\omega^0 - \varepsilon^2\,\omega^0\,\mathbf{\Omega}\,\omega^0\,\mathbf{\Omega}\,\omega^0 + \mathcal{O}(\varepsilon^3)\, .$$

where

$$\mathbf{\Omega} = \mathbf{\Omega}_0(q) + \varepsilon\,\chi'(|p - \varepsilon\, A(q)|^2)\,\mathbf{\Omega}_1(q,p) + \varepsilon\,\chi''(|p - \varepsilon\, A(q)|^2)\,\mathbf{\Omega}_{\mathrm{cut}}(q,p)\, .$$

A straight forward computation shows

$$\omega^0\,\mathbf{\Omega}_0(q)\,\omega^0 = \begin{pmatrix} 0 & 0 \\ 0 & -\Omega_0(q)\end{pmatrix}\, , \qquad \omega^0\,\mathbf{\Omega}_0(q)\,\omega^0\,\mathbf{\Omega}_0(q)\,\omega^0 = 0\, ,$$

$$\omega^0\,\mathbf{\Omega}_1(q,p)\,\omega^0 = \begin{pmatrix} 0 & -W(q) \\ W(q) & -\Omega_1(q, p - \varepsilon\, A(q))\end{pmatrix}$$

and

$$\omega^0\,\mathbf{\Omega}_{\mathrm{cut}}(q,p)\,\omega^0 = \begin{pmatrix} 0 & -\Omega_{\mathrm{cut}}(q,p) \\ \Omega_{\mathrm{cut}}^T(q,p) & 0\end{pmatrix}\, .$$

Combining the above results shows (B.31). The Hamiltonian equations are given by

$$\begin{pmatrix}\dot{q} \\ \dot{p}\end{pmatrix} = -(\omega^\varepsilon)^{-1}(q,p)\ \begin{pmatrix}\partial_q h(q,p) \\ \partial_p h(q,p)\end{pmatrix}$$

Here, a simple computation shows that

$$\begin{aligned}\partial_{q_i} h(q,p) = &- \varepsilon\, \chi'(|p-\varepsilon\, A(q)|^2)\, \partial_i A(q)\, (p-\varepsilon\, A(q)) + \partial_i e_v(q) \\ &+ \tfrac{1}{2}\, \varepsilon^2\, \chi'(|p-\varepsilon\, A(q)|^2)^2\, \langle\, p-\varepsilon\, A(q)\,,\, \partial_i W(q)\, (p-\varepsilon\, A(q))\,\rangle \\ &+ \mathcal{O}(\varepsilon^3)\end{aligned}$$

as well as

$$\begin{aligned}\partial_{p_i} h(q,p) = &\ \chi'(|p-\varepsilon\, A(q)|^2)\, (p-\varepsilon\, A(q))_i \\ &+ \varepsilon^2\, \chi'(|p-\varepsilon\, A(q)|^2)^2\, W_{ij}(q)\, (p-\varepsilon\, A(q))_j \\ &+ \varepsilon^2\, \chi'(|p-\varepsilon\, A(q)|^2)\, \chi''(|p-\varepsilon\, A(q)|^2)\, (p-\varepsilon\, A(q))_i \\ &\qquad \langle\, p-\varepsilon\, A(q)\,,\, W(q)\, (p-\varepsilon\, A(q))\,\rangle + \mathcal{O}(\varepsilon^3)\,.\end{aligned}$$

Thus, we get

$$\begin{aligned}\dot{q} &= \chi'(|p-\varepsilon\, A(q)|^2)\, (p-\varepsilon\, A(q)) + \varepsilon^2\, \chi'(|p-\varepsilon\, A(q)|^2)^2\, W(q)\, (p-\varepsilon\, A(q)) \\ &\quad + \varepsilon^2\, \chi'(|p-\varepsilon\, A(q)|^2)\, \chi''(|p-\varepsilon\, A(q)|^2) \\ &\qquad (p-\varepsilon\, A(q))\, \langle\, p-\varepsilon\, A(q)\,,\, W(q)\, (p-\varepsilon\, A(q))\,\rangle \\ &\quad - \varepsilon^2\, \chi'(|p-\varepsilon\, A(q)|^2)^2\, W(q)\, (p-\varepsilon\, A(q)) \\ &\quad - \varepsilon^2\, \chi'(|p-\varepsilon\, A(q)|^2)\, \chi''(|p-\varepsilon\, A(q)|^2) \\ &\qquad \Big((p-\varepsilon\, A(q))\, \otimes\, \Big(W(q)\, (p-\varepsilon\, A(q))\Big)\Big)\, (p-\varepsilon\, A(q)) + \mathcal{O}(\varepsilon^3) \\ &= \chi'(|p-\varepsilon\, A(q)|^2)\, (p-\varepsilon\, A(q)) + \mathcal{O}(\varepsilon^3)\end{aligned}$$

where in the last equality we used that

$$\begin{aligned}&\Big((p-\varepsilon\, A(q))\, \otimes\, \Big(W(q)\, (p-\varepsilon\, A(q))\Big)\Big)\, (p-\varepsilon\, A(q)) \\ &\qquad = (p-\varepsilon\, A(q))\, \langle\, p-\varepsilon\, A(q)\,,\, W(q)\, (p-\varepsilon\, A(q))\,\rangle\,.\end{aligned}$$

The momentum $p$ solves the equation

$$\begin{aligned}\dot{p}_i = &- \partial_i e_v(q) + \varepsilon\, \chi'(|p-\varepsilon\, A(q)|^2)\, \langle \partial_i A(q)\,,\, (p-\varepsilon\, A(q))\rangle \\ &- \varepsilon\, \chi'(|p-\varepsilon\, A(q)|^2)\, \Omega_{ij}(q,p)\, (p-\varepsilon\, A(q))_j \\ &+ \varepsilon^2\, \chi'(|p-\varepsilon\, A(q)|^2)\, W_{ij}(q)\, \partial_j e_v(q) \\ &- \tfrac{1}{2}\, \varepsilon^2\, \chi'(|p-\varepsilon\, A(q)|^2)^2\, \langle\, p-\varepsilon\, A(q)\,,\, \partial_i W(q)\, (p-\varepsilon\, A(q))\,\rangle \\ &+ \varepsilon^2\, \chi''(|p-\varepsilon\, A(q)|^2)\, \langle p-\varepsilon\, A(q)\,,\, \nabla e_v(q)\rangle\, W_{ij}(q)\, (p-\varepsilon\, A(q))_j + \mathcal{O}(\varepsilon^3)\end{aligned}$$

where we used the fact that

$$\Omega^T_{\mathrm{cut}}(q,p)\,\nabla e_v(q) = \langle p - \varepsilon\, A(q)\,,\, \nabla e_v(q)\rangle\; W(q)\,(p - \varepsilon\, A(q))\,.$$

□

**Lemma B.7** *Let the Hamiltonian symbol* $H : \mathbb{R}^{2n} \to \mathcal{B}_{\mathrm{sa}}(\mathcal{H}_{\mathrm{f}}); (r,k) \mapsto H_0(k - A(r)) + \phi(r)$ *where* $H_0 : \mathbb{R}^n \to \mathcal{B}_{\mathrm{sa}}(\mathcal{H}_{\mathrm{f}})$ *be smooth and bounded with all its derivatives. In addition, assume the magnetic vector potential* $A : \mathbb{R}^n \to \mathbb{R}^n$ *to be of the form* $A(r) = A_b(r) + \mathbf{b}\, r$ *with* $\mathbf{b} \in \mathbb{R}^{n\times n}$ *and* $A_b : \mathbb{R}^n \to \mathbb{R}^n$ *smooth and bounded with all its derivatives and the electric potential* $\phi : \mathbb{R}^n \to \mathbb{R}$ *given as* $\phi(r) = \phi_b(r) + \mathcal{E}\cdot r$ *with* $\phi_b : \mathbb{R}^n \to \mathbb{R}$ *smooth and bounded with all its derivatives and* $\mathcal{E} \in \mathbb{R}^n$*. Moreover, let* $e_0 : \mathbb{R}^n \to \mathbb{R}$ *be a continuous, non-degenerate eigenvalue of* $H_0$ *satisfying the uniform gap condition (2.82) and* $P_0(k)$ *the eigenprojection of* $H_0(k)$ *to the eigenvalue* $e_0(k)$*. Then,* $H$ *is a Weyl-symbol in* $S^0(\mathcal{B}_{\mathrm{sa}}(\mathcal{H}_{\mathrm{f}}))$ *and* $E(r,k) := \tilde{e}(r,k) + \phi(r) := e_0(k - A(r)) + \phi(r)$ *is a isolated, smooth and non-degenerate eigenvalue of* $H(r,k)$ *with eigenprojection* $\tilde{P}_0(r,k) := P_0(k - A(r))$*. The associated classical Hamiltonian is given by*

$$\tilde{h}(r,k) = h(r, k - A(r)) + \mathcal{O}(\varepsilon^3) \tag{B.32}$$

*where*

$$\begin{aligned} h(r,\kappa) = {}& e_0(\kappa) + \phi(r) + \varepsilon\, \mathrm{Tr}_n(\mathbf{B}(r)\, M(\kappa))\Big(1 - \tfrac{1}{4}\,\varepsilon\, \mathrm{Tr}_n(\mathbf{B}(r)\, \mathbf{\Omega}_0(\kappa))\Big) \\ & + \varepsilon^2 \Big( \tfrac{1}{2}\langle\, \mathcal{F}_{\mathrm{Lor}}(r,\kappa)\,,\, W(\kappa)\, \mathcal{F}_{\mathrm{Lor}}(r,\kappa)\,\rangle \\ & - \mathrm{tr}_{\mathcal{H}_{\mathrm{f}}}\Big(\mathrm{Tr}_n(\mathbf{B}(r)\, M^{op}(\kappa))\,(H_0 - e_0)^{-1}(\kappa)\, \mathrm{Tr}_n((\mathbf{B}(r)\, M^{op}(\kappa))^*)\, P_0(\kappa)\Big) \\ & - \tfrac{\mathrm{i}}{2}\, \mathrm{tr}_{\mathcal{H}_{\mathrm{f}}}\Big(\langle\, \mathbf{B}(r)\, \partial_\kappa \mathrm{Tr}_n(\mathbf{B}(r)\, M^{op}(\kappa))\,,\, \nabla P_0(\kappa)\,\rangle\, P_0(\kappa)\Big) \\ & + \tfrac{\mathrm{i}}{2}\, \mathrm{tr}_{\mathcal{H}_{\mathrm{f}}}\Big(\langle\, \partial_r \mathrm{Tr}_n(\mathbf{B}(r)\, M^{op}(\kappa))\,,\, \nabla P_0(\kappa)\,\rangle\, P_0(\kappa)\Big) \\ & + \tfrac{1}{8}\, \mathrm{tr}_{\mathcal{H}_{\mathrm{f}}}\Big(\mathrm{Tr}_n(\, \mathbf{B}(r)\, \nabla^2 P_0(\kappa)\, \mathbf{B}(r)\, \nabla^2 (H_0 - e_0)(\kappa)\,)\, P_0(\kappa)\Big) \\ & + \tfrac{1}{8}\, \mathrm{tr}_{\mathcal{H}_{\mathrm{f}}}\Big(\mathrm{Tr}_n(\, \nabla^2 P_0(\kappa)\, (\nabla^2 A(r)\, \nabla^2 (H_0 - e_0)(\kappa))\,)\, P_0(\kappa)\Big) \\ & + \tfrac{1}{8}\, \mathrm{tr}_{\mathcal{H}_{\mathrm{f}}}\Big(\mathrm{Tr}_n(\, (\nabla^2 A(r)\, \nabla^2 P_0(\kappa))\, \nabla^2 (H_0 - e_0)(\kappa)\,)\, P_0(\kappa)\Big)\,. \end{aligned} \tag{B.33}$$

*with Berry curvature*

$$\mathbf{\Omega}_0^{ij}(\kappa) := -\mathrm{i}\, \mathrm{tr}_{\mathcal{H}_{\mathrm{f}}}\Big([\, \partial_i P_0\,,\, \partial_j P_0\,]\, P_0\Big)(\kappa)\,, \tag{B.34}$$

*Magnetic field*

$$\mathbf{B}(r) := \nabla A(r) - (\nabla A(r))^T\,, \tag{B.35}$$

*Lorentz force*

$$\mathcal{F}_{\mathrm{Lor}}(r,\kappa) := -\nabla\phi(r) + \mathbf{B}(r)\,\nabla e_0(\kappa)\,, \tag{B.36}$$

*effective magnetic moment*

$$M_{ij}(\kappa) := \tfrac{\mathrm{i}}{2}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big(\partial_i P_0\,(H_0 - e_0)\,\partial_j P_0\Big)(\kappa)$$

*as well as*

$$W_{ij}(\kappa) := \mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big([\,\partial_i P_0 \,|\, (H_0 - e_0)^{-1} \,|\, \partial_j P_0\,]_+\Big)(\kappa) \tag{B.37}$$

*and*

$$M_{ij}^{op}(\kappa) := -\tfrac{\mathrm{i}}{2}\,\partial_i P_0(\kappa)\,\partial_j (H_0 - e_0)(\kappa)\,.$$

*The associated symplectic form $\tilde{\omega}^\varepsilon$ is given by*

$$\begin{aligned}\tilde{\omega}^\varepsilon(r,k) &= \omega^0 + \varepsilon\,\tilde{\Omega}(r,k) = \omega^0 + \varepsilon\,\tilde{\Omega}_0(r,k) + \varepsilon^2\,\tilde{\Omega}_1(r,k) + \mathcal{O}(\varepsilon^3)\\ &= \omega^0 + \varepsilon\,\Omega_0(r,k-A(r)) + \varepsilon^2\,\Omega_1(r,k-A(r)) + \mathcal{O}(\varepsilon^3)\end{aligned} \tag{B.38}$$

*where $\Omega_0$ is*

$$\Omega_0(r,\kappa) = \begin{pmatrix} \nabla A(r)\,\mathbf{\Omega}_0(\kappa)\,(\nabla A(r))^T & -\nabla A(r)\,\mathbf{\Omega}_0(\kappa) \\ -\mathbf{\Omega}_0(\kappa)\,(\nabla A(r))^T & \mathbf{\Omega}_0(\kappa)\,. \end{pmatrix}$$

*For*

$$\Omega_1(r,\kappa) = \begin{pmatrix} \Omega_1^{rr}(r,\kappa) & \Omega_1^{r\kappa}(r,\kappa) \\ \Omega_1^{\kappa r}(r,\kappa) & \Omega_1^{\kappa\kappa}(r,\kappa) \end{pmatrix}$$

*we have*

$$\begin{aligned}\Omega_1^{\kappa\kappa}(r,\kappa) &= \mathbf{\Omega}_1(r,\kappa)\,,\\ \Omega_1^{r\kappa}(r,\kappa) &= -\nabla A(r)\,\mathbf{\Omega}_1(r,\kappa) + \mathbf{L}(r,\kappa)\,,\\ \Omega_1^{\kappa r}(r,\kappa) &= -\mathbf{\Omega}_1(r,\kappa)\,(\nabla A(r))^T - \mathbf{L}^T(r,\kappa)\,,\end{aligned}$$

*and*

$$\begin{aligned}\Omega_1^{rr}(r,\kappa) = &\ \nabla A(r)\,\mathbf{\Omega}_1(r,\kappa)\,(\nabla A(r))^T\\ &- \mathbf{L}(r,\kappa)\,(\nabla A(r))^T + \nabla A(r)\,\mathbf{L}^T(r,\kappa)\end{aligned}$$

*where*

$$\mathbf{\Omega}_1^{ij}(r,\kappa) := \partial_{\kappa_i} S_j^B(r,\kappa) - \partial_{\kappa_j} S_i^B(r,\kappa) + \partial_l\phi(r)\,(\partial_i W_{lj}(\kappa) - \partial_j W_{li}(\kappa)) \tag{B.39}$$

*and*

$$\mathbf{L}(r,\kappa) := (\partial_r S^B)(r,\kappa) + \nabla^2\phi(r)\,W(\kappa)$$

*with*

$$S_j^B(r,\kappa) = \mathfrak{Re}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big(\langle\, \mathbf{B}(r)\, \nabla P_0(\kappa)\,,\, \nabla(H_0+e_0)(\kappa)\,\rangle \\ (H_0-e_0)^{-1}(\kappa)\,\partial_j P_0(\kappa)\, P_0(\kappa)\Big)\,. \tag{B.40}$$

*The corresponding equations of motion are*

$$\begin{pmatrix} \dot r \\ \dot k \end{pmatrix} = \Big(\omega^0 + \varepsilon\,(-\tilde\omega^\varepsilon(r,k)^{-1})_1 + \varepsilon^2\,(-\tilde\omega^\varepsilon(r,k)^{-1})_2\Big) \begin{pmatrix} \partial_r \tilde h(r,k) \\ \partial_k \tilde h(r,k) \end{pmatrix} \tag{B.41}$$

*where*

$$(-\tilde\omega^\varepsilon(r,k)^{-1})_1 = \begin{pmatrix} -\tilde\Omega^{kk}(r,k) & \tilde\Omega^{kr}(r,k) \\ \tilde\Omega^{rk}(r,k) & -\tilde\Omega^{rr}(r,k) \end{pmatrix}$$

*and*

$$(-\tilde\omega^\varepsilon(r,k)^{-1})_2 = \begin{pmatrix} -\tilde{\mathbf{\Omega}}^2_{\mathbf{B}}(r,k) & -\tilde{\mathbf{\Omega}}^2_{\mathbf{B}}(r,k)\,(\nabla A)^T(r) \\ -\nabla A(r)\,\tilde{\mathbf{\Omega}}^2_{\mathbf{B}}(r,k) & -\nabla A(r)\,\tilde{\mathbf{\Omega}}^2_{\mathbf{B}}(r,k)\,(\nabla A)^T(r) \end{pmatrix}$$

*Here, $\tilde{\mathbf{\Omega}}^2_{\mathbf{B}}(r,k)$ is defined as*

$$\tilde{\mathbf{\Omega}}^2_{\mathbf{B}}(r,k) := \mathbf{\Omega}^2_{\mathbf{B}}(r,k-A(r))$$

*where*

$$\mathbf{\Omega}^2_{\mathbf{B}}(r,\kappa) := \mathbf{\Omega}_0(\kappa)\,\mathbf{B}(r)\,\mathbf{\Omega}_0(\kappa)\,.$$

*The Liouville measure associated to $\tilde\Omega$ is given by*

$$\tilde\lambda^\varepsilon = (\nu^\varepsilon(r,k-A(r)) + \mathcal{O}(\varepsilon^3))\,\mathrm{d}r_1\wedge\cdots\wedge\mathrm{d}k_n \tag{B.42}$$

*with density*

$$\nu^\varepsilon(r,\kappa) = 1 - \tfrac{1}{2}\,\varepsilon\,\mathrm{Tr}_n(\mathbf{B}(r)\,\mathbf{\Omega}(r,\kappa)) + \varepsilon^2\,\mathrm{Tr}_n(\mathbf{L}(r,\kappa)) \\ + \tfrac{1}{8}\,\varepsilon^2\,\mathrm{Tr}_n(\mathbf{B}(r)\,\mathbf{\Omega}_0(\kappa))^2 - \tfrac{1}{4}\,\varepsilon^2\,\mathrm{Tr}_n(\mathbf{B}(r)\,\mathbf{\Omega}_0(\kappa)\,\mathbf{B}(r)\,\mathbf{\Omega}_0(\kappa)) \tag{B.43}$$

*where $\mathbf{\Omega}(r,\kappa) := \mathbf{\Omega}_0(\kappa) + \varepsilon\,\mathbf{\Omega}_1(r,\kappa)$.*

PROOF Before we start with the actual proof we show some simple identities. Let $R, Q \in S_0(\mathcal{B}(\mathcal{H}_\mathrm{f}))$ and $\tilde R, \tilde Q$ be given by $\tilde R(r,k) = R(r,k-A(r))$ and $\tilde Q(r,k) = Q(r,k-A(r))$, respectively. Then, an application of the chain rule yields

$$\nabla\tilde R(r,k) = \left(\begin{smallmatrix} 1 & -\nabla A(r) \\ 0 & 1 \end{smallmatrix}\right)\,(\nabla R)(r,k-A(r)) \tag{B.44}$$

and

$$\begin{aligned}&\Big\langle \omega^0\,\nabla\tilde{R}(r,k)\,,\,\nabla\tilde{Q}(r,k)\Big\rangle\\&\quad=\Big\langle\Big(\begin{smallmatrix}\mathbf{1}_n & 0\\ -(\nabla A(r))^T & \mathbf{1}_n\end{smallmatrix}\Big)\,\omega^0\,\Big(\begin{smallmatrix}\mathbf{1}_n & -\nabla A(r)\\ 0 & \mathbf{1}_n\end{smallmatrix}\Big)\,(\nabla R)(r,k-A(r))\,,\,(\nabla Q)(r,k-A(r))\Big\rangle\\&\quad=\Big\langle\Big(\begin{smallmatrix}0 & 1\\ -1 & \mathbf{B}(r)\end{smallmatrix}\Big)\,(\nabla R)(r,k-A(r))\,,\,(\nabla Q)(r,k-A(r))\Big\rangle\end{aligned}$$

In the special case where $R$ and $Q$ are functions mapping from $\mathbb{R}^n$ to $\mathcal{B}(\mathcal{H}_\mathrm{f})$ and $\tilde{R}(r,k)=R(k-A(r))$ as well as $\tilde{Q}(r,k)=Q(k-A(r))$ we get

$$\nabla\tilde{R}(r,k)=\Big(\begin{smallmatrix}-\nabla A(r)\\ \mathbf{1}_n\end{smallmatrix}\Big)\,(\nabla R)(r,k-A(r)) \tag{B.45}$$

and

$$\Big\langle\omega^0\,\nabla\tilde{R}(r,k)\,,\,\nabla\tilde{Q}(r,k)\Big\rangle=\langle\mathbf{B}(r)\,(\nabla R)(k-A(r))\,,\,(\nabla Q)(k-A(r))\rangle\;. \tag{B.46}$$

We start by computing the symplectic form. By definition (3.70)

$$\tilde{\Omega}_0^{ij}(r,k)=-\mathrm{i}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big([\,\partial_i\tilde{P}_0\,,\partial_j\tilde{P}_0\,]\,\tilde{P}_0\Big)(r,k)\,.$$

It follows directly that

$$\tilde{\Omega}_0^{k_ik_j}(r,k)=-\mathrm{i}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big([\,\partial_iP_0\,,\partial_jP_0\,]\,P_0\Big)(k-A(r))=\mathbf{\Omega}_0^{ij}(k-A(r))\,. \tag{B.47}$$

By (B.45) we have $\partial_{r_j}P_0(k-A(r))=-\partial_jA_\mu(r)\,\partial_\mu P_0(k-A(r))$. Thus,

$$\begin{aligned}\tilde{\Omega}_0^{r_ik_j}(r,k)&=-\mathrm{i}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big([\,\partial_{r_i}P_0(k-A(r))\,,\partial_{k_j}P_0(k-A(r))\,]\,P_0(k-A(r))\Big)\\&=-\partial_jA_\mu(r)\,\mathbf{\Omega}_0^{\mu j}(k-A(r))\end{aligned}$$

and therefore

$$\tilde{\Omega}_0^{rk}(r,k)=-\nabla A(r)\,\mathbf{\Omega}_0(k-A(r))\,.$$

Similarly we get

$$\tilde{\Omega}_0^{kr}(r,k)=-\mathbf{\Omega}_0(k-A(r))\,(\nabla A(r))^T$$

and

$$\tilde{\Omega}_0^{rr}(r,k)=\nabla A(r)\,\mathbf{\Omega}_0(k-A(r))\,(\nabla A(r))^T\,. \tag{B.48}$$

Regarding $\tilde{\Omega}_1$, substituting the definition of $S^B$ (B.40) and $W$ (B.37) into $\boldsymbol{\Omega}_1^{ij}$ (B.39) we get

$$\begin{aligned}
\boldsymbol{\Omega}_1^{ij}(r,\kappa) &= \partial_{\kappa_i} S_j^B(r,\kappa) - \partial_{\kappa_j} S_i^B(r,\kappa) + \partial_l \phi(r)\,(\partial_i W_{lj}(\kappa) - \partial_j W_{li}(\kappa)) \\
&= \partial_{\kappa_i} \mathfrak{Re}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\langle\, \mathbf{B}(r)\,\nabla P_0\,,\, \nabla(H_0+e_0)\,\rangle\,(H_0-e_0)^{-1}\,\partial_j P_0\, P_0)(\kappa) \\
&\quad + 2\,\partial_l\phi(r)\,\partial_i \mathfrak{Re}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\partial_l P_0\,(H-e)^{-1}\,\partial_j P_0\, P_0)(\kappa) \\
&\quad - \partial_{\kappa_j} \mathfrak{Re}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\langle\, \mathbf{B}(r)\,\nabla P_0\,,\, \nabla(H_0+e_0)\,\rangle\,(H_0-e_0)^{-1}\,\partial_i P_0\, P_0)(\kappa) \\
&\quad - 2\,\partial_l\phi(r)\,\partial_j \mathfrak{Re}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\partial_l P_0\,(H-e)^{-1}\,\partial_i P_0\, P_0)(\kappa)\,.
\end{aligned} \tag{B.49}$$

On the other hand, by (3.71)

$$\tilde{\Omega}_1^{ij}(r,k) = -2\,\partial_i \mathfrak{Re}(\mathrm{i}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\tilde{P}_1\,\partial_j\tilde{P}_0\,\tilde{P}_0))(r,k) + 2\,\partial_j \mathfrak{Re}(\mathrm{i}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\tilde{P}_1\,\partial_i\tilde{P}_0\,\tilde{P}_0))(r,k)\,. \tag{B.50}$$

Also, by (3.11)

$$\begin{aligned}
\tilde{P}_1(r,k) &= \tfrac{\mathrm{i}}{2}\Big(\tilde{P}_0\,\langle\,\omega^0\,\nabla\tilde{P}_0\,,\,\nabla(H+\tilde{e})\,\rangle\,(H-\tilde{e})^{-1}\Big)(r,k) \\
&\quad + \mathrm{i}\,\Big(\tilde{P}_0\,\langle\,\nabla\phi(r)\,,\,\partial_k\tilde{P}_0\,\rangle\,(H-\tilde{e})^{-1}\Big)(r,k) \\
&\quad - \tfrac{\mathrm{i}}{2}\Big((H-\tilde{e})^{-1}\,\langle\,\nabla(H+\tilde{e})\,,\,\omega^0\,\nabla\tilde{P}_0\,\rangle\,\tilde{P}_0\Big)(r,k) \\
&\quad - \mathrm{i}\,\Big((H-\tilde{e})^{-1}\,\langle\,\partial_k\tilde{P}_0\,,\,\nabla\phi(r)\,\rangle\,\tilde{P}_0\Big)(r,k)\,.
\end{aligned} \tag{B.51}$$

Substituting (B.51) into (B.50) we get

$$\begin{aligned}
\tilde{\Omega}_1^{ij}(r,k) &= \partial_i \mathfrak{Re}\Big(\mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big(\langle\,\omega^0\,\nabla\tilde{P}_0\,,\,\nabla(H+\tilde{e})\,\rangle\,(H-\tilde{e})^{-1}\,\partial_j\tilde{P}_0\,\tilde{P}_0\Big)\Big)(r,k) \\
&\quad + 2\,\partial_i \mathfrak{Re}\Big(\mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big(\langle\,\nabla\phi(r)\,,\,\partial_k\tilde{P}_0\,\rangle\,(H-\tilde{e})^{-1}\,\partial_j\tilde{P}_0\,\tilde{P}_0\Big)\Big)(r,k) \\
&\quad - \partial_j \mathfrak{Re}\Big(\mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big(\langle\,\omega^0\,\nabla\tilde{P}_0\,,\,\nabla(H+\tilde{e})\,\rangle\,(H-\tilde{e})^{-1}\,\partial_i\tilde{P}_0\,\tilde{P}_0\Big)\Big)(r,k) \\
&\quad - 2\,\partial_j \mathfrak{Re}\Big(\mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big(\langle\,\nabla\phi(r)\,,\,\partial_k\tilde{P}_0\,\rangle\,(H-\tilde{e})^{-1}\,\partial_i\tilde{P}_0\,\tilde{P}_0\Big)\Big)(r,k)\,.
\end{aligned} \tag{B.52}$$

Applying (B.46) to (B.52) and comparing with (B.49) we conclude

$$\tilde{\Omega}_1^{k_i k_j}(r,k) = \boldsymbol{\Omega}_1^{ij}(r,k-A(r))\,.$$

Next, we compute $\tilde{\Omega}_1^{rk}(r,k)$. By (B.46)

$$\begin{aligned}
&\partial_{r_i}\mathfrak{Re}\Big(\mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big(\langle\,\omega^0\,\nabla\tilde{P}_0\,,\,\nabla(H+\tilde{e})\,\rangle\,(H-\tilde{e})^{-1}\,\partial_{k_j}\tilde{P}_0\,\tilde{P}_0\Big)\Big)(r,k)\\
&\quad=-\partial_i A_\mu(r)\,\Big[\partial_{\kappa_\mu}\,\mathfrak{Re}\Big(\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big(\langle\,\mathbf{B}(r)\,\nabla P_0\,,\,\nabla(H_0+e_0)\,\rangle\\
&\qquad\qquad(H_0-e_0)^{-1}\,\partial_j P_0\,P_0\Big)\Big)\Big](k-A(r))\\
&\qquad+\Big[\partial_{r_i}\,\mathfrak{Re}\Big(\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big(\langle\,\mathbf{B}(r)\,\nabla P_0\,,\,\nabla(H_0+e_0)\,\rangle\\
&\qquad\qquad(H_0-e_0)^{-1}\,\partial_j P_0\,P_0\Big)\Big)\Big](k-A(r))\\
&\quad=-\partial_i A_\mu(r)\,(\partial_{\kappa_\mu}S_j^B)(r,k-A(r))+(\partial_{r_i}S_j^B)(r,k-A(r))
\end{aligned}\tag{B.53}$$

as well as

$$\begin{aligned}
&\partial_{k_j}\mathfrak{Re}\Big(\mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big(\tilde{P}_0\,\langle\,\omega^0\,\nabla\tilde{P}_0\,,\,\nabla(H+\tilde{e})\,\rangle\,(H-\tilde{e})^{-1}\,\partial_{r_i}\tilde{P}_0\,\tilde{P}_0\Big)\Big)(r,k)\\
&\quad=\Big[\partial_{\kappa_j}\,\mathfrak{Re}\Big(\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big(P_0\,\langle\,\mathbf{B}(r)\,\nabla P_0\,,\,\nabla(H_0+e_0)\,\rangle\\
&\qquad\qquad(H_0-e_0)^{-1}\,(-\partial_i A_\mu(r))\,\partial_\mu P_0\,P_0\Big)\Big)\Big](k-A(r))\\
&\quad=-\partial_i A_\mu(r)\,(\partial_{\kappa_j}S_\mu^B)(r,k-A(r))\,.
\end{aligned}\tag{B.54}$$

Moreover, combining (B.46) and the product rule

$$\begin{aligned}
&2\,\partial_{r_i}\mathfrak{Re}\Big(\mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big(\tilde{P}_0\,\langle\,\nabla\phi(r)\,,\,\partial_k\tilde{P}_0\,\rangle\,(H-\tilde{e})^{-1}\,\partial_{k_j}\tilde{P}_0\,\tilde{P}_0\Big)\Big)(r,k)\\
&\quad=2\,\partial_{il}^2\phi(r)\,\mathfrak{Re}\Big(\mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big(\partial_l P_0\,(H_0-e_0)^{-1}\,\partial_j P_0\,P_0\Big)\Big)(k-A(r))\\
&\qquad-2\,\partial_l\phi(r)\,\partial_i A_\mu(r)\,\partial_{\kappa_\mu}\mathfrak{Re}\Big(\mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big(\partial_l P_0\,(H_0-e_0)^{-1}\,\partial_j P_0\,P_0\Big)\Big)(k-A(r))\\
&\quad=\partial_{il}^2\phi(r)\,W_{lj}(k-A(r))-\partial_l\phi(r)\,\partial_i A_\mu(r)\,\partial_\mu W_{lj}(k-A(r))
\end{aligned}\tag{B.55}$$

and similarly

$$\begin{aligned}
&2\,\partial_{k_j}\mathfrak{Re}\Big(\mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big(\tilde{P}_0\,\langle\,\nabla\phi(r)\,,\,\partial_k\tilde{P}_0\,\rangle\,(H-\tilde{e})^{-1}\,\partial_{r_i}\tilde{P}_0\,\tilde{P}_0\Big)\Big)(r,k)\\
&\quad=-2\,\partial_l\phi(r)\,\partial_i A_\mu(r)\,\partial_j\mathfrak{Re}\Big(\mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big(P_0\,\partial_l P_0\,(H_0-e_0)^{-1}\,\partial_\mu P_0\,P_0\Big)\Big)(k-A(r))\\
&\quad=-\partial_l\phi(r)\,\partial_i A_\mu(r)\,\partial_j W_{l\mu}(k-A(r))
\end{aligned}\tag{B.56}$$

Combining (B.53) - (B.56) with (B.52) we obtain

$$\begin{aligned}
\tilde{\Omega}_1^{r_ik_j}(r,k)=&-\partial_i A_\mu(r)\,(\partial_{\kappa_\mu}S_j^B(r,k-A(r))-\partial_{\kappa_j}S_\mu^B(r,k-A(r))\\
&-\partial_i A_\mu(r)\,\partial_l\phi(r)\,\Big(\partial_\mu W_{lj}(k-A(r))-\partial_j W_{l\mu}(k-A(r))\Big)\\
&+(\partial_{r_i}S_j^B)(r,k-A(r))+\partial_{il}^2\phi_b(r)\,W_{lj}(k-A(r))
\end{aligned}$$

which can be reformulated to

$$\begin{aligned}\tilde{\Omega}_1^{rk}(r,k) = &-\nabla A(r)\,\mathbf{\Omega}_1(r,k-A(r))\\ &+(\partial_r S^B)(r,k-A(r)) + \nabla^2\phi(r)\,W(k-A(r))\,.\end{aligned}$$

Similarly we obtain

$$\begin{aligned}\tilde{\Omega}_1^{kr}(r,k) = &-\mathbf{\Omega}_1(r,k-A(r))\,(\nabla A(r))^T\\ &-(\partial_r S^B)^T(r,k-A(r)) - W(k-A(r))\,\nabla^2\phi(r)\end{aligned}$$

and

$$\begin{aligned}\tilde{\Omega}_1^{rr}(r,k) = {}&\nabla A(r)\,\mathbf{\Omega}_1(r,k-A(r))\,(\nabla A(r))^T\\ &-(\partial_r S^B)(r,k-A(r))\,(\nabla A(r))^T - \nabla^2\phi(r)\,W(k-A(r))\,(\nabla A(r))^T\\ &+\nabla A(r)\,(\partial_r S^B)^T(r,k-A(r)) + \nabla A(r)\,W(k-A(r))\,\nabla^2\phi(r)\,.\end{aligned}$$

By (3.75) the Liouville measure associated to $\tilde{\Omega}$ is given by

$$\lambda^\varepsilon = \tilde{\nu}^\varepsilon(r,k)\,\mathrm{d}r_1\wedge\cdots\wedge\mathrm{d}k_n$$

where

$$\begin{aligned}\tilde{\nu}^\varepsilon(r,k) = 1 &- \varepsilon\,\tfrac{1}{2}\,\mathrm{Tr}_{2n}(\omega^0\,\tilde{\Omega}_0(r,k)) - \varepsilon^2\,\tfrac{1}{2}\,\mathrm{Tr}_{2n}(\omega^0\,\tilde{\Omega}_1(r,k))\\ &+\varepsilon^2\,\tfrac{1}{8}\,\mathrm{Tr}_{2n}(\omega^0\,\tilde{\Omega}_0(r,k))^2 - \varepsilon^2\,\tfrac{1}{4}\,\mathrm{Tr}_{2n}(\omega^0\,\tilde{\Omega}_0(r,k)\,\omega^0\,\tilde{\Omega}_0(r,k))\\ &+\mathcal{O}(\varepsilon^3)\end{aligned}$$

It is easy to see that

$$\mathrm{Tr}_{2n}(\omega^0\,\tilde{\Omega}_0)(r,k) = \mathrm{Tr}_n(\tilde{\Omega}_0^{kr}(r,k) - \tilde{\Omega}_0^{rk}(r,k)) = \mathrm{Tr}_n(\mathbf{B}(r)\,\mathbf{\Omega}_0(k-A(r)))$$

and

$$\begin{aligned}\mathrm{Tr}_{2n}(\omega^0\,\tilde{\Omega}_1(r,k)) &= \mathrm{Tr}_n(\tilde{\Omega}_1^{kr}(r,k) - \tilde{\Omega}_1^{rk}(r,k))\\ &= \mathrm{Tr}_n(\mathbf{B}(r)\,\mathbf{\Omega}_1(r,k-A(r))) - 2\,\mathrm{Tr}_n((\partial_r S^B)(r,k-A(r)))\\ &\quad - 2\,\mathrm{Tr}_n(\nabla^2\phi(r)\,W(k-A(r)))\,.\end{aligned}$$

Moreover,

$$\begin{aligned}\mathrm{Tr}_{2n}(\omega^0\,\tilde{\Omega}_0(r,k)\,\omega^0\,\tilde{\Omega}_0(r,k)) &= \mathrm{Tr}_n(\tilde{\Omega}_0^{kr}(r,k)\,\tilde{\Omega}_0^{kr}(r,k) - \tilde{\Omega}_0^{kk}(r,k)\,\tilde{\Omega}_0^{rr}(r,k)\\ &\qquad - \tilde{\Omega}_0^{rr}(r,k)\,\tilde{\Omega}_0^{kk}(r,k) + \tilde{\Omega}_0^{rk}(r,k)\,\tilde{\Omega}_0^{rk}(r,k))\\ &= \mathrm{Tr}_n(\mathbf{B}(r)\,\mathbf{\Omega}_0(k-A(r))\,\mathbf{B}(r)\,\mathbf{\Omega}_0(k-A(r)))\,.\end{aligned}$$

Then

$$\tilde{\nu}^\varepsilon(r,k) = \nu^\varepsilon(r,k-A(r)) + \mathcal{O}(\varepsilon^3)$$

where

$$\begin{aligned}\nu^\varepsilon(r,\kappa) = 1 &- \tfrac{1}{2}\,\varepsilon\,\mathrm{Tr}_n(\mathbf{B}(r)\,\mathbf{\Omega}_0(\kappa)) - \tfrac{1}{2}\,\varepsilon^2\,\mathrm{Tr}_n(\mathbf{B}(r)\,\mathbf{\Omega}_1(r,\kappa))\\ &+ \varepsilon^2\,\mathrm{Tr}_n(\nabla^2\phi(r)\,W(\kappa)) + \varepsilon^2\,\mathrm{Tr}_n((\partial_r S^B)(r,\kappa))\\ &+ \tfrac{1}{8}\,\varepsilon^2\,\mathrm{Tr}_n(\mathbf{B}(r)\,\mathbf{\Omega}_0(\kappa))^2 - \tfrac{1}{4}\,\varepsilon^2\,\mathrm{Tr}_n(\mathbf{B}(r)\,\mathbf{\Omega}_0(\kappa)\,\mathbf{B}(r)\,\mathbf{\Omega}_0(\kappa))\end{aligned}$$

By Corollary 3.8 the effective Hamiltonian $\tilde{h}(r,k)$ associated to $H(r,k)$ is given by

$$\begin{aligned}\tilde{h}(r,k) = &\,\tilde{e}(r,k) + \varepsilon\,\mathrm{Tr}_{2n}(\omega^0\,\tilde{M})(r,k)\,\Big(1 - \tfrac{1}{4}\,\varepsilon\,\mathrm{Tr}_{2n}(\omega^0\,\tilde{\Omega}_0)(r,k)\Big)\\ &+ \varepsilon^2\,\Big(\tfrac{1}{2}\,\langle\,\omega^0\,\nabla\tilde{e}\,,\,\tilde{W}\,\omega^0\,\nabla\tilde{e}\,\rangle(r,k)\\ &- \mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big((\,\mathrm{Tr}_{2n}(\omega^0\,\tilde{M}^{op}))\,(H_0-\tilde{e})^{-1}\,(\,\mathrm{Tr}_{2n}((\omega^0\,\tilde{M}^{op})^*\,))\,\tilde{P}_0\Big)(r,k)\\ &- \tfrac{\mathrm{i}}{2}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big(\langle\,\omega^0\,\nabla\mathrm{Tr}_{2n}(\omega^0\,\tilde{M}^{op})\,,\,\nabla\tilde{P}_0\,\rangle\,\tilde{P}_0\Big)(r,k)\\ &+ \tfrac{1}{8}\,\Big(\mathrm{Tr}_{2n}(\,\omega^0\,\nabla^2\tilde{P}_0\,\omega^0\,\nabla^2(H-\tilde{e})\,)\,\tilde{P}_0\Big)(r,k) + \mathcal{O}(\varepsilon^3)\end{aligned}$$

where

$$\begin{aligned}\tilde{M}^{op}_{ij}(r,k) &= -\tfrac{\mathrm{i}}{2}\,\partial_i\tilde{P}_0(r,k)\,\partial_j(H-\tilde{e})(r,k)\,,\\ \tilde{M}_{ij}(r,k) &:= \tfrac{\mathrm{i}}{2}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big(\partial_i\tilde{P}_0\,(H-\tilde{e})\,\partial_j\tilde{P}_0\Big)(r,k)\end{aligned}$$

and

$$\tilde{W}_{ij}(r,k) := \mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big([\,\partial_i\tilde{P}_0\,|\,(H-\tilde{e})^{-1}\,|\,\partial_j\tilde{P}_0\,]_+\Big)(r,k)\,.$$

Then a simple computation similar to above results in (B.32). The details of this computation are left to the reader. What is left is to derive the equations of motion (B.41). By a simple computation using (5.4) we have

$$\begin{aligned}\tilde{\omega}^\varepsilon(r,k)^{-1} = &-\omega^0 + \varepsilon\,\begin{pmatrix}\tilde{\Omega}^{kk} & -\tilde{\Omega}^{kr}\\ -\tilde{\Omega}^{rk} & \tilde{\Omega}^{rr}\end{pmatrix}(r,k)\\ &+ \varepsilon^2\,\begin{pmatrix}\tilde{\Omega}_0^{kr}\,\tilde{\Omega}_0^{kk} - \tilde{\Omega}_0^{kk}\,\tilde{\Omega}_0^{rk} & \tilde{\Omega}_0^{kk}\,\tilde{\Omega}_0^{rr} - \tilde{\Omega}_0^{kr}\,\tilde{\Omega}_0^{kr}\\ \tilde{\Omega}_0^{rk}\,\tilde{\Omega}_0^{rk} - \tilde{\Omega}_0^{rr}\,\tilde{\Omega}_0^{kk} & \tilde{\Omega}_0^{rr}\,\tilde{\Omega}_0^{kr} - \tilde{\Omega}_0^{rk}\,\tilde{\Omega}_0^{rr}\end{pmatrix}(r,k) + \mathcal{O}(\varepsilon^3)\,.\end{aligned}$$

Then, (B.41) follows by substituting (B.47) - (B.48) into to above equation and using the definition of $\mathbf{B}(r)$ (B.35), which finishes the proof. □

**Lemma B.8** *Let the assumptions of Lemma B.7 hold. Then, a change of coordinates to kinetic momentum $\kappa = k - A(r)$ in the equations of motion (B.41) associated to $H(r,k)$ with eigenvalue $\tilde{e}(r,k) + \phi(r)$ yields*

$$\begin{pmatrix} \dot{r} \\ \dot{\kappa} \end{pmatrix} = -(\omega^{\varepsilon}_{\mathrm{KM}})^{-1}(r,\kappa) \begin{pmatrix} \partial_r h(r,\kappa) \\ \partial_\kappa h(r,\kappa) \end{pmatrix} \tag{B.57}$$

*with classical Hamiltonian $h(r,\kappa)$ given by (B.33). The symplectic form $\omega^{\varepsilon}_{\mathrm{KM}}(r,\kappa)$ satisfies*

$$\omega^{\varepsilon}_{\mathrm{KM}} = \begin{pmatrix} -\mathbf{B} & \mathbf{1}_n \\ -\mathbf{1}_n & \varepsilon\,\mathbf{\Omega} \end{pmatrix} + \varepsilon^2 \begin{pmatrix} 0 & \mathbf{L} \\ -\mathbf{L}^T & 0 \end{pmatrix} \tag{B.58}$$

*and its inverse has an expansion given by*

$$\begin{aligned}(\omega^{\varepsilon}_{\mathrm{KM}})^{-1} = &\begin{pmatrix} \varepsilon\,\mathbf{\Omega} & -\mathbf{1}_n \\ \mathbf{1}_n & -\mathbf{B} \end{pmatrix} + \varepsilon \begin{pmatrix} \varepsilon\,\mathbf{\Omega}\,\mathbf{B}\,\mathbf{\Omega} & -\mathbf{\Omega}\,\mathbf{B} \\ \mathbf{B}\,\mathbf{\Omega} & -\mathbf{B}\,\mathbf{\Omega}\,\mathbf{B} \end{pmatrix} \\ &+ \varepsilon^2 \begin{pmatrix} 0 & -(\mathbf{\Omega}\,\mathbf{B})^2 \\ (\mathbf{B}\,\mathbf{\Omega})^2 & -(\mathbf{B}\,\mathbf{\Omega})^2\,\mathbf{B} \end{pmatrix} + \varepsilon^2 \begin{pmatrix} 0 & \mathbf{L}^T \\ -\mathbf{L} & \mathbf{B}\,\mathbf{L}^T + \mathbf{L}\,\mathbf{B} \end{pmatrix} + \mathcal{O}(\varepsilon^3)\,. \end{aligned} \tag{B.59}$$

*Here, $\mathbf{B}(r)$ is defined by (B.35) and*

$$\mathbf{L}(r,\kappa) := \nabla^2\phi(r)\,W(\kappa) + (\partial_r S^B)(r,\kappa)$$

*where $W(\kappa)$ and $S^B(r,\kappa)$ are defined by (B.37) and (B.40), respectively. The coefficient matrix of the modified Berry curvatures $\mathbf{\Omega}(r,\kappa)$ is given by*

$$\mathbf{\Omega}(r,\kappa) = \mathbf{\Omega}_0(r,\kappa) + \varepsilon\,\mathbf{\Omega}_1(r,\kappa) \tag{B.60}$$

*with $\mathbf{\Omega}_0(r,\kappa)$ and $\mathbf{\Omega}_1(r,\kappa)$ given by (B.34) and (B.39). The Liouville measure of $\omega^{\varepsilon}_{\mathrm{KM}}(r,\kappa)$ is*

$$\lambda^{\varepsilon} = (\nu^{\varepsilon}(r,\kappa) + \mathcal{O}(\varepsilon^3))\,\mathrm{d}r_1 \wedge \cdots \wedge \mathrm{d}\kappa_n \tag{B.61}$$

*with density $\nu^{\varepsilon}(r,\kappa)$ given by (B.43).*

PROOF By definition $\tilde{h}(r,k) = h(r, k - A(r))$. Then, (B.44) yields

$$\begin{pmatrix} \partial_r \tilde{h}(r,k) \\ \partial_k \tilde{h}(r,k) \end{pmatrix} = \begin{pmatrix} \mathbf{1}_n & -\nabla A(r) \\ 0 & \mathbf{1}_n \end{pmatrix} \begin{pmatrix} (\partial_r h)(r, k - A(r)) \\ (\partial_\kappa h)(r, k - A(r)) \end{pmatrix} .$$

In addition, a simple computation shows

$$\begin{pmatrix} \dot{r} \\ \dot{\kappa} \end{pmatrix} = \begin{pmatrix} \mathbf{1}_n & 0 \\ -(\nabla A(r))^T & \mathbf{1}_n \end{pmatrix} \begin{pmatrix} \dot{r} \\ \dot{k} \end{pmatrix} .$$

Moreover, by (B.38) we have

$$\tilde{\omega}^\varepsilon(r,k) = \omega^\varepsilon(r, k - A(r))$$

where

$$\omega^\varepsilon(r,\kappa) := \omega^0 + \varepsilon\, \Omega_0(r,\kappa) + \varepsilon^2\, \Omega_1(r,\kappa) .$$

Substituting the result above into the equations of motion (B.41) we obtain

$$\begin{pmatrix} \dot{r} \\ \dot{\kappa} \end{pmatrix} = - \begin{pmatrix} \mathbf{1}_n & 0 \\ -(\nabla A(r))^T & \mathbf{1}_n \end{pmatrix} (\omega^\varepsilon(r,\kappa))^{-1} \begin{pmatrix} \mathbf{1}_n & -\nabla A(r) \\ 0 & \mathbf{1}_n \end{pmatrix} \begin{pmatrix} \partial_r h(r,\kappa) \\ \partial_\kappa h(r,\kappa) \end{pmatrix}$$

Since

$$\left( \begin{smallmatrix} \mathbf{1}_n & 0 \\ -(\nabla A(r))^T & \mathbf{1}_n \end{smallmatrix} \right)^{-1} = \left( \begin{smallmatrix} \mathbf{1}_n & 0 \\ (\nabla A(r))^T & \mathbf{1}_n \end{smallmatrix} \right) \quad \text{and} \quad \left( \begin{smallmatrix} \mathbf{1}_n & -\nabla A(r) \\ 0 & \mathbf{1}_n \end{smallmatrix} \right)^{-1} = \left( \begin{smallmatrix} \mathbf{1}_n & \nabla A(r) \\ 0 & \mathbf{1}_n \end{smallmatrix} \right)$$

we get

$$\begin{pmatrix} \dot{r} \\ \dot{\kappa} \end{pmatrix} = -(\omega^\varepsilon_{\mathrm{KM}}(r,\kappa))^{-1} \begin{pmatrix} \partial_r h(r,\kappa) \\ \partial_\kappa h(r,\kappa) \end{pmatrix}$$

where

$$\omega^\varepsilon_{\mathrm{KM}}(r,\kappa) = \left( \begin{smallmatrix} \mathbf{1}_n & \nabla A(r) \\ 0 & \mathbf{1}_n \end{smallmatrix} \right) \omega^\varepsilon(r,\kappa) \left( \begin{smallmatrix} \mathbf{1}_n & 0 \\ (\nabla A(r))^T & \mathbf{1}_n \end{smallmatrix} \right) . \tag{B.62}$$

Then, a simple computation shows that for any $R \in \mathbb{R}^{n\times n}$ we have

$$\left( \begin{smallmatrix} \mathbf{1}_n & \nabla A(r) \\ 0 & \mathbf{1}_n \end{smallmatrix} \right) \left( \begin{smallmatrix} \nabla A(r)\, R\, (\nabla A(r))^T & -\nabla A(r)\, R \\ -R\, (\nabla A(r))^T & R \end{smallmatrix} \right) \left( \begin{smallmatrix} \mathbf{1}_n & 0 \\ (\nabla A(r))^T & \mathbf{1}_n \end{smallmatrix} \right) = \left( \begin{smallmatrix} 0 & 0 \\ 0 & R \end{smallmatrix} \right)$$

as well as

$$\left( \begin{smallmatrix} \mathbf{1}_n & \nabla A(r) \\ 0 & \mathbf{1}_n \end{smallmatrix} \right) \left( \begin{smallmatrix} \nabla A(r)\, R^T - R\, (\nabla A(r))^T & R \\ -R^T & 0 \end{smallmatrix} \right) \left( \begin{smallmatrix} \mathbf{1}_n & 0 \\ (\nabla A(r))^T & \mathbf{1}_n \end{smallmatrix} \right) = \left( \begin{smallmatrix} 0 & R \\ -R^T & 0 \end{smallmatrix} \right) .$$

In addition,

$$\left( \begin{smallmatrix} \mathbf{1}_n & \nabla A(r) \\ 0 & \mathbf{1}_n \end{smallmatrix} \right) \omega^0 \left( \begin{smallmatrix} \mathbf{1}_n & 0 \\ (\nabla A(r))^T & \mathbf{1}_n \end{smallmatrix} \right) = \left( \begin{smallmatrix} -\mathbf{B}(r) & \mathbf{1}_n \\ -\mathbf{1}_n & 0 \end{smallmatrix} \right) .$$

Then, (B.58) follows by replacing $\omega^\varepsilon(r,\kappa)$ in (B.62) by its explicit expression and using the results above. To compute the inverse of $\omega^\varepsilon(r,\kappa)$ we again make use of a Neumann series. We have

$$(\omega^\varepsilon_{\mathrm{KM}}(r,\kappa))^{-1} = \begin{pmatrix} -\mathbf{B}(r) & \mathbf{1}_n \\ -\mathbf{1}_n & 0 \end{pmatrix}^{-1} \sum_{j=1}^{\infty} \left( -\,\varepsilon \begin{pmatrix} 0 & \varepsilon\,\mathbf{L}(r,\kappa) \\ -\varepsilon\,\mathbf{L}^T(r,\kappa) & \mathbf{\Omega}(r,\kappa) \end{pmatrix} \begin{pmatrix} -\mathbf{B}(r) & \mathbf{1}_n \\ -\mathbf{1}_n & 0 \end{pmatrix}^{-1} \right)^j .$$

Then, making use of the fact that

$$\begin{pmatrix} -\mathbf{B}(r) & \mathbf{1}_n \\ -\mathbf{1}_n & 0 \end{pmatrix}^{-1} = \begin{pmatrix} 0 & -\mathbf{1}_n \\ \mathbf{1}_n & -\mathbf{B}(r) \end{pmatrix}$$

a straight forward computation shows (B.59). Clearly, (B.61) directly follows from (B.42) by transformation to kinetic momentum, which finishes the proof. □

**Lemma B.9** *Let the assumptions of Lemma B.7 hold. In addition assume $f \in \mathcal{A}$. Then, the associated Fubini-Study metric is given by*

$$\tilde g(r,k) = \begin{pmatrix} \nabla A(r)\, g_0(k - A(r))\, (\nabla A(r))^T & -\nabla A(r)\, g_0(k - A(r)) \\ -g_0(k - A(r))\, (\nabla A(r))^T & g_0(k - A(r)) \end{pmatrix} + \mathcal{O}(\varepsilon)\,. \tag{B.63}$$

*where*

$$g_0^{ij}(\kappa) := \mathrm{tr}_{\mathcal{H}_\mathrm{f}}([\,\partial_i P_0\,, \partial_j P_0\,]\, P_0)(\kappa)\,.$$

*Moreover, for the classical Hamiltonian $\tilde h$ given by (B.32) and $\tilde Q(\tilde h_0, \tilde P_0)$ defined by*

$$\tilde Q(\tilde h_0, \tilde g_0)(r,k) = \tfrac{1}{2}\, \mathrm{Tr}_{2n}(\omega^0\, \nabla (f'(\tilde h_0(r,k))\, \tilde g_0(r,k)\, \omega^0\, \nabla \tilde h_0(r,k))\,)$$

*we have*

$$\tilde Q(\tilde h_0, \tilde g_0)(r,k) = Q(h_0, g_0)(r, k - A(r)) \tag{B.64}$$

*where*

$$Q(h_0, g_0)(r,\kappa) := \tfrac{1}{2}\, \mathrm{Tr}_n\Big(\partial_\kappa \mathcal{N}_1^Q(r,\kappa) - \partial_r \mathcal{N}_2^Q(r,\kappa) + \nabla A(r)\, \partial_\kappa \mathcal{N}_2^Q(r,\kappa)\Big) \tag{B.65}$$

*with*

$$\mathcal{N}^Q(r,\kappa) := \begin{pmatrix} \mathcal{N}_1^Q \\ \mathcal{N}_2^Q \end{pmatrix}(r,\kappa) := f'(h_0(r,\kappa)) \begin{pmatrix} -\nabla A(r)\, g_0(\kappa)\, \mathcal{F}_{\mathrm{Lor}}(r,\kappa) \\ g_0(\kappa)\, \mathcal{F}_{\mathrm{Lor}}(r,\kappa) \end{pmatrix}. \tag{B.66}$$

*Here, the Lorentz force $\mathcal{F}_{\mathrm{Lor}}$ is given by (B.36). Furthermore, for*

$$\tilde f^\varepsilon(h,\pi)(r,k) = f(\tilde h(r,k)) + \varepsilon^2\, \tilde f^{\mathrm{sc}}(\tilde h)(r,k) + \varepsilon^2\, \tilde f^{\mathrm{adi}}(\tilde h, \tilde \pi)(r,k)$$

*with*

$$\tilde{f}^{\rm sc}(\tilde{h})(r,k) = -\tfrac{1}{24}\,\mathrm{Tr}_{2n}\Big(\omega^0\,\nabla(f''(\tilde{h}_0(r,k))\,\nabla^2\tilde{h}_0(r,k)\,\omega^0\,\nabla\tilde{h}_0(r,k))\Big) + \tfrac{1}{48}\,f''(\tilde{h}_0(r,k))\,\mathrm{Tr}_{2n}(\omega^0\,\nabla^2\tilde{h}_0(r,k)\,\omega^0\,\nabla^2\tilde{h}_0(r,k)) + \mathcal{O}(\varepsilon)$$

*and*

$$\tilde{f}^{\rm adi}(\tilde{h},\tilde{\pi}) = -\tfrac{1}{4}\,f''(\tilde{h}_0(r,k))\,\|\omega^0\,\nabla\tilde{h}_0(r,k)\|^2_{\tilde{g}_0(r,k)} + \mathcal{O}(\varepsilon)\,.$$

*we have*

$$\tilde{f}^{\varepsilon}(\tilde{h},\tilde{\pi})(r,k) = f^{\varepsilon}(h,\pi)(r,k-A(r))$$

*where*

$$f^{\varepsilon}(h,\pi)(r,\kappa) = f(h(r,\kappa)) + \varepsilon^2\,f^{\rm sc}(r,\kappa) - \tfrac{1}{4}\,\varepsilon^2\,f''(h_0(r,\kappa)\,\|\mathcal{F}_{\rm Lor}(r,\kappa)\|^2_{g_0(\kappa)} + \mathcal{O}(\varepsilon^3) \tag{B.67}$$

*with*

$$\begin{aligned} f^{\rm sc}(r,\kappa) = &-\tfrac{1}{24}\,\mathrm{Tr}_n\Big(\partial_\kappa\mathcal{N}_1^{\rm sc}(r,\kappa) - \partial_r\mathcal{N}_2^{\rm sc}(r,\kappa) + \nabla A(r)\,\partial_\kappa\mathcal{N}_2^{\rm sc}(r,\kappa)\Big)\\ &+ \tfrac{1}{48}\,f''(h_0(r,\kappa))\,\mathrm{Tr}_n(\mathbf{B}(r)\,\nabla^2 e_0(\kappa)\,\mathbf{B}(r)\,\nabla^2 e_0(\kappa))\\ &- \tfrac{1}{24}\,f''(h_0(r,\kappa))\,\mathrm{Tr}_n(\nabla^2 e_0(\kappa)\,\nabla^2\phi(r))\\ &+ \tfrac{1}{24}\,f''(h_0(r,\kappa))\,\mathrm{Tr}_n(\nabla^2 e_0(\kappa)\,\nabla^2 A(r)\,\nabla e_0(\kappa)) \end{aligned} \tag{B.68}$$

*Here,*

$$\mathcal{N}_1^{\rm sc}(r,\kappa) := f''(h_0(r,\kappa))\,\Big(-\nabla A(r)\,\nabla^2 e_0(\kappa)\,\mathcal{F}_{\rm Lor}(r,\kappa) - \Big\langle\nabla e_0(\kappa)\,,\,\nabla^2 A(r)\,\nabla e_0(\kappa)\Big\rangle + \nabla^2\phi(r)\,\nabla e_0(\kappa)\Big)$$

*and* (B.69)

$$\mathcal{N}_2^{\rm sc}(r,k) := f''(h_0(r,\kappa))\,\nabla^2 e_0(\kappa)\,\mathcal{F}_{\rm Lor}(r,\kappa)\,.$$

*Note, in (B.68) and (B.69) we denote* $\langle\nabla e_0\,,\,\nabla^2 A\,\nabla e_0\rangle_i = \partial_j e_0\,\partial^2_{ji}A_l\,\partial_l e_0$ *and* $(\nabla^2 e_0\,\nabla^2 A\,\nabla e_0)_{ij} = \partial^2_{i\mu}e_0\,\partial^2_{\mu j}A_l\,\partial_l e_0$*.*

PROOF By (3.72) the expansion of the Fubini-Study metric starts with

$$\tilde{g}^{ij}(r,k) = \tilde{g}_0^{ij}(r,k) + \mathcal{O}(\varepsilon) = \mathrm{tr}_{\mathcal{H}_{\rm f}}([\,\partial_i\tilde{P}_0\,,\partial_j\tilde{P}_0\,]\,\tilde{P}_0)(r,k) + \mathcal{O}(\varepsilon)\,.$$

Therefore, (B.63) is a direct consequence of the chain rule. The expression (B.64) for $\tilde{Q}$ follows by a straight forward computation using the explicit expression (B.63) for the Fubini-Study metric $\tilde{g}$ and the fact that

$$\nabla\tilde{h}_0(r,k) = \begin{pmatrix} \nabla e_0(k - A(r)) \\ \nabla A(r)\,\nabla e_0(k - A(r)) - \nabla\phi(r) \end{pmatrix} \tag{B.70}$$

as well as the definition of the magnetic field

$$\mathbf{B}(r) = \nabla A(r) - (\nabla A)^T(r)\,.$$

Regarding, $\tilde{f}^{\mathrm{sc}}(\tilde{h})(r,k)$ recall that

$$\begin{aligned} \tilde{f}^{\mathrm{sc}}(\tilde{h})(r,k) = &-\tfrac{1}{24}\,\mathrm{Tr}_{2n}\Big(\omega^0\,\nabla\big(f''(\tilde{h}_0)\,\nabla^2\tilde{h}_0\,\omega^0\,\nabla\tilde{h}_0\big)\Big)(r,k) \\ &+\tfrac{1}{48}\,f''(\tilde{h}_0)\,\mathrm{Tr}_{2n}(\omega^0\,\nabla^2\tilde{h}_0\,\omega^0\,\nabla^2\tilde{h}_0)(r,k) + \mathcal{O}(\varepsilon)\,. \end{aligned}$$

Here, we have

$$\nabla^2_{rr}\tilde{h}_0 = \begin{pmatrix} \nabla^2_{rr}\tilde{h}_0 & \nabla^2_{rk}\tilde{h}_0 \\ \nabla^2_{kr}\tilde{h}_0 & \nabla^2_{kk}\tilde{h}_0 \end{pmatrix}$$

with

$$\begin{aligned} \nabla^2_{rr}\tilde{h}_0(r,k) = &\,\nabla A(r)\,\nabla^2 e_0(k - A(r))\,(\nabla A)^T(r) \\ &- \nabla^2 A(r)\,\nabla e_0(k - A(r)) + \nabla^2\phi(r)\,, \end{aligned}$$

$$\nabla^2_{rk}\tilde{h}_0(r,k) = -\nabla A(r)\,\nabla^2 e_0(k - A(r))\,,$$

$$\nabla^2_{kr}\tilde{h}_0(r,k) = -\nabla^2 e_0(k - A(r))\,(\nabla A)^T(r)\,,$$

and

$$\nabla^2_{kk}\tilde{h}_0(r,k) = \nabla^2 e_0(k - A(r))\,.$$

Hence, (B.68) follows by additionally using (B.70) and the definition of the Lorentz force. Finally, recall that $\tilde{f}^{\mathrm{adi}}(\tilde{h}_0,\tilde{P}_0)$ is

$$\tilde{f}^{\mathrm{adi}}(\tilde{h},\tilde{\pi})(r,k) = -\tfrac{1}{4}\,f''(\tilde{h}_0)(r,k)\,\|\omega^0\,\nabla\tilde{h}_0(r,k)\|^2_{\tilde{g}_0(r,k)} + \mathcal{O}(\varepsilon)\,.$$

A straight forward computation similar to above shows

$$\tilde{f}^{\mathrm{adi}}(\tilde{h},\tilde{\pi})(r,k) = -\tfrac{1}{4}\,\varepsilon^2\,f''(h_0(r,k - A(r))\,\|\mathcal{F}_{\mathrm{Lor}}(r,k - A(r))\|^2_{g_0(k-A(r))}$$

which finishes the proof. □

**Lemma B.10** *Let* $\tilde{a}, \tilde{b} \in S_0(\mathbb{C})$ *and* $\tilde{P} \in S_0(\mathcal{B}(\mathcal{H}_{\mathrm{f}}))$ *of the form* $\tilde{P}(r,k) = P(k - A(r))$ *where* $A : \mathbb{R}^n \to \mathbb{R}^n; r \mapsto -\frac{1}{2}\,\mathbf{b}\,r$ *with* $\mathbf{b} \in \mathbb{R}^{n\times n}$ *skew-symmetric. Then for* $a(r,\kappa) := \tilde{a}(r, \kappa + A(r))$ *and* $o(r,\kappa) := \tilde{o}(r,\kappa + A(r))$ *we have*

$$\begin{aligned}
\Big\{\{\tilde{a}\,,\tilde{P}\,\}\,,\{\tilde{o}\,,\tilde{P}\,\}\Big\}\,(r,k) = \\
= \Big( &\Big\langle \mathcal{M}^{\mathbf{b}}\,\nabla(\mathcal{D}^{\mathbf{b}}_i a)\,,\,\nabla(\mathcal{D}^{\mathbf{b}}_j o)\Big\rangle_{2n}\,\partial_{\kappa_i}P\,\partial_{\kappa_j}P \\
&+ \Big\langle (\mathcal{D}^{\mathbf{b}})^2 a\,\nabla P\,,\,\nabla^2 P\,\mathcal{D}^{\mathbf{b}} o\Big\rangle_n \\
&- \Big\langle \nabla^2 P\,\mathcal{D}^{\mathbf{b}} a\,,\,(\mathcal{D}^{\mathbf{b}})^2 o\,\nabla_\kappa P\Big\rangle_n \\
&+ \Big\langle \mathbf{b}\,\nabla^2 P\,\mathcal{D}^{\mathbf{b}} a\,,\,\nabla^2 P\,\mathcal{D}^{\mathbf{b}} o\Big\rangle_n\Big)(r, k - A(r))
\end{aligned}$$

*and*

$$\{\tilde{a}\,,\tilde{o}\}_3\,(r,k) = \tfrac{\mathrm{i}}{24}\,\mathcal{M}^{\mathbf{b}}_{\alpha_1\beta_1}\,\mathcal{M}^{\mathbf{b}}_{\alpha_2\beta_2}\,\mathcal{M}^{\mathbf{b}}_{\alpha_3\beta_3}\,\Big(\partial^{(r,\kappa),3}_{\beta_1\beta_2\beta_3} a\;\partial^{(r,\kappa),3}_{\alpha_1\alpha_2\alpha_3} o\Big)(r, k - A(r))\,.$$

*where*

$$\mathcal{M}^{\mathbf{b}} := \begin{pmatrix} 0 & \mathbf{1}_n \\ -\mathbf{1}_n & \mathbf{b} \end{pmatrix}.$$

*The differential operator* $\mathcal{D}^{\mathbf{b}} : S^0(\mathbb{C}) \to S^0(\mathbb{C}^n)$ *acts on* $c \in S^0(\mathbb{C})$ *by*

$$\mathcal{D}^{\mathbf{b}}\,c(r,\kappa) = \mathbf{b}\,\partial_\kappa c(r,\kappa) - \partial_r c(r,\kappa)\,.$$

*Hereto,* $(\mathcal{D}^{\mathbf{b}})^2 : S^0(\mathbb{C}) \to S^0(\mathbb{C}^{n\times n})$ *satisfies*

$$(\mathcal{D}^{\mathbf{b}})^2_{ij}\,c(r,\kappa) = \mathcal{D}^{\mathbf{b}}_i\,\mathcal{D}^{\mathbf{b}}_j\,c(r,\kappa) = \mathcal{D}^{\mathbf{b}}_j\,\mathcal{D}^{\mathbf{b}}_i\,c(r,\kappa)\,.$$

PROOF We start with the following observation

$$\nabla_{(r,k)}\tilde{a}(r,k) = M^A\,\nabla_{(r,\kappa)} a(r, k - A(r))$$

where

$$M^A := \begin{pmatrix} \mathbf{1}_n & -\nabla A(r) \\ 0 & \mathbf{1}_n \end{pmatrix} = \begin{pmatrix} \mathbf{1}_n & \frac{1}{2}\,\mathbf{b}^T \\ 0 & \mathbf{1}_n \end{pmatrix} = \begin{pmatrix} \mathbf{1}_n & -\frac{1}{2}\,\mathbf{b} \\ 0 & \mathbf{1}_n \end{pmatrix}.$$

In addition, for $\omega^0 = \left(\begin{smallmatrix} 0 & \mathbf{1}_n \\ -\mathbf{1}_n & 0 \end{smallmatrix}\right)$ we have

$$(M^A)^T\,\omega^0\,M^A = \begin{pmatrix} 0 & \mathbf{1}_n \\ -\mathbf{1}_n & \nabla A(r) - (\nabla A(r))^T \end{pmatrix} = \begin{pmatrix} 0 & \mathbf{1}_n \\ -\mathbf{1}_n & \mathbf{b} \end{pmatrix} = \mathcal{M}^{\mathbf{b}}\,.$$

Also, for arbitrary $\tilde{c} \in S_0(\mathbb{C})$ and $c(r, \kappa) = c(r, \kappa + A(r))$ it holds that

$$
\begin{aligned}
\{\tilde{c}\,, \tilde{P}\,\}(r, k) &= \left\langle \omega^0\, M^A\, \nabla_{(r,\kappa)} c\,,\; M^A\, \nabla_{(r,\kappa)} P \right\rangle_{2n} (r, k - A(r)) \\
&= \left\langle \mathcal{M}^{\mathbf{b}}\, \nabla_{(r,\kappa)} c\,,\; \nabla_{(r,\kappa)} P \right\rangle_{2n} (r, k - A(r)) \\
&= \left\langle \mathcal{D}^{\mathbf{b}} c\,,\; \partial_\kappa P \right\rangle_n (r, k - A(r))\,.
\end{aligned}
$$

where we used the fact that $\partial_r P(\kappa) = 0$. Hence,

$$
\left\{\tilde{a}\,, \tilde{P}\right\}(r, k) = \left\langle \mathcal{D}^{\mathbf{b}} a\,,\; \partial_\kappa P \right\rangle_n (r, k - A(r))\,.
$$

and

$$
\left\{\tilde{o}\,, \tilde{P}\right\}(r, k) = \left\langle \mathcal{D}^{\mathbf{b}} o\,,\; \partial_\kappa P \right\rangle_n (r, k - A(r))\,.
$$

Thus,

$$
\begin{aligned}
&\left\{\left\{\tilde{a}\,, \tilde{P}\right\}\,, \left\{\tilde{o}\,, \tilde{P}\right\}\right\}(r, k) \\
&\quad = \omega^0_{ij}\, \partial^{(r,k)}_j \left\langle \mathcal{D}^{\mathbf{b}} a\,,\; \partial_\kappa P \right\rangle_n (r, k - A(r)) \\
&\qquad\quad \partial^{(r,k)}_i \left\langle \mathcal{D}^{\mathbf{b}} o\,,\; \partial_\kappa P \right\rangle_n (r, k - A(r)) \\
&\quad = \mathcal{M}^{\mathbf{b}}_{\nu\mu} \Big( \left\langle \partial^{(r,\kappa)}_\mu \mathcal{D}^{\mathbf{b}} a\,,\; \partial_\kappa P \right\rangle_n \left\langle \partial^{(r,\kappa)}_\nu \mathcal{D}^{\mathbf{b}} o\,,\; \partial_\kappa P \right\rangle_n \\
&\qquad\quad + \left\langle \partial^{(r,\kappa)}_\mu \mathcal{D}^{\mathbf{b}} a\,,\; \partial_\kappa P \right\rangle_n \left\langle \mathcal{D}^{\mathbf{b}} o\,,\; \partial^{(r,\kappa)}_\nu \partial_\kappa P \right\rangle_n \\
&\qquad\quad + \left\langle \mathcal{D}^{\mathbf{b}} a\,,\; \partial^{(r,\kappa)}_\mu \partial_\kappa P \right\rangle_n \left\langle \partial^{(r,\kappa)}_\nu \mathcal{D}^{\mathbf{b}} o\,,\; \partial_\kappa P \right\rangle_n \\
&\qquad\quad + \left\langle \mathcal{D}^{\mathbf{b}} a\,,\; \partial^{(r,\kappa)}_\mu \partial_\kappa P \right\rangle_n \left\langle \mathcal{D}^{\mathbf{b}} o\,,\; \partial^{(r,\kappa)}_\nu \partial_\kappa P \right\rangle_n \Big) \\
&\qquad \circ (r, k - A(r))
\end{aligned}
$$

which we reformulate to

$$
\begin{aligned}
&\left\{\left\{\tilde{a}\,, \tilde{P}\right\}\,, \left\{\tilde{o}\,, \tilde{P}\right\}\right\}(r, k) \\
&\quad = \Big( \left\langle \mathcal{M}^{\mathbf{b}}\, \nabla_{(r,\kappa)} \mathcal{D}^{\mathbf{b}}_i a\,,\; \nabla_{(r,\kappa)} \mathcal{D}^{\mathbf{b}}_j o \right\rangle_{2n} \partial_{\kappa_i} P\, \partial_{\kappa_j} P \\
&\qquad + \left\langle \mathcal{D}^{\mathbf{b}} \mathcal{D}^{\mathbf{b}} a\, \nabla_\kappa P\,,\; \nabla^2_\kappa P\, \mathcal{D}^{\mathbf{b}} o \right\rangle_n \\
&\qquad - \left\langle \nabla^2_\kappa P\, \mathcal{D}^{\mathbf{b}} a\,,\; \mathcal{D}^{\mathbf{b}} \mathcal{D}^{\mathbf{b}} o\, \nabla_\kappa P \right\rangle_n \\
&\qquad + \left\langle \mathbf{b}\, \nabla^2_\kappa P\, \mathcal{D}^{\mathbf{b}} a\,,\; \nabla^2_\kappa P\, \mathcal{D}^{\mathbf{b}} o \right\rangle_n \Big)(r, k - A(r))\,.
\end{aligned}
$$

Regarding $\{\tilde{a}\,,\tilde{o}\}_3\,(r,k)$, by (2.5)

$$\begin{aligned}
&\{\tilde{a}\,,\tilde{o}\}_3\,(r,k)\\
&\quad = \tfrac{\mathrm{i}}{24}\,\omega^0_{\alpha_1\beta_1}\,\omega^0_{\alpha_2\beta_2}\,\omega^0_{\alpha_3\beta_3}\,\nabla^{(r,k),3}_{\beta_1\beta_2\beta_3}\tilde{a}(r,k)\,\nabla^{(r,k),3}_{\alpha_1\alpha_2\alpha_3}\tilde{b}(r,k)\\
&\quad = \tfrac{\mathrm{i}}{24}\,\mathcal{M}^{\mathbf{b}}_{\alpha_1\beta_1}\,\mathcal{M}^{\mathbf{b}}_{\alpha_2\beta_2}\,\mathcal{M}^{\mathbf{b}}_{\alpha_3\beta_3}\left(\nabla^{(r,\kappa),3}_{\beta_1\beta_2\beta_3}a\,\nabla^{(r,\kappa),3}_{\alpha_1\alpha_2\alpha_3}o\right)\circ(r,k-A(r))
\end{aligned}$$

where we used that $\mathcal{M}^{\mathbf{b}}$ is independent of $r$ and $k$. □

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