Semiclassical Wave Packets on Riemannian Manifolds

Dissertation

zur Erlangung des akademischen Grades
eines Doktors der Naturwissenschaften
(Dr. rer. nat.)

eingereicht an der
Mathematisch-Naturwissenschaftlichen Fakultät
der Eberhard Karls Universität Tübingen

vorgelegt von
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Tübingen
2015

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

Tag der mündlichen Qualifikation: 18.11.2016

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Prof. Dr. Wolfgang Rosenstiel

Danksagung

Ich bedanke mich an dieser Stelle ganz herzlich bei allen, die mich beim Schreiben dieser Arbeit begleitet und unterstützt haben.

Zuerst möchte ich mich bei Stefan Teufel bedanken, der mir die Möglichkeit gegeben hat, dieses interessante Thema zu bearbeiten. Seine fachlich hervorragende Betreuung half mir stets auch die kritischen Phasen einer Promotion gut zu meistern.

Darüber hinaus bedanke ich mich bei Christian Lubich, der sich dazu bereit erklärt hat, das Zweitgutachten zu übernehmen.

Daneben möchte ich mich bei allen anderen Mitgliedern der Arbeitsgruppe Mathematische Physik für die sehr angenehme Arbeitsatmosphäre bedanken. Hervorzuheben sind hier meine Zimmerkollegen Jonas Lampart, dessen tiefes mathematisches Verständnis mir sehr geholfen hat, und Johannes von Keler, mit dem ich durch das ein oder andere Tief gegangen bin. Außerdem danke ich Stefan Keppeler für die immer interessanten Gespräche.

Zu guter Letzt gilt mein besonderer Dank meiner Frau Julia und meinen Söhnen Emil, Timo und Linus für ihre Unterstützung, Ausdauer und Ablenkung.

Contents

Zusammenfassung

Ein Hauptinteresse der Quantenmechanik ist die Analyse der Schrödinger Gleichung

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\Psi + V\Psi\,, \qquad \Psi|_{t_0} \in L^2(\mathcal{M}, \mathrm{d}\mu)$$

wobei $\hbar$ die Planck Konstante, m die Masse und Δ der Laplace Operator sind. Diese Gleichung beschreibt die Dynamik einer komplexwertigen Wellenfunktion. Man möchte einerseits die Struktur der Gleichung untersuchen, andererseits analytische und numerische Lösungen finden.

Auch wenn die mathematische Struktur der Schrödinger Gleichung oft recht einfach erscheint, so macht der hochdimensionale Konfigurationsraum $\mathcal{M}$ und die stark oszillierende Wellenfunktion das Lösen sogar für moderne Superrechner nahezu unmöglich. Daher ist es notwendig die analytische Struktur des Systems zu untersuchen, um Möglichkeiten einer Dimensionsreduktion und vorteilhafte numerische Eigenschaften zu finden. Dies führt dann zu effektiven Gleichungen und Näherungslösungen für die ursprüngliche Schrödinger Gleichung. Im Euklidischen Fall, $\mathcal{M} = \mathbb{R}^n$, existiert dazu sowohl in der Analysis als auch in der Numerik eine Fülle an Literatur.

Zwei grundlegende Methoden der Mathematischen Physik zur Dimensionsreduktion komplexer Quantensysteme sind die Adiabatische Störungstheorie und die Semiklassik, bei denen man unterschiedliche Skalen identifiziert und das System entsprechend separiert. Dies reduziert die physikalisch relevanten Freiheitsgrade und vereinfacht die Komplexität eines solchen Systems. Eines der bekanntesten Beispiele ist die Born-Oppenheimer Näherung. Für den Euklidischen Fall siehe [Teu03].

Aus numerischer Sicht gibt Lubichs Blaues Buch [Lub08] eine exzellente Übersicht über die Numerische Analysis.

In dieser Arbeit kombinieren wir analytische und numerische Interessen und verwenden Techniken aus der Differentialgeometrie, der Funktionalanalysis, der Mathematischen Physik und der Numerischen Analysis. Zunächst sind wir daran interessiert, eine passende approximative, explizite Lösung für die Schrödinger Gleichung, zu finden und herzuleiten, jedoch in einer semiklassischen Skalierung, wobei $\mathcal{M}$ eine Riemannsche Mannigfaltigkeit mit Metrik g ist:

$$\mathrm{i}\varepsilon \frac{\partial \Psi}{\partial t} = -\frac{\varepsilon^2}{2m} \Delta_{LB} \Psi + V\Psi , \qquad \Psi|_{t_0} \in L^2(\mathcal{M}, g)$$

mit einem kleinen, positiven Parameter ε, dem Laplace-Beltrami Operator Δ_{LB} und einer reellwertigen Funktion V, genannt Potential, multipliziert mit ε.

Diese Struktur erscheint in vielen, unterschiedlichen physikalischen Situationen, wie zum Beispiel in der Moleküldynamik, in chemischen Reaktionen, in der Festkörperphysik oder der Quantenoptik, insbesondere bei Quantenwellenleitern.

Wachsmuth und Teufel [[Wac10], [WT10]] und Lampart and Teufel [LT14] lieferten entscheidende Beiträge zur Analyse solcher Quantensystem mit Zwangsbedingungen auf Mannigfaltigkeiten und lieferten Beweise für effektive Gleichungen und Lösungen. In [HLT14] sind weitere Resultate für verallgemeinerte Wellenleiter zu finden.

Des Weiteren soll diese explizite Lösung numerisch attraktiv sein. Das bedeutet, dass es möglich sein soll, sie in numerischen Algorithmen als Basisfunktionen zu verwenden und dass sie als Anfangsbedingung für Modelle solch erwähnter physikalischer Systeme genommen werden kann.

Um dies zu erreichen beschränken wir uns auf Riemannsche Mannigfaltigkeiten von beschränkter Geometrie und führen Normalkoordinaten ein, auch bekannt als geodätische oder Riemann Koordinaten. Als Anfangsbedingung wählen wir einen bestimmten Typ von Gaussschem Wellenpaket, ein sogenanntes Hagedornsches Wellenpaket, und verwenden Hagedorns Vorgehen von [Hag80], ausführlich erweitert in [Hag98]. Da wir auch an einer numerischen Verwendung interessiert sind, nutzen wir die Notation und Schritte von [FGL09], jedoch angepasst an den Riemmanschen Fall.

In der Literatur finden sich unterschiedliche Ansätze Hagedornsche Wellenpakete aus geometrische Sicht zu analysieren sowie numerisch anwendbare Lösungen der Schrödinger Gleichung auf Riemannschen Mannigfaltigkeiten in Form von Wellenpaketen herzuleiten. Dell'Antonio und Tenuta [DT04] leiten mittels der Methoden von Hagedorn einen effektiven Hamilton Operator her und konstruieren Näherungslösungen, aber ohne Normalkoordinaten zu verwenden. Ohsawa und Leok [OL13] geben eine symplektische und stärker geometrische Sicht auf Gausssche Wellenpakete mit einigen alternativen Sichtweisen auf die Resultate, die in [Lub08] zusammengestellt sind.

Der Aufbau der Arbeit ist wie folgt. Kapitel 2 führt kurz in die Grundlagen semiklassischer Wellenpakete in Hagedorns Notation auf $\mathbb{R}^n$ sowie Riemannscher Geometrie und Normalkoordinaten ein.

Die Hauptresultate werden in Kapitel 3 dargelegt. Nach einem kurzem Umriss der Idee, führen wir modifizierte Hagedorn Wellenpakete ψ auf Riemannschen Mannigfaltigkeiten $\mathcal{M}$ mit Metrik g ein.

Zuletzt erwähnen wir im Ausblick 4 nach unserem Fazit Ansätze für Leiteroperatoren und die Verwendung in numerischen Algorithmen.

Jetzt möchten wir eine kurze Zusammenfassung der Hauptresultate geben, ohne dabei auf mathematische Vollständigkeit zu bestehen. Letzteres wird ausführlich im erwähnten Kapitel getan.

Seit $q(t)$ eine glatte Kurve in $\mathcal{M}$ für $t \in [0, T]$ und sei $p(t)$ ein Vektorfeld. Seien P, Q komplexe $1, 1$-Tensorfelder über $T\mathcal{M}$ entlang $q(t)$, die eine bestimmte Symmetriebedingung punktweise erfüllen. Ein komplexes Gauss Wellenpaket in Hagedorns Parametrisierung auf $\mathcal{M}$ entlang $q(t)$

mit Parametern $[q(t), p(t), Q(t), P(t)]$ ist definiert als

$$\begin{aligned}
&\psi[q(t), p(t), Q(t), P(t)](x) \\
&\quad := \chi^r_{q(t)}(x)\,(\pi\,\varepsilon)^{-n/4}\,(\operatorname{tr} Q(t))^{-1/2}\ \times \\
&\qquad \exp\Bigg(\frac{\mathrm{i}}{2\,\varepsilon}\,g\left(\exp^{-1}_{q(t)}(x), P(t)\,Q(t)^{-1}\exp^{-1}_{q(t)}(x)\right) + \\
&\qquad\qquad \frac{\mathrm{i}}{\varepsilon}\,g\left(p(t), \exp^{-1}_{q(t)}(x)\right)\Bigg).
\end{aligned}$$

mit entsprechender Abschneidefunktion $\chi^r_{q(t)}(x)$.

Dies ergibt ein semiklassisches komplexes Gauss Wellenpaket in Normalkoordinaten y auf $\mathbb{R}^n$, welches durch die Abbildung $\Phi_{q(t)}$ mit $\mathcal{M}$ identifiziert wird:

$$\begin{aligned}
&\varphi[p(t), Q(t), P(t)](y, t) := \psi[q(t), p(t), Q(t), P(t)]\left(\Phi_{q(t)}(y)\right) \\
&\quad = \tilde{\chi}^r_{q(t)}(y)\,(\pi\,\varepsilon)^{-n/4}\,(\det Q)^{-1/2} \times \\
&\qquad \exp\left(\frac{\mathrm{i}}{2\,\varepsilon}\,y^a\,\left(P\,Q^{-1}\right)_{ab}\,y^b + \frac{\mathrm{i}}{\varepsilon}\,p_c\,y^c\right).
\end{aligned}$$

mit der Abschneidefunktion $\tilde{\chi}^r_{q(t)}(y) = \chi^r_{q(t)}\left(\exp_{q(t)}(y)\right)$ entsprechend den Normalkoordinaten und $p_c = g_{cd}p^d$.

Das vollständige Gauss Wellenpaket ist dann

$$\begin{aligned}
&\phi[p(t), Q(t), P(t)](y, t) \\
&\quad = \exp\left(\frac{\mathrm{i}}{\varepsilon}\,S(t)\right)\,\varphi[p(t), Q(t), P(t)](y, t),
\end{aligned}$$

mit dem klassischen Wirkungsintegral $S(t) = \int_0^t \frac{(\delta_{ab}p^a p^b)(s)}{2m}\mathrm{d}s$ entlang $q(t)$.

Um die Schrödingergleichung in Normalkoordinaten formulieren zu können, berechnen wir dann die Zeitableitung der Abbildung $\Phi^{-1}_{q(t)}$ auf eben diese Koordinaten. Dies erlaubt uns unser Haupttheorem über diese Wellenpakete als approximative Lösungen der freien Schrödinger Gleichung auf $\mathcal{M}$ zu beweisen. Abgekürzt besagt es das Folgende.

Sind die Parameter $[q(t), p(t), Q(t), P(t)]$ Lösungen der angepassten klassischen Bewegungsgleichungen

$$
\begin{aligned}
\dot{q} &= \nabla_t\, q = \frac{p}{m} = g(p, \cdot) \\
\dot{p} &= \nabla_t\, p = \nabla_t \dot{q} = 0 \\
\dot{Q} &= \nabla_t\, Q = \frac{P}{m} \\
\dot{P} &= \nabla_t\, P = -\left(R(p, \cdot)\cdot, p\right) Q
\end{aligned}
$$

wobei die letzte Gleichung ausgedrückt in Normalkoordinaten besagt,

$$\dot{P}^c_e = -R_a{}^c{}_{bd}\, p^a p^b\, Q^d_e\,,$$

dann ist $\phi_t(y)$ eine approximative Lösung der Ordnung $\mathcal{O}\left(\varepsilon^{3/2}\right)$ von

$$\mathrm{i}\,\varepsilon \frac{\partial}{\partial t}\phi_t(y) + \frac{\varepsilon^2}{2m}\,\Delta^{nc}_{LB}\,\phi_t(y) = \mathcal{O}\left(\varepsilon^{3/2}\right)\ .$$

mit dem Laplace-Beltrami Operator $\Delta^{\mathrm{nc}}_{\mathrm{LB}}$ in Normalkoordinaten. Ausgedrückt in Pullbacks

$$\Phi^*_{q(t)}\,\mathrm{i}\varepsilon \frac{\mathrm{d}}{\mathrm{d}t}\left({\Phi^{-1}_{q(t)}}^*\phi_t\right) - \Phi^*_{q(t)}\, H\, {\Phi^{-1}_{q(t)}}^*\phi_t = \mathcal{O}\left(\varepsilon^{3/2}\right)$$

bedeutet es, dass die Näherungslösung auch eine approximative Lösung der zeitabhängigen Schrödingergleichung auf $\mathcal{M}$ (3.3) ist.

Nachdem der Hauptunterschied zum Resultat in flachen Raum, hauptsächlich Krümmungseffekte, erläutert wurde, machen wir eine erste Fehleranalyse. Als Resultat ergibt sich, dass das modifzierte Hagedorn Wellenpaket die volle Lösung der Schrödingergleichung auf einer Riemannschen Mannigfaltigkeit mit beschränkter Geometrie bis auf $C\,\varepsilon^{1/2}$ für jedes t in einem geschlossen Intervall approximiert, wobei C unabhängig von ε ist.

1 Introduction

In quantum mechanics one primary interest lies in the analysis of the Schrödinger equation,

$$i\hbar\frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\,\Delta\,\Psi + V\Psi\,, \qquad \Psi|_{t_0} \in L^2(\mathcal{M}, \mathrm{d}\mu) \tag{1.1}$$

where $\hbar$ is Planck's constant, m is the mass and Δ is the Laplacian. This equation describes the dynamics of a complex-valued wave function. One main part is analyzing the structure of this equation, another one is finding solutions to it, analytically and numerically.

The mathematical structure of the Schrödinger equation (1.1) may be quite simple, but often the high dimensional configuration space $\mathcal{M}$ and the highly oscillating wave function makes even a numerical solution nearly impossible, yet with modern high performance computers. Therefore it is necessary to search for analytical structural properties of the system to reduce the dimension and to find numerical appealing characteristics. This leads to effective equations to and approximate solutions of the original Schrödinger equation. In the Euclidian case, $\mathcal{M} = \mathbb{R}^n$, there exists plenty of literature for both analysis and numerics.

Two main approaches of mathematical physics for reducing the dimension of complex quantum systems are adiabatic perturbation theory and semiclassical analysis, where one identifies different scalings and separate the systems according to these scales. This reduces the physically relevant degrees of freedom and simplifies the complexity of such a system. One of the most prominent examples is the Born-Oppenheimer approximation. For the Euclidian case see [Teu03].

From a numerics point of view Lubich's Blue Book [Lub08] gives an excellent overview of the numerical analysis of such quantum dynamical systems.

In this thesis we combine analytical and numerical interests and use techniques from differential geometry, functional analysis, mathematical physics and numerical analysis. First we are interested in finding and deriving a suitable approximative explicit solution to (1.1), but in a semiclassical scaling and where $\mathcal{M}$ is a Riemannian manifold with metric g:

$$\mathrm{i}\varepsilon \frac{\partial \Psi}{\partial t} = -\frac{\varepsilon^2}{2m} \Delta_{LB} \Psi + V\Psi , \qquad \Psi|_{t_0} \in L^2(\mathcal{M}, g)$$

where ε is a small positive parameter, Δ_{LB} is the Laplace-Beltrami operator and V is, multiplied by ε, a real valued function, called potential.

This structure appears in several different physical situations, such as molecular dynamics, chemical reactions, solid-state physics or quantum optics, especially quantum wave guides.

Wachsmuth and Teufel [[Wac10], [WT10]] and Lampart and Teufel [LT14] made a huge contribution in analysing such constraint quantum system for manifolds and proved effective equations and solutions for them. In [HLT14] further results on generalized quantum wave guides can be found.

Second this explicit solution has to be numerically attractive. This means, that it should be possible to use it in numerical algorithms as basis functions and that it could be taken as initial data for modelling such above mentioned physical systems.

To accomplish that, we restrict to Riemannian manifolds of bounded geometry and introduce normal coordinates, also known as geodesic or Riemann coordinates. As initial data we use a special type of Gaussian wave packet, called Hagedorn wave packet, and stick to Hagedorn's procedure introduced in [Hag80] and elaborated in [Hag98]. As we are also interested in a numerical application, we follow closely the notation and steps of the review in [FGL09], but adopted to the Riemannian case.

Different approaches to analysing Hagedorn wave packets from a geometric perspective and deriving a numerically applicable solution to the Schrödinger equation on Riemannian manifolds in form of wave packets have been done. Dell'Antonio and Tenuta [DT04] derive an effective Hamiltonian and construct approximate solutions also using Hagedorn's technique, but without normal coordinates. Ohsawa and Leok [OL13] provide a symplectic and more geometric view of Gaussian wave packets with some alternative views of the results compiled in [Lub08].

The structure of this work is as follows. Chapter 2 introduces shortly the basics about semiclassical wave packets in Hagedorn's notation in $\mathbb{R}^n$ and the background of Riemannian geometry and normal coordinates.

The main results are presented in chapter 3. After a sketch of the idea, we introduce modified Hagedorn wave packets ψ on a Riemannian manifold $\mathcal{M}$ with metric g.

At last, after the conclusion, we mention some ideas about ladder operators and numerical algorithms in our outlook, chapter 4.

Now we summarize briefly our main results without mathematical completeness. This will be done in the chapter mentioned.

Let $q(t)$ be a smooth curve in $\mathcal{M}$ for $t \in [0, T]$ and let $p(t)$ be a vector field. Let P, Q be complex 1,1-tensorfields above $T\mathcal{M}$ along $q(t)$, satisfying a symmetry condition pointwise. Then a complex Gaussian wave packet in Hagedorn's parametrization on $\mathcal{M}$ along $q(t)$ with parameters $[q(t), p(t), Q(t), P(t)]$ is defined as

$$\begin{aligned}
&\psi[q(t), p(t), Q(t), P(t)](x) \\
&\quad := \chi^r_{q(t)}(x)\,(\pi\,\varepsilon)^{-n/4}\,(\operatorname{tr} Q(t))^{-1/2} \times \\
&\qquad \exp\Bigg(\frac{\mathrm{i}}{2\,\varepsilon}\, g\left(\exp^{-1}_{q(t)}(x), P(t)\,Q(t)^{-1}\exp^{-1}_{q(t)}(x)\right) + \\
&\qquad\qquad \frac{\mathrm{i}}{\varepsilon}\, g\left(p(t), \exp^{-1}_{q(t)}(x)\right)\Bigg).
\end{aligned}$$

with an appropriate smooth cutoff $\chi^r_{q(t)}(x)$.

This yields a semiclassical complex Gaussian wave packet in Riemannian normal coordinates y on $\mathbb{R}^n$ identified by a mapping $\Phi_{q(t)}$ with $\mathcal{M}$:

$$\begin{aligned}
&\varphi[p(t),Q(t),P(t)](y,t) := \psi[q(t),p(t),Q(t),P(t)]\left(\Phi_{q(t)}(y)\right) \\
&\quad = \tilde{\chi}^r_{q(t)}(y)\,(\pi\,\varepsilon)^{-n/4}\,(\det Q)^{-1/2} \times \\
&\qquad \exp\left(\frac{\mathrm{i}}{2\,\varepsilon}\,y^a\,\left(P\,Q^{-1}\right)_{ab}\,y^b + \frac{\mathrm{i}}{\varepsilon}\,p_c\,y^c\right).
\end{aligned}$$

with $\tilde{\chi}^r_{q(t)}(y) = \chi^r_{q(t)}\left(\exp_{q(t)}(y)\right)$ the cutoff according to normal coordinates and $p_c = g_{cd}\,p^d$.

The full semiclassical Gaussian wave packet then is

$$\begin{aligned}
&\phi[p(t),Q(t),P(t)](y,t) \\
&\quad = \exp\left(\frac{\mathrm{i}}{\varepsilon}\,S(t)\right)\,\varphi[p(t),Q(t),P(t)](y,t),
\end{aligned}$$

with the classical action integral $S(t) = \int_0^t \frac{(\delta_{ab}p^a p^b)(s)}{2m}\mathrm{d}s$ along $q(t)$.

We then calculate the time-derivative of the mapping $\Phi^{-1}_{q(t)}$ to normal coordinates to be able to formulate the Schrödinger equation in such coordinates. This allows to prove our main theorem about those wave packets in geodesic coordinates as an approximate solution of the free Schrödinger equation on $\mathcal{M}$. Shortly this is the following.

If the parameters $[q(t),p(t),Q(t),P(t)]$ are solutions to the adapted classical equations of motion

$$\begin{aligned}
\dot{q} &= \nabla_t\,q = \frac{p}{m} = g(p,\cdot) \\
\dot{p} &= \nabla_t\,p = \nabla_t \dot{q} = 0 \\
\dot{Q} &= \nabla_t\,Q = \frac{P}{m}
\end{aligned}$$

$$\dot{P} = \nabla_t P = -\left(R(p,\cdot)\cdot, p\right) Q$$

where the last equation reads in normal coordinates

$$\dot{P}_e^c = -R_{a\ \,bd}^{\ c}\, p^a p^b Q_e^d\,,$$

then $\phi_t(y)$ is an approximate solution of order $\mathcal{O}\left(\varepsilon^{3/2}\right)$ to

$$\mathrm{i}\,\varepsilon \frac{\partial}{\partial t}\phi_t(y) + \frac{\varepsilon^2}{2m}\,\Delta_{LB}^{nc}\,\phi_t(y) = \mathcal{O}\left(\varepsilon^{3/2}\right)\ .$$

with $\Delta_{\mathrm{LB}}^{\mathrm{nc}}$ the Laplace-Beltrami operator in normal coordinates. In terms of pull backs this equation reads

$$\Phi_{q(t)}^{*}\,\mathrm{i}\varepsilon\frac{\mathrm{d}}{\mathrm{d}t}\left({\Phi_{q(t)}^{-1}}^{*}\phi_t\right) - \Phi_{q(t)}^{*}\,H\,{\Phi_{q(t)}^{-1}}^{*}\phi_t = \mathcal{O}\left(\varepsilon^{3/2}\right)$$

meaning that this approximate solution is also an approximate solution to the time-dependent Schrödinger equation on $\mathcal{M}$ (3.3).

After identifying the main difference to the results in flat space, mainly curvature effects, we give a first error analysis. As a result the modified Hagedorn wave packet approximates the full solution of the Schrödinger equation on a Riemannian manifold of bounded geometry up to $C\,\varepsilon^{1/2}$ for any t in a closed interval with C independent of ε.

2 Technical Preliminaries

2.1 Semiclassical Wave Packets: A Summary

In this section we want to give a short summary of semiclassical wave packets, one part of the main background of this thesis. A more detailed description, overview and proof of results of such wave packets can be found in [Lub08]. Semiclassical wave packets are useful approximate solutions to describe the dynamics of a quantum-mechanical system. Here the wave function as a solution to the Schrödinger equation is replaced by a function that depends only on a finite number of complex parameters. By the time-dependent variational principle one gets evolution equations for these parameters. A standard example are Gaussian wave packets parametrized using position, momentum and complex width. Their equations of motion in the classical limit are just the classical equations of motion by Newton.

Let us consider a Schrödinger equation in the so called semiclassical scaling. That means let $0 < \varepsilon \ll 1$ be the semiclassical parameter and

$$\mathrm{i}\varepsilon \frac{\partial \Psi}{\partial t} = -\frac{\varepsilon^2}{2m} \Delta \Psi + V \Psi , \qquad \Psi|_{t_0} \in L^2(\mathbb{R}^n) \tag{2.1}$$

with potential V as a multiplication operator. This situation can be found for example in the Born-Oppenheimer approximation for the motion of nuclei, where ε^2 stands for the ratio of nuclei and electron masses. This approximation is mostly used in many chemical and physical calculations.

It is well known that typical solutions to (2.1) highly oscillate with wavelength $\sim \varepsilon$. This makes a numerical approach difficult.

In 1976, Heller, [Hel76], proposed that using a Gaussian wave packet in (2.1)

$$\begin{aligned}\Psi(x,t) &\approx u(x,t)\\ &= \exp\left(\frac{\mathrm{i}}{\varepsilon}\left(\frac{1}{2}\left(x-q(t)\right)^T C(t)\left(x-q(t)\right)\right.\right.\\ &\qquad\left.\left.+\,p(t)\cdot\left(x-q(t)\right)+\zeta(t)\right)\right)\end{aligned}$$

with position average $q(t)\in\mathbb{R}^n$ and momentum average $p(t)\in\mathbb{R}^n$ of the wave packet, the time dependent variational approximation of (2.1) can be achieved. The complex symmetric matrix $C(t)\in\mathbb{C}^{n\times n}$ describes the width of the packet and has a positive definite imaginary part. At last, the wave packet is normalized by the phase parameter $\zeta(t)\in\mathbb{C}$.

Later in 1980 [Hag80], Hagedorn introduced his notation for such Gaussian wave packets and elaborated it in many papers, especially in [Hag98]. He factorizes the complex width matrix $C(t)$ into two complex matrices $A(t)$ and $\mathrm{i}B(t)$ satisfying special symplectic properties. This leads to important insights about the properties of the parameters of a Gaussian wave packet.

Here we want to briefly review these results using again a slightly different notation for the matrices $A=Q$ and $\mathrm{i}B=P$, introduced in [FGL09] and [Lub08]. This notation resembles the symmetry between the position and momentum parameters and their width matrices.

First we state without proof the matrix factorization lemma, taken from [Lub08] and compare [Hag98].

Lemma 1. *Let $P,Q\in\mathbb{C}^{n\times n}$ satisfy*

$$\begin{aligned}Q^TP-P^TQ&=0\\ Q^*P-P^*Q&=2\mathrm{i}\mathbf{1}\,,\end{aligned}\tag{2.2}$$

then Q and P are invertible and

$$C=PQ^{-1}$$

is complex symmetric, that is $C^T = C$, with positive definite imaginary part

$$\operatorname{Im} C = (QQ^*)^{-1} .$$

Conversely, every complex symmetric matrix C with positive definite imaginary part can be written as $C = PQ^{-1}$ with matrices Q and P satisfying (2.2).

The semiclassical wave packet in Hagedorn's notation is a complex Gaussian of unit L^2-norm parametrized as

$$\begin{aligned} &\varphi[q,p,Q,P](x) \\ &\quad = (\pi\varepsilon)^{-n/4} (\det Q)^{-1/2} \times \\ &\qquad \exp\left(\frac{\mathrm{i}}{2\varepsilon} (x-q)^T PQ^{-1} (x-q) + \frac{\mathrm{i}}{\varepsilon} p^T (x-q) \right) \end{aligned}$$

where $p, q \in \mathbb{R}^n$ are the momentum and position average of the wave packet respectively. $P, Q \in \mathbb{C}^{n\times n}$ are two parameters satisfying (2.2).

The most appealing fact about semiclassical Gaussian wave packets is that they are exact solutions to the time-dependent Schrödinger equation in case of a quadratic potential, if the parameters are propagated by the standard classical equations of motion associated with (2.1):

$$\begin{aligned} \dot{q} &= \frac{p}{m} \\ \dot{p} &= -\nabla V(q) \\ \dot{Q} &= \frac{P}{m} \\ \dot{P} &= -\nabla^2 V(q) Q \end{aligned} \tag{2.3}$$

where $\nabla^2 V(q)$ is the Hessian matrix.

Considering the classical action integral

$$S(t) = \int_0^t \frac{|p|^2(s)}{2m} - V\left(q(s)\right) \mathrm{d}s \tag{2.4}$$

the following basic result for semiclassical Gaussian wave packets in Hagedorn's parametrization is valid (taken from [Lub08], see [Hag80]).

Theorem 2 (Gaussian Wave Packets in a Quadratic Potential, Hagedorn 1980)**.** *Let V be a quadratic potential and let $\big(q(t), p(t), Q(t), P(t)\big)$ be a solution to the classical equations* (2.3) *for time $0 < t < T$ and let $S(t)$ be the corresponding action* (2.4)*. Assuming that $Q(0)$ and $P(0)$ satisfy* (2.2) *it follows that $Q(t)$ and $P(t)$ satisfy* (2.2) *for all times t and*

$$\psi(x,t) = \exp\left(\frac{\mathrm{i}S(t)}{\varepsilon}\right) \varphi[q(t), p(t), Q(t), P(t)](x)$$

is a solution to the semiclassical, time-dependent Schrödinger equation (2.1)*.*

According to this result, it is possible to get a time-propagated solution to (2.1), without solving this Schrödinger equation, but by solving the set of ordinary differential equations (2.3) for the Gaussian parameters. Furthermore this shows that the wave packet moves along classical trajectories.

2.2 Riemannian Geometry

Before we will discuss the general idea for semiclassical wave packets in Hagedorn's notation on Riemannian manifolds, we recall some basics about Riemannian geometry, manifolds of bounded geometry and geodesics. This is the natural setting for the framework of this work. All theorems will be given without a proof and for further information see most standard textbooks about these topics. Here we refer to [FK03, Lan99, Ber03].

2.2.1 Riemannian Manifolds

Definition 1. Let $\mathcal{M}$ be a manifold of dimension n with a $(0,2)$-tensor field g, that means, for any $x \in \mathcal{M}$ there exists a bilinear form g_x on the tangent space $\mathrm{T}_x\,\mathcal{M}$. Furthermore $x \mapsto g_x(X_x, Y_x)$ is $C^\infty(\mathcal{M})$ for any pair of vector fields $X, Y \in V\mathcal{M}$ on $\mathcal{M}$.

Then we call the pair $(\mathcal{M}, g)$ a *Riemannian manifold* with Riemannian metric g if for any point $x \in \mathcal{M}$ the bilinear form $g_x = \langle\cdot,\cdot\rangle_x$ is a scalar product on $T_x\mathcal{M}$, that means, it is positive definit and symmetric.

We denote coordinate systems on $\mathcal{M}$ with $x = (x^1, \dots, x^n)$ and we use the Einstein summation convention, which implies a summation over double repeated indices as superscript and subscript in a single term.

The coefficients of the metric g can be calculated using the basis vector fields $\partial_i = \frac{\partial}{\partial x^a}$ belonging to a chart (U, x) :

$$g_{ab} := \left\langle \partial_a, \partial_b \right\rangle \quad \text{for any } x.$$

Using the local expression on U for vector fields $X = \zeta^a \partial_a$ and $Y = \eta^b \partial_b$ it directly follows

$$\langle X, Y\rangle = \left\langle \zeta^a \partial_a, \eta^b \partial_b \right\rangle = \zeta^a \eta^b \left\langle \partial_a, \partial_b \right\rangle = g_{ab} \zeta^a \eta^b$$

After these basics we introduce the covariant derivative on $\mathcal{M}$, which is the Levi-Cevita connection ∇.

Definition 2. Let $\mathcal{M}$ be a Riemannian manifold with metric g. Let X, Y, Z be smooth vector fields on $\mathcal{M}$ and f be a smooth function on $\mathcal{M}$. Then the *covariant derivative* on $\mathcal{M}$ is the Levi-Cevita connection

$$\nabla \colon V\mathcal{M} \times V\mathcal{M} \to V\mathcal{M}, \quad X, Y \mapsto \nabla_X Y$$

with the following properties

$$\begin{aligned}
&\nabla_{fX} Y = f \nabla_X Y \\
&\nabla_X \left(f Y\right) = \mathrm{d}f(X)\, Y + f \left(\nabla_X Y\right) \\
&\nabla_Z \langle X, Y\rangle = \left\langle \nabla_Z X, Y \right\rangle + \left\langle X, \nabla_Z Y \right\rangle \\
&\nabla_X Y - \nabla_Y X = [X, Y]
\end{aligned}$$

where $[X, Y] f := X\left(Y f\right) - Y\left(X f\right)$ is the Lie-bracket for vector fields.

In local coordinates $x = (x^1, \dots, x^n)$ with basis vector fields $\partial_1, \cdots, \partial_n$ the covariant derivative is

$$\nabla_{\partial_a} \partial_b = \Gamma^c_{ab} \partial_c$$

with Γ^c_{ab} the Christoffel symbols of the second kind.

Additionally the Levi-Cevita connection as an affine connection defines a derivative along curves.

Definition 3. Let $c(\alpha)$ be a smooth curve and X be a vector field on $(\mathcal{M}, g)$. Then the derivate of X along $c(\alpha)$ is defined as

$$\nabla_\alpha X = \nabla_{\dot{c}(\alpha)} X.$$

This directly gives a notion of a parallel vector field.

Definition 4. A vector field X is called *parallel* along a curve $c(\alpha)$, if

$$\nabla_{\dot{c}(\alpha)} X = 0.$$

For parallel vector fields the following theorem of existence and uniqueness holds.

Theorem 3. *Let $c(\alpha)$ be a smooth curve on $\mathcal{M}$ with $\alpha \in I \subset \mathbb{R}$ and v be a vector in $T_{c(0)}\mathcal{M}$. Then there exists one and only one vector field X parallel to c with $X(c(0)) = v$.*

Now we can define the parallel transport which gives the possibility to transport geometric object along curves.

Definition 5 (Parallel transport)**.** Let $c(\alpha)$ be a smooth curve on $\mathcal{M}$ with $\alpha \in I \subset \mathbb{R}$ and v be a vector in $T_{c(0)}\mathcal{M}$. The *parallel transport* $P_c(\alpha)$: $T_{c(0)}\mathcal{M} \mapsto T_{c(\alpha)}\mathcal{M}$ transports v parallel along c and is defined as

$$P_{c(\alpha)} v := X(c(\alpha)), \tag{2.5}$$

X being the vector field parallel to c with $X(c(0)) = v$.

Before we turn to the notion of curvature, we do need a generalization of the second order differential operator appearing in the Schrödinger equation on Riemannian manifolds, which is the

Definition 6 (Laplace-Beltrami operator)**.** Let ∂_a, $a = 1, \cdots, n$ be a set of coordinate vector fields for a chart U of $\mathcal{M}$. We denote with g^{ab} the metric tensor in this coordinate frame. Then the Laplace-Beltrami operator on a Riemannian manifold $\mathcal{M}$ with metric g for a smooth scalar function f is defined as

$$\Delta_{\mathrm{LB}} f := \operatorname{div} \operatorname{grad} f = \frac{1}{\sqrt{g}} \partial_a \sqrt{g}\, g^{ab}\, \partial_b f$$

with $\sqrt{g} = \sqrt{|g|}$ and $|g| = \det(g^{ab})$.

2.2.2 Riemannian Curvature

Now we define the Riemann curvature tensor, which expresses the curvature of a Riemannian manifold. Different definitions of the Riemann tensor yield opposite signs in a metric expansion and different arranging of indices in index notation. There are at least three different definitions, the one used here (see [FK03]) and often found in the physics literature. Then one can change the order of slots within the tensor, changing the order of indices in a natural way, yielding a $+$ sign in the metric expansion, (see [Lan99]). Third, changing the sign in the Riemann tensor definition and getting a normal order in the index notation, (see [Mil63]).

Here we use the following definition of the Riemann tensor:

Definition 7. Let $(\mathcal{M}, g)$ be a Riemannian manifold with metric g and Levi-Civita connection or covariant derivative ∇. Let X, Y, Z be vector fields with Lie-bracket $[\cdot, \cdot]$. Then we can define the following terms:

- The *curvature* is defined as

$$R(X, Y)Z := \nabla_X \nabla_Y Z - \nabla_Y \nabla_X Z - \nabla_{[X,Y]} Z.$$

- The coefficients of the curvature are given by

  $$R(\partial_b, \partial_d)\partial_c = R^a{}_{cbd}\partial_a$$

  with basis vector fields ∂_e corresponding to a map (U, x).

- In terms of Christoffel symbols the coefficients can be written as

  $$R^a{}_{cbd} = \partial_b \Gamma^a{}_{dc} - \partial_d \Gamma^a{}_{bc} + \Gamma^e{}_{dc}\Gamma^a{}_{be} - \Gamma^e{}_{bc}\Gamma^a{}_{de}.$$

The following properties and identities of the curvature and its coefficients will be used often throughout this work, especially in subsection 3.4.1 and 3.4.2, where the normal coordinate expansion of g and Δ_{LB} are derived. Therefore we only give them in coordinate form.

- We often use the abbreviation:

  $$R_{acbd} = g_{ae}R^e{}_{cbd}.$$

- Antisymmetry in both the first two and last two arguments

  $$\begin{aligned} R^a{}_{cbd} &= -R^a{}_{cdb} \\ R_{acbd} &= -R_{cabd}. \end{aligned}$$

- Symmetry of both blocks

  $$R_{acbd} = R_{bdac}.$$

- Dependent on index position, contraction over two indices yields

  $$\begin{aligned} \mathrm{Ric}_{cd} &= R^a{}_{cad} && \text{Ricci curvature tensor} \\ 0 &= R^a{}_{acb} && \text{trace of antisymmetric tensor.} \end{aligned}$$

- Bianchi identity for Riemann tensor

  $$R^a{}_{cbd} + R^a{}_{bdc} + R^a{}_{dcb} = 0$$

  and this means that

  $$R_{acba} = -R_{abac} + \underbrace{R_{aacb}}_{=0} = -R_{abac} = \mathrm{Ric}_{bc}\,.$$

2.2.3 Geodesics and Exponential Mapping

In this subsection we introduce a notion of straight lines for Riemannian manifolds and state some direct consequences. We denote the derivative with respect to a parameter $\alpha \in \mathbb{R}$ with $\dot{}$.

Definition 8 (Geodesics)**.** A smooth curve $\gamma\colon I \mapsto \mathcal{M}$ is called a *geodesic* if its tangent vector field is parallel, that means

$$\nabla_{\dot{\gamma}}\dot{\gamma} = 0.$$

Then the following basic theorem about the existence of geodesics is fundamental for the introduction of normal coordinates.

Theorem 4. *Let $\mathcal{M}$ be a Riemannian manifold and $T_x\mathcal{M}$ be the tangent space at point $x \in \mathcal{M}$. For any point $x \in \mathcal{M}$ and any vector $v \in T_x\mathcal{M}$ there exists a unique maximal defined geodesic $\gamma = \gamma_{x,v}\colon I \mapsto \mathcal{M}$ on an open interval $I \in \mathbb{R}$ with*

$$\gamma(0) = x\,, \quad \dot{\gamma}(0) = v\,.$$

Now for every fixed t on a curve $q(t)$, $q(t)$ is also a point on $\mathcal{M}$ and according to theorem 4 there exists a neighbourhood $U_{q(t)}$, such that for any point $x \in U_{q(t)}$ there is a unique geodesic of minimal length $\gamma_{q(t),x}$ in $U_{q(t)}$ joining $q(t)$ and x. If we set $\gamma_{q(t),x}(1) = x$, then $\left|\frac{\partial}{\partial s}\gamma_{q(t),x}(s)|_{s=0}\right|$ is the length of the geodesic. The following definition gives us the possibility to map those geodesics onto straight lines on $T_{q(t)}\mathcal{M}$.

Theorem 5 (Exponential Mapping)**.** *Again let $\mathcal{M}$ be a Riemannian manifold and $T_x\mathcal{M}$ be the tangent space at point $x \in \mathcal{M}$. For a sufficient small neighbourhood of the origin $V \subset T_x\mathcal{M}$ the mapping*

$$\exp_x : V \mapsto \mathcal{M}\,, \quad v \mapsto \gamma_{x,v}(1)$$

is a diffeomorphism between V and the neighbourhood $U := \exp_x(V)$ of x.

Using this theorem the following line is true,

$$\exp_{q(t)}: V \subset T_{q(t)}\mathcal{M} \to U_{q(t)}, \exp_{q(t)} y_{q(t)}(x) = \gamma_{q(t),y}(1) = x$$

by identifying x and $y_{q(t)}(x) := \dot{\gamma}_{q(t),x}(0)$.

2.2.4 Riemann Normal Coordinates

We now introduce normal coordinates on $\mathcal{M}$. In this work we will make extensive use of these natural coordinates, as they give us the possibility to calculate on $\mathbb{R}^n$ like in the flat case, but with extra terms dependent on the curvature of $\mathcal{M}$. Furthermore they will allow us to define wave packets analogue to those of Hagedorn.

First we need to restrict the exponential mapping $\exp_{q(t)}$ to a ball of size r smaller than the injectivity radius ρ_t.

Definition 9 (Injectivity Radius)**.** Let $\mathcal{M}$ be a Riemannian manifold and $\exp_x$ be the exponential mapping at point $x \in \mathcal{M}$. Then the injectivity radius is defined as

$$\rho_x := \sup \varepsilon$$

such that $\exp_x : B_0^\varepsilon \to B_x^\varepsilon$ is a diffeomorphism, where B_x^r is a ball around x with radius r.

Thus by definition $\exp_{q(t)}$ is a diffeomorphism along $\gamma_{q(t)}$ and the inverse mapping

$$\exp_{q(t)}^{-1} : B_{q(t)}^\rho \subset \mathcal{M} \to B_0 \subset T_{q(t)}\mathcal{M}$$

exists. This restriction is done by a smooth cutoff function.

Definition 10 (Normal cutoff)**.** Choose $0 < r < \rho_{q(t)}$ for any $0 < t < T$ with $\rho_{q(t)}$ the injectivity radius of the exponential mapping at $q(t)$, definition 9. Then we can define the smooth cutoff function $\chi^r_{q(t)} \in C^\infty(\mathcal{M})$ with $\chi^r_{q(t)}(x) \in [0,1]$ as

$$\chi^r_{q(t)}(x) := \begin{cases} 0 & \text{for } \operatorname{dist}\left(x, q(t)\right) > \rho_{q(t)} \\ 1 & \text{for } \operatorname{dist}\left(x, q(t)\right) < r < \rho_{q(t)} . \end{cases}$$

In addition to the restricted exponential mapping and its inverse mentioned above, choosing an orthonormal basis $e = (e_a)_{a\leq n}$ of $T_{q(t)}\mathcal{M}$ leads to normal coordinates $y = (y^a_{q(t)})_{a\leq n}$ on $U_{q(t)}$ via

Definition 11 (Riemann normal coordinates)**.**

$$y^a_{q(t)}(x) := g\left(\exp^{-1}_{q(t)}(x), e_a\right) = g\left(\dot{\gamma}_{q(t),x}(0), e_a\right).$$

Choosing an orthonormal basis allows us to identify $T_{q(t)}\mathcal{M}$ with $\mathbb{R}^n$ and map $\mathcal{M}$ to $\mathbb{R}^n$ by a simple coordinate change.

Because in these coordinates $y_{q(t)}\left(q(t)\right) = 0$ and $\frac{\partial}{\partial y^a_{q(t)}}\Big|_{q(t)} = e_a$ the coefficients of the metric tensor at point $q(t)$ are

$$g_{ab}\left(q(t)\right) = g(e_a, e_b) = \delta_{ab},$$

which simplifies raising and lowering indices at $q(t)$.

Furthermore we are able to define a notion of distance for expanding relevant terms in order of normal coordinates.

Definition 12 (Distance)**.** Let $y = \exp^{-1}_{q(t)}(x)$ be a point on $T_{q(t)}\mathcal{M}$. By introducing Riemann normal coordinates geodesics are straight lines through 0 on $\mathbb{R}$ identified with $T_{q(t)}\mathcal{M}$ and the geodesic distance is in leading order equal to the euclidian distance. Thus we can define

$$|y| := \operatorname{dist}(y, 0) = \sqrt{g_{ab}y^a y^b} = \sqrt{\delta_{ab}y^a y^b}$$

Of course by the definition 11 the coordinate functions $y^a_{q(t)}$ depend on the choice of the orthonormal basis e at point $q(t)$. But a comparison of normal coordinate systems at different points $q(t)$ and $q(t+\Delta t)$ with small Δt is possible by choosing a basis at for example $q(t)$ and the basis induced by the parallel transported basis to the point $q(t+\Delta t)$. Therefore we define an orthonormal frame $E_{q(t)}$ of $T_{q(t)}\mathcal{M}$ using the parallel transport along $q(t)$ (2.5) by

Definition 13 (Parallel transported orthonormal frame)**.** Let e be an orthonormal system for $T_{q(0)}\mathcal{M}$, then the orthonormal frame for $q(t)$ is given by

$$E_{q(t)} := P_{q(t)}e$$

This frame allows us to move the chosen basis at $q(t)$ for sufficiently small Δt and to keep track of the normal coordinate systems. This is necessary because in the next section we want to define a mapping from $\mathcal{M}$ to $\mathbb{R}^n$ for each point $q(t)$, which later transforms the generally defined wave packets on $\mathcal{M}$ into wave packets similar to those of Hagedorn's type on $\mathbb{R}^n$.

2.2.5 Definition of the Mapping $\Phi^{-1}_{q(t)}$

Using the cutoff function, the exponential mapping for the coordinate transformation is a diffeomeorphism and together with the parallel transported frame it can be used to define the following mapping

Definition 14 (Normal coordinate mapping $\Phi^{-1}_{q(t)}$)**.** Let

$$\exp^{-1}_{q(t)}(x) \colon B^r_{q(t)} \subset \mathcal{M} \to B_0 \subset T_{q(t)}\mathcal{M}$$

be the inverse exponential mapping and $E_{q(t)}$ the parallel transported orthonormal frame of $T_{q(t)}\mathcal{M}$ both at point $q(t)$. Then

$$\Phi^{-1}_{q(t)} \colon B^r_{q(t)} \subset \mathcal{M} \to \mathbb{R}^n\,,\ \Phi^{-1}_{q(t)}(x) = E_{q(t)} \circ \exp^{-1}_{q(t)}(x) = y$$

is a differentiable mapping from arbitrary coordinates $x \in B^r_{q(t)} \subset \mathcal{M}$ to normal coordinates y on $T_{q(t)}\mathcal{M}$ identified with $\mathbb{R}^n$.

Furthermore as we restrict to open balls $B^r_{q(t)}$ it is a diffeomorphism and its inverse $\Phi_{q(t)}$ with

$$\Phi_{q(t)} \colon \mathbb{R}^n \to B^r_{q(t)} \subset \mathcal{M}\,,\ \Phi_{q(t)}(y) = x$$

exists and is differentiable.

Using these coordinate transformations we are now able to apply the associated pull backs and push forwards to smoothly go back and forth between our Riemannian manifold $\mathcal{M}$ and $\mathbb{R}^n$. The pull back $\Phi^*_{q(t)}$ maps a smooth function $f(x) \colon \mathcal{M} \to \mathbb{R}$ on $\mathcal{M}$ to a function $g(y) \colon \mathbb{R}^n \to \mathbb{R}$ on $\mathbb{R}^n$ via $g(y) = \left(\Phi^*_{q(t)} f\right)(y) = f\left(\Phi_{q(t)}(y)\right)$ and of course the other way around using the pull back Φ^{-1^*}. This is the necessary tool to get a Hagedorn wave packet in its regular form on $\mathbb{R}^n$ in normal coordinates, which is the topic of the next chapter.

2.2.6 Bounded Geometry

To finish our review about Riemannian geometry, we explain shortly manifolds of bounded geometry. Those provide an obvious framework for our setting. More about this can be found in [Shu92].

Definition 15 (Bounded Geometry)**.** Let $(\mathcal{M}, g)$ be a Riemannian manifold and let ρ_x be the injectivity radius at $x \in \mathcal{M}$. We define $\rho_{\mathcal{M}} := \inf_x \rho_x$. Then $\mathcal{M}$ is of *bounded geometry* if

1. $\rho_{\mathcal{M}} > 0$
2. Every transition function between two normal coordinate charts has bounded derivatives up to any order.

This definition implies two useful consequences:

- $\mathcal{M}$ is complete because $\rho_{\mathcal{M}} > 0$, which means, that every geodesic can be extended infinitely.

- The coefficients of the curvature and metric tensors together with any of their covariant derivatives are bounded by global constants, when expressed in normal coordinates.

3 Semiclassical Gaussian Wave Packets on Riemannian Manifolds

3.1 General Idea for the Formulation on Riemannian Manifolds

After the Introduction and a short review of the basic fundamentals needed, we now turn to the main part of this thesis. Our goal is to construct an approximate solution to the linear Schrödinger equation on a Riemannian manifold and to show that those are also an approximation to the full solution. They shall be approximate in a semiclassical sense, that means we give error terms in order of a small scaling parameter. Furthermore the solutions have to be in an appropriate form to be handled numerically.

Here we want to introduce our general idea for modifying semiclassical wave packets in Hagedorn's parametrization on Riemannian manifolds. Throughout the thesis let $\mathcal{M}$ be a Riemannian manifold of bounded geometry. We denote the metric on $\mathcal{M}$ with g and write $(\mathcal{M}, g)$. Often we only write $\mathcal{M}$, unless it is unclear.

At first we have a look at the Schrödinger equation, which has to be solved.

3.1.1 Schrödinger Equation on Riemannian Manifolds

We want to approximate solutions to the linear Schrödinger equation in semiclassical scaling on a Riemannian manifold $\mathcal{M}$ with metric g and volume measure $\mathrm{d}\mu$ by using semiclassical wave packets.

The general time-dependent, linear Schrödinger equation on $\mathcal{M}$ in semiclassical scaling with Hamilton operator H is

$$\begin{aligned} \mathrm{i}\varepsilon \frac{\partial \Psi}{\partial t} &= H\Psi \\ &= -\frac{\varepsilon^2}{2m} \Delta_{LB} \Psi + V\Psi , \qquad \Psi|_{t_0} \in L^2(\mathcal{M}, \mathrm{d}\mu) \end{aligned} \tag{3.1}$$

with a small, so called semiclassical parameter ε and mass m. The scaling parameter ε gives the order of a separation of scales within the quantum mechanical system. For example in many cases in physics, it is just Planck's constant $\hbar$.

The potential V is just a multiplication operator on $\mathcal{M}$ and can be handled similar to the Euclidian case when $\mathcal{M} = \mathbb{R}^n$. So the potential will give no further differences.

The Laplace-Beltrami operator, definition 6, page 25 is the generalized second order differential operator on a manifold with metric, similar to the Laplace operator in Euclidian space.

For simplicity we will first restrict to the free Schrödinger equation with Laplace-Beltrami operator Δ_{LB} , because a smooth potential V will add no additional difficulties.

The solution Ψ to (3.1) exists and is unique because Δ_{LB} is a self-adjoint operator on the second Sobolev space $H^2(M, g)$ for $\mathcal{M}$ being a Riemannian manifold with bounded geometry, see [Shu92].

3.1.2 Sketching the Idea

Before going into technical details, now we want to illustrate the general idea how to formulate semiclassical or Hagedorn wave packets on Riemannian manifolds. An overview of the scheme is shown in figure 3.1.

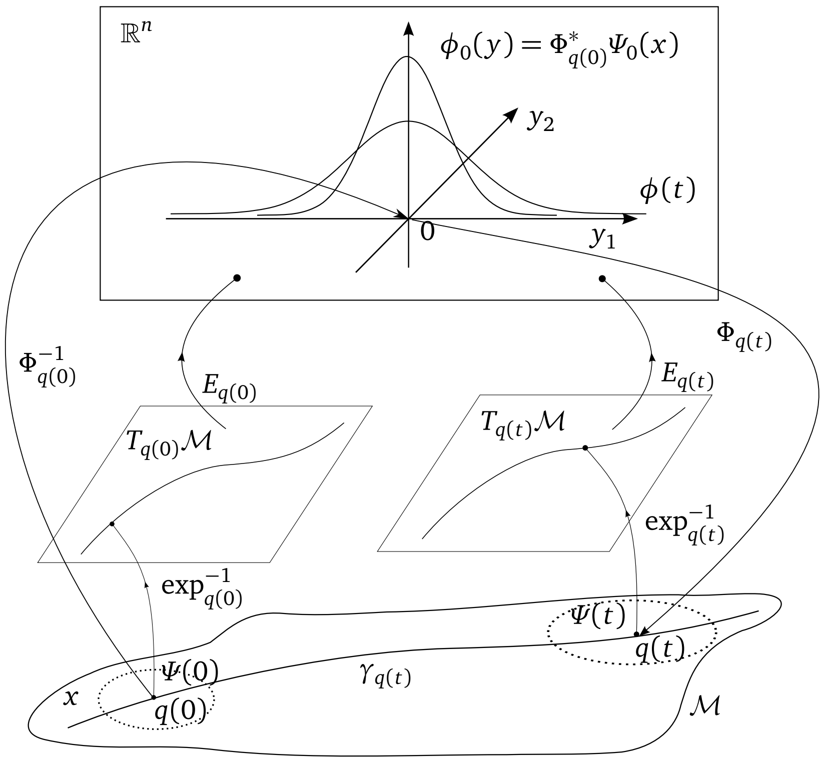

Figure 3.1: Scheme of setting

First we start with the definition of a modified Gaussian wave packet Ψ in Hagedorn's parametrization on a Riemannian manifold. Then we introduce a mapping $\Phi_{q(t)}$ along a curve $\gamma_{q(t)} \in \mathcal{M}$ and identify the tangent space $T_{q(t)}\mathcal{M}$ with $\mathbb{R}^n$, by using the exponential mapping and choosing an orthonormal frame $E_{q(t)}$. This introduces normal coordinates y, also known as geodesic or Riemann coordinates. Using this mapping we are able to transform Ψ into a modified Gaussian wave packet ϕ in Hagedorn's parametrization similar to $\mathbb{R}^n$. For ϕ we formulate a Schrödinger equation in normal coordinates. Therefor we expand the Laplace-Beltrami operator in normal coordinates up to order $\mathcal{O}\left(y^3\right)$. This leads to a theorem similar to Hagedorn's about solutions for classical parameter equations and wave packets. Using a cutoff function the effective solution can be remapped to $\mathcal{M}$ which gives an approximate solution to the Schrödinger equation on $\mathcal{M}$.

3.2 Hagedorn Wave Packets on Riemannian Manifolds

3.2.1 The Setting

As seen in the flat case a semiclassical wave packet in Hagedorn's parametrization is originally defined as

$$\begin{aligned}
&\varphi[q,p,Q,P](x,t) \\
&\quad = (\pi\varepsilon)^{-n/4}\left(\det Q(t)\right)^{-1/2} \times \\
&\qquad \exp\left(\frac{\mathrm{i}}{2\varepsilon}\left(x-q(t)\right)^T P(t)Q(t)^{-1}\left(x-q(t)\right)+\frac{\mathrm{i}}{\varepsilon}p^T\left(x-q(t)\right)\right)
\end{aligned}$$

with $p(t), q(t) \in \mathbb{R}^n$ the momentum and position respectively. The two complex matrices $P(t), Q(t) \in \mathbb{C}^{n\times n}$, satisfying condition 2.2, represent the momentum and position covariances respectively. The wave packet is centralized around and moves along the curve $q(t)$ in $\mathbb{R}^n$. A short summary can be found in section 2.1.

Now we want to recall again our setting for the reformulation of semiclassical wave packets on Riemannian manifolds. Let $\mathcal{M}$ be a Riemannian manifold of bounded geometry and with metric g, see definitions 1 and 15. $x \in \mathcal{M}$ is an arbitrary point on $\mathcal{M}$ and $q(t)$ a curve in $\mathcal{M}$ with $t \in I \subset \mathbb{R}$.

In general in $\mathcal{M}$ one cannot say what $x - q(t)$ means, because $\mathcal{M}$ has no vector space structure. To be able to define a wave packet on $\mathcal{M}$, we have to clarify that and choose appropriate coordinates.

Therefore we use the exponential mapping, introduced in section 2.2, definition 5. It identifies straight lines on $T_{q(t)}\mathcal{M}$ with geodesics through $q(t)$ on $\mathcal{M}$. Now we can give $|x - q(t)|$ a meaning: it is just the length of the geodesic between x and $q(t)$.

3.2.2 Gaussian Wave Packets in Hagedorn's Parametrization

Following our idea above, we can now define a general complex Gaussian wave packet in Hagedorn's parametrization on a Riemannian manifold $\mathcal{M}$ using the restricted exponential mapping. Because our wave packet is $\sqrt{\varepsilon}$-localized around $q(t)$ we choose an appropriate size r of the cutoff function, see definition 10, and apply the exponential mapping to formulate a Gaussian wave packet on $\mathcal{M}$. A deeper error analysis will be done in section 3.6.

Definition 16 (Gaussian wave packet on a Riemannian manifold)**.** Let $q\colon I \to \mathcal{M}$ be a smooth curve and let $\exp^{-1}_{q(t)}(x)\colon B^r_{q(t)} \to T_{q(t)}\mathcal{M}$ be the inverse exponential mapping at point $q(t)$ for any $t \in I$. Let $p(t) \in T_{q(t)}\mathcal{M}$ be a vectorfield along $q(t)$ and let $P, Q \in \Gamma(q^* \operatorname{End}(T\mathcal{M}) \otimes \mathbb{C})$ be complex $1,1$-tensorfields above $T\mathcal{M}$ along $q(t)$, satisfying condition (2.2) pointwise. Then a complex Gaussian wave packet in Hagedorn's parametrization on a Riemannian manifold $\mathcal{M}$ along $q(t)$ with parameters $[q(t), p(t), Q(t), P(t)]$ is defined as

$$
\begin{aligned}
&\psi[q(t), p(t), Q(t), P(t)](x) \qquad\qquad (3.2)\\
&\quad := \chi^r_{q(t)}(x)\,(\pi\,\varepsilon)^{-n/4}\,(\operatorname{tr} Q(t))^{-1/2} \times \\
&\qquad \exp\Bigg(\frac{\mathrm{i}}{2\,\varepsilon}\, g\left(\exp^{-1}_{q(t)}(x), P(t)Q(t)^{-1}\exp^{-1}_{q(t)}(x)\right) + \\
&\qquad\qquad \frac{\mathrm{i}}{\varepsilon}\, g\left(p(t), \exp^{-1}_{q(t)}(x)\right)\Bigg).
\end{aligned}
$$

The full semiclassical wave packet, which later will be the basis for the

Hagedorn wave packets, then is given as

$$\begin{aligned}&\Psi[q(t),p(t),Q(t),P(t)](x,t)\\&\quad=\exp\left(\frac{\mathrm{i}}{\varepsilon}S(t)\right)\psi[q(t),p(t),Q(t),P(t)](x),\end{aligned}$$

with the classical action integral

$$S(t)=\int_0^t\frac{g(p,p)(s)}{2m}\mathrm{d}s.$$

The main part of this work is to show that by choosing the parameters $[q(t),p(t),Q(t),P(t)]$ properly, this wave packet $\Psi(x,t)$ is an approximate solution to the free Schrödinger equation

$$\begin{aligned}\mathrm{i}\varepsilon\frac{\partial\Psi}{\partial t}&=H\Psi\\&=-\frac{\varepsilon^2}{2}\Delta_{LB}\Psi,\qquad\Psi|_{t_0}\in L^2(\mathcal{M},\mathrm{d}\mu)\end{aligned}\tag{3.3}$$

and also approximates the full solution. In which sense is the main topic of this thesis and will be elaborated in the following sections.

3.3 Modified Hagedorn Wave Packets in Normal Coordinates

By applying the pull back $\Phi^*_{q(t)}$ we are able to define modified Hagedorn wave packets in normal coordinates coming from a complete Riemannian manifold $\mathcal{M}$. Be aware that along $q(t)$ the metric simplifies to $g(\partial_a,\partial_b)=\delta_{ab}$ because $q(t)$ is at any time the basis point for choosing Riemann normal coordinates.

Definition 17 (Modified Hagedorn basis wave packet in normal coordinates). Let $\psi[q(t),p(t),Q(t),P(t)](x)$ be the Gaussian wave packet on

$\mathcal{M}$ as defined in (3.2) and $\Phi^*_{q(t)}$ be the pull back according to the normal coordinate mapping, definition (14). Then a complex Gaussian in Riemann normal coordinates on $\mathbb{R}^n$ identified by $\Phi_{q(t)}$ with $\mathcal{M}$ in Hagedorn's parametrization is defined as:

$$\begin{aligned}
\varphi[p(t),Q(t),P(t)](y,t) &:= \left(\Phi^*_{q(t)}\psi[q(t),p(t),Q(t),P(t)]\right)(y) \\
&= \psi[q(t),p(t),Q(t),P(t)]\left(\Phi_{q(t)}(y)\right) \\
&= \tilde{\chi}^r_{q(t)}(y)\,(\pi\,\varepsilon)^{-n/4}\,(\det Q(t))^{-1/2}\times \\
&\quad \exp\left(\frac{\mathrm{i}}{2\,\varepsilon}\,y^a\,\left(P(t)Q(t)^{-1}\right)_{ab}\,y^b+\frac{\mathrm{i}}{\varepsilon}\,p_c\,y^c\right).
\end{aligned}$$

with $\tilde{\chi}^r_{q(t)}(y)=\chi^r_{q(t)}\left(\exp_{q(t)}(y)\right)$ the cutoff according to normal coordinates and $p_c=g_{cd}p^d$.

Again the full semiclassical Gaussian wave packet then is

$$\begin{aligned}
&\phi[p(t),Q(t),P(t)](y,t) \\
&\quad=\exp\left(\frac{\mathrm{i}}{\varepsilon}\,S(t)\right)\,\varphi[p(t),Q(t),P(t)](y,t),
\end{aligned}$$

with the classical action integral $S(t)=\int_0^t \frac{(\delta_{ab}p^a p^b)(s)}{2m}\mathrm{d}s$ along $q(t)$.

As can be seen from above and in contrary to the flat case, $q(t)$ no longer is a parameter within the Hagedorn parametrization of a wave packet, but comes indirectly with the mapping $\Phi_{q(t)}$.

The properties of this wave packet in normal coordinates are similar to those of a regular Hagedorn wave packet on $\mathbb{R}^n$. First P,Q are symplectic complex matrices and they have to obey the same symplectic relations like (2.2)

$$\begin{aligned}
Q^T P - P^T Q &= 0 \\
Q^* P - P^* Q &= 2\mathrm{i}\mathbf{1}\,.
\end{aligned} \tag{3.4}$$

Second the wave packet is concentrated in position around zero and in momentum around p with uncertainty widths

$$\sigma_y = \sqrt{\mathrm{Var}(y)} = \sqrt{\frac{\varepsilon}{2}}\ \det Q \qquad (3.5)$$
$$\sigma_p = \sqrt{\mathrm{Var}(p)} = \sqrt{\frac{\varepsilon}{2}}\ \det P\,.$$

This can be easily verified by calculating the appropriate variances. Again, the first equation means that the main part of the wave packet is centered around zero with width $|y| \sim \sqrt{\varepsilon}$. As we are interested in error terms up to order ε, this is the reason why we expanded all terms in normal coordinates up to order $|y|^2$ or $|y|^3$, depending on preceding derivatives. In lemma 16, page 70, we prove this well known property of Gaussian wave packets for a multiplication of y up to any order.

To show that this wave packet is an approximate solution to the Schrödinger equation (3.3) mapped to $\mathbb{R}^n$ with $\Phi_{q(t)}$ and expanded in normal coordinates, we just put it into the equation and check whether we can choose the parameters $[q(t), p(t), Q(t), P(t)]$ appropriately. Thus it is necessary to have the Laplace-Beltrami operator in normal coordinates. Before we will derive that, we first have to analyze the derivative with respect to t of the mapping $\Phi^{-1}_{q(t)}$, because of the time-derivative in the Schrödinger equation. In normal coordinates with a parallel transported orthonormal frame the derivative with respect to t of a vector field $p(t)$ is just $\partial_t p(t) = \nabla_{\dot q(t)} p(t) = \nabla_t p(t)$, compare page 24. The same is valid for the derivative of the tensor fields $P(t), Q(t)$.

3.3.1 Jacobi Fields and the Derivative of $\Phi^{-1}_{q(t)}$

The following basics about Jacobi fields can be found in any textbook on differential geometry. The latter calculations for the Jacobi initial value problem follow closely [Wit08]. Throughout this subsection we denote differentiation with respect to α by a prime $'$ and with respect to β by a dot $\dot{}$, respectively. Moreover, we always suppose $I, J \subset \mathbb{R}$ to be an open neighbourhood of the zero element.

Definition 18 (Geodesic variation)**.** Let $c\colon I \mapsto \mathcal{M}$ be a smooth curve on a Riemannian manifold $(\mathcal{M}, g)$.

- A *geodesic variation* of c is a differentiable map $F(\alpha,\beta)\colon I \times J \mapsto \mathcal{M}$ with $F(\alpha,0) = c(\alpha)$ such that

  $$F(\alpha,\cdot) =: \gamma_\alpha(\cdot).$$

  is a geodesic for every α.

- The associated *variational vector field* X along γ is defined as

  $$\beta \mapsto X(\beta) := \frac{\partial F}{\partial \alpha}(\alpha,\beta)\bigg|_{\alpha=0}$$

Proposition 6 (Jacobi equation)**.** *For any geodesic variation $\gamma_\alpha(\cdot)$ of c the corresponding variational vector field satisfies the linear differential equation called Jacobi equation for any β*

$$\ddot{X} + R(X,\dot{\gamma})\gamma = 0\,. \tag{3.6}$$

where $\dot{}$ is short for $\nabla_\beta = \nabla_{\dot{\gamma}(\beta)}$. The solutions of the Jacobi equation are called Jacobi fields along γ.

Proposition 7 (Jacobi initial value problem)**.** *Let $c\colon\ I \mapsto \mathcal{M}$ be a curve and $Y \in \Gamma(c^*(T\mathcal{M}))$. Consider a family of geodesics $\{\gamma_\alpha\colon\ J \mapsto \mathcal{M}|\ \alpha \in I\}$ such that*

$$\gamma_\alpha(0) = c(\alpha) \quad , \quad \dot{\gamma}_\alpha(0) = Y(\alpha)\,.$$

Then we can define the geodesic variation $F(\alpha,\beta) := \gamma_\alpha(\beta)$ according to definition 18, and the corresponding variational vector field

$$X(\beta) := \frac{\partial F}{\partial \alpha}(\alpha,\beta)\bigg|_{\alpha=0}$$

and $X \in \Gamma(\gamma_0^*(T\mathcal{M}))$ *is a Jacobi field along* γ_0*, solving the initial value problem*

$$(\nabla_\beta)^2 X = R(\dot{\gamma}_0, X)\dot{\gamma}_0$$

with initial data

$$X(0) = c'(0) \quad , \quad (\nabla_\beta X)(0) = (\nabla_\alpha Y)(0) \tag{3.7}$$

where $\nabla_\alpha = \nabla_{c'(\alpha)}$ *and* $\nabla_\beta = \nabla_{\dot{\gamma}_0(\beta)}$

Proof. The first part of this proposition is just a restatement of definition 18 and proposition 6 that is F is a variation of γ_0 through geodesics γ_α and X is a Jacobi field along γ_0 (remember that $R(\cdot,\cdot)$ is antisymmetric). For a sketch overview see figure 3.2.

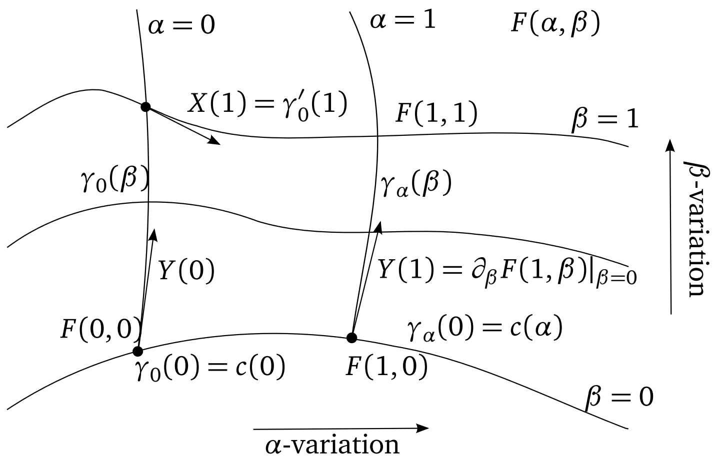

Figure 3.2: Jacobi field variation

Furthermore, we can calculate the initial conditions for X:

$$\begin{aligned}
X(0) &= \frac{\partial}{\partial \alpha} F(\alpha,0)\bigg|_{\alpha=0} = \frac{\partial}{\partial \alpha}\gamma_\alpha(0)\bigg|_{\alpha=0} = \frac{\mathrm{d}}{\mathrm{d}\alpha}\gamma_\alpha(0)\bigg|_{\alpha=0} \\
&= \frac{\mathrm{d}}{\mathrm{d}\alpha} c(\alpha)\bigg|_{\alpha=0} = c'(0)
\end{aligned}$$

and by use of the torsion-freeness of ∇ together with $[\partial_\beta, \partial_\alpha] = 0$:

$$\begin{aligned}
(\nabla_\beta X)(0) &= \left(\nabla_\beta \frac{\partial F}{\partial \alpha}(\alpha,\beta)\bigg|_{\alpha=0}\right)_{\beta=0} = \left(\nabla_\alpha \frac{\partial F}{\partial \beta}(\alpha,\beta)\bigg|_{\beta=0}\right)_{\alpha=0} \\
&= \left(\nabla_\alpha \frac{\partial}{\partial \beta}\gamma_\alpha(\beta)\bigg|_{\beta=0}\right)_{\alpha=0} = \nabla_\alpha \dot{\gamma}_\alpha(0)\big|_{\alpha=0} = \nabla_\alpha Y(\alpha)\big|_{\alpha=0} \\
&= (\nabla_\alpha Y)(0) \, .
\end{aligned}$$

□

Next steps include the Jacobi field Taylor expansion, which later gives the opportunity to reorder terms according to the exponential mapping. Let $P_{\gamma_0}(\beta)\colon T_{\gamma_0(0)}\mathcal{M} \to T_{\gamma_0(\beta)}\mathcal{M}$ denote the parallel transport along γ_0 (see definition 13). This yields a Taylor expansion for $X(\beta)$:

$$\begin{aligned}
X(\beta) \;=\; & P_{\gamma_0}(\beta)\Big\{X(0) + \beta(\nabla_\beta X)(0) + \frac{\beta^2}{2}\left((\nabla_\beta)^2 X\right)(0) \\
& \qquad + \frac{\beta^3}{6}\left((\nabla_\beta)^3 X\right)(0) + \mathcal{O}\left(\beta^4\right)\Big\} \\
\overset{(3.6)}{=} \; & P_{\gamma_0}(\beta)\Big\{X(0) + \beta(\nabla_\beta X)(0) + \frac{\beta^2}{2} R\big(\dot{\gamma}_0(0), X(0)\big)\dot{\gamma}_0(0) \\
& \qquad + \frac{\beta^3}{6}\nabla_\beta|_{\beta=0}\Big(R\big(\dot{\gamma}_0(\beta), X(\beta)\big)\dot{\gamma}_0(\beta)\Big) \\
& \qquad + \mathcal{O}\left(\beta^4\right)\Big\}
\end{aligned}$$

$$
\begin{aligned}
= P_{\gamma_0}(\beta)\Big\{ & X(0) + \beta(\nabla_\beta X)(0) + \frac{\beta^2}{2} R\big(\dot\gamma_0(0), X(0)\big)\dot\gamma_0(0) \\
& + \frac{\beta^3}{6}\Big(\big(\nabla_\beta|_{\beta=0} R\big)\big(\dot\gamma_0(0), X(0)\big)\dot\gamma_0(0) \\
& \qquad + R\big(\dot\gamma_0(0), (\nabla_\beta X)(0)\big)\dot\gamma_0(0)\Big) \\
& + \mathcal{O}(\beta^4)\Big\}
\end{aligned}
$$

where we used the geodesic equation $\nabla_\beta \dot\gamma_0 = 0$ and

$$
\begin{aligned}
\nabla_\beta\big(R(\dot\gamma_0, X)\dot\gamma_0\big) = (\nabla_\beta R)(\dot\gamma_0, X)\dot\gamma_0 + \underbrace{R(\nabla_\beta\dot\gamma_0, X)\dot\gamma_0}_{=0} \\
+ R(\dot\gamma_0, \nabla_\beta X)\dot\gamma_0 + \underbrace{R(\dot\gamma_0, X)\nabla_\beta\dot\gamma_0}_{=0} .
\end{aligned}
\tag{3.8}
$$

If we finally use the initial data (3.7) and the definition of the vector field Y, we obtain

$$
\begin{aligned}
X(\beta) = P_{\gamma_0}(\beta)\Big\{ & c'(0) + \beta(\nabla_\alpha Y)(0) + \frac{\beta^2}{2} R\big(Y(0), c'(0)\big)Y(0) \\
& + \frac{\beta^3}{6}\Big(\big(\nabla_\beta|_{\beta=0} R\big)\big(Y(0), c'(0)\big)Y(0) \\
& \qquad + R\big(Y(0), (\nabla_\alpha Y)(0)\big)Y(0)\Big) \\
& + \mathcal{O}(\beta^4)\Big\} .
\end{aligned}
\tag{3.9}
$$

In our case we now choose $c(\alpha) = q(t)$ and $Y(t) = \exp^{-1}_{q(t)}(x)$ as well as

$$
F(t,\beta) := \exp_{q(t)}(\beta Y(t))
$$

such that $F(t,0) = q(t)$ and most important $F(t,1) = x$. The last property means, that the geodesic variation along t at $\beta = 1$ is equal to fixed $x \in \mathcal{M}$, our standard arbitrary point on the manifold. This leads to

$$
\left.\frac{\partial F}{\partial t}(t,1)\right|_{t=0} = \frac{\partial}{\partial t}\exp_{q(t)}(Y(t)) = \frac{\partial x}{\partial t} = 0 = X(1) \tag{3.10}
$$

according to Proposition 7 (p. 41). Compare figure 3.3

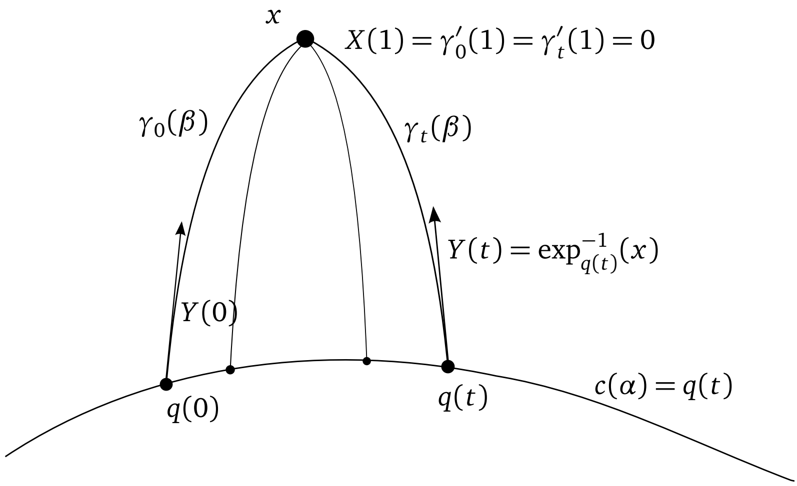

Figure 3.3: Gedoesic variation

Lemma 8 (Derivative of $\exp^{-1}_{q(t)}(x)$). *Given the above settings, the derivative of the exponential mapping* $\exp^{-1}_{q(t)}(x)$ *is*

$$\frac{\partial}{\partial t}\exp^{-1}_{q(t)}(x) = \frac{\partial}{\partial t}Y(t) = -\dot{q}(t) - \frac{1}{3}R(Y(t), \dot{q}(t))Y(t) + \mathcal{O}\left(Y^3\right)$$

Proof. Using (3.9) together with (3.10) and $P_{\gamma_0}(1) = \mathrm{id}$, we can move all terms except $(\nabla_t Y)(0)$ to the left hand side, which is zero according to (3.10). Then the derivative of $Y(t)$ along t is

$$\begin{aligned}(\nabla_t Y)(0) = \frac{\partial}{\partial t}Y(t) = \Big\{ & -c'(0) - \frac{1}{2}R\big(Y(0), c'(0)\big)Y(0) \\ & - \frac{1}{6}\Big(\big(\nabla_\beta|_{\beta=0}R\big)\big(Y(0), c'(0)\big)Y(0) \\ & + R\big(Y(0), (\nabla_t Y)(0)\big)Y(0)\Big) + \dots\Big\}\,. \end{aligned} \tag{3.11}$$

Because $c(\alpha) = q(t)$ it directly follows that $c'(0) = \dot{q}(0)$.

Furthermore the last two terms can also be rewritten in orders of Y. First $(\nabla_t Y)(0) = -\dot{q}(0) + \mathcal{O}\left(Y^2\right)$ leaving the last term similar to the second one except of higher orders in Y.

The third term contains $\left(\nabla_\beta|_{\beta=0} R\right)$ which is again of order Y because $\nabla_\beta|_{\beta=0} = Y(t)$ and derivatives of R being bounded by definition 15. Any further terms of the original Taylor series of $X(\beta)$ are of the same structure as the β^3-terms containing higher derivatives of R similar to (3.8) and hence can be neglected. □

3.4 The Schrödinger Equation in Normal Coordinates

Because we want to solve the Schrödinger equation on $\mathcal{M}$ as well as in Riemann coordinates, we need the Laplace-Beltrami operator and therefore also the metric g expanded in normal coordinates.

3.4.1 Expansion of the Metric in Normal Coordinates

We restrict to terms up to order $\mathcal{O}\left(y^3\right)$. The following explicit expansion can be found mostly in physics literature, mainly [Bre09, CV10, MSvdV99, Nes99]. Here we refer to these but also to [BGV92], where a concise proof can be looked up.

Proposition 9. *Let $x \in \mathcal{M}$ be a arbitrary point on a Riemannain manifold with metric g. Let y be normal coordinates centered at x according to definition 11. The metric g expanded in these normal coordinates around* 0 *is*

$$g_{ab}(y) = \delta_{ab} - \frac{1}{3} y^c y^d R_{acbd} - \frac{1}{6} y^c y^d y^e \partial_c R_{adbe} + \mathcal{O}\left(|y|^4\right) \qquad (3.12)$$

with the Euclidian distance $|y| = \mathrm{dist}(y_0, y)$ see definition 12 and $y_0 = \exp_{q_0}^{-1}(x) = 0$.

Further terms according to metric g in normal coordinates will be needed later and are calculated in the next few lines.

With the following expansion of the determinant of a tensor

$$\det(\mathrm{id} + \varepsilon A) = 1 + \varepsilon \operatorname{tr} A + \mathcal{O}\left(\varepsilon^2\right)$$

and the relation $\operatorname{tr} T^a{}_b = T^a{}_a$ we are able to expand the determinant of g. Note that we expand around $x \in \mathcal{M}$ in normal coordinates, which essentially means around $y_0 = \exp_{q_0}^{-1}(x) = 0$, where $g(x) = \delta^a_b$.

$$\begin{aligned}\det g &= 1 - \frac{1}{3} y^c y^d R^a{}_{cad} - \frac{1}{6} y^c y^d y^e \partial_c R^a{}_{dae} + \mathcal{O}\left(|y|^4\right) \\ &= 1 - \frac{1}{3} y^c y^d \operatorname{Ric}_{cd} - \frac{1}{6} y^c y^d y^e \partial_c \operatorname{Ric}_{de} + \mathcal{O}\left(|y|^4\right)\end{aligned}$$

where we used the contraction $R^a{}_{cad} = \operatorname{Ric}_{cd}$. Taking the square root of $\det g$ in form of a taylor series gives

$$\sqrt{g} = 1 - \frac{1}{6} y^c y^d \operatorname{Ric}_{cd} - \frac{1}{12} y^c y^d y^e \partial_c \operatorname{Ric}_{de} + \mathcal{O}\left(|y|^4\right)$$

and taking the inverse of a Taylor series gives

$$\frac{1}{\sqrt{g}} = 1 + \frac{1}{6} y^c y^d \operatorname{Ric}_{cd} + \frac{1}{12} y^c y^d y^e \partial_c \operatorname{Ric}_{de} + \mathcal{O}\left(|y|^4\right)$$

For completeness we write

$$g^{ab}(y) = \delta^{ab} + \frac{1}{3} y^c y^d R^a{}_c{}^b{}_d + \frac{1}{6} y^c y^d y^e \partial_c R^a{}_d{}^b{}_e + \mathcal{O}\left(|y|^4\right).$$

3.4.2 Laplace-Beltrami in Riemann Normal Coordinates

To expand the Laplace-Beltrami operator in normal coordinates, we use the metric expansion of g in normal coordinates (3.12) and all other related equations from 3.4.1. Using these we can state the following

Proposition 10. *Again let $x \in \mathcal{M}$ be an arbitrary point on a Riemannian manifold with metric g. Let y be normal coordinates centered at x according to definition 11. The Laplace-Beltrami operator expanded in normal coordinates up to order $\mathcal{O}\left(|y|^3\right)$ is*

$$\begin{aligned}\Delta^{\mathrm{nc}}_{\mathrm{LB}} = {} & \delta^{ab}\partial_a\partial_b \\ & - \frac{2}{3} y^c \operatorname{Ric}_{cb} \partial_b \\ & + y^c y^d \left(\frac{1}{3} R^a{}_c{}^b{}_d \,\partial_a - \frac{5}{6}\partial_c \operatorname{Ric}_{bd} + \frac{5}{12}\left(\partial_b \operatorname{Ric}_{cd}\right)\right)\partial_b \\ & + \mathcal{O}\left(|y|^3\right)\end{aligned}$$

Proof. The Laplace-Beltrami operator (see definition 6, page 25) is defined as

$$\Delta_{\mathrm{LB}} := \frac{1}{\sqrt{g}}\,\partial_a \sqrt{g}\, g^{ab}\partial_b = g^{ab}\,\partial_a\partial_b + (\partial_a g^{ab})\partial_b + \frac{1}{\sqrt{g}}\, g^{ab}\,(\partial_a \sqrt{g}\,)\partial_b\,.$$

To get the Laplace-Beltrami operator expanded in normal coordinates

$$\Delta^{\mathrm{nc}}_{\mathrm{LB}} = \Phi^*_{q(t)}\Delta_{\mathrm{LB}}\Phi^{-1\,*}_{q(t)}$$

we calculate each term using the metric normal expansion. To begin with we take the first part of the last term

$$\begin{aligned}\frac{1}{\sqrt{g}}\, g^{ab}(y) = \delta^{ab} & + \frac{1}{3} y^c y^d R^a{}_c{}^b{}_d + \frac{1}{6} y^c y^d y^e \partial_c R^a{}_d{}^b{}_e \\ & + \frac{1}{6} y^c y^d \operatorname{Ric}_{cd}\delta^{ab} + \frac{1}{12} y^c y^d y^e \partial_c \operatorname{Ric}_{de}\delta^{ab} \\ & + \mathcal{O}\left(|y|^4\right)\end{aligned} \tag{3.13}$$

Now we calculate each term explicitly. The first term reads

$$g^{ab}\,\partial_a\partial_b = \left(\delta^{ab} + \frac{1}{3} y^c y^d R^a{}_c{}^b{}_d\right)\partial_a\partial_b + \mathcal{O}\left(|y|^3\right)$$

For terms with derivatives falling on the metric g we need the following Bianchi identitiy for a derivative of the Riemann tensor

$$
\begin{aligned}
\partial_a R^{a\ \ b}_{\ c\ \ d} = R^{a\ \ b}_{\ c\ \ d,a} &\overset{g_{ab}|_{y_0}=\delta^b_a}{=} R_{acbd,a} \overset{\text{Bianchi}}{=} -R_{acab,d} - R_{acda,b} \\
&= -\partial_d \operatorname{Ric}_{cb} + \partial_b \operatorname{Ric}_{cd} \\
&= -\partial_d \operatorname{Ric}_{bc} + \left(\partial_a \operatorname{Ric}_{cd}\right)\delta^{ab} \\
&= -\partial_c \operatorname{Ric}_{bd} + \left(\partial_a \operatorname{Ric}_{cd}\right)\delta^{ab}
\end{aligned}
\tag{3.14}
$$

For $\partial_a g^{ab}$ we have a separate look at each derivative falling on the $y's$ because $\partial_a y^c = \delta^{ac}$. Furthermore as the Riemann tensor is antisymmetric in its first and second pairs of indices respectively and the trace of an antisymmetric operator is zero.

$$
\begin{aligned}
&\frac{1}{3}(\partial_a y^c) y^d R^{a\ \ b}_{\ c\ \ d} = \frac{1}{3}\delta^{ac} y^d R^{a\ \ b}_{\ c\ \ d} = \frac{1}{3} y^d R^{a\ \ b}_{\ a\ \ d} = 0 \\
&\frac{1}{3} y^c (\partial_a y^d) R^{a\ \ b}_{\ c\ \ d} = \frac{1}{3} y^c \delta^{ad} R^{a\ \ b}_{\ c\ \ d} = \frac{1}{3} y^c R^{a\ \ b}_{\ c\ \ a} = -\frac{1}{3} y^c \operatorname{Ric}_{cb} \\
&\frac{1}{3} y^c y^d \partial_a R^{a\ \ b}_{\ c\ \ d} \overset{(3.14)}{=} -\frac{1}{3} y^c y^d \partial_c \operatorname{Ric}_{bd} + \frac{1}{3} y^c y^d \left(\partial_a \operatorname{Ric}_{cd}\right)\delta^{ab}
\end{aligned}
$$

Furthermore the second order terms

$$
\begin{aligned}
\frac{1}{6}(\partial_a y^c) y^d y^e \partial_c R^{a\ \ b}_{\ d\ \ e} = \frac{1}{6}\delta^{ac} y^d y^e \partial_c R^{a\ \ b}_{\ d\ \ e} &= \frac{1}{6} y^d y^e \partial_a R^{a\ \ b}_{\ d\ \ e} \\
&\overset{(3.14)}{=} -\frac{1}{6} y^d y^e \partial_d \operatorname{Ric}_{be} + \frac{1}{6} y^d y^e \left(\partial_a \operatorname{Ric}_{de}\right)\delta^{ab} \\
&= -\frac{1}{6} y^c y^d \partial_c \operatorname{Ric}_{bd} + \frac{1}{6} y^c y^d \left(\partial_a \operatorname{Ric}_{cd}\right)\delta^{ab} \\
\frac{1}{6} y^c (\partial_a y^d) y^e \partial_c R^{a\ \ b}_{\ d\ \ e} = \frac{1}{6} y^c \delta^{ad} y^e \partial_c R^{a\ \ b}_{\ d\ \ e} &= \frac{1}{6} y^c y^e \partial_c R^{a\ \ b}_{\ a\ \ e} = 0 \\
\frac{1}{6} y^c y^d (\partial_a y^e) \partial_c R^{a\ \ b}_{\ d\ \ e} = \frac{1}{6} y^c y^d \delta^{ae} \partial_c R^{a\ \ b}_{\ d\ \ e} &= \frac{1}{6} y^c y^d \partial_c R^{a\ \ b}_{\ d\ \ a} \\
&= -\frac{1}{6} y^c y^d \partial_c \operatorname{Ric}_{db}
\end{aligned}
$$

At last we need the terms from $\partial_a \sqrt{g}$

$$\partial_a \sqrt{g} = -\frac{1}{3} y^c \operatorname{Ric}_{ca} - \frac{1}{6} y^c y^d \partial_c \operatorname{Ric}_{ad} - \frac{1}{12} y^d y^e \left(\partial_a \operatorname{Ric}_{de}\right)$$

and then we multiply by (3.13) and get

$$\begin{aligned}\frac{1}{\sqrt{g}} g^{ab} (\partial_a \sqrt{g}) \partial_b = \Bigg(-\frac{1}{3} y^c \operatorname{Ric}_{cb} - \frac{1}{6} y^c y^d \partial_c \operatorname{Ric}_{bd} \\ - \frac{1}{12} y^d y^e \left(\partial_a \operatorname{Ric}_{de}\right) \delta^{ab} \Bigg) \partial_b + \mathcal{O}\left(|y|^3\right)\end{aligned}$$

The Laplace-Beltrami operator expanded in normal coordinates is then fully stated as

$$\begin{aligned}\Phi^*_{q(t)} \Delta_{\mathrm{LB}} \Phi^{-1}_{q(t)}{}^* = \Delta^{\mathrm{nc}}_{\mathrm{LB}} &= \frac{1}{\sqrt{g}} \partial_a \sqrt{g}\, g^{ab} \partial_b \\
&= g^{ab} \partial_a \partial_b + (\partial_a g^{ab}) \partial_b + \frac{1}{\sqrt{g}} g^{ab} (\partial_a \sqrt{g}) \partial_b \\
&= \left(\delta^{ab} + \frac{1}{3} y^c y^d R^{a\ \ b}_{\ c\ \ d} \right) \partial_a \partial_b \\
&\quad + \Bigg(-\frac{1}{3} y^c \operatorname{Ric}_{cb} + \frac{1}{3} y^c y^d \partial_a R^{a\ \ b}_{\ c\ \ d} \\
&\qquad + \frac{1}{6} y^d y^e \partial_a R^{a\ \ b}_{\ d\ \ e} - \frac{1}{6} y^c y^d \partial_c \operatorname{Ric}_{db} \Bigg) \partial_b \\
&\quad + \Bigg(-\frac{1}{3} y^c \operatorname{Ric}_{cb} - \frac{1}{6} y^c y^d \partial_c \operatorname{Ric}_{bd} \\
&\qquad - \frac{1}{12} y^d y^e \left(\partial_a \operatorname{Ric}_{de}\right) \delta^{ab} \Bigg) \partial_b + \mathcal{O}\left(|y|^3\right) \\
&= \delta^{ab} \partial_a \partial_b \\
&\quad - \frac{2}{3} y^c \operatorname{Ric}_{cb} \partial_b \\
&\quad + y^c y^d \Bigg(\frac{1}{3} R^{a\ \ b}_{\ c\ \ d} \partial_a + \frac{1}{6} \partial_a R^{a\ \ b}_{\ c\ \ d} + \frac{1}{3} \partial_a R^{a\ \ b}_{\ c\ \ d} \\
&\qquad - \frac{1}{3} \partial_c \operatorname{Ric}_{bd} - \frac{1}{12} \left(\partial_a \operatorname{Ric}_{cd}\right) \delta^{ab} \Bigg) \partial_b + \mathcal{O}\left(|y|^3\right)\end{aligned}$$

$$
\begin{aligned}
&= \delta^{ab}\partial_a\partial_b \\
&\quad - \frac{2}{3} y^c \operatorname{Ric}_{cb} \partial_b \\
&\quad + y^c y^d \left(\frac{1}{3} R^a{}_c{}^b{}_d \, \partial_a - \frac{5}{6} \partial_c \operatorname{Ric}_{bd} + \frac{5}{12} \left(\partial_b \operatorname{Ric}_{cd} \right) \right) \partial_b \\
&\quad + \mathcal{O}\left(|y|^3 \right)
\end{aligned}
$$

□

3.5 Main Results

Here we show the main results of this thesis. First we state and prove the main solution theorem, then we give results about the the packets following geodesics, formulate an effective Schrödinger equation and describe the main difference to the flat case.

3.5.1 Modified Gaussian Wave Packets as Approximate Solutions

Ordinary Gaussian wave packets with parameters appropriately adopted, solve the time-dependent Schrödinger equation exactly. Within the Hagedorn parametrization the equations of motion for the parameters become the standard classical equations of motion for a potential V (see section 2.1). In our case of modified Hagedorn wave packets on Riemannian manifolds we end up with slightly modified classical equations of motion.

Let $q(t)$ be a smooth curve in $\mathcal{M}$ for $t \in [0, T]$ and let $p(t)$ be a vector field as above. Let $P, Q \in \Gamma(q^* \operatorname{End}(T\mathcal{M}) \otimes \mathbb{C})$ be complex 1, 1-tensorfields above $T\mathcal{M}$ along $q(t)$, satisfying condition 2.2 pointwise. Then the adapted classical equations of motion for $V = 0$ are

$$
\begin{aligned}
\dot{q} &= \nabla_t q = \frac{p}{m} = g(p,\cdot) \\
\dot{p} &= \nabla_t p = \nabla_t \dot{q} = 0 \\
\dot{Q} &= \nabla_t Q = \frac{P}{m} \\
\dot{P} &= \nabla_t P = -\big(R(p,\cdot)\cdot, p\big)\, Q
\end{aligned}
\tag{3.15}
$$

where the last equation reads in normal coordinates

$$
\dot{P}^c_e = -R_a{}^c{}_{bd}\, p^a p^b\, Q^d_e \,.
$$

Solutions to these equations exist because g and R fulfill global Lipschitz conditions due to $\mathcal{M}$ being of bounded geometry and thus the Picard-Lindelöf theorem is applicable, keeping in mind that p is constant.

Before we can state our theorem about our modified Gaussians as approximate solutions, we have to say something about the properties of Q and P under the influence of a time-derivative. The following goes analogue to the flat case and is strongly adopted from Lemma 1.4 in [Lub08]. As we finally work on $\mathbb{R}^n$, it is just a rewriting and a restatement for $Q, P \in \Gamma(q^* \operatorname{End}(T\mathcal{M}) \otimes \mathbb{C})$.

Lemma 11. *Let $Q, P \in \Gamma(q^* \operatorname{End}(T\mathcal{M}) \otimes \mathbb{C})$ and let $Q(t), P(t) \in \mathbb{C}^{n\times n}$ be their expression on the normal coordinate frame relative to $\Phi_{q(t)}$. Suppose they satisfy*

$$
\begin{aligned}
\dot{Q}(t) &= F(t)P(t) \\
\dot{P}(t) &= G(t)Q(t)
\end{aligned}
$$

with real symmetric matrices $F(t), G(t)$. If relations (3.4) *hold at $t = 0$, then they hold for all t.*

Proof. We simply calculate the time-derivative

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\left(Q^*P - P^*Q\right) &= \dot{Q}^*P + Q^*\dot{P} - \dot{P}^*Q - P^*\dot{Q} \\ &= P^*FP - Q^*GQ - Q^*GQ - P^*FP \\ &= 0\end{aligned}$$

and the same yields for $\frac{\mathrm{d}}{\mathrm{d}t}\left(Q^TP - P^TQ\right) = 0$ □

Now we have all parts together to formulate our theorem about approximate solutions on $\mathbb{R}^n$. We show that ϕ_t approximately fulfills a local Schrödinger equation as partial differential equation on regions $\Phi^{-1}_{q(t)}(B^{\rho/2})$ where the cutoff is equal to one.

Theorem 12 (Main Solution Theorem). *Let* $[q(t), p(t), Q(t), P(t)]$ *be as above and for* $0 \le t \le T$ *be a solution of the equations of motion* (3.15) *with* $S(t)$ *the corresponding action* (2.4) *and initial conditions* $q(0), p(0), S(0)$ *and* $Q(0), P(0)$ *satisfying the relations* (3.4). *Then the modified Hagedorn Gaussian in the normal coordinate system* y *on* $\mathbb{R}^n$,

$$\begin{aligned}\phi_t(y) &= \phi[p(t), Q(t), P(t)](y,t) \\ &= \exp\left(\frac{\mathrm{i}}{\varepsilon}S(t)\right)\varphi[p(t), Q(t), P(t)](y,t)\end{aligned}$$

with

$$\begin{aligned}&\varphi[p(t), Q(t), P(t)](y,t) = \\ &\qquad (\pi\,\varepsilon)^{-n/4}(\det Q)^{-1/2}\exp\left(\frac{\mathrm{i}}{2\,\varepsilon}\,y^a\,\left(P\,Q^{-1}\right)_{ab}\,y^b + \frac{\mathrm{i}}{\varepsilon}\,p_c\,y^c\right)\end{aligned}$$

and $p_c = g_{cd}p^d$, *is an approximate solution of order* $\mathcal{O}\left(\varepsilon^{3/2}\right)$ *to this partial differential equation on* $\Phi^{-1}_{q(t)}(B^{\rho/2})$

$$\mathrm{i}\,\varepsilon\frac{\partial}{\partial t}\phi_t(y) + \frac{\varepsilon^2}{2m}\,\Delta^{nc}_{LB}\,\phi_t(y) = \mathcal{O}\left(\varepsilon^{3/2}\right)\,. \tag{3.16}$$

Remark 1. We do all calculation within the region of mapped $B^{\rho/2} := B^{\rho/2}_{q(t)}$ where the cutoff $\tilde{\chi}_{q(t)} = 1$. We show later in 3.6 that all other regions do not contribute.

Remark 2. In terms of pull backs this equation reads

$$\Phi^*_{q(t)}\,\mathrm{i}\varepsilon\frac{\mathrm{d}}{\mathrm{d}t}\left({\Phi^{-1}_{q(t)}}^*\phi_t\right) - \Phi^*_{q(t)}\,H\,{\Phi^{-1}_{q(t)}}^*\phi_t = \mathcal{O}\left(\varepsilon^{3/2}\right)$$

meaning that this approximate solution is also an approximate solution to the time-dependent Schrödinger equation on $\mathcal{M}$ (3.3). This will be shown later in theorem 14, page 65.

Remark 3. Remember again that in normal coordinates along $q(t)$ we can easily move indices up and downwards by using that $g_{ab}\left(q(t)\right) = \delta^b_a$. We will heavily make use of that property in the following calculations.

Proof Main Solution Theorem. We show by a direct calculation that ϕ obeys the Schrödinger equation up to order $\mathcal{O}\left(\varepsilon^{3/2}\right)$ comparing terms of every order of y. Keeping in mind that Gaussian wave packets are centered around 0 with $|y| \sim \sqrt{\varepsilon}$, this means that $\left\|y\,\phi_t\right\| = \mathcal{O}\left(\sqrt{\varepsilon}\right)$ and similar for higher orders. A profound argument about this property can be found in lemma 15, page 67. Furthermore, because $\mathcal{M}$ is of bounded geometry, all curvature components and their derivatives are bounded. This altogether leads to the equations of motion (3.15).

Because we have to deal with an exponential Gaussian function, we can simply divide by ϕ after executing the derivatives, leaving just the derivatives of the exponents. These can be ordered up to y^2 and compared separately. So in the following we write down the derivatives according to t and y separately and then we compare real and imaginary parts of each side and order.

First we start with the right hand side, calculating the Laplace-Beltrami operator in normal coordinates acting on the modified Hagedorn wave packet.

$$-\frac{\varepsilon^2}{2m}\,\Delta^{nc}_{LB}\,\phi = -\frac{\varepsilon^2}{2m}\Big[\delta^{ab}\partial_a\partial_b + y^c y^d \frac{1}{3}R^{a\ \ b}_{\ c\ \ d}\,\partial_a\partial_b \qquad (3.17)$$
$$- y^c\,\frac{2}{3}\,\mathrm{Ric}_{cb}\,\partial_b$$
$$+ y^c y^d\left(-\frac{5}{6}\partial_c\,\mathrm{Ric}_{bd} + \frac{5}{12}\left(\partial_b\,\mathrm{Ric}_{cd}\right)\right)\partial_b\Big]\phi$$
$$+\mathcal{O}\left(|y|^3\right)$$

Here we reordered the terms according to their contribution to $\mathcal{O}\left(|y|^n\right)$. In fact only the first two terms are needed. The second and third line of the equation above only have one y-derivatives acting on ϕ leading to terms of higher order. This can be shown exemplarily using the second line.

Differentiating the exponent leads to

$$\frac{\varepsilon^2}{2m}\,y^a\,\frac{2}{3}\,\mathrm{Ric}_{ab}\,\partial_b\left(\frac{\mathrm{i}}{2\,\varepsilon}\,y^c\,\left(P\,Q^{-1}\right)_{cd}\,y^d + \frac{\mathrm{i}}{\varepsilon}\,p_e\,y^e\right)$$
$$= \frac{\mathrm{i}\,\varepsilon}{6m}\,y^a\,\mathrm{Ric}_{ab}\,\delta^c_b\,\left(P\,Q^{-1}\right)_{cd}\,y^d$$
$$+\frac{\mathrm{i}\,\varepsilon}{6m}\,y^a\,\mathrm{Ric}_{ab}\,y^c\,\left(P\,Q^{-1}\right)_{cd}\,\delta^d_b$$
$$+\frac{\mathrm{i}\,\varepsilon}{3m}\,y^a\,\mathrm{Ric}_{ab}\,p_e\delta^e_b$$

Investigating the different orders we clearly see that the first two terms are of order $\mathcal{O}\left(\varepsilon\cdot y^2\right) = \mathcal{O}\left(\varepsilon^2\right)$, keeping in mind that $y = \mathcal{O}\left(\sqrt{\varepsilon}\right)$. The third term then is of order $\mathcal{O}\left(\varepsilon\cdot y\right) = \mathcal{O}\left(\varepsilon^{3/2}\right)$. So whenever there is only one derivative with respect to y within the Laplace-Beltrami operator falling on the wave packet in (3.17) it yields terms of higher order.

This leaves only the second order derivatives. Of course the single second order Laplace term reproduces the same terms as the flat case. So we get as zeroth order in y:

$$\frac{p_a^2}{2m} - \frac{\mathrm{i}\,\varepsilon}{2m}\left(P\,Q^{-1}\right)_{aa}$$

Now we apply to the time-derivative on the left-hand side the same procedure of ordering terms according to their contribution to $\mathcal{O}\left(|y|^n\right)$:

$$\begin{aligned}\mathrm{i}\,\varepsilon\frac{\mathrm{d}}{\mathrm{d}t}\phi(t,y) &= \mathrm{i}\,\varepsilon\frac{\mathrm{d}}{\mathrm{d}t}\phi(t,\Phi_{q(t)}^{-1}(x)) \\ &= \mathrm{i}\,\varepsilon\frac{\partial}{\partial t}\phi + \mathrm{i}\,\varepsilon\frac{\partial}{\partial y}\phi\cdot\frac{\partial}{\partial t}\Phi_{q(t)}^{-1}(x) \end{aligned} \tag{3.18}$$

Continuing with the first term

$$\begin{aligned}\mathrm{i}\,\varepsilon\frac{1}{\phi}\frac{\partial}{\partial t}\phi = &-\dot{S} + (\det Q)^{1/2}\,\mathrm{i}\,\varepsilon\frac{\mathrm{d}}{\mathrm{d}t}(\det Q)^{-1/2} \\ &+\mathrm{i}\,\varepsilon\frac{\partial}{\partial t}\left(\frac{\mathrm{i}}{2\,\varepsilon}y^c\left(P\,Q^{-1}\right)_{cd}y^d + \frac{\mathrm{i}}{\varepsilon}p_e y^e\right)\end{aligned} \tag{3.19}$$

with $-\dot{S} = -\frac{p_a^2}{2m}$.

Furthermore the derivative of $\det Q(t)$ can be calculated according to Jacobi's formula

$$\begin{aligned}\mathrm{i}\,\varepsilon\frac{\mathrm{d}}{\mathrm{d}t}(\det Q)^{-1/2} &= -\mathrm{i}\,\varepsilon\frac{1}{2}(\det Q)^{-3/2}\frac{\mathrm{d}}{\mathrm{d}t}(\det Q) \\ &= -\mathrm{i}\,\varepsilon\frac{1}{2}(\det Q)^{-1/2}\,\mathrm{tr}\left(Q^{-1}\frac{\mathrm{d}}{\mathrm{d}t}Q(t)\right) \\ &= -\frac{\mathrm{i}\,\varepsilon}{2m}\left(P\,Q^{-1}\right)_{aa}(\det Q)^{-1/2}\end{aligned}$$

where we used that $\dot{Q}(t) = P(t)/m$ and the last factor goes back into the normalization of ϕ.

Now we can proceed according to section 3.3.1 with the second term of (3.18). As we choose the vector field $Y(t)$ to be the exponential mapping, i. e. $Y(t) = \exp_{q(t)}^{-1}(x)$, we get the Riemann normal coordinates by choosing a basis for $T\mathcal{M}$ and calculating $y^i(t) = \langle Y(t), e_i(t) \rangle$. Hence the derivative according to t can be calculated as

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\phi(t, \langle Y(t), e_i(t)\rangle) &= \frac{\partial}{\partial t}\phi + \frac{\partial}{\partial y}\phi \cdot \frac{\partial}{\partial t}\langle Y(t), e_i(t)\rangle \\
&= \frac{\partial}{\partial t}\phi + \frac{\partial}{\partial y}\phi \cdot \left(\left\langle \frac{\partial}{\partial t} Y(t), e_i(t) \right\rangle + \left\langle Y(t), \frac{\partial}{\partial t} e_i(t) \right\rangle \right) \\
&= \frac{\partial}{\partial t}\phi + \frac{\partial}{\partial y}\phi \cdot \left\langle \frac{\partial}{\partial t} Y(t), e_i(t) \right\rangle
\end{aligned}
$$

Because the frame $e_i(t)$ is parallel transported along the geodesic on $\mathcal{M}$, its t-derivation is zero on $T\mathcal{M}$.

So we just need the derivation of the exponential mapping $\frac{\partial}{\partial t} Y(t) = \frac{\partial}{\partial t} \exp^{-1}_{q(t)}(x)$ derived above in (3.11) rewritten directly in normal coordinates.

$$
\begin{aligned}
\frac{\partial}{\partial t}\Phi^{-1}_{q(t)}(x) = \frac{\mathrm{d}}{\mathrm{d}t} y^a(t) = \left\langle \frac{\mathrm{d}}{\mathrm{d}t} Y(t), e_a \right\rangle &= \left\langle \frac{\mathrm{d}}{\mathrm{d}t} \exp^{-1}_{q(t)}(x), e_a \right\rangle \\
&= -\dot{q}^a(t) - \frac{1}{3} R_{acdb} y^c y^d \dot{q}^b + \mathcal{O}\left(y^3\right) \qquad (3.20)
\end{aligned}
$$

Finally we have calculated all terms of the time-derivative according to third y-order. Using only the zeroth order, $\mathrm{i}\,\varepsilon \partial_a \phi = -p_a$ and $-\dot{q}^a(t) = \frac{-p_a}{m}$ we reproduce the same terms as for the Laplacian side and the equation is fulfilled.

Now we can proceed with the terms of first order in y. Again only the zeroth order Laplacian term with the single second order derivative leads to terms. For the second order derivation of the exponential according to y only the mixed terms contribute

$$
\begin{aligned}
&\frac{-\varepsilon^2}{2m} \partial_a^2 \left(\frac{\mathrm{i}}{2\,\varepsilon} y^c \left(P Q^{-1}\right)_{cd} y^d + \frac{\mathrm{i}}{\varepsilon} p_e y^e \right) \\
&\qquad = \frac{-\varepsilon^2}{2m} \left(\frac{\mathrm{i}}{2\,\varepsilon} y^c \left(P Q^{-1}\right)_{ca} + \frac{\mathrm{i}}{2\,\varepsilon} \left(P Q^{-1}\right)_{ad} y^d \right) \cdot \left(\frac{\mathrm{i}}{\varepsilon} p_a \right) \\
&\qquad = \frac{p_a}{2m} y^c \left(P Q^{-1}\right)_{ca} + \frac{p_a}{2m} \left(P Q^{-1}\right)_{ad} y^d
\end{aligned}
$$

In case of the time-derivative only terms of the third part of (3.19) and first part of (3.20) give higher order terms in y.

$$\begin{aligned}
&\mathrm{i}\,\varepsilon\frac{\partial}{\partial t}\left(\frac{\mathrm{i}}{2\,\varepsilon}y^c\left(PQ^{-1}\right)_{cd}y^d+\frac{\mathrm{i}}{\varepsilon}p_e y^e\right)+\mathrm{i}\,\varepsilon\partial_a\phi\frac{\partial}{\partial t}\Phi^{-1}_{q(t)}(x)\\
&=-\dot{p^a}y_a+\mathrm{i}\,\varepsilon\partial_a\left(\frac{\mathrm{i}}{2\,\varepsilon}y^c\left(PQ^{-1}\right)_{cd}y^d+\frac{\mathrm{i}}{\varepsilon}p_e y^e\right)\cdot\left(-\dot{q^a}(t)\right)\\
&=-\dot{p^a}y_a+\frac{p_a}{2m}y^c\left(PQ^{-1}\right)_{ca}+\frac{p_a}{2m}\left(PQ^{-1}\right)_{ad}y^d
\end{aligned}$$

again with $-\dot{q^a}(t)=\frac{-p_a}{m}$. According to our initial value with fixed p and $V=0$, the equation is fulfilled with $\dot{p}=0$, (3.15).

At last the terms of second order in y coming from the Laplacian look like

$$\frac{1}{2m}y^a\left(PQ^{-1}\right)^2_{ab}y^b+y^c y^d\frac{1}{6m}R^{a\ \,b}_{\ c\ \,d}p_a p_b$$

Furthermore for the terms of second order in y coming from the time-derivative, we have to calculate a bit more.

$$\begin{aligned}
&-\frac{1}{2}y^a\frac{\mathrm{d}}{\mathrm{d}t}\left(PQ^{-1}\right)_{ab}y^b+p_a\frac{1}{3}R^a_{cdb}y^c y^d\dot{q}^b\\
&=-\frac{1}{2}y^a\left(\dot{P}Q^{-1}\right)_{ab}y^b-\frac{1}{2}y^a\left(P\dot{Q}^{-1}\right)_{ab}y^b+p_a\frac{1}{3m}R^{a\ \,d}_{\ c\ \,b}y^c y^d p_b\\
&=\frac{1}{2m}y^a\left(PQ^{-1}\right)^2_{ab}y^b-\frac{1}{2}y^a\left(\dot{P}Q^{-1}\right)_{ab}y^b-p_a\frac{1}{3m}R^{a\ \,b}_{\ c\ \,d}y^c y^d p_b
\end{aligned}$$

The last step included first a index exchange in the last pair of the Riemann tensor, and second the following simple calculation:

$$\frac{\mathrm{d}}{\mathrm{d}t}Q^{-1}(t)=-Q^{-2}(t)\dot{Q}(t)=-Q^{-2}(t)\frac{1}{m}P.$$

This leaves the last equation for the proof of the main theorem:

$$
\begin{aligned}
y^c y^d \frac{1}{6m} R^{a\ \ b}_{\ c\ \ d} p_a p_b &= -\frac{1}{2} y^c \left(\dot{P} Q^{-1}\right)_{cd} y^d - p_a \frac{1}{3m} R^{a\ \ b}_{\ c\ \ d} y^c y^d p_b \\
\frac{1}{2} \left(\dot{P} Q^{-1}\right)_{cd} &= -\frac{1}{2} R^{a\ \ b}_{\ c\ \ d} p_a p_b \\
\dot{P}^c_e &= -R_{a\ \ bd}^{\ \ c} p^a p^b Q^d_e .
\end{aligned}
$$

Now if we rewrite every particular equation in a coordinate free form, the equations of motion (3.15) are reproduced. □

3.5.2 The Geodesic Equation

The proof shows that the equation necessary for $p(t)$ parallel transported along $q(t)$ is $\dot{p} = \nabla_t p = 0$. Furthermore the proof gives $\dot{q} = p/m$. So together it holds that $\nabla_t \dot{q}=0$.

Because $q(0)$ is the base point for the definition of the Riemann coordinate mapping $\Phi_{q(0)}$ and so is $q(t)$ and $\Phi_{q(t)}$. This means that for $V = 0$ the curve $q(t)$ on $\mathcal{M}$ is determined by the geodesic equation on $\mathcal{M}$ within U_{q_0}

$$
\ddot{q}^m + \Gamma^m_{kl} \dot{q}^k \dot{q}^l = 0
$$

where Γ^m_{kl} are the Christoffel symbols and $q^k(t)$ are the coordinate curves of $q(t)$ in Riemann normal coordinates. The Christoffels are zero in q_0, leaving

$$
\ddot{q}^m(t_0) = \nabla_t \dot{q} = 0 \tag{3.21}
$$

and thus $q(t)$ has to be a geodesic for $t \in I$, solving the geodesic equation. This also means that the modified Hagedorn wave packet follows straight lines on $\mathcal{M}$ which are the geodesics, similar to the flat case.

3.5.3 The Effective Schrödinger Equation for Modified Hagedorn Wave Packets

Analysing the calculations for proving the main theorem, one can state an effective Schrödinger-type like partial differential equation for the modified Hagedorn wave packets in normal coordinates.

Remark 4. Let φ be a wave packet according to our definition (17) and $\phi|_{t_0} \in L^2(\mathbb{R}^n)$ be the full Hagedorn wave packet. Furthermore we assume the same conditions as in theorem (12), especially the ones for the Hagedorn parameters. Then $\phi_t(y)$ approximately solves

$$\mathrm{i}\varepsilon \frac{\partial}{\partial t} \phi_t(y) = -\frac{\varepsilon^2}{2m} \Bigg[\underbrace{\delta^{ab} \partial_a \partial_b + y^c y^d \frac{1}{3} R^a{}_c{}^b{}_d \, \partial_a \partial_b}_{=: \Delta^{nc}_{LB,\mathrm{eff}}} \Bigg] \phi_t(y) + \mathcal{O}\left(\varepsilon^{3/2}\right) .$$

This is just a close follow up to the calculations done in the previous proof. Only those terms of the Laplace-Beltrami operator in normal coordinates contribute which contain second order derivatives in y.

3.5.4 Difference to the Flat Case: Sectional Curvature

If we compare the new equations of motion for the Hagedorn parameter to the flat case, where $\mathcal{M} = \mathbb{R}^n$ we see that only the equation for P changes. It now involves a curvature dependent term. Here we want to shortly analyze what this term could mean. Therefore we give a definition for the sectional curvature, one way to describe curvature of Riemannian manifolds.

Definition 19 (Sectional Curvature)**.** Let $\mathcal{M}$ be a Riemannian manifold of dimension $n \geq 2$. For $x \in M$ given a two-dimensional subspace $\sigma \subset T_x\mathcal{M}$, spanned by u, v, the sectional curvature is defined as

$$K(u,v) := \frac{\langle R(u,v)v, u\rangle}{\|u\|^2 \, \|v\|^2 - \langle u,v\rangle^2}$$

If the sectional curvature K is constant, that means for all $x \in \mathcal{M}$ and u, v resp. all two-dimensional subspaces $\sigma \subset T_x\mathcal{M}$

$$K(u,v) = K = \text{const.}$$

then the Riemannian can be written as

$$R(u,v)w = K \cdot \Big(\langle w, v\rangle\, u - \langle w, u\rangle\, v \Big) \quad \text{for } u, v, w \in \mathrm{T}_x\,\mathcal{M}$$

Using coordinates this is similar to

$$\begin{aligned} R^a_{cbd}\,\partial_a &= R(\partial_b, \partial_d)\partial_c = K \cdot \Big(\big\langle \partial_c, \partial_d \big\rangle\, \partial_b - \big\langle \partial_c, \partial_b \big\rangle\, \partial_d \Big) \\ &= K \cdot \Big(g_{cd}\,\delta^a_b - g_{cb}\,\delta^a_d \Big)\partial_a \end{aligned}$$

which yields

$$\begin{aligned} R^a_{cbd} &= K \cdot \Big(g_{cd}\,\delta^a_b - g_{cb}\,\delta^a_d \Big) \\ R_a{}^c{}_{bd} &= K \cdot \Big(g^c_d\,\delta_{ab} - g^c_b\,\delta_{ad} \Big) \end{aligned}$$

Thus the equation of motion for P on Riemannian manifolds with constant sectional curvature can be associated with the sectional curvature K.

$$\dot{P} = -\,\big\langle R(\cdot, p)p, \cdot \big\rangle\, Q$$

in normal coordinates

$$\dot{P}^c_e = -R_a{}^c{}_{bd}\, p^a p^b\, Q^d_e = -K \cdot \Big(g^c_d\,\delta_{ab} - g^c_b\,\delta_{ad} \Big) p^a p^b\, Q^d_e$$

Because P is connected with the packet momentum width (3.5), we can observe the following for the change of the momentum width in time

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\sigma_p &= \sqrt{\frac{\varepsilon}{2}}\frac{\mathrm{d}}{\mathrm{d}t}\det P \\ &= \sqrt{\frac{\varepsilon}{2}}\det P\;\mathrm{tr}(P^{-1}\dot{P}) \text{ which is proportional to } -K. \end{aligned} \tag{3.22}$$

For Riemannian manifolds with constant sectional curvature, there exist three possible cases

- negative curvature, hyperbolic geometry, e. g. hyperbolic space, geodesics diverge
- zero curvature, Euclidian geometry, e. g. Euclidian space, geodesics are straight lines
- positive curvature, spherical space, e. g. unit sphere, geodesics converge

If $K > 0$ then the change of momentum width (3.22) seems to be negative and the momentum width decreases, which means that the wave packet gets narrower. As on elliptic manifolds geodesics converge and the wave packet moves along those geodesics, this behavior agrees with our formula for $\dot{P}$.

Vice versa if $K < 0$, the change of momentum width seems to be positive and the momentum width increases, which means that the wave packet spreads. This fits the behavior of our wave packets on hyperbolic manifolds, following diverging geodesics.

We neglected in this discussion the sign of the other terms appearing in (3.22), which must be calculated in coordinates, but we haven't done it rigorously.

In conclusion the extra term in the equation of motion for P compared to the flat case, should agree with the dynamics of an Hagedorn wave packet following geodesics on Riemannian manifolds with constant sectional curvature.

3.5.5 About Solutions for Potentials

Our main result is about the free Schrödinger equation on the Riemannian manifold $\mathcal{M}$ without any potential. We restricted the main part of this thesis to the free case, because new insights only arise from the curvature and an additional potential term would have created less focus. In this subsection we shortly want to mention the case with a potential.

If $\mathcal{M} = \mathbb{R}^n$ a Hagedorn wave packet still is an exact solution to the Schrödinger equation, if a potential V is quadratic. If V is cubic or higher, one can still prove an error bound ([Hag98]).

If $\mathcal{M}$ is a Riemannian manifold with constant curvature and bounded geometry, then even if there is no potential, a modified Hagedorn wave packet in normal coordinates is an approximation to the full solution and the parameters have to solve slightly modified equations. In this case, $q(t)$ is a geodesic and obeys the geodesic equation (3.21). The first point is still valid, if there is a potential $V \neq 0$ and the only additional terms are the same as in the flat case. But now, $q(t)$ is no longer a geodesic, but has to solve a potential equation. So, consider the following equations of motion,

$$
\begin{aligned}
\dot{q} &= \nabla_t q = \frac{p}{m} = g(p,\cdot) \qquad (3.23)\\
\dot{p} &= \nabla_t p = \nabla_t \dot{q} = -\nabla V(q)\\
\dot{Q} &= \nabla_t Q = \frac{P}{m}\\
\dot{P} &= \nabla_t P = -\big(R(p,\cdot)\cdot, p\big)\, Q - \nabla^2 V(q)
\end{aligned}
$$

where V is a multiplication operator with linearization along $q(t)$.

Then, a similar result for the approximated solution like before is possible.

Corollary 13. *Let $V \neq 0$ be a potential with $V \in C^\infty(\mathcal{M})$. Let the parameters $[q(t), p(t), Q(t), P(t)]$ be as above and for $0 \leq t \leq T$ be a solution of the equations of motion* (3.23) *with $S(t)$ the corresponding action* (2.4) *and initial conditions $q(0), p(0), S(0)$ and $Q(0), P(0)$ satisfying the relations* (3.4)*. Then the modified Hagedorn Gaussian*

$$\phi[p(t), Q(t), P(t)](y, t) = \exp\left(\frac{\mathrm{i}}{\varepsilon} S(t)\right) \varphi[p(t), Q(t), P(t)](y, t)$$

with

$$\varphi[p(t),Q(t),P(t)](y,t) = \\ (\pi\,\varepsilon)^{-n/4}(\det Q)^{-1/2}\,\exp\left(\frac{\mathrm{i}}{2\,\varepsilon}\,y^a\,\left(P\,Q^{-1}\right)_{ab}\,y^b + \frac{\mathrm{i}}{\varepsilon}\,p_c\,y^c\right)$$

is an approximate solution of order $\mathcal{O}\left(\varepsilon^{3/2}\right)$ the following partial differential equation on $\Phi^{-1}_{q(t)}(B^{\rho/2}) \subset \mathbb{R}^n$

$$\mathrm{i}\,\varepsilon\frac{\partial}{\partial t}\phi_t(y) = (-\frac{\varepsilon^2}{2m}\,\Delta^{nc}_{LB} + V)\phi_t(y) + \mathcal{O}\left(\varepsilon^{3/2}\right)$$

Proof. First we expand the potential in orders of the normal coordinate y.

$$V(q) = V(q) + (\nabla V)(q)y + (\nabla^2 V)(q)y^2 + \mathcal{O}\left(|y|^3\right)$$

Then we mimic the proof of our main theorem 12 and keep track of the order terms of V. This yields after a similar lengthy calculation as in 12, that the equations of motion (3.23) are valid. □

3.6 Error Analysis

In this section we want to give an error approximation for the modified Hagedorn wave packet on manifolds. The focus lies on a first analysis without optimality of constants or error size. For notational simplicity any constant C can be different.

3.6.1 Error for the Solution on $\mathcal{M}$

We present an upper error bound which clearly is not optimal, but sufficient for a first impression. For the error bound we start with an initial wave packet on $\mathbb{R}^n$, which is an approximate solution to (3.16), as shown in theorem 12. Now we show that it also approximates the full solution on $\mathcal{M}$.

We choose ρ to be independent of t by

$$\rho = \min \rho_{q(t)} \quad \text{for all } t \in [0, T].$$

Furthermore we choose a smooth time-independent cutoff χ_r, satisfying definition (10). This leads to the following main error statement about our modified Hagedorn wave packet.

Theorem 14 (Main Error Theorem). *Let ϕ_0 be the initial Hagedorn wave packet on $\mathbb{R}^n$ and $\Psi_0(x) = {\Phi_{q(0)}^{-1}}^* \chi_r \phi_0(y)$ with cutoff χ_r the mapped initial wave packet on $\mathcal{M}$. Let $q(t)$ be a solution to the geodesic equation on $\mathcal{M}$. Furthermore let Ψ_t be the solution to the full Schrödinger equation on $\mathcal{M}$* (3.3) *with initial wave function $\Psi_0 = \Psi_0$. Let $\Psi_{t,\text{trunc}} = {\Phi_{q(t)}^{-1}}^* \phi_{t,\text{trunc}} = {\Phi_{q(t)}^{-1}}^* \chi_r \phi_t$ the truncated and mapped wave packet with ϕ_t fulfilling* (3.16) *of our main solution theorem 12. Then a bound for the approximation error on $\mathcal{M}$ with $r = \rho/2$ is given by*

$$\left\| \Psi_t - \Psi_{t,\text{trunc}} \right\|_{L^2(\mathcal{M})} \leq C \varepsilon^{1/2}$$

for any $t \in [0, T]$ with C a constant independent of ε.

Proof. We use a standard Duhamel type argument also known as variation of constants formula.

$$\begin{aligned}
&\left\| \Psi_t - \Psi_{t,\text{trunc}} \right\|_{L^2(\mathcal{M})} = \\
&= \left\| \mathrm{e}^{-\mathrm{i}/\varepsilon\, t H} \Psi_0 - {\Phi_{q(t)}^{-1}}^* \phi_{t,\text{trunc}} \right\|_{L^2(\mathcal{M})} \\
&= \left\| \mathrm{e}^{-\mathrm{i}/\varepsilon\, t H} {\Phi_{q(0)}^{-1}}^* \chi_r \phi_0 - {\Phi_{q(t)}^{-1}}^* \phi_{t,\text{trunc}} \right\| \\
&= \left\| {\Phi_{q(0)}^{-1}}^* \chi_r \phi_0 - \mathrm{e}^{\mathrm{i}/\varepsilon\, t H} {\Phi_{q(t)}^{-1}}^* \phi_{t,\text{trunc}} \right\| \\
&= \left\| \int_0^t \frac{\mathrm{d}}{\mathrm{d}s} \left({\Phi_{q(0)}^{-1}}^* \chi_r \phi_0 - \mathrm{e}^{\mathrm{i}/\varepsilon s H} {\Phi_{q(s)}^{-1}}^* \phi_{s,\text{trunc}} \right) \mathrm{d}s \right\| \\
&= \left\| \int_0^t -\mathrm{e}^{\mathrm{i}/\varepsilon s H} \left(\frac{\mathrm{i}}{\varepsilon} H {\Phi_{q(s)}^{-1}}^* \phi_{s,\text{trunc}} + {\dot{\Phi}_{q(s)}^{-1}}{}^* \phi_{s,\text{trunc}} + {\Phi_{q(s)}^{-1}}^* \dot{\phi}_{s,\text{trunc}} \right) \mathrm{d}s \right\|
\end{aligned}$$

$$
\begin{aligned}
&\leq t \sup_{s\in[0,t]} \left\| \frac{\mathrm{i}}{\varepsilon} \Phi_{q(s)}^{-1}{}^{*} \left(\Phi_{q(s)}^{*} H \, \Phi_{q(s)}^{-1}{}^{*} \phi_{s,\mathrm{trunc}} - \Phi_{q(s)}^{*} \, \mathrm{i}\varepsilon \dot{\Phi}_{q(s)}^{-1}{}^{*} \phi_{s,\mathrm{trunc}} - \mathrm{i}\varepsilon \dot{\phi}_{s,\mathrm{trunc}} \right) \right\| \\
&\leq \frac{t}{\varepsilon} \sup_{s\in[0,t]} \left\| \Phi_{q(s)}^{*} H \, \Phi_{q(s)}^{-1}{}^{*} \phi_{s,\mathrm{trunc}} - \Phi_{q(s)}^{*} \, \mathrm{i}\varepsilon \frac{\mathrm{d}}{\mathrm{d}s} \left(\Phi_{q(s)}^{-1}{}^{*} \phi_{s,\mathrm{trunc}} \right) \right\|_{L^2(\mathcal{M})} \\
&= \frac{t}{\varepsilon} \sup_{s\in[0,t]} \left\| \Phi_{q(s)}^{*} H \, \Phi_{q(s)}^{-1}{}^{*} \phi_{s,\mathrm{trunc}} - \Phi_{q(s)}^{*} \, \mathrm{i}\varepsilon \frac{\mathrm{d}}{\mathrm{d}s} \left(\Phi_{q(s)}^{-1}{}^{*} \phi_{s,\mathrm{trunc}} \right) \right\|_{L^2(B^{\rho})} \\
&\leq \frac{t}{\varepsilon} \sup_{s\in[0,t]} \left\| \Phi_{q(s)}^{*} H \, \Phi_{q(s)}^{-1}{}^{*} \phi_{s,\mathrm{trunc}} - \Phi_{q(s)}^{*} \, \mathrm{i}\varepsilon \frac{\mathrm{d}}{\mathrm{d}s} \left(\Phi_{q(s)}^{-1}{}^{*} \phi_{s,\mathrm{trunc}} \right) \right\|_{L^2(B^{\rho/2})} \\
&\quad + \frac{t}{\varepsilon} \sup_{s\in[0,t]} \left\| \Phi_{q(s)}^{*} H \, \Phi_{q(s)}^{-1}{}^{*} \phi_{s,\mathrm{trunc}} - \Phi_{q(s)}^{*} \, \mathrm{i}\varepsilon \frac{\mathrm{d}}{\mathrm{d}s} \left(\Phi_{q(s)}^{-1}{}^{*} \phi_{s,\mathrm{trunc}} \right) \right\|_{L^2(B^{\rho}/B^{\rho/2})} \\
&\leq C \, \varepsilon^{1/2}
\end{aligned}
$$

for any $t \in [0,T]$ and $B^{\rho} := B^{\rho}_{q(s)} \subset \mathcal{M}$.

The third step can be done because the propagator of $H = \frac{-\varepsilon^2}{2m} \Delta_{\mathrm{LB}}$ is unitary on $\mathcal{M}$. Furthermore $\Phi_{q(s)}^{-1}{}^{*}$ is bounded because it is a mapping on a manifold of bounded geometry.

Then for the eighth step, because we are only dealing with functions living on B^{ρ} we can restrict the norm to $L^2(B^{\rho})$. This is remarkable and due to our construction of the modified Gaussian wave packet.

For $L^2(B^{\rho/2})$ we can directly substitute $\phi_{s,\mathrm{trunc}}$ with ϕ_s, which satisfies (3.16) , because within the ball of radius $\rho/2$ they are equal by construction. Then the expression in the norm fulfills theorem 12, p. 53 and is of order $\mathcal{O}\left(\varepsilon^{3/2}\right)$.

Each term in the second norm is small on its own and the last step follows using the lemmas down below. □

Thus our modified Hagedorn wave packet is not an exact solution to the free Schrödinger equation on $\mathcal{M}$ like in the flat case on $\mathbb{R}^n$, but an approximation of order $\mathcal{O}\left(\varepsilon^{1/2}\right)$. Nonetheless for most practical purposes, where one starts with a wave packet and is interested in its dynamics and centre of mass, our approximation gives a good result.

3.6.2 Necessary Bounds

In this subsection we give additional approximations needed for the main error. The first one is the most important one, because all other approximations can be tracked back to this. It further gives the reason for expanding up to orders of y in all our previous results.

Lemma 15. *Let ϕ_t be the wave packet fulfilling* (3.16) *on $\mathbb{R}^n$ of our main theorem 12 with initial condition ϕ_0. Let $\alpha = (\alpha_1, \ldots, \alpha_n)$ be a multiindex with $|\alpha| = \alpha_1 + \cdots + \alpha_n$. Then the norm of ϕ_t multiplied by any y^α outside a ball of radius $\rho/2$ is exponentially small,*

$$\left\| y^\alpha \phi_t \right\|_{L^2\left(\mathbb{R}^n \backslash B_0^{\rho/2}\right)} \leq C_n \exp(c_n/\varepsilon)$$

for any n.

Proof.

$$\begin{aligned}
&\left\| y^\alpha \phi_t \right\|_{L^2\left(\mathbb{R}^n \backslash B_0^{\rho/2}\right)} = \\
&= \left\| (\pi\,\varepsilon)^{-n/4} (\det Q)^{-1/2}\, y^\alpha \exp\left(\underbrace{\frac{\mathrm{i}}{2\,\varepsilon}\, y^T P\, Q^{-1}\, y}_{\in \mathbb{R}^n} + \frac{\mathrm{i}}{\varepsilon}\, p\, y \right) \right\| \\
&= (\pi\,\varepsilon)^{-n/2} (\det Q)^{-1} \int_{L^2\left(\mathbb{R}^n \backslash B_0^{\rho/2}\right)} y^\alpha \exp\left(\frac{\mathrm{i}}{\varepsilon}\, y^T P\, Q^{-1}\, y \right) \mathrm{d}y \\
&\overset{1}{\leq} (\pi\,\varepsilon)^{-n/2} (\det Q)^{-1} \int_{L^2\left(\mathbb{R}^n \backslash B_0^{\rho/2}\right)} y^\alpha \exp\left(-\frac{1}{\varepsilon} \lambda y^2 \right) \mathrm{d}y \\
&\overset{2}{=} (\pi\,\varepsilon)^{-n/2} (\det Q)^{-1} S_n \int_{\rho/2}^{\infty} r^{|\alpha|+n-1} \exp\left(-\frac{1}{\varepsilon} \lambda r^2 \right) \mathrm{d}r \\
&\overset{3}{=} \varepsilon^{|\alpha|/2} (\pi)^{-n/2} (\det Q)^{-1} S_n \int_{\frac{\rho}{2}/\sqrt{\varepsilon}}^{\infty} \bar{r}^{|\alpha|+n-1} \exp\left(-\lambda \bar{r}^2 \right) \mathrm{d}\bar{r}
\end{aligned}$$

$$
\begin{aligned}
&\overset{4}{=} C_n \varepsilon^{|\alpha|/2} \begin{cases} \frac{\partial^{k/2}}{\partial \lambda^{k/2}} \lambda^{-1/2} \int_{\frac{\rho}{2}\sqrt{\lambda/\varepsilon}}^{\infty} \exp\left(-\tilde{r}^2\right) \mathrm{d}\tilde{r} & \text{for } k \text{ even} \\ \frac{\partial^{(k-1)/2}}{\partial \lambda^{(k-1)/2}} \lambda^{-1} \int_{\frac{\rho}{2}\sqrt{\lambda/\varepsilon}}^{\infty} \tilde{r} \exp\left(-\tilde{r}^2\right) \mathrm{d}\tilde{r} & \text{for } k \text{ odd} \end{cases} \\
&\overset{5}{=} C_n \varepsilon^{|\alpha|/2} \begin{cases} \frac{\partial^{k/2}}{\partial \lambda^{k/2}} \lambda^{-1/2} \frac{\sqrt{\pi}}{2} \operatorname{erfc}\left(\frac{\rho}{2}\sqrt{\lambda/\varepsilon}\right) & \text{for } k \text{ even} \\ \frac{\partial^{(k-1)/2}}{\partial \lambda^{(k-1)/2}} \lambda^{-1} \left[-\frac{1}{2} \exp\left(-\tilde{r}^2\right)\right]_{\frac{\rho}{2}\sqrt{\lambda/\varepsilon}}^{\infty} & \text{for } k \text{ odd} \end{cases} \\
&\overset{6}{\leq} C_n \varepsilon^{|\alpha|/2} \begin{cases} \frac{\partial^{k/2}}{\partial \lambda^{k/2}} \lambda^{-1/2} \frac{\sqrt{\pi}}{2} \exp\left(-\frac{\lambda \rho^2}{4\varepsilon}\right) & \text{for } k \text{ even} \\ \frac{\partial^{(k-1)/2}}{\partial \lambda^{(k-1)/2}} \lambda^{-1} \frac{1}{2} \exp\left(-\frac{\lambda \rho^2}{4\varepsilon}\right) & \text{for } k \text{ odd} \end{cases} \\
&\leq C_n \exp(c_n/\varepsilon)
\end{aligned}
$$

where we define $C_n := (\pi)^{-n/2} (\det Q)^{-1} S_n$, $k := |\alpha| + n - 1$ and $c_n = \frac{-\lambda\rho^2}{4}$. The numbered steps use the following relations:

1. The exponent can be estimated by the smallest eigenvalue λ of the positive symmetric matrix PQ^{-1}:

   $$\mathrm{i}\, y^T PQ^{-1} y \leq -\lambda y^2$$

2. By using spherical coordinates we reduce the integral to a radius dependent one and separate the area of the hypersurface S_n from the volume of the multidimensional sphere or hypersphere V_n with radius R.

   $$V_n = \int_0^R S_n r^{n-1} \mathrm{d}r$$

where S_n can be calculated using the gamma function, resulting in

$$S_n = \begin{cases} \frac{2^{(n+1)/2}\pi^{(n-1)/2}}{(n-2)!!} & \text{for } n \text{ odd} \\ \\ \frac{2\pi^{n/2}}{(\frac{1}{2}n-1)!} & \text{for } n \text{ even} \end{cases}$$

3. Now we use the substitution

$$\begin{aligned} \bar{r} &= \varepsilon^{-1/2} r & r^{(|\alpha|+n-1)} &= \varepsilon^{(|\alpha|+n-1)/2}\,\bar{r} \\ \mathrm{d}\bar{r} &= \varepsilon^{-1/2}\mathrm{d}r & \rho &\mapsto \rho/\sqrt{\varepsilon} \end{aligned}$$

   This gives a single ε-dependency within the integral lower limit.

4. The integral can be evaluated by the following identities:

$$\begin{aligned} &\int_{\rho/\sqrt{\varepsilon}}^{\infty} \bar{r}^k \exp\left(-\lambda \bar{r}^2\right) \mathrm{d}\bar{r} = \\ &= -\int_{\rho/\sqrt{\varepsilon}}^{\infty} -\bar{r}^2 \exp\left(-\lambda \bar{r}^2\right) \bar{r}^{k-2}\mathrm{d}\bar{r} \\ &= -\frac{\partial}{\partial \lambda}\int_{\rho/\sqrt{\varepsilon}}^{\infty} \exp\left(-\lambda \bar{r}^2\right) \bar{r}^{k-2}\mathrm{d}\bar{r} \\ &= \left(-\frac{\partial}{\partial \lambda}\right)^2 \int_{\rho/\sqrt{\varepsilon}}^{\infty} \exp\left(-\lambda \bar{r}^2\right) \bar{r}^{k-4}\mathrm{d}\bar{r} \\ &= \cdots = \begin{cases} \left(-\frac{\partial}{\partial \lambda}\right)^{k/2} \int_{\rho/\sqrt{\varepsilon}}^{\infty} \exp\left(-\lambda \bar{r}^2\right) \mathrm{d}\bar{r} & \text{for } k \text{ even} \\ \\ \left(-\frac{\partial}{\partial \lambda}\right)^{(k-1)/2} \int_{\rho/\sqrt{\varepsilon}}^{\infty} \bar{r} \exp\left(-\lambda \bar{r}^2\right) \mathrm{d}\bar{r} & \text{for } k \text{ odd} \end{cases} \end{aligned}$$

5. Using the definition of the error function

$$\mathrm{erf}(x) := \frac{2}{\sqrt{\pi}} \int_0^x \exp(-t^2)\mathrm{d}t$$

one can define the complementary error function

$$\begin{aligned}\operatorname{erfc}(x) &:= 1 - \operatorname{erf}(x)\\ &= \frac{2}{\sqrt{\pi}} \int_x^\infty \exp(-t^2)\mathrm{d}t\end{aligned}$$

This yields the case $n-1$ even.

For $n-1$ odd the integral can be easily solved.

6. For the complementary error function an exponential bound can be found in [AS72] and stronger ones, if necessary, in [CDS03], which further can be approximated for our needs

$$\operatorname{erfc}(x) \leq \frac{1}{2}\mathrm{e}^{-2x^2} + \frac{1}{2}\mathrm{e}^{-x^2} \leq \mathrm{e}^{-x^2}, \qquad x > 0$$

□

Lemma 16. *For a semiclassical Gaussian wave packet ϕ_t a multiplication by y^α, α being a multiindex like above, gives*

$$\left\| y^\alpha \phi_t \right\|_{L^2(\mathbb{R}^n)} \leq C_n \varepsilon^{|\alpha|/2}$$

Proof. This is a direct consequence of lemma 15, choosing $\rho = 0$. □

Lemma 17. *Let ϕ_t be the wave packet fulfilling* (3.16) *on $\mathbb{R}^n$ of our main solution theorem 12 with initial condition ϕ_0. Furthermore by applying the cutoff χ_r, definition* (10) *with $r = \rho/2$, let $\phi_{t,\text{trunc}} = \chi_r \phi_t$ be the truncated wave packet which can be mapped by $\Phi_{q(t)}$ to $\mathcal{M}$. Then the difference between those two functions is exponentially small, clearly*

$$\left\| \phi_t - \phi_{t,\text{trunc}} \right\| \leq C_n \exp(c_n/\varepsilon)$$

for any n.

Proof.

$$\left\|\phi_t - \phi_{t,\text{trunc}}\right\| = \left\|\phi_t - \chi\phi_t\right\| = \left\|(1-\chi)\phi_t\right\| \leq \left\|\phi_t\right\|_{L^2\left(\mathbb{R}^n \setminus B_0^{\rho/2}\right)}$$

Thus the problem reduces to the calculation of the norm of ϕ_t outside the cutoff radius, see lemma 15. □

Furthermore we need a bound for the time derivative of the modified Hagedorn wave packet.

Lemma 18. *Let ϕ_t be the wave packet fulfilling* (3.16) *on $\mathbb{R}^n$ of our main theorem 12 with initial condition ϕ_0. Then the time-derivative is bounded by*

$$\left\|\frac{\mathrm{d}}{\mathrm{d}t}\phi_t[p(t),Q(t),P(t)]\right\|_{L^2(\mathbb{R}^n)} \leq C_n \left\|\phi_t\right\|_{L^2(\mathbb{R}^n)}$$

Proof. The time-derivative acting on ϕ_t only yields again a Gaussian wave packet either multiplied by y, by bounded matrices $P(t), Q(t)$ or bounded $p(t)$, being solutions of ordinary differential equations. Thus the statement directly follows. □

The next lemma gives error bounds for derivatives of $\phi_{t,\text{trunc}}$.

Lemma 19. *Again let ϕ_t be the wave packet fulfilling* (3.16) *on $\mathbb{R}^n$ of our main theorem 12 with initial condition ϕ_0. Furthermore by applying the cutoff χ_r, definition* (10) *with $r = \rho/2$, let $\phi_{t,\text{trunc}} = \chi_r\phi_t$ be the truncated wave packet which can be mapped by ${\Phi_{q(t)}^{-1}}^*$ to $\mathcal{M}$. Let $\alpha = (\alpha_1, \ldots, \alpha_n)$ be a multiindex with $|\alpha| = \alpha_1 + \cdots + \alpha_n$. Then the following bounds hold:*

$$\left\|\frac{\mathrm{d}}{\mathrm{d}t}\phi_{t,\text{trunc}}\right\|_{L^2\left(B^\rho \setminus B^{\rho/2}\right)} \leq C_n \exp(c_n/\varepsilon)$$

$$\left\|\frac{\partial^\alpha}{\partial y^\alpha}\phi_{t,\text{trunc}}\right\|_{L^2\left(B^\rho \setminus B^{\rho/2}\right)} \leq C_n \exp(c_n/\varepsilon)$$

for any n.

Proof. The first inequation is calculated by

$$\begin{aligned}\left\|\frac{\mathrm{d}}{\mathrm{d}t}\phi_{t,\mathrm{trunc}}\right\|_{L^2\left(B^\rho\setminus B^{\rho/2}\right)} &= \left\|\frac{\mathrm{d}}{\mathrm{d}t}\left(\chi_r\phi_t\right)\right\| = \left\|\dot{\chi}_r\phi_t + \chi_r\dot{\phi}_t\right\| = \left\|\chi_r\dot{\phi}_t\right\| \\ &\leq C_n \left\|\phi_t\right\|_{L^2\left(B^\rho\setminus B^{\rho/2}\right)} \\ &\leq C_n \left\|\phi_t\right\|_{L^2\left(\mathbb{R}^n\setminus B^{\rho/2}\right)} \\ &\leq C_n \exp(c_n/\varepsilon)\end{aligned}$$

using lemma 18 and lemma 15.

The second bound is proved similarly.

$$\begin{aligned}\left\|\frac{\partial^\alpha}{\partial y^\alpha}\phi_{t,\mathrm{trunc}}\right\|_{L^2\left(B^\rho\setminus B^{\rho/2}\right)} &= \left\|\frac{\partial^\alpha}{\partial y^\alpha}\left(\chi_r\phi_t\right)\right\| \\ &= \left\|\left(\frac{\partial^\alpha}{\partial y^\alpha}\chi_r\right)\phi_t + \chi_r\left(\frac{\partial^\alpha}{\partial y^\alpha}\phi_t\right)\right\| \\ &\leq C_n \left\|y^\alpha\phi_t\right\|_{L^2\left(\mathbb{R}^n\setminus B^{\rho/2}\right)} \\ &\leq C_n \exp(c_n/\varepsilon)\end{aligned}$$

using that χ_r is a smooth bounded function and that y-derivatives acting on ϕ_t again only yield either a multiplication of a Gaussian wave packet by y^α, by bounded matrices $P(t), Q(t)$ or bounded $p(t)$, being solutions to the classical equations of motion. $\square$

4 Conclusion and Outlook

Here we want to summarize the results of this thesis and give a short outlook.

4.1 Conclusion

In this work we introduce semiclassical Gaussian wave packets and show that they are approximate solutions to the Schrödinger equation in semiclassical scaling on Riemannian manifolds of bounded geometry, see theorem 12, page 53. Furthermore we show that they are an approximation to the full solution and give first error bounds, see theorem 14, page 65.

To achieve these goals, we have to modify semiclassical Gaussian wave packets in a specific notation, first introduced by Hagedorn [Hag80] and altered in a way presented here in [FGL09], see section 2.1. The modifications are due to a change of the space, the wave packets live on. That is, instead of flat Euclidian space $\mathbb{R}^n$, our wave packets live on a Riemannian manifold $\mathcal{M}$ with metric g. For this purpose we introduce so called normal or geodesic coordinates by using the exponential mapping and formulate the packets and the Schrödinger equation in terms of those, see definition 17, page 38.

We prove that these modified Hagedorn wave packets are approximate solutions to the Schrödinger equation in normal coordinates and that their parameters have to fulfill similar classical equations as in the Euclidian case, see (3.15), page 52. The only difference to the flat case arises in one equation of motion, which can be traced back to a change of the width of momentum due to curvature, see subsection 3.5.4, page 60.

A first error analysis shows that the modified Hagedorn wave packets approximate the solution on the manifold in order $\varepsilon^{1/2}$, for time $t \in [0, T]$ and the small semiclassical parameter $\varepsilon > 0$.

4.2 Outlook

At last we want to give a short outlook of what can be possibly done with our results. This summary consists of two aspects, a generalization of the modified Gaussian to full wave packets and a proposal for a numerical usage.

First our modified Hagedorn wave packet can be extended to general wave packets similar to Hagedorn's results in [Hag98]. It seems possible to alter the raising and lowering operators $A^\dagger$ and A by a term proportional to $\frac{1}{3} y\, R\, \partial$, leading to a slight change in the commutator of H^{nc} with $A^\dagger$, canceling the extra terms arising. This should give a similar result about the created wave packets as approximate solutions to the Schrödinger equation in normal coordinates.

Second, it should be possible to introduce a numerical algorithm, similar to the one of Fayou, Gradinaru and Lubich [FGL09], because it still suffices to solve the ordinary differential equations of the parameters to get a time-propagated wave packet. In our free case the geodesic equation for $q(t), p(t)$ and the classical equations of motions for $P(t)$ and $Q(t)$ on $\mathbb{R}^n$ have to be solved. This should lead to a similar Galerkin type approximation, even in the case of $V = 0$, because the additional terms of the Laplace-Beltrami operator could be treated similar to potential terms. One has to be aware, that this results in space-dependent terms in front of a differential operator, which cannot be solved via a standard splitting procedure but eventually with a Krylov type solution, see [Lub08].

Bibliography

[AS72] Milton Abramowitz and Irene A Stegun, *Handbook of mathematical functions: with formulas, graphs, and mathematical tables*, no. 55, Courier Dover Publications, 1972.

[Ber03] Marcel Berger, *A panoramic view of riemannian geometry*, Springer, 2003.

[BGV92] N. Berline, E. Getzler, and M. Vergne, *Heat kernels and dirac operators*, Grundlehren Text Editions, Springer Berlin Heidelberg, 1992.

[Bre09] Leo Brewin, *Riemann normal coordinate expansions using cadabra*, Classical and Quantum Gravity **26** (2009), no. 17, 175017.

[CDS03] Marco Chiani, Davide Dardari, and Marvin K Simon, *New exponential bounds and approximations for the computation of error probability in fading channels*, Wireless Communications, IEEE Transactions on **2** (2003), no. 4, 840–845.

[CV10] Pavel Castro-Villarreal, *Brownian motion meets riemann curvature*, Journal of Statistical Mechanics: Theory and Experiment **2010** (2010), no. 08, P08006.

[DT04] GF Dell'Antonio and Lucattilio Tenuta, *Semiclassical analysis of constrained quantum systems*, Journal of Physics A: Mathematical and General **37** (2004), no. 21, 5605.

[FGL09] Erwan Faou, Vasile Gradinaru, and Christian Lubich, *Computing semiclassical quantum dynamics with hagedorn wavepackets*, SIAM Journal on Scientific Computing **31** (2009), no. 4, 3027–3041.

[FK03] Helmut Fischer and Helmut Kaul, *Mathematik für physiker: Band 3*, vol. 3, Teubner, Wiesbaden, 2003.

[GH12] V Gradinaru and GA Hagedorn, *A time–splitting for the semiclassical schrödinger equation*.

[Hag80] George A Hagedorn, *Semiclassical quantum mechanics*, Communications in Mathematical Physics **71** (1980), no. 1, 77–93.

[Hag98] ______, *Raising and lowering operators for semiclassical wave packets*, Annals of Physics **269** (1998), no. 1, 77–104.

[Hel76] Eric J Heller, *Time dependent variational approach to semiclassical dynamics*, The Journal of Chemical Physics **64** (1976), no. 1, 63–73.

[Her25] G Herglotz, *Über die bestimmung eines linienelementes in normalkoordinaten aus dem riemannschen krümmungstensor*, Mathematische Annalen **93** (1925), no. 1, 46–53.

[HLT14] Stefan Haag, Jonas Lampart, and Stefan Teufel, *Generalised quantum waveguides*, arXiv preprint arXiv:1402.1067 (2014).

[Lan99] S. Lang, *Fundamentals of differential geometry*, vol. 191, Springer, 1999.

[LT14] Jonas Lampart and Stefan Teufel, *The adiabatic limit of schrödinger operators on fibre bundles*, arXiv preprint arXiv:1402.0382 (2014).

[Lub08] Christian Lubich, *From quantum to classical molecular dynamics: Reduced models and numerical analysis*, Zurich Lectures in Advanced Mathematics, European Mathematical Society, 2008.

[Mil63] John Willard Milnor, *Morse theory*, no. 51, Princeton university press, 1963.

[MSvdV99] Uwe Muller, Christian Schubert, and Anton EM van de Ven, *A closed formula for the riemann normal coordinate expansion*, General Relativity and Gravitation **31** (1999), no. 11, 1759–1768.

[Nes99] Alexander I Nesterov, *Riemann normal coordinates, fermi reference system and the geodesic deviation equation*, Classical and Quantum Gravity **16** (1999), no. 2, 465.

[OL13] Tomoki Ohsawa and Melvin Leok, *Symplectic semiclassical wave packet dynamics*, Journal of Physics A: Mathematical and Theoretical **46** (2013), no. 40, 405201.

[RS72] M. Reed and B. Simon, *Methods of modern mathematical physics I: Functional analysis*, Academic Press, 1972.

[RS75] M. Reed and B. Simon, *Methods of modern mathematical physics II: Fourier analysis, selfadjointness*, Academic Press, Inc., 1975.

[Shu92] M. A. Shubin, *Spectral theory of elliptic operators on non-compact manifolds*, Astérisque (1992), no. 207, 37–108.

[Teu03] Stefan Teufel, *Adiabatic perturbation theory in quantum dynamics*, Lecture Notes in Mathematics, vol. 1821/2003, Springer Berlin / Heidelberg, 2003.

[Wac10] J. Wachsmuth, *Effective Schrödinger equations on submanifolds*, Ph.D. thesis, Eberhard-Karls-Universität Tübingen, 2010.

[Wit08] O. Wittich, *L^2-homogenization of heat equations on tubular neighborhoods*, ArXiv e-prints (2008).

[Wit11] Olaf Wittich, *A homogenization result for laplacians on tubular neighbourhoods of closed riemannian submanifolds*, Shaker, 2011.

[WT10] J. Wachsmuth and S. Teufel, *Constrained quantum systems as an adiabatic problem*, Physical Review A **82** (2010), no. 2.