

**On the Nonrelativistic Limit of  
Quantum Electrodynamics:**  
From the Matter–Antimatter–Photon  
Quantum Field Hybrid  
to Charged, Massive and Spinning Particles  
Interacting with Photons

**Dissertation**

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## Abstract

In the context of this dissertation the nonrelativistic Limit of Quantum Electrodynamics (QED) is derived by the help of the Wegner flow equation. Thereby all constituents of the QED Quantum field can be treated on equal footing, leading to the fundamental Hamiltonian of light–matter interactions for a plurality of electrons and positrons as classical point–like particles carrying mass, charge and spin.

The QED quantum field is a hybrid which is composed of the matter– and antimatter quantum fields and the photon quantum field. Additionally, the coupling of the matter– and antimatter quantum fields to classical external potentials is considered. The constituents of this hybrid are initially inextricably interwoven with each other.

Starting from the hybrid QED field (represented in the Coulomb gauge), firstly, it is shown that the physical problem is that the respective QED Hamiltonian does not commute with the QED particle number operator. The latter is defined via the occupation number of the matter– and antimatter modes. This lack of commutation is the reason why the QED Hamiltonian can not be retranslated to first quantization, where one would sum over individual point–like particles.

The fact that the QED Hamiltonian does not commute with the particle number operator means that the particle number is not a conserved quantity. This property fundamentally separates the physics of QED from the nonrelativistic physics on the atomic scale. Therefore a unitary transformation of the QED Hamiltonian is performed such that a unitarily equivalent QED Hamiltonian arises which conserves the particle number. Proceeding in this way, the classical or quantum mechanical concept of a point particle with the attributes mass, charge and spin is put in the center as *the essential* property of the non-relativistic limit of QED.

The unitary transformation of the hybrid QED quantum field is performed by the help of the Wegner flow equation. In general, the flow equation is a differential equation that provides a method for (block)diagonalizing an operator in a continuous manner by means of a generator adapted to the problem.

In the context of the thesis problem, the generator of the flow equation is constructed in such a way as to eliminate, the pair terms of the QED Coulomb interaction and those of the coupling to external c-number potentials, and the high-energy photons. High-energy photons in this context are the X-ray photons and the gamma ray photons.

The flow equation which follows from this generator is given by a nonlinear ordinary differential equation and can thus only be solved perturbatively. For this the QED Hamiltonian is expanded with respect to the (dimensionless) finestructure constant. This has the consequence that the originally nonlinear differential equation decomposes into a system of (still nonlinear) coupled differential equations. Since the zeroth order differential equation of this system can be solved exactly there follows for all higher orders coupled linear differential equations for which a solution can be found.

The QED Hamiltonian transformed in this way is manifestly particle number conserving, however, it cannot be translated back into the first quantization yet. The reason for this is that in this QED Hamilton operator preserving the particle number, still the matter and antimatter degrees of freedom are coherently superposed. This is due to the fact that the QED field operators are still given in the so-called Dirac representation.

By the help of the Eriksen transformation it is possible to decouple the matter- and antimatter degrees of freedom in the particle number conserving QED quantum field. The Eriksen transformation is a unitary transformation that transforms the single-particle Dirac Hamiltonian in such a way that the resulting Hamiltonian – the so-called Newton-Wigner Hamiltonian – is of blockdiagonal shape. Furthermore, the Eriksen transformation is defined by the property that it is energy separating. This means that first, the eigenfunctions of the single-particle Dirac Hamiltonian, the four-component Dirac spinors, become the Newton-Wigner spinors. The latter have, for the matter degrees of freedom, entries in the upper two components, whereas the lower components are zero. For the antimatter degrees of freedom it is vice versa: their Newton-Wigner spinors have entries in the lower two components, whereas the upper components are zero. Secondly, in the Newton-Wigner representation, the energy eigenvalue problem is separated in such a way that there is one for matter and antimatter separately (with the respective minus sign for antimatter).

Therefore the Eriksen transformation guarantees that the matter– and antimatter degrees of freedom are completely decoupled in the Newton–Wigner representation. This enables to express the Newton–Wigner spinors by the Pauli eigenfunctions of nonrelativistic atomic physics (as solutions for the electrons as well as for the positrons), which vary slowly on the length scale of the Bohr radius (with respect to the Compton wavelength of the electron).

Going now, with respect to the unitarily equivalent QED quantum field preserving the particle number, from the Dirac representation of the field operators to the Newton-Wigner representation, the matrix elements can be evaluated as gradient expansion with respect to the slowly varying Newton-Wigner field operators. The solution is constructed up to the second order in the finestructure constant such that the first relativistic corrections to the Pauli Hamiltonian of light–matter interaction of atomic physics occur.

The Wegner flow equation also yields self energy terms resulting first from the QED Coulomb interaction (longitudinal interaction), and second from the interaction of the matter– and antimatter quantum fields with high-energy photons (transversal interaction). These describe the renormalization of the bare mass of the fermion. Their evaluation leads then also to a renormalization of the magnetic moment of the fermions which is in agreement with the result of J. Schwinger. Moreover, all effective one– and two–particle interactions known from the light–matter interaction of atomic physics arise in this way. The longitudinal QED Coulomb interaction leads, in addition to the Coulomb interaction between two fermions, to the Darwin term and the spin–orbit interaction in the field of another fermion. The transversal QED interaction leads to the orbit–orbit interaction between two fermions, to their magnetic dipole–dipole interaction, and their spin–other–orbit interaction.

It is finally possible to express the unitarily equivalent, particle number conserving QED Hamiltonian, represented in the Newton–Wigner representation, in first quantization. Proceeding in this guise the goal is achieved to find a nonrelativistic Hamiltonian of light–matter interactions describing classical, point–like particles carrying mass, charge and spin interacting with low–energy photons.





## Zusammenfassung

Im Rahmen dieser Dissertation wird der nichtrelativistische Limes der Quantenelektrodynamik (QED) mit Hilfe der Wegnerschen Flussgleichung hergeleitet. Dabei können alle Konstituenten des QED Quantenfeldes gleich behandelt werden, sodass es sich bei dem Ergebnis um den echten, fundamentalen Hamiltonoperator der Licht–Materie Wechselwirkung handelt, und zwar für eine Pluralität von Elektronen und Positronen als klassische Punktteilchen die Masse, Ladung und Spin tragen.

Bei dem QED Quantenfeld handelt es sich um ein Hybrid aus Materiequantenfeldern, Antimateriequantenfeldern und Photonquantenfeldern, wobei zusätzlich die Kopplung der Materie– und Antimateriequantenfelder an äußere klassische Potentiale berücksichtigt wird. Die Konstituenten dieses Hybrids sind zunächst untrennbar miteinander verwoben.

Ausgehend von diesem hybriden QED Quantenfeld (dargestellt in der Coulomb–Eichung) wird zunächst ausführlich aufgezeigt, dass das physikalische Problem dasjenige ist, dass der entsprechende QED Hamiltonoperator nicht mit dem Teilchenzahloperator vertauscht (letzterer ist, in der Modendarstellung, durch die Besetzungszahl der Materie– und der Antimateriemoden definiert). Dieses Nichtvertauschen ist die Ursache dafür, dass der QED Hamiltonoperator nicht in die erste Quantisierung zurück übersetzt werden kann, in der man über individuelle Punktteilchen summiert. Das Nichtvertauschen des QED Hamiltonoperators mit dem Teilchenzahloperator bedeutet, dass die Teilchenzahl keine Erhaltungsgröße in der QED ist. Diese Eigenschaft trennt die Physik der QED radikal von der nichtrelativistischen Physik auf atomarer Skala.

Daher wird eine unitäre Transformation des QED Hamiltonoperators dergestalt durchgeführt, dass ein unitär äquivalenter QED Hamiltonoperator zu Tage tritt, der die Teilchenzahl erhält. Zugleich wird auf diese Weise das klassische bzw. quantenmechanische Punktteilchen mit den Attributen Masse, Ladung und Spin als zentrale Eigenschaft des nichtrelativistischen Limes der QED in den Mittelpunkt gestellt.

Die unitäre Transformation des hybriden QED Quantenfeldes wird mit Hilfe der Wegnerschen Flussgleichung durchgeführt. Allgemein handelt es sich bei dieser Flussgleichung um eine Differential-

gleichung, die mit Hilfe eines die Fragestellung angepassten Generators einen gegebenen Operator unitär äquivalent transformiert bzw. blockdiagonalisiert, und zwar auf kontinuierliche Art und Weise.

Im Rahmen des Problems dieser Dissertation wird der Generator der Flussgleichung dergestalt konstruiert, dass erstens die Paarsterme der QED Coulomb–Wechselwirkung und diejenigen der Kopplung an äußere  $c$ -Zahl Potentiale, und zweitens die hochenergetischen Photonen eliminiert werden. Bei den letzteren handelt es sich um Röntgenphotonen und Gammaphotonen.

Die mit diesem Generator konstruierte Flussgleichung führt auf eine nichtlineare, gewöhnliche Differentialgleichung und kann daher nur perturbativ gelöst werden. Der QED Hamiltonoperator wird dazu in eine Reihe bezüglich der (dimensionslosen) Feinstrukturkonstante entwickelt. Dadurch zerfällt die ursprünglich nichtlineare Differentialgleichung in ein System gekoppelter (zunächst nichtlinearer) Differentialgleichungen. Da jedoch die nullte Ordnung dieses Systems gekoppelter Differentialgleichungen exakt lösbar ist, resultieren für alle höheren Ordnungen nunmehr lineare gekoppelte Differentialgleichungen, für die eine Lösung gefunden werden kann.

Der auf diese Weise unitär transformierte QED Hamiltonoperator ist manifest teilchenzahlerhaltend, allerdings lässt er sich noch nicht in die erste Quantisierung zurück übersetzen. Die Ursache dafür ist dass in diesem die Teilchenzahl erhaltenden QED Hamiltonoperator noch immer die Materie– und Antimateriefreiheitsgrade kohärent überlagert sind. Dies liegt daran dass die QED Feldoperatoren in der Dirac Darstellung vorliegen.

Mit Hilfe der Eriksen–Transformation gelingt es im unitär äquivalenten, die Teilchenzahl erhaltenden QED Quantenfeld die Materie– und Antimateriefreiheitsgrade zu entkoppeln. Die Eriksen–Transformation transformiert erstens den Einteilchen Dirac–Hamiltonian unitär äquivalent auf einen blockdiagonalen Dirac–Hamiltonoperator, den so genannten Newton–Wigner Hamiltonoperator. Zweitens wird die Eriksen Transformation dadurch definiert, energieseparierend zu sein. Dies bedeutet, dass die Eigenfunktionen des Einteilchen Dirac–Hamiltonians, die vierkomponentigen Dirac–Spinoren, in der Newton–Wigner Darstellung in (nach wie vor vierkomponentige) Spinoren übergehen, die für die Materie Einträge in

den beiden oberen Komponenten aufweisen, und für die Antimaterie Einträge in den beiden unteren Komponenten. Zudem wird das Energieeigenwertproblem separiert, sodass es für Materie und Antimaterie getrennt gültig ist (mit dem entsprechenden Minus für die Antimaterie). Auf diese Weise ist sichergestellt, dass Materie- und Antimateriefreiheitsgrade in der Newton–Wigner Darstellung vollständig entkoppelt sind. Mit Hilfe der Eriksen Transformation ist es dann möglich, die Newton–Wigner Spinoren durch die Pauli Eigenfunktionen der nichtrelativistischen Atomphysik auszudrücken (sowohl als Lösungen für Elektronen, als auch für Positronen), die auf der Skala des Bohrschen Radius langsam variierende Funktionen sind (relativ zur Compton–Wellenlänge des Elektrons).

Geht man nun bezüglich des die Teilchenzahl erhaltenden QED Quantenfeldes von der Dirac–Darstellung der Feldoperatoren in die Newton–Wigner Darstellung, so lassen sich die Matrixelemente als Gradiententwicklung bezüglich der langsam variierenden Newton–Wigner Feldoperatoren auswerten. Die Lösung wird bis zur zweiten Ordnung in der Feinstrukturkonstanten konstruiert, sodass die ersten relativistischen Korrekturen zum Pauli Hamiltonoperator der Licht–Materie Atomphysik in Erscheinung treten.

Die durch die Wegnersche Flussgleichung erhaltenen Selbstenergieterme, resultierend erstens aus der QED Coulomb–Wechselwirkung (longitudinale Wechselwirkung), und zweitens aus der Wechselwirkung der Materie– und Antimateriefelder mit hochenergetischen Photonen (transversale Wechselwirkung) renormalisieren die nackte Masse des Elektrons. Deren Auswertung führt daher auf eine Renormalisierung des magnetischen Moments der Fermionen, die in Übereinstimmung mit dem Resultat von J. Schwinger ist.

Darüber hinaus entstehen sämtliche effektive Ein– und Zweiteilchenwechselwirkungsterme wie sie aus der Licht–Materie Wechselwirkung der Atomphysik bekannt sind. Die longitudinale QED Coulomb–Wechselwirkung führt, neben der Coulomb–Wechselwirkung zwischen zwei Fermionen, zum Darwin–Term und zur Spin–Bahn Wechselwirkung im Feld eines anderen Fermions. Die transversale QED Wechselwirkung führt auf die Orbit–Orbit Wechselwirkung, die magnetische Dipol–Dipol Wechselwirkung und die Spin–Other–Orbit Wechselwirkung.

Zusammenfassend ist es so möglich, den unitär äquivalenten, die Teilchenzahl erhaltenden QED Hamiltonoperator in die erste Quantisierung zurück zu übersetzen. Auf diese Weise wird das Ziel erreicht, einen nichtrelativistischen Hamiltonoperator der Licht–Materie Wechselwirkung zu erhalten, der Punktteilchen (Elektronen und Positronen) mit Masse, Ladung und Spin in Wechselwirkung mit niederenergetischen Photonen beschreibt.

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# 1 Introduction

Quantum Electrodynamics (QED) is a quantum field theory. It is the theory of light–matter interactions in second quantization. This means that it is not only the electromagnetic field that is described by the occupation number of its modes, or by the creation and annihilation operators of the (massless) photons. In QED also the particles are described by the excitation and deexcitation of modes, however, of matter and antimatter modes. Thus, also the massive particles, the fermions, are described by creation and annihilation operators.

QED has been born by Paul Dirac in 1928 [1], and it has been raised by Julian Schwinger, Richard Feynman and Shin ichiro Tomonaga. For sure, there were many other physicists who contributed to the development of QED, or even laid the foundations of the theory, as for example Pascual Jordan, its "unsung hero" [2].

Nevertheless, Paul Dirac is known to be "the founding father and guiding spirit" of QED [2]. He laid the foundations of the theory by trying to unite the principles of quantum mechanics with the special theory of relativity. This led him to the discovery that relativistic quantum mechanics must at least be four dimensional as it is described by the Dirac–Hamiltonian, which has a representation as a  $4 \times 4$  matrix operator. Up to then it was thought that it was sufficient to describe the nonrelativistic electron interacting with electromagnetic fields by the  $2 \times 2$  Schrödinger–Pauli Hamiltonian. However, the additional two dimensions in the Dirac–Hamiltonian held a problem ready: the negative energy solutions. These are problematic because of the interactions of the electron with electromagnetic fields. The electron could in principle occupy these states of increasingly negative energy by emitting photons, and in this way lower its energy further and further. This is then an infinite process and therefore it is surely not physical. Thus, Dirac applied the Pauli principle and postulated that the ground state of relativistic quantum mechanics is of such nature that all states of negative energies are occupied, whereas all states of positive energies are empty. He then interpreted the excitations of this ground state as holes in the Dirac–sea. In that way he discovered the antiparticle of the electron, the hole. This is the famous hole theory [3, 4, 5, 2]. Later on, the hole in the Dirac–sea became renowned as the positron. Now with the introduction of the positron into QED

the problem of negative energy solutions has finally been removed [3, 4, 5, 2]. An in-depth introduction into the history of QED can be found in [2].

So in textbook QED we are dealing with quantum fields for both, matter, antimatter and light. This immediately brings a philosophical or semantic trick box into play, and to say it right away, I believe that this trick box is in a sense central to the problem posed in this dissertation. Why is that?

Now, as is stated by Silvan Schweber [2], "The history of elementary particles can be analyzed in terms of oscillations between two viewpoints: one which takes fields as fundamental, in which particles are the quanta of the fields; and the other which takes particles as fundamental, and in which fields are macroscopic coherent states." Obviously, Dirac favored the particle point of view! Nevertheless, in the beginning it was mentioned that QED is a quantum *field* theory. Now take a look at the following picture in figure 1:

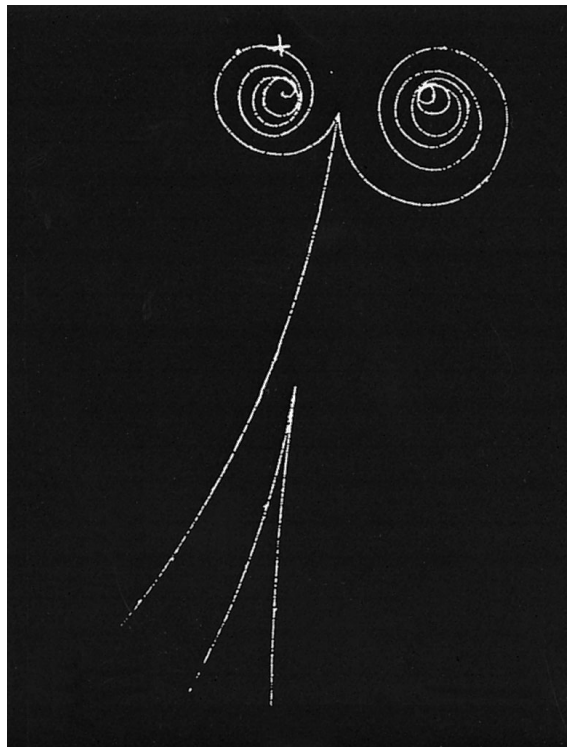


Figure 1: Bubble chamber trajectories of an electron and a positron

Here you can see the trajectories of an electron and a positron moving in a static magnetic induction field of a bubble chamber. The (classical, Newtonian!) Lorentz force forces the **particles** onto spiral paths, however, since the electron carries charge  $q = -|e|$ , and the

positron carries charge  $q = +|e|$ , one of them goes around left, the other goes around right. The intricate point is that one (reasonably) presupposes that point particles are moving here which create the tracks, not quantum fields!

*Oh no!*, you might think now, *not the old, boring dispute regarding the particle–wave dualism!* Yes, obviously, the problem runs through to quantum field theories! But I am not going to philosophize wildly, on the contrary: the problem is approached very formally. It is therefore important to point out how here the philosophical or semantic trick box is **related to an actual, formal “problem” of QED: the lack of particle number conservation**. Yes, in QED, the particle number is not conserved!

Now, saying that in a quantum field theory the particle number is not a conserved quantity might be confusing. *How can the particle number be not conserved in QED when there are no particles, only quantized (anti–)matter fields?* This mystery can be solved at least formally: it is possible to define a particle number operator  $\hat{N}$  that counts the number of occupied matter and antimatter modes. And this particle number operator **does not commute with the Hamiltonian  $\hat{\mathcal{H}}_{QED}$  of QED**,  $[\hat{N}, \hat{\mathcal{H}}_{QED}] \neq \hat{0}$ ! For explaining this in more detail take a look at the QED Hamiltonian in the Coulomb gauge [6]

$$\hat{\mathcal{H}}_{QED} = \hat{\mathcal{H}}_D + \hat{\mathcal{H}}_{rad} + \hat{\mathcal{V}}_{ext} + \hat{\mathcal{H}}_{\perp} + \hat{\mathcal{V}}_C \quad (1)$$

The first term  $\hat{\mathcal{H}}_D$  is the single–particle Dirac Hamiltonian in its second quantized guise. The single–particle Dirac Hamiltonian describes the Dirac–particle in a static external magnetic induction field. It comprises the kinetic energy of the Dirac–particle, its Zeeman energy and its rest energy. The second term  $\hat{\mathcal{H}}_{rad}$  describes the quantized electromagnetic field. The term  $\hat{\mathcal{V}}_{ext}$  describes the interaction of the quantized matter and antimatter fields with external electrostatic sources. The term  $\hat{\mathcal{H}}_{\perp}$  describes the interaction between (anti–)matter fields and photons, and finally, the term  $\hat{\mathcal{V}}_C$  describes the interaction between the (anti–)matter fields, namely the QED Coulomb interaction.

At a first glance, the Hamiltonian (1) looks more or less like the ordinary Hamiltonian of light–matter interactions. And if it would

not be for the hats, one could really confuse them. Therefore, it has to be mentioned again, that all of these contributions in (1) are quantized operator valued fields. And this fact creates an (at least until now) unbridgeable rift between the world of QED and the nonrelativistic description of the interactions between light and matter. For sure, in our classical, nonrelativistic world, the particle number is a well defined, conserved quantity and we observe electrons carrying a fixed mass  $m_e$ , charge  $q = -|e|$  and spin  $s_z = \pm \frac{\hbar}{2}$  (or positrons with fixed mass  $m_e$ , charge  $q = +|e|$  and spin  $s_z = \mp \frac{\hbar}{2}$ )! The nonrelativistic Hamiltonian  $\hat{H}_{LM}^{(el)}$  of electrons interacting with light (or the one of positrons  $\hat{H}_{LM}^{(pos)}$  interacting with light) should really conserve the particle number iff it describes the particles causing the trajectories in figure 1.

Therefore we ask: what is the relation between the QED Hamiltonian (8) and the nonrelativistic Hamiltonian  $\hat{H}_{LM}$  describing point-like fermions interacting with light?

The answer will be given throughout this dissertation. The result regarding the electrons assumes the following guise [7, 8]

$$\hat{H}_{LM}^{(el)} = \hat{H}_{SP}^{(el)} + \hat{H}_{\perp}^{(low,el)} + \hat{V}_{C,ee} + \hat{V}_{\perp,ee} + H_{rad} + \hat{V}_{ext}^{(el)} \quad (2)$$

where [7, 8]

$$\hat{H}_{SP}^{(el)} = \sum_{j=1}^N \left( \begin{aligned} & m_e c^2 + \frac{(\Pi_b^{(j)})(\Pi_b^{(j)})}{2m_e} - \frac{1}{8} \frac{1}{m_e^3 c^2} \left( \Pi_b^{(j)} \right)^4 \\ & + \left( 2 + \frac{\alpha_{FS}}{\pi} \right) \left( \frac{q_e \hbar}{2m_e} B_b^{(ext)} \sigma_b^{(P,j)} \right)_{s,s'} \end{aligned} \right) \quad (3)$$

is the nonrelativistic Schrödinger–Pauli Hamiltonian.  $\Pi_b^{(j)}$  is the gauge invariant velocity of the electrons, and  $\sigma_b^{(P,j)}$  are the Pauli matrices.  $\left( 2 + \frac{\alpha_{FS}}{\pi} \right)$  is the Schwinger result of the anomalous magnetic moment of the electron. Note that  $N$  is the total number of electrons, hence, these can be counted!

Now [7, 8]

$$\hat{H}_{\perp}^{(low,el)} = -\frac{1}{m_e c^2} \sum_{j=1}^N \hat{j}_b^{(e)} \left( \mathbf{r}^{(j)} \right) \hat{\mathcal{A}}_b \left( \mathbf{r}^{(j)} \right) \quad (4)$$

where  $\sum_{j=1}^N \hat{j}_b^{(e)}(\mathbf{r}^{(j)})$  is the nonrelativistic current density caused by a plurality of point electrons interacting with low-energy photons. The latter are described by the vector potential  $\mathfrak{A}_b(\mathbf{r}^{(j)})$ .

The term [7, 8]

$$\hat{V}_{C,ee} = \frac{1}{2} \sum_{j \neq j'}^N \left( \begin{array}{c} \frac{q_e^2}{4\pi\epsilon_0 |\mathbf{r}^{(j')} - \mathbf{r}^{(j)}|} \\ -\frac{q_e^2}{4\pi\epsilon_0} \left( \frac{\hbar}{m_e c} \right)^2 \pi \delta^{(3)}(\mathbf{r}^{(j)} - \mathbf{r}^{(j')}) \\ -\frac{q_e^2}{8\pi\epsilon_0} \frac{\hbar}{m_e c} \sigma_{b''}^{(P,j)} \epsilon_{bb'b''} \frac{r_b^{(j)} - r_b^{(j')}}{|\mathbf{r}^{(j)} - \mathbf{r}^{(j')}|^3} \frac{\Pi_{b'}^{(j)}}{m_e c} \end{array} \right) \quad (5)$$

describes the Coulomb interaction between the electrons, their Darwin interaction and their spin-orbit interaction due to the presence of the other electrons.

The following term [7, 8]

$$\hat{V}_{ext}^{(el)} = \frac{Z |q_e|}{4\pi\epsilon_0} \sum_{j=1}^N \left( \begin{array}{c} \frac{1}{4\pi |\mathbf{R} - \mathbf{r}^{(j)}|} \\ -\frac{1}{8} \frac{\hbar}{m_e c} \frac{\hbar}{m_e c} \delta^{(3)}(\mathbf{R} - \mathbf{r}^{(j)}) \\ +\frac{1}{4} \frac{\hbar}{m_e c} \epsilon_{bb'b''} \left( \frac{R_b - r_b^{(j)}}{4\pi |\mathbf{R} - \mathbf{r}^{(j)}|^3} \right) \left( \frac{\Pi_{b'}}{m_e c} \sigma_{b''}^{(P,j)} \right)_{\mu, \mu'} \end{array} \right) \quad (6)$$

describes the interaction of the electrons with external c-number sources, the respective Darwin term, and the spin-orbit interaction in the external electric field.

The effective interaction term [7, 8]

$$\hat{V}_{\perp,ee} = \frac{1}{2} \sum_{j \neq j'}^N \left( \begin{array}{c} \left( -\frac{q_e^2}{4\pi\epsilon_0} \right) \frac{1}{2} \left( \frac{\delta_{a,b}}{|\mathbf{r}^{(j)} - \mathbf{r}^{(j')}|} + \frac{(r_a^{(j)} - r_a^{(j')})(r_b^{(j)} - r_b^{(j')})}{|\mathbf{r}^{(j)} - \mathbf{r}^{(j')}|^3} \right) \frac{\Pi_b^{(j')}}{m_e c} \frac{\Pi_a^{(j)}}{m_e c} \\ + \left( -\frac{q_e^2}{4\pi\epsilon_0} \right) \frac{1}{4} \left( \frac{\hbar}{m_e c} \right)^2 \left( \begin{array}{c} \frac{8}{3} \pi \delta^{(3)}(\mathbf{r}^{(j)} - \mathbf{r}^{(j')}) \delta_{a,b} \\ + \frac{3(r_a^{(j)} - r_a^{(j')})(r_b^{(j)} - r_b^{(j')}) - 3|\mathbf{r}^{(j)} - \mathbf{r}^{(j')}|^2 \delta_{a,b}}{|\mathbf{r}^{(j)} - \mathbf{r}^{(j')}|^5} \end{array} \right) \sigma_b^{(P,j')} \sigma_a^{(P,j)} \\ + \frac{1}{2} \frac{\hbar}{m_e c} \frac{q_e^2}{4\pi\epsilon_0} \frac{r_b^{(j)} - r_b^{(j')}}{|\mathbf{r}^{(j)} - \mathbf{r}^{(j')}|^3} \epsilon_{b',b,b''} \left( \Pi_b^{(j')} \sigma_{b''}^{(P,j)} - \Pi_b^{(P,j)} \sigma_{b''}^{(j')} \right) \end{array} \right) \quad (7)$$

comprises the orbit–orbit interaction, the magnetic dipole–dipole interaction, and the spin–other orbit interaction between the electrons. Finally,  $H_{rad}$  is the radiation field of the photons.

The corresponding Hamiltonian  $\hat{H}_{LM}^{(pos)}$  thus describes point positrons interacting with light.

Now for going from the QED Hamiltonian (8) to the nonrelativistic Hamiltonian (2) it would be necessary to retranslate the QED Hamiltonian to first quantization, e.g. as a discrete sum over individual particles. However, that is not possible, because the particle number is not conserved, as can be seen from the nonvanishing commutator of the QED Hamiltonian (1) with the particle number operator  $\hat{N}$ . And the reason why the QED particle number operator does not commute with the QED Hamiltonian is the interaction terms  $\hat{\mathcal{H}}_{\perp}$ ,  $\hat{\mathcal{V}}_C$  and  $\hat{\mathcal{V}}_{ext}$ . Vividly spoken it is the interaction of the (anti–)matter fields with the high energy photons which allows for processes during which matter or antimatter or photons are created and annihilated, and the pair terms in the QED Coulomb interaction and in the coupling to external sources, such that there is no way to fix the particle number in QED.

It seems like an irresolvable philosophical or semantic contradiction: one has to talk about particles all the time although they are described by quantum fields! For the time being, however, the following conception seems to make sense: QED does not describe interacting point particles. It also does not describe pure quantum fields. What QED is is hard to say. The clearest picture to think of is that QED describes a **hybrid** between matter, antimatter and light (somewhat loosely expressed, I sometimes call it the QED soup!). This hybrid has physical properties which stand for themselves, and which have nothing to do with the physical properties of classical, nonrelativistic point particles.

As is shown throughout this dissertation, the fact that the properties of this light–(anti–)matter hybrid stand for themselves is reflected in the necessity of renormalization of the attributes of its constituents, the renormalization of the bare mass  $m_0$  and the  $g$ –factor of the fermions. By deducing the nonrelativistic limit of QED, renormalization is really required!

To briefly summarize what has been said so far: in QED, which is

a field theory, the particle number is not a conserved quantity. This fact harbors a philosophical or semantic contradiction connected to the particle–wave dualism. Moreover, this fact absolutely separates QED from our nonrelativistic world. So how can one understand the trajectories in figure 1 when the particles which create them are being described by Quantum Electrodynamics as a high–energy field theory? The question can also be formulated differently: **how can one derive the nonrelativistic limit of Quantum Electrodynamics**, so that the hybrid is unwound and disintegrates into its components: nonrelativistic particles and low–energy photons? How can one come from the QED Hamiltonian  $\hat{\mathcal{H}}_{QED}$  with the property  $[\hat{N}, \hat{\mathcal{H}}_{QED}] \neq \hat{0}$  to the nonrelativistic Hamiltonian of light–matter interactions  $\hat{\mathcal{H}}_{LM} = \hat{\mathcal{H}}_{LM}^{(el)} + \hat{\mathcal{H}}_{LM}^{(pos)}$  for which  $[\hat{N}, \hat{\mathcal{H}}_{LM}] = \hat{0}$ ?

As it becomes obvious from these questions, the ancient dispute regarding the particle–wave dualism is not only a philosophical or semantic one. In QED it gets a technical face in the form of a non-vanishing commutator. Obviously, for answering the question above one needs to address the non-vanishing commutator  $[\hat{N}, \hat{\mathcal{H}}_{QED}] \neq \hat{0}$ ! So in fact, the deduction of the nonrelativistic limit of QED is obviously closely interwoven with the question of the relation between classical point particles and quantum fields. It disposes of a formal expression,  $[\hat{N}, \hat{\mathcal{H}}_{QED}] \neq \hat{0}$ , and this has the consequence that one can ask: **is there a unitary transformation of the QED Hamiltonian  $\hat{\mathcal{H}}_U$  such that  $[\hat{N}, \hat{\mathcal{H}}_U] = \hat{0}$ ?** hence, such that  $\hat{\mathcal{H}}_U$  conserves the particle number? And if so, how is  $\hat{\mathcal{H}}_U$  related to  $\hat{\mathcal{H}}_{LM}$ , and can one express this unitarily equivalent Hamiltonian  $\hat{\mathcal{H}}_{LM}$  in first quantization, where one can **sum over individual particles with their attributes mass  $m_e$ , charge  $q$  and spin  $s_z$ ?**

Now this is a very formal question that can be attacked in a technically and methodologically crystal clear manner. This is exactly what was done in the context of this dissertation. And yes, finding a unitarily equivalent Hamiltonian  $\hat{\mathcal{H}}_U$  which conserves the particle number  $\hat{N}$  is indeed possible! However, it will turn out that it is not sufficient to find such a Hamiltonian  $\hat{\mathcal{H}}_U$  which preserves the particle number for the goal of describing point particles. This is because in  $\hat{\mathcal{H}}_U$ , **the matter and antimatter modes are still coherently superposed,**



which means that one cannot reexpress  $\hat{\mathcal{H}}_U$  in first quantization.

However, one can also solve this problem technically in a clean way. Now the reason for this coherent superposition of matter and antimatter degrees of freedom lies in the properties of the single-particle Dirac Hamiltonian and the reinterpretation of the Dirac-hole as the positron. In the so-called Dirac representation, in which  $\hat{\mathcal{H}}_{QED}$  must therefore naturally be, and in which its sister  $\hat{\mathcal{H}}_U$  still is, electrons and positrons are still present as a matter-antimatter hybrid.

This means that one has yet to pass from the Dirac representation of  $\hat{\mathcal{H}}_U$  to the so-called the Newton Wigner representation [9, 10, 7]. The Newton-Wigner representation is closely related to the nonrelativistic limit of the single-particle Dirac Hamiltonian, and it is only in this representation in which a classical interpretation is possible, hence, in which we find the nonrelativistic Hamiltonian  $\hat{\mathcal{H}}_{LM}$  of light-matter interactions (for both electrons and positrons). Technically the Newton-Wigner representation can be brought about by another unitary transformation, the so-called Eriksen transformation [11, 10, 7]. Expressing the Hamiltonian  $\hat{\mathcal{H}}_U$  in the Newton-Wigner representation indeed makes it possible to derive the nonrelativistic limit of QED as a many-fermion Hamiltonian  $\hat{\mathcal{H}}_{LM}$  describing the interactions of fermions as point particles, their interactions with each other, and their interactions **with low-energy photons**. The Hamiltonian  $\hat{\mathcal{H}}_{LM}$  can then be retranslated to first quantization, hence, from this Hamiltonian then follows  $\hat{H}_{LM}$  and thus the Hamiltonian (2)!

It has to be emphasised, however, that it is an interesting feature, given the history of QED as "oscillating between the two viewpoints", that one can answer the question of how one can derive the nonrelativistic or classical limit from QED in a physically sensible way by answering the question **how can one regain the classical point particle carrying mass, charge and spin** from QED.

To give an answer to this question by defining the essential properties of point-like nonrelativistic particles is the bridge between QED and nonrelativistic light-matter interactions, and this bridge is nothing but the nonrelativistic limit of QED.

Fritz Rohrlich [12] already regretted in 1980 that "there does not exist up to date a clean proof of this [nonrelativistic...] limit,



[although] this notion is logically very reasonable and my view philosophically necessary because QED without [its nonrelativistic limit] is incomplete.”

Now the inspiration to the question of how one can derive the nonrelativistic limit of QED came from the pioneering work of Takashi Itoh [13]. He was the first who deduced from the Hamiltonian of QED the nonrelativistic many-body Hamiltonian of electrons interacting with each other in case of a static external electromagnetic field. Methodologically, the work unfortunately leaves something to be desired, because the positrons are not treated properly. Itoh often neglects terms in his derivation which violate particle number conservation and provides unclear arguments for this (at least for me). Itoh also eliminates all photons from the QED Hamiltonian, such that he cannot implement the necessity of renormalization. With that it is not possible to achieve the anomalous magnetic moment of the electron.

Claude Cohen-Tannoudji et. al. have also faced this question in their book *Photons and Atoms. Introduction to Quantum Electrodynamics* [6]. There they deduce the nonrelativistic limit from the QED Hamiltonian starting by two-component formalism of the field operators. This means that their field operators describe already on the QED level particles and antiparticles separately. They argue that the coupling between the matter and antimatter degrees of freedom is small, but neglecting this coupling from the beginning is not satisfactory because again, in that way it is not possible to treat the positrons on equal footing. Obviously, the positrons are particles equal to the electron, see again figure 1! However, with their method of perturbation theory, they are able to derive the Schrödinger–Pauli Hamiltonian of the electron in first order of their expansion. For higher order calculations they refer to the work of Iwo Bialynicki–Birula *The Hamiltonian of Quantum Electrodynamics* [14]. There Bialynicki–Birula unitarily transforms the QED Hamiltonian with a Foldy–Wouthuysen transformation adapted to the formalism of field theory. With that he gets as the most important representative of the relativistic corrections to the Schrödinger–Pauli-Hamiltonian the spin-orbit interaction of the fermions (electrons and positrons) with the electromagnetic field. However, he also does not consider (small) terms which violate the particle number conservation from the

beginning by starting from Dirac field operators which describe matter and antimatter separately. Furthermore, the relativistic correction to the kinetic energy is missing.

In another work of Bialynicki–Birula [15], starting with the sentence “The relationship between quantum and classical electrodynamics is a complex subject, with many aspects, not all of which are at present well understood.”, the focus has been laid on the classical limit of the radiation or electromagnetic field *interacting with a plurality of charged particles*. The approach taken in this dissertation shows, however, that it is very important to consider the whole QED hybrid, to take it radically serious as an object that has nothing to do with its constituents arising from it in the nonrelativistic limit, e.g. that it is *not made of particles and the radiation field as distinguishable objects*. This makes it possible to focus on how to get back to the classical point particle carrying mass, charge and spin, interacting with low–energy photons, by attacking the problem of particle number conservation violation (which is a problem insofar as it is not understable in classical terms).

Therefore, in this dissertation, a different approach for deriving the nonrelativistic limit from QED is taken. Thereby it is shown that it is not necessary to put particle number conservation into it from the beginning, or to drop small, however existent, particle number violating terms <sup>1</sup>. All constituents of QED shall be treated on equal footing. Therefore, for deriving the classical, nonrelativistic limit from QED, use is made of the so–called Wegner flow equation [16]. The Wegner flow equation (or the flow equation) is a tool for unitarily transforming a given matrix or an operator in a continuous manner. It is a differential equation generated by a generator which has to be chosen on the basis of physical considerations.

Hence, a unitary transformation of the QED Hamiltonian is to be sought such that the resulting Hamiltonian  $\hat{\mathcal{H}}_U$  conserves the particle number. It now turns out that one has to choose the generator of the related flow equation such that the pair terms in the QED Coulomb interaction as well as the high energy photons are eliminated from the QED Hamiltonian! It will be shown that high–energy photons are those whose wave number  $q$  is larger than  $\alpha_{FS}m_e c^2$ , where  $\alpha_{FS}$

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<sup>1</sup>It has to be emphasised that with such an intuitive approach, one can not be sure that terms, which actually belong to the result in this order, are suppressed.

is the finestructure constant. Thus, it is the hard X-ray photons and the gamma rays which are being eliminated. Only then the resulting Hamiltonian preserves the particle number. Unfortunately this generator generates a nonlinear differential equation that one cannot solve exactly. This reflects the fact that, as is generally known, real interactions can only be treated in terms of perturbation theory. This means that one has to expand the QED Hamiltonian in terms of a dimensionless coupling constant, which is the fine structure constant  $\alpha_{FS}$ . The resulting system of coupled **linear** differential equations can then be solved in principle in any order, and here it is solved up to the order  $\alpha_{FS}^2$ .

Now this has also the consequence that the bare mass  $m_0$  occurring as a parameter in the QED Hamiltonian will be changed during the process of taking the nonrelativistic limit from it. This is also known as renormalization. The  $g$ -factor of the fermions is also renormalized. In that way one finds the Schwinger result of the anomalous  $g$ -factor [17].

However, as has already been mentioned, the aspect of particle number conservation this is not the only one of the story. The particle number conserving Hamiltonian  $\hat{\mathcal{H}}_U$  is not yet expressible in first quantization. Due to the fact that the QED Hamiltonian is built upon the properties of the nondiagonal single-particle Dirac Hamiltonian, in QED, the matter and antimatter degrees of freedom are superposed, and this coherent superposition is independent of the aspect of particle number conservation. Therefore, in a second step, one has to decouple the matter and antimatter degrees of freedom in  $\hat{\mathcal{H}}_U$ . This can be done by the help of the Erikson transformation [11, 10, 7], which is a unitary transformation generalizing the Foldy-Whouthuysen transformation [18]. It is a unitary transformation that blockdiagonalizes the single-particle Dirac Hamiltonian in an external static magnetic field, and with that it enables to express the Dirac operators in the so-called Newton-Wigner representation. Now in the Newton-Wigner representation the Dirac operators decompose into matter and antimatter degrees of freedom separately, hence allowing for a classical interpretation [19, 9, 10]. There are several works which are concerned with this de-facto blockdiagonalization of the single-particle Dirac Hamiltonian, see for example [20, 21, 22, 23, 24, 25, 11, 26, 27, 28, 29]. However, in none of them but in the one of Bylev and Pirner [26] use

is made of a flow equation based approach. But Bylev and Pirner have not solved the related flow equation exactly, only perturbatively. It is, however, possible to solve this flow equation exactly.

All of this is explained in detail in the following sections. Finally it should be said that with the path outlined here it is possible to derive the nonrelativistic limit of QED for both electrons *and* positrons *and* their interactions in a completely symmetric fashion. With that it is possible to answer the urgent question of T. Padmanabhan of "What happens to the antiparticles when you take the non-relativistic limit of QFT?" [30].

It was Ettore Majorana who emphasised already in 1937 that "The prescriptions to cast the [Dirac] theory into a symmetric form, in conformity with its content, are however not entirely satisfactory, because one always starts from an asymmetric form or because symmetric results are obtained only after one applies appropriate procedures such as the cancellation of divergent constants, that one should possibly avoid." [31]. In this work he then clarified that four degrees of freedom are needed for *both* matter and antimatter, so  $4 + 4 = 8$  degrees of freedom altogether.

However, in this dissertation, the final result for the *many-body - Schrödinger-Pauli Hamiltonian* is only presented for the electrons. Unfortunately, there was no time left for the (completeley) analog evaluation of the positrons.

Furthermore, this dissertation was completed in July 2022. In the meantime, the results have been extended by Nils Schopohl so that the renormalization of the bare charge  $q_0$  and the Lamb shift are now also available as the result of a unitary transformation of the QED Hamiltonian based on Wegner's flow equation [8].

Now the structure of the work is as follows: in section 2 the reader is introduced to the Hamiltonian of QED in the Coulomb gauge. Then the relation between QED and the classical limit problem is discussed, and the Newton-Wigner representation of single-particle Dirac Hamiltonian is briefly sketched.

In section 3 the method of unitarily transforming matrices or operators by the help of the Wegner flow equation is presented, and then the method is discussed in the context of the question of how to deduce the classical limit from QED.

Next in the first part of the solution to the classical limit problem of QED 4 the flow equation that generates particle number conservation is set up and solved by the help of perturbation theory. In that way one achieves a unitarily equivalent QED Hamiltonian  $\hat{\mathcal{H}}_U$  which conserves the particle number, and in which all constituents, fermions, photons, and their interactions, occur in a completely symmetric fashion.

Then in the section 5 the Eriksen transformation is introduced as the unitary transformation which blockdiagonalizes the single-particle Dirac Hamiltonian, and which decouples matter and antimatter degrees of freedom. Then the single-particle Dirac Hamiltonian in the Newton-Wigner representation, which follows from the Eriksen transformation, is discussed.

In the second part of the solution to the classical limit problem of QED 6 it is shown how one can retranslate the results achieved so far to first quantization by applying the Eriksen transformation to  $\hat{\mathcal{H}}_U$ . At this point the positrons are not further considered, the evaluation is only done for the part describing the electrons. Thereby it is shown how the renormalization of the electron properties come into play: one part comes from the interaction with the high-energy photons. This is referred to as transversal renormalization. The other contributions to the renormalization, the longitudinal contribution, is due to the QED Coulomb interaction. As will become clear, it stems from the necessity of normal ordering the QED Coulomb interaction. Next the effective Schrödinger-Pauli Hamiltonian is derived. Finally the nonrelativistic Hamiltonian of light-matter interaction in first quantization for a plurality of electrons is presented and the results are being discussed.

The appendix is intended as an auxiliary tool for those who wish to follow long calculations in detail. There is, however, one appendix section which stands alone. In section J it is shown how the Maxwell Equations of the operator valued fields describing the photons as well as their coupling to sources can be derived.

This dissertation was developed over a period of four years in close collaboration with my supervisor Prof. Dr. Nils Schopohl. Most of the calculations in this dissertation have been developed by my supervisor while it was an indispensable part of mine to carefully check all these calculations independently.

Furthermore it was an essential part of my mine to critically question

the physical ideas which we have developed and discussed together, and to insist on a physically coherent picture (or to be taught better, i.e. to learn). In that way I have made several important contributions concerning the physical coherence of the overall work. This concerns, first, referring strictly to graph 1, the insistence that all constituents of the QED soup must be treated equally, which has led to the realization that it is inconsistent to introduce two separate components for matter and antimatter from the beginning for the QED field operators.

Second, it was my insistence that we live in a world where there are always photons that laid the basis for finding a generator for the flow equation that allows to eliminate only a certain part of the photons, namely the high-energy photons, from the QED Hamiltonian.

Third, it was unclear for a long time how to get from the four-dimensional Dirac Hamiltonian to the nonrelativistic two-dimensional Schrödinger–Pauli Hamiltonian. By reading McKellar’s extremely insightful paper [9] I was able to make it clear that also in the nonrelativistic limit the formalism will be four-dimensional, however, it has somehow to be given by the diagonal Dirac  $\beta$  matrix. With this insight it became possible to solve the flow equation for the Eriksen transformation exactly and, indeed, the nonrelativistic limit of the Dirac Hamiltonian was found to be given by  $\beta$  times the two-dimensional Schrödinger–Pauli Hamiltonian, hence, as a four-dimensional, blockdiagonal Hamiltonian.

Fourth, in the long discussions on how to choose the cut-off of the renormalization terms to get a physically consistent picture, I was able to make a decisive contribution by insisting that it is inconsistent to say on the one hand that the correct cut-off must be made Lorentz invariant, but on the other hand it was clear that the anomalous  $g$ -factor has nothing at all to do with Lorentz invariance. This led to the idea, following Paul Dirac [32], to implement a physical cut-off which consists in limiting both the photon energy and the kinetic energy of the fermions. This in turn led to the correct renormalization of the bare mass  $m_0$  of the fermions and therefore to the Schwinger result for the  $g$ -factor.

Finally, I realized that one does not have to do the evaluation for the part with the positrons all over again, but that one can also obtain the positron Hamiltonian using the charge conjugation operator, which

makes sense since, of course, the fermions should be renormalized in a symmetric way.

There have been many other contributions I could make during the long and intensive discussions, here I have listed the most important ones.



## 2 Quantum Electrodynamics (QED) in the Coulomb Gauge

### 2.1 Introduction to QED in the Coulomb Gauge

There are several highly recommendable books on QED [6, 32, 33, 4, 34, 5, 35, 36, 37, 38], where each book has a different focus, making it worthwhile to read each one in order to understand and learn about quantum field theories and Quantum Electrodynamics. Since for the derivation of the nonrelativistic limit of the QED Hamiltonian its representation in the Coulomb gauge is the most convenient one, the representation from [6] has been mostly adopted.

As already indicated in the introduction, the hybrid quantum field of QED consists of a charged (anti-)matter quantum field, a radiation field, and their interaction fields. It can be represented by the following Hamiltonian in the Coulomb gauge <sup>2</sup>: [6]

$$\hat{\mathcal{H}}_{QED} = \hat{\mathcal{H}}_D + \hat{\mathcal{H}}_{rad} + \hat{\mathcal{V}}_{ext} + \hat{\mathcal{H}}_{\perp} + \hat{\mathcal{V}}_C \quad (8)$$

The interpretation of these terms goes as follows: the first term  $\hat{\mathcal{H}}_D$  is the second quantized Dirac Hamiltonian. It comprises the rest energy, the kinetic energy and the Zeeman energy of the charged (anti-)matter quantum fields. The second term  $\hat{\mathcal{H}}_{rad}$  is the radiation field or the quantized electromagnetic field. The term  $\hat{\mathcal{V}}_{ext}$  is the potential energy of the charged (anti-)matter quantum field in an external static classical source  $\Phi^{(ext)}(\mathbf{r})$ . The last two terms  $\hat{\mathcal{H}}_{\perp}$  and  $\hat{\mathcal{V}}_C$  are the essential terms of QED.  $\hat{\mathcal{V}}_C$  comprises the Coulomb interaction of the charged (anti-)matter quantum fields, and  $\hat{\mathcal{H}}_{\perp}$  describes the interaction of the charged matter quantum fields with the radiation field or the photons.

One could think that the QED Hamiltonian (8) is not Lorentz invariant, since the decomposition of the electromagnetic quantum

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<sup>2</sup>The reason why the Hamiltonian (8) is referred to as "in the Coulomb gauge" is that the Coulomb interaction between the (anti-)matter fields appears explicitly. In a representation without a choice of gauge the Hamiltonian of classical light-matter interactions consists of the kinetic energy of the electrons plus the energy of the electromagnetic field. Decomposing the latter into longitudinal and transversal parts then the Coulomb interaction as the longitudinal interaction of light-matter interactions, as well as the coupling to the light, the transversal part of light-matter interactions, appears. This is because light and matter are related by the Maxwell equations, which also decompose into longitudinal and transversal parts [6].



field into longitudinal and transversal parts is not. However, as has already been shown by W. Heisenberg and W. Pauli in 1930 the total Hamiltonian (8) is Lorentz invariant [39]. A nice summary of their arguments can also be found in [14].

The various terms of (8) and their properties are discussed in more detail in the following.

### The Second Quantized Single-Particle Dirac Hamiltonian

The second quantized Dirac Hamiltonian  $\hat{\mathcal{H}}_D$  is given as

$$\hat{\mathcal{H}}_D = \int d^3r \sum_{\mu, \mu' \in \{1,2,3,4\}} \frac{1 - \mathcal{C}_F}{2} \left( \hat{\Psi}_\mu^\dagger(\mathbf{r}) \mathbf{H}_{\mu, \mu'}^{(D)} \hat{\Psi}_{\mu'}(\mathbf{r}) \right) \quad (9)$$

It contains the integral kernel  $\mathbf{H}_{\mu, \mu'}^{(D)}$ , which is the single-particle Dirac Hamiltonian in a static external magnetic induction field  $B_b^{(ext)} = \text{rot } A_b^{(ext)}(\mathbf{r})$ . It is given by

$$\mathbf{H}^{(D)} = m_0 c^2 \beta + \sum_{b \in \{x, y, z\}} c \alpha_b \left( \hat{\mathbf{p}}_b - q_e A_b^{(ext)}(\mathbf{r}) \right) \quad (10)$$

The four by four diagonal Dirac  $\beta$  matrix and the non-diagonal Dirac  $\alpha_b$  matrix obey to the algebraic relations

$$\begin{aligned} \beta \alpha_a + \alpha_a \beta &= 0_{4 \times 4} \\ \beta^2 &= 1_{4 \times 4} \\ \alpha_a \alpha_b &= \delta_{a,b} 1_{4 \times 4} + i \varepsilon_{abc} \sigma_c \\ a, b &\in \{x, y, z\} \end{aligned} \quad (11)$$

These are diagonal or non-diagonal with respect to a chosen representation [5]. In our case this is the so-called Dirac representation:

$$\begin{aligned} \alpha_a &= \sigma_x^{(P)} \otimes \sigma_a^{(P)} \\ \beta &= \sigma_z^{(P)} \otimes 1_{2 \times 2} \end{aligned} \quad (12)$$

where matrices  $\sigma_a^{(P)}$  are the Pauli matrices in their standard representation, thus

$$\begin{aligned}\sigma_x^{(P)} &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ \sigma_y^{(P)} &= \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \\ \sigma_z^{(P)} &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\end{aligned}\tag{13}$$

The first term in the single-particle Dirac Hamiltonian (10) describes the rest energy of the Dirac fermion, whereas the second term describes its kinetic energy and its Zeeman energy. (In the Heisenberg picture of  $\mathbf{H}^{(D)}$  one finds that the velocity  $\hat{v}_a$  of the Dirac particle is  $c\alpha_a$ .) Please note the rest mass  $m_0$ , which is the **bare mass** of the Dirac fermion!

In the appendix sections A, C and D the properties of the single particle Dirac Hamiltonian  $\mathbf{H}^{(D)}$  are discussed in more detail. An extensive introduction to (the history of) the Dirac Hamiltonian can be found in [3, 40, 5, 40, 41].

The (anti-)matter field operators  $\hat{\Psi}_\mu$  and  $\hat{\Psi}_\mu^\dagger(\mathbf{r})$ , the so called Dirac spinors, are given by

$$\begin{aligned}\hat{\Psi}_\mu(\mathbf{r}) &= \sum_k \left( U_\mu(\mathbf{r}; k) \hat{c}_k + V_\mu(\mathbf{r}; k) \hat{b}_{\tilde{k}}^\dagger \right) \\ \hat{\Psi}_\mu^\dagger(\mathbf{r}) &= \sum_k \left( U_\mu^*(\mathbf{r}; k) \hat{c}_k^\dagger + V_\mu^*(\mathbf{r}; k) \hat{b}_{\tilde{k}} \right) \\ \mu &\in \{1, 2, 3, 4\}\end{aligned}\tag{14}$$

The operators  $\hat{c}_k^\dagger$ ,  $\hat{c}_k$  and  $\hat{b}_{\tilde{k}}^\dagger$ ,  $\hat{b}_{\tilde{k}}$  are creation and annihilation operators ( $k$  is a multi index counting the modes of the Dirac eigenvalue problem). They operate on the matter sector of the Fock space of QED, and they obey to the anti-commutation relations for spin- $\frac{1}{2}$  particles [4, 5]:

$$\begin{aligned}
\{\hat{c}_k, \hat{c}_{k'}^\dagger\} &= \delta_{k,k'} \hat{1} = \{\hat{b}_{\tilde{k}}, \hat{b}_{\tilde{k}'}^\dagger\} \\
\{\hat{c}_k, \hat{c}_{k'}\} &= \hat{0} = \{\hat{c}_k^\dagger, \hat{c}_{k'}^\dagger\} \\
\{\hat{b}_{\tilde{k}}, \hat{b}_{\tilde{k}'}\} &= \hat{0} = \{\hat{b}_{\tilde{k}}^\dagger, \hat{b}_{\tilde{k}'}^\dagger\} \\
\{\hat{b}_{\tilde{k}}, \hat{c}_{k'}\} &= \hat{0} = \{\hat{b}_{\tilde{k}}^\dagger, \hat{c}_{k'}^\dagger\} \\
\{\hat{b}_{\tilde{k}}^\dagger, \hat{c}_{k'}\} &= \hat{0} = \{\hat{b}_{\tilde{k}}^\dagger, \hat{c}_{k'}^\dagger\}
\end{aligned} \tag{15}$$

$U_\mu(\mathbf{r}; k)$  is the  $\mu$ -th component of a Dirac amplitude belonging to the positive energy  $E_k > 0$ , whereas  $V_\mu(\mathbf{r}; k)$  is the  $\mu$ -th component of a Dirac amplitude belonging to the negative energy  $-E_k < 0$ .

$$\begin{aligned}
\mathbf{H}_{\mu,\mu'}^{(D)} U_{\mu'}(\mathbf{r}; k) &= E_k U_\mu(\mathbf{r}; k) \\
\mathbf{H}_{\mu,\mu'}^{(D)} V_{\mu'}(\mathbf{r}; k) &= -E_k V_\mu(\mathbf{r}; k)
\end{aligned} \tag{16}$$

The Dirac amplitudes comprise four components for *both* matter and antimatter [31]!

Please notice that in case the Dirac Hamiltonian comprises an external *electric* field  $E^{(ext)}$  the charge conjugation symmetry is broken. This is because the matter is attracted by the electric field, the Lorentz force being  $F^{(e)} = -|e|E^{(ext)}$ , whereas the antimatter is repulsed by the electric field  $F^{(p)} = +|e|E^{(ext)}$ . In that case the set of modes  $k$  and  $\tilde{k}$  are not necessarily of the same scope and one would have to introduce a summation over the mode indices  $\tilde{k}$  in the part describing the negative energy solutions in 16 [10].

From the requirement that the Dirac Hamiltonian (10) must be hermitian, the amplitudes  $U_\mu^*(\mathbf{r}; k)$ ,  $U_\mu(\mathbf{r}; k')$  and  $V_\mu^*(\mathbf{r}; k)$ ,  $V_\mu(\mathbf{r}; k')$  obey to the following orthogonality relations:

$$\begin{aligned}
\int d^3r \sum_{\mu} U_{\mu}^{\star}(\mathbf{r}; k) U_{\mu}(\mathbf{r}; k') &= \delta_{k,k'} \\
\int d^3r \sum_{\mu} V_{\mu}^{\star}(\mathbf{r}; k) V_{\mu}(\mathbf{r}; k') &= \delta_{k,k'} \\
\int d^3r \sum_{\mu} U_{\mu}^{\star}(\mathbf{r}; k) V_{\mu}(\mathbf{r}; k') &= 0 \\
\int d^3r \sum_{\mu} V_{\mu}^{\star}(\mathbf{r}; k) U_{\mu}(\mathbf{r}; k') &= 0
\end{aligned} \tag{17}$$

From which the completeness relation of the Dirac modes follows as

$$\sum_k (U_{\mu}(\mathbf{r}; k) U_{\mu'}^{\star}(\mathbf{r}'; k) + V_{\mu}(\mathbf{r}; k) V_{\mu'}^{\star}(\mathbf{r}'; k)) = \delta_{\mu,\mu'} \delta^{(3)}(\mathbf{r} - \mathbf{r}') \tag{18}$$

And the anti commutation relations of the creation and annihilation operators of the fermions imply

$$\begin{aligned}
\{\hat{\Psi}_{\mu}(\mathbf{r}), \hat{\Psi}_{\mu'}^{\dagger}(\mathbf{r}')\} &= \delta_{\mu,\mu'} \delta^{(3)}(\mathbf{r} - \mathbf{r}') \hat{1} \\
\{\hat{\Psi}_{\mu}(\mathbf{r}), \hat{\Psi}_{\mu'}(\mathbf{r}')\} &= \hat{0} = \{\hat{\Psi}_{\mu}^{\dagger}(\mathbf{r}), \hat{\Psi}_{\mu'}^{\dagger}(\mathbf{r}')\}
\end{aligned} \tag{19}$$

It can be shown that the relation (19) is a necessary consequence if one requires that the momentum operator  $\hat{\Psi}_{\mu}$  generates translations in spacetime  $x$  [5].

The operation  $\frac{1-\mathcal{C}_F}{2}$  in (9) ensures that the Dirac quantum field is symmetric under charge conjugation [33]. It is explained in more detail below, where the QED current density operator  $\hat{j}_b(\mathbf{r})$  and the QED charge density operator  $\hat{\rho}(\mathbf{r})$  are introduced, and also in the appendix section F. It has to be mentioned that the operation  $\frac{1-\mathcal{C}_F}{2}$  removes an (infinite) constant being not observable [4].

The most important operators of QED, besides the Hamiltonian (8), are the particle number operator  $\hat{N}$  and the charge number operator  $\hat{Q}$ .

$$\begin{aligned}
\hat{N} &= \hat{N}^{(e)} + \hat{N}^{(p)} = \sum_k \left( \hat{c}_k^\dagger \hat{c}_k + \hat{b}_{\tilde{k}}^\dagger \hat{b}_{\tilde{k}} \right) \\
\hat{N}^{(e)} &= \sum_k \hat{c}_k^\dagger \hat{c}_k \\
\hat{N}^{(p)} &= \sum_k \hat{b}_{\tilde{k}}^\dagger \hat{b}_{\tilde{k}}
\end{aligned} \tag{20}$$

$\hat{N}^{(e)}$  is given by the mode occupation number  $\hat{c}_k^\dagger \hat{c}_k$ . It counts the occupied Dirac-modes of  $\mathbf{H}^{(D)}$  with mode index  $k$  and positive energy eigenvalue  $E_k > 0$ .  $\hat{N}^{(p)}$  is given by the mode occupation number  $\hat{b}_{\tilde{k}}^\dagger \hat{b}_{\tilde{k}}$ . It counts its occupied Dirac-modes with mode index  $\tilde{k}$  and negative energy eigenvalue  $-E_k < 0$ .

Hence, the charge number operator  $\hat{Q}$  is defined by

$$\hat{Q} = q_e \left( \hat{N}^{(e)} - \hat{N}^{(p)} \right) \tag{21}$$

Now the most important properties of these two operators for the question posed in this dissertation are [8]

$$\begin{aligned}
\left[ \hat{Q}, \hat{\mathcal{H}}_{QED} \right] &= \hat{0} \\
\left[ \hat{N}, \hat{\mathcal{H}}_{QED} \right] &\neq \hat{0}
\end{aligned} \tag{22}$$

Like in our classical physical world, the charge number  $\hat{Q}$  is a conserved quantity in QED. What separates QED from our world is the *lacking of particle number conservation*. The reason for the latter is the fact that in QED the energy can be so high that there are processes which allow to *convert photons into fermion pairs and vice versa*. Actually, the particle number operator  $\hat{N}$  does not commute with  $\hat{\mathcal{H}}_{QED}$  because of the interaction terms  $\hat{\mathcal{H}}_{\perp}$  and  $\hat{\mathcal{V}}_C$ .

If one wishes to rebuild our classical world from QED or to regain the nonrelativistic limit from it, one has to handle the lack of particle number conservation. In subsection 2.2 a closer look is taken at the properties (22).

## The Radiation Field

The quantized radiation field can be represented according to [6]

$$\hat{\mathcal{H}}_{rad} = \frac{1}{2} \int d^3r' \sum_{b \in \{x,y,z\}} \left( \hat{E}_b^{(T)}(\mathbf{r}') \varepsilon_0 \hat{E}_b^{(T)}(\mathbf{r}') + \hat{B}_b(\mathbf{r}') \frac{1}{\mu_0} \hat{B}_b(\mathbf{r}') \right) \quad (23)$$

In this representation it resembles its classical counterpart, the classical electromagnetic field, the most. However, (23) is an operator valued field. For understanding this better it is convenient to represent the electromagnetic field by a linear superposition of creation and annihilation operators  $\hat{a}_{\mathbf{q},\lambda}^\dagger$  and  $\hat{a}_{\mathbf{q},\lambda}$  describing the creation and annihilation of the particle of the electromagnetic field, the photon, with polarization  $\lambda \in \{I, II\}$  and wavevector  $\mathbf{q}$

$$\hat{A}_b^{(T)}(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{q}} \sum_{\lambda \in \{I, II\}} \mathcal{A}_b(\mathbf{q}, \lambda) \left( e^{i\mathbf{q}\cdot\mathbf{r}} \hat{a}_{\mathbf{q},\lambda} + e^{-i\mathbf{q}\cdot\mathbf{r}} \hat{a}_{\mathbf{q},\lambda}^\dagger \right) \quad (24)$$

$$\mathcal{A}_b(\mathbf{q}, \lambda) = \sqrt{\frac{\hbar}{2\varepsilon_0\omega(\mathbf{q})}} u_b(\mathbf{q}, \lambda)$$

$$\hat{E}_b^{(T)}(\mathbf{r}) = \frac{i}{\sqrt{V}} \sum_{\mathbf{q}} \sum_{\lambda \in \{I, II\}} \mathcal{E}_b(\mathbf{q}, \lambda) \left( e^{i\mathbf{q}\cdot\mathbf{r}} \hat{a}_{\mathbf{q},\lambda} - e^{-i\mathbf{q}\cdot\mathbf{r}} \hat{a}_{\mathbf{q},\lambda}^\dagger \right) \quad (25)$$

$$\mathcal{E}_b(\mathbf{q}, \lambda) = \sqrt{\frac{\hbar\omega(\mathbf{q})}{2\varepsilon_0}} u_b(\mathbf{q}, \lambda)$$

$$\hat{B}_b^{(T)}(\mathbf{r}) = \frac{i}{\sqrt{V}} \sum_{\mathbf{q}} \sum_{\lambda \in \{I, II\}} \mathcal{B}_b(\mathbf{q}, \lambda) \left( e^{i\mathbf{q}\cdot\mathbf{r}} \hat{a}_{\mathbf{q},\lambda} - e^{-i\mathbf{q}\cdot\mathbf{r}} \hat{a}_{\mathbf{q},\lambda}^\dagger \right) \quad (26)$$

$$\mathcal{B}_b(\mathbf{q}, \lambda) = \sqrt{\frac{\hbar\omega(\mathbf{q})}{2c^2\varepsilon_0}} \varepsilon_{bb'b''} \frac{q_{b'}}{q} u_{b''}(\mathbf{q}, \lambda)$$

This mode expansion of the quantized electromagnetic field relates to a Volume  $V$  with periodic boundary conditions. One has to keep

in mind that in the end of all calculations one has to take the limit  $V \rightarrow \infty$ .

As photons are bosons, their related creation and annihilation operators obey to commutation relations

$$\begin{aligned} [\hat{a}_{\mathbf{q},\lambda}, \hat{a}_{\mathbf{q}',\lambda'}] &= \hat{0} = [\hat{a}_{\mathbf{q},\lambda}^\dagger, \hat{a}_{\mathbf{q}',\lambda'}^\dagger] \\ [\hat{a}_{\mathbf{q},\lambda}, \hat{a}_{\mathbf{q}',\lambda'}^\dagger] &= \delta_{\lambda,\lambda'} \delta_{\mathbf{q},\mathbf{q}'} \hat{1} \end{aligned} \quad (27)$$

The wavevector  $q_b$  and the related polarization vectors  $u_a(\mathbf{q}, I)$  and  $u_a(\mathbf{q}, II)$  form a complete orthonormal basis in the Fock space of the photons. For *linearly* polarized photons there holds

$$\begin{aligned} u_b^*(\mathbf{q}, \lambda) &= u_b(\mathbf{q}, \lambda) \\ \sum_a u_a(\mathbf{q}, I) u_a(\mathbf{q}, I) &= 1 = \sum_a u_a(\mathbf{q}, II) u_a(\mathbf{q}, II) \\ \sum_a u_a(\mathbf{q}, I) u_a(\mathbf{q}, II) &= 0 \\ \sum_a u_a(\mathbf{q}, I) q_a &= 0 = \sum_a u_a(\mathbf{q}, II) q_a \end{aligned} \quad (28)$$

The commutation relations (27) imply for the transversal vector potential  $\hat{A}_a^{(T)}(\mathbf{r})$  and the transversal electrical field  $\hat{E}_a^{(T)}(\mathbf{r})$

$$\begin{aligned} [\hat{A}_a^{(T)}(\mathbf{r}), \hat{E}_b^{(T)}(\mathbf{r}')] &= \frac{1}{\varepsilon_0} \frac{\hbar}{i} \delta_{ab}^{(T)}(\mathbf{r} - \mathbf{r}') \hat{1} \\ [\hat{A}_a^{(T)}(\mathbf{r}), \hat{A}_b^{(T)}(\mathbf{r}')] &= \hat{0} = [\hat{E}_a^{(T)}(\mathbf{r}), \hat{E}_b^{(T)}(\mathbf{r}')] \end{aligned} \quad (29)$$

The integral kernel  $\delta_{ab}^{(T)}(\mathbf{r} - \mathbf{r}')$ , the so-called transversal delta function [6], is given by

$$\begin{aligned} \delta_{ab}^{(T)}(\mathbf{r} - \mathbf{r}') &= \frac{2}{3} \delta_{ab} \delta^{(3)}(\mathbf{r} - \mathbf{r}') - \lim_{\eta \rightarrow 0^+} \Theta(|\mathbf{r} - \mathbf{r}'| - \eta) \frac{\delta_{ab} |\mathbf{r} - \mathbf{r}'|^2 - 3(\mathbf{r} - \mathbf{r}')_a (\mathbf{r} - \mathbf{r}')_b}{4\pi |\mathbf{r} - \mathbf{r}'|^5} \\ &= \lim_{\xi \rightarrow 0} \int \frac{d^3 q}{(2\pi)^3} \frac{e^{i\mathbf{q} \cdot (\mathbf{r} - \mathbf{r}')}}{1 + q^2 \xi^2} \left( \delta_{a,b} - \frac{q_a q_b}{|\mathbf{q}|^2} \right) \end{aligned} \quad (30)$$

Together with its complement, the longitudinal delta function

$$\begin{aligned}
\delta_{ab}^{(L)}(\mathbf{r} - \mathbf{r}') &= -\frac{\partial^2}{\partial r_a \partial r_b} \frac{1}{4\pi |\mathbf{r} - \mathbf{r}'|} \\
&= \frac{1}{3} \delta_{ab} \delta^{(3)}(\mathbf{r} - \mathbf{r}') + \lim_{\eta \rightarrow 0^+} \Theta(|\mathbf{r} - \mathbf{r}'| - \eta) \frac{\delta_{ab} |\mathbf{r} - \mathbf{r}'|^2 - 3(\mathbf{r} - \mathbf{r}')_a (\mathbf{r} - \mathbf{r}')_b}{4\pi |\mathbf{r} - \mathbf{r}'|^5} \\
&= \lim_{\xi \rightarrow 0} \int \frac{d^3 q}{(2\pi)^3} \frac{e^{i\mathbf{q} \cdot (\mathbf{r} - \mathbf{r}')}}{1 + q^2 \xi^2} \left( \delta_{a,b} - \frac{q_a q_b}{|\mathbf{q}|^2} \right)
\end{aligned} \tag{31}$$

one finds

$$\delta_{ab}^{(L)}(\mathbf{r} - \mathbf{r}') + \delta_{ab}^{(T)}(\mathbf{r} - \mathbf{r}') = \delta_{ab} \delta^{(3)}(\mathbf{r} - \mathbf{r}') \tag{32}$$

With  $a, b \in \{x, y, z\}$  there holds

$$\hat{B}_a(\mathbf{r}) = \varepsilon_{abc} \nabla_b \hat{A}_c^{(T)}(\mathbf{r}) = \left( \text{rot} \hat{\mathbf{A}}^{(T)}(\mathbf{r}) \right)_a \tag{33}$$

and

$$\nabla_a \hat{A}_a^{(T)}(\mathbf{r}) = \hat{0} = \nabla_a \hat{E}_a^{(T)}(\mathbf{r}) \tag{34}$$

With these relations one can represent the radiation field Hamiltonian (23) by the occupation number operator  $\hat{a}_{\mathbf{q},\lambda}^\dagger \hat{a}_{\mathbf{q},\lambda}$  for the photons according to

$$\hat{\mathcal{H}}_{rad} = \sum_{\mathbf{q}} \sum_{\lambda \in \{I, II\}} \hbar \omega(\mathbf{q}) \left( \hat{a}_{\mathbf{q},\lambda}^\dagger \hat{a}_{\mathbf{q},\lambda} + \frac{1}{2} \hat{1} \right) \tag{35}$$

The photon number operator is thus given by

$$\hat{N}^{(ph)} = \sum_{\mathbf{q}} \sum_{\lambda \in \{I, II\}} \hat{a}_{\mathbf{q},\lambda}^\dagger \hat{a}_{\mathbf{q},\lambda} \equiv \sum_q \hat{a}_q^\dagger \hat{a}_q \tag{36}$$

In the appendix it is shown that the operator valued electromagnetic field obeys to the Maxwell equations and that we can also deduce the quantum analogue wave equation by the help of the Heisenberg equations of motion for the fields  $\hat{E}_b^{(T)}(\mathbf{r})$  and  $\hat{B}_b^{(T)}(\mathbf{r})$ , see section J.



## The Coupling of the Charged Matter and Antimatter Quantum Field to an External Electric c-Number Field

The coupling to an external potential  $\Phi^{(ext)}(\mathbf{r})$  is given by the contribution

$$\hat{\mathcal{V}}_{ext} = \int d^3r \hat{\rho}(\mathbf{r}) \Phi^{(ext)}(\mathbf{r}) \quad (37)$$

Here,  $\hat{\rho}(\mathbf{r})$  is the QED current density operator as introduced below in (43).  $\hat{\mathcal{V}}_{ext}$  describes, for example, the interaction of electrons and positrons with the Coulomb field of an atomic nucleus with charge number  $Z$  at the position  $\mathbf{R}$  according to

$$\Phi^{(ext)}(\mathbf{r}) = \frac{Z |q_e|}{4\pi\epsilon_0} \frac{1}{|\mathbf{r} - \mathbf{R}|} \quad (38)$$

The potential (38) breaks the charge conjugation symmetry because it is attractive for the electrons but repulsive for the positrons.

The Fourier representation of the potential  $\Phi^{(ext)}(\mathbf{q}) = \frac{Z|q_e|}{4\pi\epsilon_0} e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{R})} \frac{1}{|\mathbf{q}|^2}$  and of the QED charge density operator  $\tilde{\rho}(\mathbf{q}) = \int d^3r e^{-i\mathbf{q}\cdot\mathbf{r}} \hat{\rho}(\mathbf{r})$  will be very useful later on:

$$\begin{aligned} \hat{\mathcal{V}}_{ext} &= \frac{Z |q_e|}{4\pi\epsilon_0} \int \frac{d^3q}{(2\pi)^3} \frac{e^{i\mathbf{q}\cdot\mathbf{R}}}{|\mathbf{q}|^2} \int d^3r e^{-i\mathbf{q}\cdot\mathbf{r}} \hat{\rho}(\mathbf{r}) \\ &= \frac{Z |q_e|}{4\pi\epsilon_0} \int \frac{d^3q}{(2\pi)^3} \frac{e^{i\mathbf{q}\cdot\mathbf{R}}}{|\mathbf{q}|^2} \tilde{\rho}(\mathbf{q}) \end{aligned} \quad (39)$$

### Matter–Antimatter–Photon Interaction and Coulomb Interaction

The coupling between the charged (anti-)matter quantum fields and the radiation field is described by

$$\hat{\mathcal{H}}_{\perp} = - \int d^3r \hat{j}_b(\mathbf{r}) \hat{A}_b^{(T)}(\mathbf{r}) \quad (40)$$

The charge symmetrized QED current density  $\hat{j}_b(\mathbf{r})$  can be represented according to

$$\hat{j}_b(\mathbf{r}) = q_e \frac{1 - \mathcal{C}_F}{2} \sum_{\mu, \mu' \in \{1,2,3,4\}} \hat{\Psi}_\mu^\dagger(\mathbf{r}) (c\alpha_b)_{\mu, \mu'} \hat{\Psi}_{\mu'}(\mathbf{r}) \quad (41)$$

Whereas the vector potential  $\hat{A}_b^{(T)}(\mathbf{r})$  of the photons is given by (24). The Coulomb interaction can be represented by

$$\hat{\mathcal{V}}_C = \frac{1}{8\pi\epsilon_0} \int d^3r \int d^3r' \frac{\hat{\rho}(\mathbf{r}) \hat{\rho}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \quad (42)$$

Where the symmetrized charge density operator  $\hat{\rho}(\mathbf{r})$  is given by

$$\hat{\rho}(\mathbf{r}) = q_e \frac{1 - \mathcal{C}_F}{2} \sum_{\mu \in \{1,2,3,4\}} \hat{\Psi}_\mu^\dagger(\mathbf{r}) \hat{\Psi}_\mu(\mathbf{r}) \quad (43)$$

The representations of the charge density (43) and the current density (41) are according to the one proposed by Wolfgang Pauli [33].  $\mathcal{C}_F$  is the symbol for charge conjugation operation, see also appendix F. Usually, in text books on QED or quantum field theory, the current density (41) and the charge density (43) are introduced without the charge symmetry operation  $\mathcal{C}_F$  [4, 5]. However, the hint is given that the operators occurring in the respective scalars (QED charge density), vectors (QED current density) or tensors should always be considered as being *normally ordered*. This means that creation operators are shifted to the left, whereas annihilation operators are shifted to the right. Depending on the commutation relations these operators obey to there can occur minus signs during the exchange, or even  $\delta_k$ 's, where  $k$  is a multi index.

Now for example

$$\begin{aligned} \mathcal{N}(c_{k'} c_k^\dagger) &= -c_k^\dagger c_{k'} \\ \mathcal{N}(c_{k'} c_k^\dagger c_{k''}^\dagger) &= -\mathcal{N}(c_k^\dagger c_{k'} c_k^\dagger) = +c_k^\dagger c_k^\dagger c_{k'} \end{aligned} \quad (44)$$

whereas without the operation  $\mathcal{N}$  then, due to the anticommutation relations (15)

$$\begin{aligned} c_{k'} c_k^\dagger &= \delta_{k, k'} - c_k^\dagger c_{k'} \\ c_{k'} c_k^\dagger c_{k''}^\dagger &= (\delta_{k, k'} - c_k^\dagger c_{k'}) c_{k''}^\dagger \\ &= \delta_{k, k'} c_{k''}^\dagger + \delta_{k', k''} c_k + c_k^\dagger c_{k''}^\dagger c_{k'} \end{aligned} \quad (45)$$

The normal ordering operation  $\mathcal{N}$  indeed has a true *physical* meaning. In the appendix section F it is shown that the operation  $\frac{1-\mathcal{C}_F}{2}$  related to charge symmetry operation  $\mathcal{C}_F$  corresponds exactly to the normal ordering operation  $\mathcal{N}$  [7]. Moreover, these operations guarantee that in the (unfortunately unknown) QED ground state  $|G\rangle$  the expectation value of  $\hat{j}_b(\mathbf{r})$  and  $\hat{\rho}(\mathbf{r})$  vanish, which should of course be the case [4].

It has to be mentioned that it depends on the purpose which representation, the charge symmetry operation  $\frac{1-\mathcal{C}_F}{2}$  according to Pauli or the normal ordering operation  $\mathcal{N}$ , is more convenient [7].

## 2.2 QED and the Classical Limit Problem

In this subsection the reader shall be introduced in a more formal way into the two aspects which separate Quantum Electrodynamics as a field theory describing the interaction between quantized light– and matter–antimatter fields from classical light–matter interaction between fermions and photons.

The **first**, fundamental aspect is the **lack of particle number conservation** which is indicated by the non–vanishing commutator of the QED particle number operator (20) with the QED Hamiltonian (8). The physical reason for this is the fact that in the QED soup high energy photons buzz around, causing the creation and annihilation of fermions and other photons! The QED field is a quantum field consisting of matter and antimatter fields and light fields, and all these fields are inextricably interwoven with each other.

The **second** aspect is the **coherent superposition of matter and antimatter degrees of freedom** due to the definition of the Dirac field operators (14).

These two aspects are independant of each other, as will be elaborated in detail below.

Thus, in order to derive the nonrelativistic limit of QED there are two steps necessary: one **first** has to unitarily transform the QED Hamiltonian  $\hat{\mathcal{H}}_{QED}$  in such a way that it commutes with the QED particle number operator  $\hat{N}$ . This will essentially amount to eliminating the pair terms in the QED Coulomb interaction, and to eliminate the *high energy* photons. In chapter 4.1 it is specified what is

meant by high energy photons (see (85) and the following discussion): these are photons which are not important for the physics of *classical* light-matter interaction processes, because their wavelength is below the order of magnitude relevant for physics on the atomic or chemical length scale.

The resulting unitarily equivalent many-body QED Hamiltonian is a particle number conserving one for matter and antimatter fields moving at arbitrary speed and interacting with *low-energy* photons, the ones which are relevant for the classical light-matter interactions. However, this unitarily equivalent many-body Hamiltonian is *still not describing electrons and positrons separately*. That means that it is still not retranslatable to first quantization. Therefore, in a **second step**, one has to decouple the matter and antimatter degrees of freedom in this many-body QED Hamiltonian.

In the following the reader is introduced to the fundamental aspect, the lack of particle number conservation. With this, it will be shown why the QED Hamiltonian (8) is very difficult to interpret, although the contributions look very similar to their classical analogues. This is done by a discussion of the QED charge density operator (43) and the QED current density operator (41).

Then the second aspect of decoupling the matter and antimatter degrees of freedom is discussed in a more formal way, and it is elaborated why there is a strict order of procedure for addressing the two aspects.

### The Lack of Particle Number Conservation in QED

One really has to emphasize that and actually put three exclamation points on it: although the various contributions to the QED Hamiltonian (8) are very similar to their classical counterparts, one really has to be extremely careful, because these objects do not behave classically, and what is going on in QED is absolutely non-trivial. As is known, in our classical world, particle number conservation holds *strictly*, and one can sum over the individual energies of the particles (regarding their kinetic energy or their Zeeman energy), as well as over the Coulomb energy of two particles. However, there is no way to express the Hamiltonian (8) as one in which one can sum over

individual particles. Formally, this means that there is no simple way to reexpress the field theory QED Hamiltonian (8) in first quantization [7]. This point can be more clarified by the simplest possible example, by regarding the QED charge density (43).

In our classical world one could denote for the classical charge density  $\varrho^{(cl)}(\mathbf{r})$  [7]

$$\varrho^{(cl)}(\mathbf{r}) = q_e \sum_{j=1}^{N^{(e)}} \delta^{(3)}(\mathbf{r} - \mathbf{r}^{(j,e)}) - q_e \sum_{j=1}^{N^{(p)}} \delta^{(3)}(\mathbf{r} - \mathbf{r}^{(j,p)}) \quad (46)$$

where one would sum over individual electrons and even, with the respective minus sign, over individual positrons.

Writing out the QED charge density  $\hat{\varrho}(\mathbf{r})$  (using (14) and the properties (17)) and applying the normal ordering operation  $\mathcal{N}$  or charge conjugation operation  $\frac{1-\mathcal{C}_F}{2}(c_k c_{k'}^\dagger) = -c_{k'}^\dagger c_k$ , see (44), one finds [7]

$$\begin{aligned} \hat{\varrho}(\mathbf{r}) &= \hat{\varrho}_0(\mathbf{r}) + \hat{\varrho}_+(\mathbf{r}) + \hat{\varrho}_-(\mathbf{r}) \\ \hat{\varrho}_0(\mathbf{r}) &= q_e \sum_{k,k'} \sum_{\mu} \left( U_{\mu}^*(\mathbf{r}; k') U_{\mu}(\mathbf{r}; k) \hat{c}_{k'}^\dagger \hat{c}_k - V_{\mu}^*(\mathbf{r}; k) V_{\mu}(\mathbf{r}; k') \hat{b}_{k'}^\dagger \hat{b}_k \right) \\ \hat{\varrho}_+(\mathbf{r}) &= q_e \sum_{k,k'} \sum_{\mu} U_{\mu}^*(\mathbf{r}; k') V_{\mu}(\mathbf{r}; k) \hat{c}_{k'}^\dagger \hat{b}_k^\dagger \\ \hat{\varrho}_-(\mathbf{r}) &= q_e \sum_{k,k'} \sum_{\mu} V_{\mu}^*(\mathbf{r}; k) U_{\mu}(\mathbf{r}; k') \hat{b}_{k'}^\dagger \hat{c}_{k'} \end{aligned} \quad (47)$$

Comparing (46) and (47) it becomes obvious that only  $\hat{\varrho}_0$  could be a candidate for a classical interpretation, since it is proportional to the occupation number operator  $\hat{c}_{k'}^\dagger \hat{c}_k$  for matter and, with the respective minus sign, the occupation number operator  $\hat{b}_{k'}^\dagger \hat{b}_k$  for antimatter. The contributions  $\hat{\varrho}_+$  and  $\hat{\varrho}_-$  describe the creation and annihilation of an electron–positron pair, as they comprise products of matter and anti–matter creation and annihilation operators  $\hat{b}_{k'}^\dagger \hat{c}_{k'}$  and  $\hat{c}_{k'}^\dagger \hat{b}_k^\dagger$ . These contributions to the QED charge density operator cannot be interpreted classically, and there is no way to express the operator  $\hat{\varrho}(\mathbf{r})$  as one in which one can count over individual point charges as in the classical expression (46).

From the anticommutation relations (15) of the fermionic creation and annihilation operators one finds [8, 7]

$$\left[ \hat{N}, \hat{\rho}_0(\mathbf{r}) \right] = \hat{0} \quad (48)$$

and [8, 7]

$$\left[ \hat{N}, \hat{\rho}_\pm(\mathbf{r}) \right] = \pm 2\hat{\rho}_\pm(\mathbf{r}) \quad (49)$$

The same holds true for the QED current density operator [7]

$$\begin{aligned} \hat{j}_b(\mathbf{r}) &\equiv q_e \frac{1 - \mathcal{C}_F}{2} \hat{\Psi}_\mu^\dagger(\mathbf{r}) (c\alpha_b)_{\mu\nu} \hat{\Psi}_\nu(\mathbf{r}) \\ &= q_e c \sum_{\mu,\nu} \mathcal{N} \left( \sum_{k'} \left( U_\mu^*(\mathbf{r}; k') \hat{c}_{k'}^\dagger + V_\mu^*(\mathbf{r}; k') \hat{b}_{\bar{k}'}^\dagger \right) (\alpha_b)_{\mu,\nu} \sum_k \left( U_\nu(\mathbf{r}; k) \hat{c}_k + V_\nu(\mathbf{r}; k) \hat{b}_{\bar{k}}^\dagger \right) \right) \\ &= q_e c \sum_{k,k'} \sum_{\mu,\nu} (\alpha_b)_{\mu,\nu} \left\{ \begin{aligned} &U_\mu^*(\mathbf{r}; k') U_\nu(\mathbf{r}; k) \hat{c}_{k'}^\dagger \hat{c}_k - V_\mu^*(\mathbf{r}; k') V_\nu(\mathbf{r}; k) \hat{b}_{\bar{k}}^\dagger \hat{b}_{\bar{k}'} \\ &+ U_\mu^*(\mathbf{r}; k') V_\nu(\mathbf{r}; k) \hat{c}_{k'}^\dagger \hat{b}_{\bar{k}}^\dagger + V_\mu^*(\mathbf{r}; k) U_\nu(\mathbf{r}; k') \hat{b}_{\bar{k}} \hat{c}_{k'} \end{aligned} \right. \\ &= \hat{j}_b^{(0)}(\mathbf{r}) + \hat{j}_b^{(+)}(\mathbf{r}) + \hat{j}_b^{(-)}(\mathbf{r}) \end{aligned} \quad (50)$$

where again one finds [8, 7]

$$\left[ \hat{N}, \hat{j}_b^{(0)}(\mathbf{r}) \right] = \hat{0} \quad (51)$$

and [8, 7]

$$\left[ \hat{N}, \hat{j}_b^{(\pm)}(\mathbf{r}) \right] = \pm 2\hat{j}_b^{(\pm)}(\mathbf{r}) \quad (52)$$

Now this has of course implications for the QED Hamiltonian  $\hat{\mathcal{H}}_{QED}$ . The QED Coulomb interaction, for example, comprises nine terms, of which six are non-particle number conserving! For example, the contributions  $\hat{\rho}_0(\mathbf{r}) \circ \hat{\rho}_+(\mathbf{r})$  or  $\hat{\rho}_+(\mathbf{r}) \circ \hat{\rho}_+(\mathbf{r})$  are not particle number conserving. By far, written out, the QED Coulomb interaction seems to have very little in common with the classical Coulomb interaction, at least formally.

It is exactly these nonclassical properties (49) and (52) which should be eliminated from the QED Hamiltonian. The aim is to find a

physically equivalent representation of the QED Hamiltonian in which these non-particle number conserving contributions are removed. This can be achieved by eliminating the pair terms of the QED Coulomb interaction and by simultaneously eliminating the high-energy photons, which are the reason for the creation and annihilation of fermion pairs and other photons.

However, as indicated, a particle number conserving QED Hamiltonian is not the end of the story, since there is still the second aspect, the coherent superposition of matter and antimatter degrees of freedom.

### The Coherent Superposition of Matter and Antimatter Degrees of Freedom

Imagine that one has succeeded in finding a unitarily equivalent QED Hamiltonian  $\hat{\mathcal{H}}_U$  which preserves the particle number, hence  $[\hat{N}, \hat{\mathcal{H}}_U] = \hat{0}$ . In this Hamiltonian  $\hat{\mathcal{H}}_U$  all contributions with sub- or superscripts ( $\pm$ ) have vanished, while those with (0) remain (plus some corrections, as will be shown). Then, for example, the particle number conserving contribution to the QED current density (50), which couples to the low energy photons as  $-\hat{j}_b^{(0)}(\mathbf{r}) \cdot \hat{A}_b^{(T,low)}(\mathbf{r})$ , would be given as follows:

$$\hat{j}_b^{(0)}(\mathbf{r}) = \sum_{k,k'} (U_\mu^*(\mathbf{r}; k') (\alpha_b)_{\mu\nu} U_\nu(\mathbf{r}; k) \hat{c}_{k'}^\dagger \hat{c}_k - V_\mu^*(\mathbf{r}; k') (\alpha_b)_{\mu\nu} V_\nu(\mathbf{r}; k) \hat{b}_k^\dagger \hat{b}_{k'})$$

Here, the occupation number operator  $\hat{c}_{k'}^\dagger \hat{c}_k$  for the matter and  $\hat{b}_k^\dagger \hat{b}_{k'}$  for the antimatter are separated. However, in the Dirac amplitudes  $U_\mu(\mathbf{r}; k')$  and  $V_\nu(\mathbf{r}; k)$ , which are the modes of the Dirac field operators (14), the matter and antimatter degrees of freedom are **not yet** separated.

The reason why there is no clear distinction between matter and antimatter in QED as a field theory is that it is build upon the properties of the single-particle Dirac Hamiltonian (10). The amplitudes  $U_\mu(\mathbf{r}; k')$  and  $V_\mu(\mathbf{r}; k)$  both comprise four components, hence eight degrees of freedom altogether, such that the Dirac

particle itself is a hybrid of matter and antimatter degrees of freedom [31, 10, 8, 7].

In the introduction it has been mentioned that the relativistic fermion, described by the Dirac Hamiltonian (10) is necessarily a four-dimensional object [1, 31, 40], whereas the nonrelativistic fermion, described by the  $2 \times 2$  Schrödinger–Pauli Hamiltonian, is two-dimensional. But one can still insist in the four-dimensional theory that one wants an eigenvalue problem for the matter degrees of freedom and the antimatter degrees of freedom separately, no matter how many dimensions are necessary for describing the relativistic fermion! This means that the Dirac amplitudes  $U(\mathbf{r}; k')$  and  $V(\mathbf{r}; k)$  *have to decompose into upper and lower components* [10, 7]. Only then it is assured that under a temporal evolution the matter and antimatter degrees of freedom remain separated for all times [10, 7].

Hence, a unitary transformation  $\mathbb{T}$  is searched for such that for the eigenvalue problem (16) [10, 7]

$$\begin{aligned} \mathbb{T} \circ \mathbf{H}^{(D)} \circ \mathbb{T}^\dagger \circ \mathbb{T}U(\mathbf{r}; k) &= E_k \mathbb{T}U(\mathbf{r}; k) \\ \mathbb{T} \circ \mathbf{H}^{(D)} \circ \mathbb{T}^\dagger \circ \mathbb{T}V(\mathbf{r}; k) &= -E_k \mathbb{T}V(\mathbf{r}; k) \end{aligned} \tag{53}$$

where the new amplitudes  $\mathbb{T}U(\mathbf{r}; k)$  describe matter only, and the amplitudes  $\mathbb{T}V(\mathbf{r}; k)$  describe antimatter only, and the transformed Dirac Hamiltonian  $\mathbb{T} \circ \mathbf{H}^{(D)} \circ \mathbb{T}^\dagger$  is blockdiagonal. Only then is the connection to the Schrödinger–Pauli Hamiltonian visible, because it will not hurt the Schrödinger–Pauli theory if one adds two "0"-dimensions to it, meaning that the Schrödinger–Pauli Hamiltonian is extended by two blocks  $\hat{0}_{2 \times 2}$ , and the Schrödinger–Pauli eigenfunctions are extended by  $\begin{pmatrix} 0 \\ 0 \end{pmatrix}$ !

Now in case of the free Dirac Hamiltonian the decoupling of the matter and antimatter degrees of freedom can be done by the so-called Foldy–Whouthuysen transformation  $\mathbf{S}$  [18, 9, 5, 3]. In case of a Dirac particle in a static external magnetic field it is the so-called Eriksen  $\mathbb{T}$  transformation which succeeds in the decoupling [23, 11, 20, 10]. As is shown in section 5, the Eriksen transformation transforms the single-particle Dirac–Hamiltonian  $\mathbf{H}^{(D)}$  into the so-called Newton Wigner representation  $\hat{\mathbf{H}}^{(NW)} \equiv \mathbb{T} \circ \mathbf{H}^{(D)} \circ \mathbb{T}^\dagger$ , and the corresponding Newton–Wigner eigenfunctions  $\mathbb{T}U(\mathbf{r}; k)$  and  $\mathbb{T}V(\mathbf{r}; k)$



indeed decompose into upper components for the matter, and lower components for the anti-matter. This will be crucial for being able to reexpress the field theory Hamiltonian  $\hat{\mathcal{H}}_U$  that conserves the particle number in first quantization. For a recent in-depth discussion of the Eriksen transformation see [10].

As hopefully has become more clear: due to the coherent superposition of matter and anti-matter degrees of freedom in the single-particle Dirac theory, this superposition is carried into the field theory, because for the Dirac field operators (14) the Dirac amplitudes  $U_\mu(\mathbf{r}; k')$  and  $V_\nu(\mathbf{r}; k)$  serve as expansion modes. From this follows that in QED, expressed in the Dirac representation, there is also no clear distinction between electrons (matter) and positrons (antimatter). This aspect *does not have something to do with the particle number conservation*, as will be explained in more detail in the following subsection 2.3.

If one succeeds in resolving the first aspect, the lack of particle number conservation, one will have a many-body QED Hamiltonian  $\hat{\mathcal{H}}_U$  still given in the Dirac representation. This means that  $\hat{\mathcal{H}}_U$  is still expressed by the Dirac spinors (14). Hence, this Hamiltonian still couples matter and antimatter degrees of freedom.

However, one can in fact still apply the Eriksen transformation  $\mathbb{T}$ , that serves for decoupling the matter and antimatter degrees of freedom in the single particle Dirac theory, to the particle number conserving many-body Hamiltonian  $\hat{\mathcal{H}}_U$

To give an impression of how this is done, for the particle number conserving contribution to the QED current density, which remains after eliminating the particle number violating terms, this would mean that one inserts the Eriksen transformation according to  $\mathbb{T}^\dagger \mathbb{T} = \hat{1}$ :

$$\begin{aligned} \hat{j}_b^{(0)}(\mathbf{r}) = & \sum_{k, k'} \left( U_\nu^*(\mathbf{r}; k') (\mathbb{T}^\dagger)_{\nu\mu} \left( (\mathbb{T})_{\mu\nu'} (\alpha_b)_{\nu'\mu'} (\mathbb{T}^\dagger)_{\mu'\nu} \right) (\mathbb{T})_{\nu\mu} U_\mu(\mathbf{r}; k) \hat{c}_{k'}^\dagger \hat{c}_k \right. \\ & \left. - V_\nu^*(\mathbf{r}; k') (\mathbb{T}^\dagger)_{\nu\mu} \left( (\mathbb{T})_{\mu\nu'} (\alpha_b)_{\nu'\mu'} (\mathbb{T}^\dagger)_{\mu'\nu} \right) (\mathbb{T})_{\nu\mu} V_\mu(\mathbf{r}; k) \hat{b}_k^\dagger \hat{b}_{k'} \right) \end{aligned}$$

One can now *reinterpret* the amplitudes  $\mathbb{T}_{\nu\mu} U_\mu(\mathbf{r}; k) \equiv U_\nu^{(NW)}(\mathbf{r}; k)$  and  $(\mathbb{T})_{\nu\mu} V_\mu(\mathbf{r}; k) \equiv V_\nu^{(NW)}(\mathbf{r}; k)$  as Newton-Wigner amplitudes  $U_\nu^{(NW)}(\mathbf{r}; k)$  and  $V_\nu^{(NW)}(\mathbf{r}; k)$  [10, 8, 7]. The Newton-Wigner amplitudes can then be assumed to be proportional to the two-Schrödinger-Pauli amplitudes of atomic energy scales, because

the Newton–Wigner representation of the Dirac amplitudes is *the* representation for the classical interpretation of the Dirac electron [9]. They will therefore will serve as expansion coefficients for the Newton–Wigner field operators  $\Phi_\nu(\mathbf{r})$ . One can then therefore explicitly calculate the matrix elements of the form  $\mathbb{T} \circ \alpha_b \circ \mathbb{T}^\dagger$  as a gradient expansion with respect to the gauge invariant moment operators  $\hat{\Pi}_a(\mathbf{r})$ , because the latter acts, in the nonrelativistic subspace of QED, on the slowly varying Schrödinger–Pauli wave functions.

Unitarily transforming the QED Hamiltonian (8) in the manner outlined here, namely first finding a unitarily equivalent QED Hamiltonian that conserves the particle number and second applying the Eriksen transformation  $\mathbb{T}$  for decoupling matter and antimatter degrees of freedom, necessarily implies the renormalization of the bare mass  $m_0$  and the  $g$ -factor of the fermions [8, 7]. This is because QED is a field theory with true interactions. Since it is not possible to transform the QED Hamiltonian into a particle number conserving one exactly, only perturbatively, the result is valid up to a certain order in the coupling constant that one has to choose (the finestructure constant). Therefore, as will be shown, the “true” electron mass  $m_e$  and therefore the “true”  $g$ -factor of the fermions, the anomalous  $g$ -factor, only appear as classical attributes when one *renormalizes* the bare mass  $m_0$ . This means that one has to choose a cut-off for otherwise divergent integrals in terms which add up to the one-particle terms. In that guise the classical, the nonrelativistic Hamiltonian of light–matter interactions for electrons *as well as* for positrons *and* their interactions emerges.

But how can all of this be achieved? What unites the two aspects introduced above is the relation with a change of representation. In quantum mechanics, such a change of representation is done by a unitary transformation, hence, a transformation which maintains the physical content of a given Hamiltonian as the generator of the dynamics of the respective physical system. If this transformation can be performed only perturbatively, it is clear that the physical content can be maintained only up to a certain order in the perturbation method chosen.

In this dissertation the method of choice is the so-called flow equation [16]. It is a differential equation for unitarily transforming a given (Hamilton) operator in a *continuous* manner, and it is discussed in the

section 3. With the flow equation one can find a particle number conserving unitarily equivalent QED Hamiltonian  $\hat{\mathcal{H}}_U$  [8, 7].

Furthermore one can also deduce the Eriksen transformation  $\mathbb{T}$  by the help of the flow equation. The Eriksen transformation leads to the very important Newton–Wigner representation of the single–particle Dirac Hamiltonian and the related eigenfunctions [7].

Therefore, before diving into the flow equation, the Newton–Wigner representation is explained in a little more detail, because it is a very convenient representation for a classical interpretation of the single–particle Dirac Hamiltonian (and related observables) [19, 18, 9, 10]. This will help to understand why the lack of particle number conservation and the decoupling of matter and antimatter degrees of freedom are independent aspects, and why one *first* has to find a unitarily equivalent QED Hamiltonian that preserves the particle number, and *then* decouple the matter and antimatter degrees of freedom.

### 2.3 The Newton–Wigner Representation: A Short Exposure

The so–called Newton–Wigner representation  $\mathbf{H}^{(NW)} \equiv \mathbb{T} \circ \mathbf{H}^{(D)} \circ \mathbb{T}^\dagger$ , of the Dirac Hamiltonian  $\mathbf{H}^{(D)}$ , resulting from the Eriksen transformation  $\mathbb{T}$  that has been mentioned in the previous subsection, has much to do with the problem of finding the nonrelativistic limit of the QED Hamiltonian (8). As is presented in the appendix section B, the Eriksen transformation  $\mathbb{T}$  that allows the transition from the Dirac representation described by  $\mathbf{H}^{(D)}$  to the Newton–Wigner representation  $\mathbf{H}^{(NW)}$  can be found by solving the flow equation *exactly* [10, 7].

However, as has already been mentioned, the Eriksen transformation can also be applied to QED as a field theory. In this subsection a short insight into the consequences that the Eriksen transformation  $\mathbb{T}$  has for *Quantum Electrodynamics* as a many–body theory shall be given. For this the QED particle number operator  $\hat{N}$  and the QED charge density operator  $\hat{\rho}(\mathbf{r})$  will be presented in the Newton–Wigner representation.

At this point one has to make a clear distinction between the single particle Dirac Hamiltonian (10) and its second quantized complement (9) regarding the way of speaking: speaking of the Dirac representation in the context of the single particle theory, the observables are transformed into one another by the unitary transformation  $\mathbb{T}$ , for example for an arbitrary operator  $\hat{\mathcal{O}}^{(D)}(\hat{x}, \hat{p})$  in the Dirac picture then

$$\hat{\mathcal{O}}^{(NW)}(\hat{x}, \hat{p}) \equiv \mathbb{T} \circ \hat{\mathcal{O}}^{(D)}(\hat{x}, \hat{p}) \circ \mathbb{T}^\dagger \quad (54)$$

Speaking of the Dirac representation in the context of QED, however, it is always referred to the second quantized observables which are described by the Dirac field operators (14). Hence,

$$\mathcal{O}^{(D)} = \int d^3r \hat{\Psi}_\mu^\dagger(\mathbf{r}) \left( \hat{\mathcal{O}}^{(D)}(\hat{x}, \hat{p}) \right)_{\mu, \mu'} \hat{\Psi}_{\mu'}(\mathbf{r}) \quad (55)$$

Accordingly, speaking of the Newton–Wigner representation in the context of QED, it is referred to the second quantized observables expressed by the so-called Newton–Wigner field operators  $\hat{\Phi}_\nu(\mathbf{r})$  introduced below (62). These *indeed* result from the Eriksen transformation  $\mathbb{T}$ :

$$\begin{aligned} \mathcal{O}^{(NW)} &= \int d^3r \hat{\Phi}_\mu^\dagger(\mathbf{r}) \left( \mathbb{T} \circ \hat{\mathcal{O}}^{(D)}(\hat{x}, \hat{p}) \circ \mathbb{T}^\dagger \right)_{\mu, \mu'} \hat{\Phi}_{\mu'}(\mathbf{r}) \\ &= \int d^3r \hat{\Phi}_\mu^\dagger(\mathbf{r}) \left( \hat{\mathcal{O}}^{(NW)}(\hat{x}, \hat{p}) \right)_{\mu, \mu'} \hat{\Phi}_{\mu'}(\mathbf{r}) \end{aligned} \quad (56)$$

As an example for switching from the Dirac representation to the Newton–Wigner representation consider the QED particle number operator  $\hat{N}$  given in (20): in the Dirac representation, it is, expressed in the position space  $\mathbf{r}$ , a highly nonlocal operator [8, 7]:

$$\begin{aligned}
\hat{N} &= \sum_k \left( \hat{c}_k^\dagger \hat{c}_k + \hat{b}_{\bar{k}}^\dagger \hat{b}_{\bar{k}} \right) \\
&= \sum_k \mathcal{N} \left( \hat{c}_k^\dagger \hat{c}_k - \hat{b}_{\bar{k}}^\dagger \hat{b}_{\bar{k}} \right) \\
&= \int d^3r \mathcal{N} \left( \sum_{\mu, \mu'} \hat{\Psi}_\mu^\dagger(\mathbf{r}) \left( \mathbf{P}^{(+)} - \mathbf{P}^{(-)} \right)_{\mu, \mu'} \hat{\Psi}_{\mu'}(\mathbf{r}) \right) \\
&= \int d^3r \mathcal{N} \left( \sum_{\mu, \mu'} \hat{\Psi}_\mu^\dagger(\mathbf{r}) \left( \frac{\mathbf{H}^{(D)}}{\sqrt{\mathbf{H}^{(D)} \circ \mathbf{H}^{(D)}}} \right)_{\mu, \mu'} \hat{\Psi}_{\mu'}(\mathbf{r}) \right)
\end{aligned} \tag{57}$$

Here use has been made of the normal ordering rule  $\mathcal{N} \left( \hat{b}_{\bar{k}}^\dagger \hat{b}_{\bar{k}} \right) = -\hat{b}_{\bar{k}} \hat{b}_{\bar{k}}^\dagger$ , for an in-depth explanation again see appendix section F.

Furthermore, the projection operators  $\mathbf{P}^{(\pm)}$  have been used, which are introduced in the appendix section A. Roughly spoken,  $\mathbf{P}^{(+)}$  projects onto eigenstates  $U_\mu(\mathbf{r}; k)$  of positive energy solutions of the single particle Dirac Hamiltonian, and  $\mathbf{P}^{(-)}$  projects onto its eigenstates of negative energy solutions  $V_\mu(\mathbf{r}; k)$ .

The exact formal identity [7, 10]

$$\left( \mathbf{P}^{(+)} - \mathbf{P}^{(-)} \right)_{\mu, \mu'} = \left( \frac{\mathbf{H}^{(D)}}{\sqrt{\mathbf{H}^{(D)} \circ \mathbf{H}^{(D)}}} \right)_{\mu, \mu'} \tag{58}$$

is also explained in detail in section A of the appendix.

As has already been mentioned, the QED particle number operator  $\hat{N}$  in the Dirac representation is *nonlocal*, meaning that the integrand in (57) cannot be interpreted as a particle density in position space  $\mathbf{r}$ .

*However*, in the Newton–Wigner representation,  $\hat{N}$  becomes local. To see this one needs the following identity [7, 10]

$$\mathbf{T}^\dagger \circ \beta \circ \mathbf{T} = \mathbf{P}^{(+)} - \mathbf{P}^{(-)} \tag{59}$$

where  $\beta$  is nothing but the Dirac  $\beta$  matrix (12) referring to the existence of matter (upper block,  $+\hat{1}_{2 \times 2}$ ) and antimatter (lower block,  $-\hat{1}_{2 \times 2}$ )! (The identity (59) is derived in section C of the appendix.)

Inserting (59) into (57) there follows [7, 8]

$$\begin{aligned}
\hat{N} &= \int d^3r \mathcal{N} \left( \sum_{\mu, \mu'} \Psi_{\mu}^{\dagger}(\mathbf{r}) \left( \frac{\mathbf{H}^{(D)}}{\sqrt{\mathbf{H}^{(D)} \circ \mathbf{H}^{(D)}}} \right)_{\mu, \mu'} \hat{\Psi}_{\mu'}(\mathbf{r}) \right) \\
&= \int d^3r \mathcal{N} \left( \sum_{\mu, \mu'} \Psi_{\mu}^{\dagger}(\mathbf{r}) (\mathbb{T}^{\dagger} \circ \beta \circ \mathbb{T})_{\mu, \mu'} \hat{\Psi}_{\mu'}(\mathbf{r}) \right) \\
&= \int d^3r \mathcal{N} \left( \sum_{\nu, \nu', \mu, \mu'} \hat{\Psi}_{\mu}^{\dagger}(\mathbf{r}) (\mathbb{T}^{\dagger})_{\mu, \nu} (\beta)_{\nu, \nu'} (\mathbb{T})_{\nu', \mu'} \hat{\Psi}_{\mu'}(\mathbf{r}) \right) \\
&= \int d^3r \mathcal{N} \left( \sum_{\nu, \nu', \mu, \mu'} (\mathbb{T}^{\dagger})_{\mu, \nu} \hat{\Psi}_{\mu}^{\dagger}(\mathbf{r}) (\beta)_{\nu, \nu'} (\mathbb{T})_{\nu', \mu'} \hat{\Psi}_{\mu'}(\mathbf{r}) \right)
\end{aligned} \tag{60}$$

In the last line it has been integrated partially with respect to  $\hat{\Psi}_{\mu}^{\dagger}(\mathbf{r})$ , such that  $\mathbb{T}^{\ddagger} = \mathbb{T}^{\dagger}(\hat{\Pi}^*)$ .

If one reinterprets the "new" field operators [7, 8]

$$\begin{aligned}
\hat{\Phi}_{\nu}(\mathbf{r}) &= \sum_{\mu' \in \{1, 2, 3, 4\}} (\mathbb{T})_{\nu, \mu'} \hat{\Psi}_{\mu'}(\mathbf{r}) \\
\hat{\Phi}_{\nu}^{\dagger}(\mathbf{r}) &= \sum_{\mu \in \{1, 2, 3, 4\}} (\mathbb{T}^{\dagger})_{\mu, \nu} \hat{\Psi}_{\mu}^{\dagger}(\mathbf{r})
\end{aligned} \tag{61}$$

as Dirac spinors *in the Newton–Wigner representation* then [7, 8]

$$\hat{N} = \int d^3r \mathcal{N} \left( \sum_{\nu, \nu'} \hat{\Phi}_{\nu}^{\dagger}(\mathbf{r}) (\beta)_{\nu, \nu'} \hat{\Phi}_{\nu'}(\mathbf{r}) \right) \tag{62}$$

becomes a *local* operator. As will be shown in section 5, the Newton–Wigner field operators  $\hat{\Phi}_{\nu}(\mathbf{r})$  are blockdiagonal meaning that the Newton–Wigner expansion amplitudes  $U_{\mu'}^{(NW)}(\mathbf{r}, k)$  to positive energy eigenvalues have entries in the upper two components, while the lower two components are zero, whereas for the Newton–Wigner expansion amplitudes  $V_{\mu'}^{(NW)}(\mathbf{r}, k)$  to negative energy eigenvalues, it is vice versa, the upper components vanish while the lower do not. Hence, the integrand can be interpreted as a true particle density

The same holds true for the QED charge density operator (43) [7, 8]:

$$\begin{aligned}
\hat{Q} &= \int d^3r q_e \mathcal{N} \left( \sum_{\mu} \Psi_{\mu}^{\dagger}(\mathbf{r}) \Psi_{\mu}(\mathbf{r}) \right) \\
&= q_e \mathcal{N} \left( \sum_{\nu, \mu, \mu'} \int d^3r \hat{\Psi}_{\mu}^{\dagger}(\mathbf{r}) (\mathbb{T}^{\dagger})_{\mu, \nu} (\mathbb{T})_{\nu, \mu'} \hat{\Psi}_{\mu'}(\mathbf{r}) \right) \\
&= q_e \mathcal{N} \left( \sum_{\nu, \mu, \mu'} \int d^3r (\mathbb{T}^{\dagger})_{\mu, \nu} \hat{\Psi}_{\mu}^{\dagger}(\mathbf{r}) (\mathbb{T})_{\nu, \mu'} \hat{\Psi}_{\mu'}(\mathbf{r}) \right) \\
&= \int d^3r q_e \mathcal{N} \left( \sum_{\nu} \hat{\Phi}_{\nu}^{\dagger}(\mathbf{r}) \hat{\Phi}_{\nu}(\mathbf{r}) \right)
\end{aligned} \tag{63}$$

One can now make the ansatz [8, 7]

$$\Phi_{\nu}(\mathbf{r}) = (\mathbb{T})_{\nu, \mu} \hat{\Psi}_{\mu}(\mathbf{r}) = \begin{pmatrix} \hat{\psi}_{+}(\mathbf{r}) \\ \hat{\psi}_{-}(\mathbf{r}) \\ \hat{\chi}_{+}^{\dagger}(\mathbf{r}) \\ \hat{\chi}_{-}^{\dagger}(\mathbf{r}) \end{pmatrix}_{\nu} \equiv \begin{pmatrix} \hat{\psi}_{+}(\mathbf{r}) \\ \hat{\psi}_{-}(\mathbf{r}) \\ 0 \\ 0 \end{pmatrix}_{\nu} + \begin{pmatrix} 0 \\ 0 \\ \hat{\chi}_{+}^{\dagger}(\mathbf{r}) \\ \hat{\chi}_{-}^{\dagger}(\mathbf{r}) \end{pmatrix}_{\nu} \tag{64}$$

where  $\hat{\psi}_{\pm}(\mathbf{r})$  and  $\hat{\chi}_{\pm}(\mathbf{r})$  are the field operators of many-body physics for electrons and positrons separately.

Therefore one finds [7]

$$\begin{aligned}
\hat{Q} &= \int d^3r q_e \mathcal{N} \left( \begin{pmatrix} \hat{\psi}_{+}^{\dagger}(\mathbf{r}) & , \hat{\psi}_{-}^{\dagger}(\mathbf{r}) & , \hat{\chi}_{+}(\mathbf{r}) & , \hat{\chi}_{-}(\mathbf{r}) \end{pmatrix} \begin{pmatrix} \hat{\psi}_{+}(\mathbf{r}) \\ \hat{\psi}_{-}(\mathbf{r}) \\ \hat{\chi}_{+}^{\dagger}(\mathbf{r}) \\ \hat{\chi}_{-}^{\dagger}(\mathbf{r}) \end{pmatrix} \right) \\
&= \int d^3r q_e \mathcal{N} \left( \sum_{\sigma} \hat{\psi}_{\sigma}^{\dagger}(\mathbf{r}) \hat{\psi}_{\sigma}(\mathbf{r}) + \sum_{\sigma} \hat{\chi}_{\sigma}(\mathbf{r}) \hat{\chi}_{\sigma}^{\dagger}(\mathbf{r}) \right) \\
&= \int d^3r q_e \left( \sum_{\sigma} \hat{\psi}_{\sigma}^{\dagger}(\mathbf{r}) \hat{\psi}_{\sigma}(\mathbf{r}) - \sum_{\sigma} \hat{\chi}_{\sigma}^{\dagger}(\mathbf{r}) \hat{\chi}_{\sigma}(\mathbf{r}) \right) \\
&\equiv \int d^3r q_e \left( \hat{n}^{(e)}(\mathbf{r}) - \hat{n}^{(p)}(\mathbf{r}) \right)
\end{aligned} \tag{65}$$

Where  $\hat{n}^{(e)}(\mathbf{r}) = \sum_{\sigma} \hat{\psi}_{\sigma}^{\dagger}(\mathbf{r}) \hat{\psi}_{\sigma}(\mathbf{r})$  is the electron particle density, whereas  $\hat{n}^{(p)}(\mathbf{r}) = \sum_{\sigma} \hat{\chi}_{\sigma}^{\dagger}(\mathbf{r}) \hat{\chi}_{\sigma}(\mathbf{r})$  is the positron particle density. Please notice the minus sign for the positrons.

Hence [7]

$$\hat{\rho}^{(NW)}(\mathbf{r}) = q_e \hat{n}^{(e)}(\mathbf{r}) - q_e \hat{n}^{(p)}(\mathbf{r}) \quad (66)$$

and for the particle density operator [8, 7]

$$\hat{n}^{(NW)}(\mathbf{r}) = \hat{n}^{(e)}(\mathbf{r}) + \hat{n}^{(p)}(\mathbf{r}) \quad (67)$$

This means that in the Newton–Wigner representation the particle density operator and the charge density operator become local operators that can be interpreted as a true particle density and a true charge density in position space. There are no oscillating, the particle number violating terms like  $\hat{\rho}_{\pm}(\mathbf{r})$  as is the case in the Dirac representation of the QED charge density operator (47). There are also no complicated operators like  $\frac{H^{(D)}}{\sqrt{H^{(D)} \circ H^{(D)}}}$  like in the QED particle number (57).

However, as has been mentioned in the last subsection, it is not sufficient to know the Newton–Wigner representation of the field operators for deducing the classical limit of QED. One might think, after having seen the Newton–Wigner representations of the QED charge and current density operators, that the Eriksen transformation  $\mathbb{T}$  should make it possible to reexpress the QED Hamiltonian  $\hat{\mathcal{H}}_{QED}$  by the Newton–Wigner field operators  $\Phi_{\nu}(\mathbf{r})$  and  $\Phi_{\nu}^{\dagger}(\mathbf{r})$  and then the QED Hamiltonian in the Newton–Wigner representation is retranslatable to first quantization yielding the classical light–matter interaction Hamiltonian. However, this is not the case, and now it is possible to understand a little more formally why that is not sufficient. It is because the particle number violating terms stemming from the interaction terms  $\hat{\mathcal{H}}_{\perp}$  and  $\hat{\mathcal{V}}_C$  are removed **too early** by replacing the Dirac field operators  $\hat{\Psi}_{\mu}(\mathbf{r})$  by the Newton–Wigner field operators  $\hat{\Phi}_{\mu}(\mathbf{r})$  in (8)! Take a look, for example, at the unitary transformation of the operator  $\alpha_b \frac{\Pi_b}{m_0 c}$ , occurring in  $\hat{\mathcal{H}}_{\perp}$ . It still has complicated form in the Newton–Wigner representation [7]:

$$\mathbb{T} \left( \alpha_b \frac{\Pi_b}{m_0 c} \right) \mathbb{T}^{\dagger} = \frac{1}{\sqrt{\mathbf{1}_{4 \times 4} + \frac{2}{m_0 c^2} \mathbf{H}_{4 \times 4}^{(P)}}} \left( \frac{\Pi_b}{m_0 c} \alpha_b + \frac{2}{m_0 c^2} \mathbf{H}_{4 \times 4}^{(P)} \beta \right) \quad (68)$$



This relation is derived in the appendix in section B. However, the term with the non-diagonal Dirac  $\alpha_b$  matrix vanishes iff it is applied to the Newton–Wigner field operators (see section 5). Hence, if one applies the Eriksen transformation before eliminating the particle number violating contributions of the transversal interaction  $\hat{\mathcal{H}}_{\perp}$  given in (40), and the QED Coulomb interaction  $\hat{\mathcal{V}}_C$  given in (42), this does not yield the correct (e.g. experimentally very well verified) light-matter interaction Hamiltonian  $\hat{H}_{LM}^{(el)}$  as presented in (2). It would yield a Hamiltonian without effective interactions, and without self-energy terms (e.g. without renormalization terms).

Therefore the aspect of particle number conservation and the aspect of decoupling the degrees of freedom of the matter and antimatter fields are independent aspects of the classical limit problem of QED. Furthermore it is necessary that one **first** finds a particle number conserving representation of the QED Hamiltonian (8), and **then** decouples the matter and antimatter degrees of freedom by reexpressing this particle–number conserving unitarily equivalent QED Hamiltonian in Newton–Wigner representation! **QED described by the Hamiltonian  $\hat{\mathcal{H}}_{QED}$  is not a many–body theory, but its particle number conserving sister  $\hat{\mathcal{H}}_U$  is, and this makes it possible to apply the Eriksen transformation.**

As has already been mentioned, the aspect of finding a unitarily equivalent QED Hamiltonian which conserves the particle number can be attacked by the help of the flow equation. The aspect of decoupling the matter and antimatter degrees of freedom can be attacked by the help of the Eriksen transformation. The matrix representation of the Eriksen transformation can be found by the help of the flow equation.

In the following section the flow equation is introduced first on a general level, then the Wegner flow equation is discussed briefly in order to present the initial idea of its inventor Franz Wegner.

Then the Brockett flow equation is discussed briefly, because this type of flow equation gives the Eriksen transformation  $\mathbb{T}$ , which enables one to decouple the matter and anti–matter degrees of freedom.

Since the Eriksen transformation is well discussed in the literature, see for example [23, 24, 25, 11, 27, 28, 29, 10], its derivation is not as fundamental as that of the particle number preserving QED Hamiltonian. But it is a nice example of how the flow equation can be

solved exactly, therefore, the solution of the flow equation which yields the Eriksen transformation is presented in section [B](#) of the appendix. As will be shown, the flow equation yielding the particle number conserving QED Hamiltonian can only be solved perturbatively.

### 3 The Flow Equation

The flow equation is a method for unitarily transforming a given (Hamilton) operator in a *continuous* manner. It has been introduced into physics by Franz Wegner in 1994 [16]. In many cases applying the flow equation in the sense envisioned by Wegner means that one searches for a unitarily equivalent Hamiltonian that is diagonal or at least blockdiagonal instead of being non-diagonal. In some sense it is the operator analogon to diagonalizing a scalar matrix, however, this (block-) diagonalization is achieved by solving a differential equation. The requirement of unitary equivalence means that the transformed Hamiltonian should describe the same physics as the original Hamiltonian by leaving physical observables related to the matrix elements of the Hamiltonian invariant.

The idea is the following. For a given Hamiltonian  $\hat{H}$  an infinitesimal shift that is guided by the flow parameter  $s$  can be expressed by [7]

$$\hat{H}(s + ds) = \exp [\hat{\eta}(s) ds] \hat{H}(s) \exp [-\hat{\eta}(s) ds] \quad (69)$$

The generator  $\hat{\eta}(s)$  of this shift must be skew-hermitian in order to keep the shifted Hamiltonian hermitean [7] :

$$\begin{aligned} \hat{\eta}(s)^\dagger &= -\hat{\eta}(s) \\ \left( \hat{H}(s + ds) \right)^\dagger &= \left( \exp [\hat{\eta}(s) ds] \hat{H}(s) \exp [-\hat{\eta}(s) ds] \right)^\dagger \\ &= \exp \left[ -\hat{\eta}^\dagger(s) ds \right] \hat{H}^\dagger(s) \exp \left[ -\hat{\eta}^\dagger(s) ds \right] \\ &= \exp [\hat{\eta}(s) ds] \hat{H} \exp [\hat{\eta}(s) ds] \\ &= \hat{H}(s + ds) \end{aligned}$$

The initial value for  $s = 0$  is given by  $\hat{H}(s = 0) = \hat{H}$ .

The flow parameter  $s$  does not have a specific physical meaning, it serves as parameter for the unitary transformation.

By making use of the Baker-Campbell-Hausdorff formula, see (629),

$$\exp(xA) \circ B \circ \exp(-xA) = \sum_{n=0}^{\infty} \frac{x^n}{n!} [A, B]^n \quad (70)$$

for operators  $A, B$ , one finds for (69) in the order  $ds$  [7]

$$\hat{H}(s + ds) = \hat{H}(s) + ds[\hat{\eta}(s), \hat{H}(s)] + \mathcal{O}((ds)^2)$$

Thus [7],

$$\frac{\hat{H}(s + ds) - \hat{H}(s)}{ds} = [\hat{\eta}(s), \hat{H}(s)] + \mathcal{O}((ds)^2)$$

In the limit  $ds \rightarrow 0$  the flow equation follows as [7]

$$\frac{d}{ds}\hat{H}(s) = [\hat{\eta}(s), \hat{H}(s)] \quad (71)$$

Now there are two questions regarding the solution of the flow equation (71). The first one is what is the suitable generator  $\hat{\eta}(s)$  that lets the initial Hamiltonian  $\hat{H}(s = 0)$  flow, for all  $s$ , towards a diagonal or at least block diagonal shape, so that finally  $\hat{H}(\infty)$  is completely (block) diagonal.

The second question is what is the right ansatz for  $\hat{H}(s)$  that fulfills the left side of the flow equation (71). This question might be answered only for a concrete problem at hand.

In the following two subsections we will discuss two possible choices of the generator  $\hat{\eta}(s)$  related to two types of flow equations: the Wegner generator  $\hat{\eta}^{(W)}(s)$  which generates a nonlinear differential equation, and the Brockett generator  $\hat{\eta}^{(B)}(s)$  which generates a linear differential equation.

### 3.1 The Wegner Flow Equation

The Wegner flow equation for an initial Hamiltonian  $\hat{H}(s)$  assumes the following guise [16]:

$$\begin{aligned} \frac{d}{ds}\hat{H}(s) &= \left[ \left[ \hat{H}^{(D)}(s), \hat{H}(s) \right], \hat{H}(s) \right] \\ \hat{H}(0) &= \hat{H} \end{aligned} \quad (72)$$

Here,  $\hat{H}^{(D)}(s)$  refers to the *diagonal* part of the initial Hamiltonian  $\hat{H}(s)$ , hence, the latter is decomposed into a diagonal part and a non-diagonal part according to

$$\hat{H}(s) = \hat{H}^{(D)}(s) + \hat{H}^{(ND)}(s) \quad (73)$$

The generator  $\hat{\eta}^{(W)}(s)$  that leads to the Wegner flow equation (72) is given by [16]

$$\hat{\eta}^{(W)}(s) = \left[ \hat{H}^{(D)}(s), \hat{H}(s) \right] \quad (74)$$

A hint that the unitarily transformed Hamiltonian  $\hat{H}(\infty)$  assumes a diagonal or at least a blockdiagonal form can be sketched by considering the trace of the square of  $\hat{H}(s)$ , which is invariant under a unitary transformation [7]:

$$\begin{aligned} \frac{d}{ds} \text{tr} \left( \hat{H}(s) \hat{H}(s) \right) &= \frac{d}{ds} \text{tr} \left( \hat{H}(0) \hat{H}(0) \right) \\ &= \frac{d}{ds} \text{tr} \left( \hat{H}^{(D)}(s) \hat{H}^{(D)}(s) \right) + \frac{d}{ds} \text{tr} \left( \hat{H}^{(ND)}(s) \hat{H}^{(ND)}(s) \right) \end{aligned} \quad (75)$$

This holds because  $\text{tr} \left( \hat{H}^{(D)}(s) \circ \hat{H}^{(ND)}(s) \right) = 0$ . Furthermore, since  $\hat{H}(0)$  is constant, there follows  $\frac{d}{ds} \text{tr} \left( \hat{H}(0) \hat{H}(0) \right) = 0$ . From this one finds [7]

$$\begin{aligned} 0 &= \frac{d}{ds} \text{tr} \left( \hat{H}^{(D)}(s) \hat{H}^{(D)}(s) \right) + \frac{d}{ds} \text{tr} \left( \hat{H}^{(ND)}(s) \hat{H}^{(ND)}(s) \right) \\ -\frac{d}{ds} \text{tr} \left( \hat{H}^{(ND)}(s) \hat{H}^{(ND)}(s) \right) &= \frac{d}{ds} \text{tr} \left( \hat{H}^{(D)}(s) \hat{H}^{(D)}(s) \right) \end{aligned} \quad (76)$$

An increase in the diagonal parts  $\hat{H}^{(D)}(s)$  of  $\hat{H}(s)$  is accompanied by a decrease in its off-diagonal parts  $\hat{H}^{(ND)}(s)$ . In the limit  $s \rightarrow \infty$  then hopefully we find  $\hat{H}^{(ND)} \rightarrow 0$ , at least approximately. As has been pointed out by Franz Wegner, it depends strongly on the initial problem how far the diagonalization can be advanced, i.e., whether the non-diagonal elements actually disappear completely or

whether small parts remains. It is also not possible to say in general whether a generator leads to complete diagonalization, or only to block diagonalization. Furthermore, there are no instructions for finding a suitable generator [42, 43]. Hence, finding the right generator is the fine art of this method of unitary transformation.

The Wegner generator  $\hat{\eta}^{(W)}$  of the flow equation allows great flexibility in the unitary transformation, however, it leads to a nonlinear differential equation that is cubic in the initial Hamiltonian  $\hat{H}(s)$  so that there does not necessarily have to be a simple solution to it.

Furthermore, it must also be noted that it depends on the choice of the base which parts of the Hamiltonian are *diagonal* or *nondiagonal*. An operator that is diagonal in one base is not necessarily diagonal in another base. In this way, the flow equation itself becomes dependent on the choice of base. This means that there could be several generators that achieve the desired blockdiagonalization, and one cannot say a priori which is the most convenient one. Now for the solution of physical problems this means that it might be that a unitarily equivalent, blockdiagonalized Hamiltonian is not physically interpretable because the chosen base does not allow for a physical interpretation. For example, the Dirac Hamiltonian describing the Dirac electron can be interpreted classically only iff one changes the representation by the help of the Foldy–Wouthuysen transformation or the Eriksen transformation. This holds true also for observables like velocity or angular moment and so on [9].

### 3.2 The Brockett Flow Equation

The Brockett flow equation for an initial Hamiltonian  $\hat{H}(s)$  assumes the following guise [44]:

$$\frac{d}{ds}\hat{H}(s) = \left[ \left[ \hat{N}, \hat{H}(s) \right], \hat{H}(s) \right] \quad (77)$$

Here,  $\hat{N}$  is some hermitian operator which does not depend on the flow parameter  $s$ .

The generator  $\hat{\eta}^{(B)}(s)$  that leads to the Brockett flow equation (77) is given by [44]

$$\hat{\eta}^{(B)}(s) = \left[ \hat{N}, \hat{H}(s) \right] \quad (78)$$

Since  $\hat{N}$  is constant, the Brockett flow equation is only quadratic in the initial Hamiltonian. The price for a simpler differential equation is that the unitarily transformed Hamiltonian  $\hat{H}(\infty)$  is not necessarily of diagonal or blockdiagonal shape. What one can show is that the Brockett generator leads to a unitarily equivalent Hamiltonian that commutes with the operator  $\hat{N}$ , which means that they share the same base.

For this consider the following functional  $\Phi(s)$  [7]

$$\Phi(s) = \text{tr} \left( \left( \hat{H}(s) - \hat{N} \right)^2 \right) \quad (79)$$

Since  $\hat{H}(s)$  and  $\hat{N}$  are both hermitian operators, the function (79) is positive semidefinite,  $\Phi(s) \geq 0$ .

For the the derivative of the functional  $\Phi(s)$  with respect to  $s$  one finds [7]

$$\begin{aligned} \frac{d}{ds} \Phi(s) &= \frac{d}{ds} \text{tr} \left[ \left( \hat{H}(s) - \hat{N} \right)^2 \right] \\ &= \frac{d}{ds} \left[ \text{tr} \left( \hat{H}(s) \hat{H}(s) \right) + \text{tr} \left( \hat{N} \hat{N} \right) - 2 \text{tr} \left( \hat{N} \hat{H}(s) \right) \right] \\ &= \frac{d}{ds} \left[ \text{tr} \left( \hat{H}(0) \hat{H}(0) \right) + \text{tr} \left( \hat{N} \hat{N} \right) - 2 \text{tr} \left( \hat{N} \hat{H}(s) \right) \right] \\ &= -2 \text{tr} \left( \hat{N} \frac{d}{ds} \hat{H}(s) \right) \end{aligned} \quad (80)$$

Here use has been made of the fact that the trace is cyclically invariant. Using furthermore the Brockett flow equation (77) one finds [7]

$$\begin{aligned}
\frac{d}{ds}\Phi(s) &= -2\text{tr}\left(\hat{N}\left[\hat{\eta}^{(B)}(s), \hat{H}(s)\right]\right) \\
&= -2\text{tr}\left(\hat{N}\left(\hat{\eta}^{(B)}(s)\hat{H}(s) - \hat{H}(s)\hat{\eta}^{(B)}(s)\right)\right) \\
&= 2\text{tr}\left(\left(\hat{N}\hat{H}(s) - \hat{H}(s)\hat{N}\right)\hat{\eta}^{(B)}(s)\right) \\
&= 2\text{tr}\left(\hat{\eta}^{(B)}(s)\hat{\eta}^{(B)}(s)\right) \\
&= -2\text{tr}\left(\hat{\eta}^{(B)}(s)\left(\hat{\eta}^{(B)}(s)\right)^\dagger\right) \leq 0
\end{aligned}$$

Since the functional is positive semidefinite,  $\Phi(s) \geq 0$ , and its derivative is negative semidefinite,  $\frac{d}{ds}\Phi(s) \leq 0$ , there follows in the limit  $s \rightarrow \infty$  [7]

$$\lim_{s \rightarrow \infty} \frac{d}{ds}\Phi(s) = 0 = \text{tr}\left(\hat{\eta}^{(B)}(\infty)\left(\hat{\eta}^{(B)}(\infty)\right)^\dagger\right)$$

And therefore [7]

$$\hat{0} = \hat{\eta}^{(B)}(\infty) = \left[\hat{N}, \hat{H}(\infty)\right]$$

As one can see, the Brockett generator achieves a unitary transformation of  $\hat{H}(s)$  such that for  $s \rightarrow \infty$  the transformed Hamiltonian  $\hat{H}(\infty)$  commutes with the operator  $\hat{N}$ . Only if  $\hat{N}$  is itself diagonal or blockdiagonal one can infer that  $\hat{H}(\infty)$  must be so!

In the following subsection the use of the Wegner flow equation in the context the problem attacked in this dissertation is briefly sketched, namely, the deduction of the nonrelativistic limit of QED.

### 3.3 Flow Equations and the Classical Limit Problem of QED

As has been elucidated in section 2.2, one has to attack two aspects regarding the deduction of the nonrelativistic limit of Quantum Electrodynamics, and there is a strict order in which to proceed: one **first** has to find a unitary transformation that gives a QED Hamiltonian  $\hat{\mathcal{H}}_U$  that is particle number conserving, thus,  $\left[\hat{N}, \hat{\mathcal{H}}_U\right] = \hat{0}$ . It is possible to find this unitarily equivalent QED Hamiltonian by the help of the Wegner flow equation.



In part one of the deduction of the nonrelativistic limit of QED the generator  $\hat{\eta}^{(LM)}(s)$ , where LM stands for light–matter, which gives a unitarily equivalent QED Hamiltonian  $\hat{\mathcal{H}}_U$  is presented. It generates a nonlinear ordinary differential equation. This can then be solved *perturbatively* by expanding the QED Hamiltonian in a series in the (dimensionless) finestructure constant  $\alpha_{FS}$ . This expansion will lead to recursive **linear** differential equations, which will be solved up to the order  $\alpha_{FS}^2$ .

The solution  $\hat{\mathcal{H}}_U$  is then given by [7, 8]

$$\lim_{s \rightarrow \infty} \hat{\mathcal{H}}_U(s) = m_0 c^2 \left( \hat{H}^{(0)} + \hat{H}^{(1)}(\infty) + \hat{H}^{(2,h)}(\infty) + \hat{H}^{(2,i)}(\infty) \dots \right) \quad (81)$$

Here,  $\hat{H}^{(1)}(\infty)$  is the first order solution, and  $\hat{H}^{(2,h)}(\infty) + \hat{H}^{(2,i)}(\infty)$  is the second order solution comprising an homogeneous part  $\hat{H}^{(2,h)}(\infty)$  and an inhomogeneous part  $\hat{H}^{(2,i)}(\infty)$ . The particle number conserving Hamiltonian  $\lim_{s \rightarrow \infty} \hat{\mathcal{H}}_U(s) = \hat{\mathcal{H}}_U(\infty) \equiv \hat{\mathcal{H}}_U$ , which will be discussed in subsection 4.2, is a many–body Hamiltonian still being expressed by the Dirac field operators  $\hat{\Psi}_\mu(\mathbf{r})$  given in (14). As has been indicated in section 2.2, these Dirac field operators superpose matter and antimatter degrees of freedom due to the Dirac amplitudes  $U_\mu(\mathbf{r}; k)$  and  $V_\mu(\mathbf{r}; k)$ . For the decoupling one can then make use of the Eriksen transformation  $\mathbb{T}$ .

## 4 Solution to the Classical Limit Problem of QED

### Part I: Applying the Flow Equation

In subsection 4.1 the generator  $\hat{\eta}^{(LM)}(s)$  for the flow equation that provides in the limit  $s \rightarrow \infty$  a unitarily equivalent QED Hamiltonian  $\hat{\mathcal{H}}_U$  that preserves the particle number is introduced. LM in  $\hat{\eta}^{(LM)}(s)$  stands for light–matter, since this unitarily equivalent QED Hamiltonian is a many–body Hamiltonian in second quantization describing the interaction between charged fermions moving at arbitrary speed and interacting with low–energy photons.

As will be shown, the generator  $\hat{\eta}^{(LM)}(s)$  depends quadratically on the initial (QED) Hamiltonian. Therefore, the related flow equation is a nonlinear differential equation.

It comprises the operator  $\hat{N}_I$  counting the number of occupied Dirac modes, and the operator  $\hat{N}_{II}$  counting the number of occupied photon modes of *high energy*. The latter means that the flow equation for constructing a light–matter interaction QED Hamiltonian  $\hat{\mathcal{H}}_U$  eliminates photons with wavenumbers larger than  $q_B = \frac{\alpha_{FS}}{\lambda_C}$ , where  $\lambda_C$  is the Compton wavelength of the electron, and  $\alpha_{FS}$  the finestructure constant. The related wavelength of the photons relevant for light–matter interaction processes is then the Bohr wavelength  $\lambda_B = \frac{2\pi}{q_B} \approx 3\text{\AA}$ . In the end one will therefore get a Hamiltonian  $\hat{\mathcal{H}}_U$  that describes processes of atomic and molecular physics, and even solid state physics.

The related flow equation decomposes into recursive differential equations by expanding the QED Hamiltonian into a series in the finestructure constant  $\alpha_{FS}$ . For solving them one has to choose the initial data, which will be done in a physically consistent manner.

The solution of the first order differential equation will be presented in full, whereas the solution of the second order differential equation is in larger parts shifted to the appendix, in order to keep the overview.

The homogeneous part of the second order differential equation is related to the QED Coulomb interaction. For solving this equation the latter should be decomposed into a normal ordered part and a self–reaction part. The decomposition is presented in section G of the appendix. The self–reaction part of the QED Coulomb interaction

yields one part of the contribution to the renormalization of the bare mass  $m_0$  of the fermions and their  $g$ -factor.

The other part of the renormalization of the fermionic attributes is due to the QED interaction with photons beyond the energy threshold  $\hbar c q_B = \alpha_{FS} m_e c^2$ . These hard X-ray photons and the higher energy ones are being eliminated from the QED Hamiltonian. This takes place by solving the inhomogeneous part of the second order differential equation.

Besides the renormalization contributions one will by that get terms describing an effective Coulomb interaction and an effective transversal interaction now with the low-energy photons.

#### 4.1 Generating Particle Number Conservation

A unitary transformation is searched for such that in the low energy sector of QED there holds particle number conservation for the fermions, and all processes during which high energy photons that are irrelevant for nonrelativistic light-matter interactions are eliminated. The flow equation for that aim is given by [8, 7]

$$\begin{aligned} \frac{d}{ds} \hat{H}(s) &= \left[ \hat{\eta}^{(LM)}(s), \hat{H}(s) \right] \\ \hat{H}(0) &= \frac{1}{m_0 c^2} \hat{\mathcal{H}}^{(QED)} \end{aligned} \tag{82}$$

The generator  $\hat{\eta}^{(LM)}(s)$  of the flow equation can be found by regarding the following positive semidefinite functional  $\Phi^{(LM)}(s) \geq 0$  [8, 7]:

$$\Phi^{(LM)}(s) = \frac{1}{2} \text{tr} \left( \left[ \hat{N}_I, \hat{H}(s) \right] \circ \left[ \hat{H}(s), \hat{N}_I \right] \right) + \frac{1}{2} \text{tr} \left( \left[ \hat{N}_{II}, \hat{H}(s) \right] \circ \left[ \hat{H}(s), \hat{N}_{II} \right] \right) \tag{83}$$

Where

$$\begin{aligned}
\hat{N}_I &= \hat{N}^{(e)} + \hat{N}^{(p)} = \sum_k \left( \hat{c}_k^\dagger \hat{c}_k + \hat{b}_{\tilde{k}}^\dagger \hat{b}_{\tilde{k}} \right) \\
\hat{N}_{II} &= N_{q_B}^{(ph)} \equiv \sum_{|\mathbf{q}| > q_B} \sum_{\lambda \in \{I, II\}} \hat{a}_{\mathbf{q}, \lambda}^\dagger \hat{a}_{\mathbf{q}, \lambda} \\
&= \sum_{\mathbf{q}, \lambda} \kappa_q \hat{a}_{\mathbf{q}, \lambda}^\dagger \hat{a}_{\mathbf{q}, \lambda} \\
&\equiv \sum_q \kappa_q \hat{a}_q^\dagger \hat{a}_q
\end{aligned} \tag{84}$$

and

$$\kappa_q = \begin{cases} 1 & \text{for } |\mathbf{q}| \geq q_B \\ 0 & \text{for } |\mathbf{q}| < q_B \end{cases} \tag{85}$$

Hence,  $\hat{N}_I$  counts the occupied fermion modes, and  $\hat{N}_{II}$  counts the occupied photon modes of photons with energies are larger than  $\hbar c q_B$ . (85) ensures that all photons with wavelength  $\lambda_B \equiv \frac{2\pi}{q_B} \gtrsim 3\text{\AA}$  and longer remain contained, whereas all photons with wavelength  $\lambda_B \lesssim \frac{2\pi}{q_B}$  are being eliminated. Hence X-ray photons and gamma photons are eliminated. Note that the Compton wavelength of the electron  $\lambda_C \approx 2.4\text{ pm}$ , indicating the range of wavelengths where pair creation starts to take place, was *not* chosen as upper limit for the photon elimination. With the choice to eliminate photons with wavelengths  $\lambda_B$  and shorter one is of order  $\lambda_B \approx \frac{\lambda_C}{\alpha_{FS}}$  well away from the pair creation threshold.

Now for the derivative with respect to  $s$  one finds for the functional (83) [8, 7]

$$\begin{aligned}
\frac{d}{ds} \Phi^{(LM)}(s) &= \begin{cases} \frac{1}{2} \text{tr} \left( \left[ \hat{N}_I, \frac{d}{ds} \hat{H}(s) \right] \circ \left[ \hat{H}(s), \hat{N}_I \right] + \left[ \hat{N}_I, \hat{H}(s) \right] \circ \left[ \frac{d}{ds} \hat{H}(s), \hat{N}_I \right] \right) \\ + \frac{1}{2} \text{tr} \left( \left[ \hat{N}_{II}, \frac{d}{ds} \hat{H}(s) \right] \circ \left[ \hat{H}(s), \hat{N}_{II} \right] + \left[ \hat{N}_{II}, \hat{H}(s) \right] \circ \left[ \frac{d}{ds} \hat{H}(s), \hat{N}_{II} \right] \right) \\ \text{tr} \left( \hat{\eta}^{(LM)}(s) \circ \left[ \hat{H}(s), \left[ \hat{N}_I, \left[ \hat{N}_I, \hat{H}(s) \right] \right] \right] \right) \\ + \text{tr} \left( \hat{\eta}^{(LM)}(s) \circ \left[ \hat{H}(s), \left[ \hat{N}_{II}, \left[ \hat{N}_{II}, \hat{H}(s) \right] \right] \right] \right) \end{cases} \\
&= \text{tr} \left( \hat{\eta}^{(LM)}(s) \circ \left[ \hat{H}(s), \left( \left[ \hat{N}_I, \left[ \hat{N}_I, \hat{H}(s) \right] \right] + \left[ \hat{N}_{II}, \left[ \hat{N}_{II}, \hat{H}(s) \right] \right] \right) \right] \right)
\end{aligned} \tag{86}$$

Iff the generator  $\hat{\eta}^{(LM)}$  is choosen according to [8, 7]

$$\hat{\eta}^{(LM)}(s) \equiv \left[ \hat{H}(s), \left( \left[ \hat{N}_I, \left[ \hat{N}_I, \hat{H}(s) \right] \right] + \left[ \hat{N}_{II}, \left[ \hat{N}_{II}, \hat{H}(s) \right] \right] \right) \right] \quad (87)$$

then  $(\hat{\eta}^{(LM)}(s))^\dagger = -\hat{\eta}^{(LM)}(s)$ , and for (86) one further finds

$$\begin{aligned} \frac{d}{ds} \Phi^{(LM)}(s) &= \text{tr} \left( \hat{\eta}^{(LM)}(s) \circ \hat{\eta}^{(LM)}(s) \right) \\ &= -\text{tr} \left( \hat{\eta}^{(LM)}(s) \circ \left( \hat{\eta}^{(LM)}(s) \right)^\dagger \right) \leq 0 \end{aligned} \quad (88)$$

Altogether then for  $s \rightarrow \infty$  there holds  $\lim_{s \rightarrow \infty} \Phi^{(LM)}(s) = 0 = \lim_{s \rightarrow \infty} \frac{d}{ds} \Phi^{(LM)}(s)$ , implying [8, 7]

$$\begin{aligned} \lim_{s \rightarrow \infty} \left[ \hat{N}_I, \hat{H}(s) \right] &= \left[ \hat{N}_I, \hat{H}(\infty) \right] = \hat{0} \\ \lim_{s \rightarrow \infty} \left[ \hat{N}_{II}, \hat{H}(s) \right] &= \left[ \hat{N}_{II}, \hat{H}(\infty) \right] = \hat{0} \end{aligned} \quad (89)$$

The generator (87) therefore generates a flow equation which, if solvable, provides in the limit  $s \rightarrow \infty$  a unitarily equivalent QED Hamiltonian  $\hat{\mathcal{H}}_U$  that conserves the particle number and that does not describe absorption and emission processes of photons with high energies  $\hbar\omega(\mathbf{q}) > \hbar c q_B$ .

#### 4.1.1 Series Expansion

It has been proven that the generator  $\hat{\eta}^{(LM)}$  allows to obtain a particle number conserving QED Hamiltonian. The related flow equation assumes the following guise [8, 7]

$$\begin{aligned} \frac{d}{ds} \hat{H}(s) &= \left[ \hat{\eta}^{(LM)}(s), \hat{H}(s) \right] \\ &= \left[ \left[ \hat{H}(s), \left( \left[ \hat{N}_I, \left[ \hat{N}_I, \hat{H}(s) \right] \right] + \left[ \hat{N}_{II}, \left[ \hat{N}_{II}, \hat{H}(s) \right] \right] \right) \right], \hat{H}(s) \right] \end{aligned} \quad (90)$$

For  $s = 0$  the initial values are given by

$$\begin{aligned}
\hat{H}(0) &= \frac{1}{m_0 c^2} \hat{\mathcal{H}}_{QED} \\
&= \frac{1}{m_0 c^2} \left( \hat{\mathcal{H}}_D + \hat{\mathcal{H}}_{rad} + \hat{\mathcal{V}}_{ext} + \hat{\mathcal{H}}_{\perp} + \hat{\mathcal{V}}_C \right)
\end{aligned} \tag{91}$$

Since the differential equation (90) is nonlinear, one can only solve it perturbatively. As a parameter for a perturbation series of  $\hat{H}(0)$  the dimensionless finestructure constant  $\alpha_{FS} = \frac{|q_e|^2}{4\pi\epsilon_0\hbar c} = \frac{1}{k_C a_B} \simeq \frac{1}{137}$  is chosen. This yields to [8, 7]

$$\hat{H}(s) = \sum_{j=0}^{\infty} \hat{H}^{(j)}(s) \tag{92}$$

Inserting this series into the differential equation (90) one find the following recursion equations [8, 7]

$$\begin{aligned}
\frac{d}{ds} \sum_{j=0}^{\infty} \hat{H}^{(j)}(s) &= \left[ \left[ \sum_{j'=0}^{\infty} \hat{H}^{(j')}(s), \left( \left[ \hat{N}_I, \left[ \hat{N}_I, \sum_{j''=0}^{\infty} \hat{H}^{(j'')}(s) \right] \right] + \left[ \hat{N}_{II}, \left[ \hat{N}_{II}, \sum_{j''=0}^{\infty} \hat{H}^{(j'')}(s) \right] \right] \right) \right], \sum_{j'''=0}^{\infty} \hat{H}^{(j''')}(s) \right] \\
&= \sum_{j'''=0}^{\infty} \sum_{j''=0}^{\infty} \sum_{j'=0}^{\infty} \sum_{j=0}^{\infty} \delta_{j,j'+j''+j'''} \left[ \left[ \hat{H}^{(j')}(s), \left( \left[ \hat{N}_I, \left[ \hat{N}_I, \hat{H}^{(j'')}(s) \right] \right] + \left[ \hat{N}_{II}, \left[ \hat{N}_{II}, \hat{H}^{(j'')}(s) \right] \right] \right) \right], \hat{H}^{(j''')}(s) \right] \\
&= \sum_{j=0}^{\infty} \sum_{j'=0}^{\infty} \sum_{j''=0}^{\infty} \Theta(j-j'-j'') \left[ \left[ \hat{H}^{(j')}(s), \left( \left[ \hat{N}_I, \left[ \hat{N}_I, \hat{H}^{(j'')}(s) \right] \right] + \left[ \hat{N}_{II}, \left[ \hat{N}_{II}, \hat{H}^{(j'')}(s) \right] \right) \right] \right], \hat{H}^{(j-j'-j'')}(s) \right]
\end{aligned} \tag{93}$$

where

$$\Theta(x) = \begin{cases} 1 & \text{for } x \geq 0 \\ 0 & \text{for } x < 0 \end{cases} \tag{94}$$

is the Heaviside step function.

Comparing the orders of  $j$  on both sides we finally find [8, 7]

$$\frac{d}{ds} \hat{H}^{(j)}(s) = \sum_{j'=0}^{\infty} \sum_{j''=0}^{\infty} \Theta(j-j'-j'') \left[ \left[ \hat{H}^{(j')}(s), \left( \left[ \hat{N}_I, \left[ \hat{N}_I, \hat{H}^{(j'')}(s) \right] \right] + \left[ \hat{N}_{II}, \left[ \hat{N}_{II}, \hat{H}^{(j'')}(s) \right] \right) \right] \right], \hat{H}^{(j-j'-j'')}(s) \right] \tag{95}$$

These recursive linear differential equations will now be solved up to the order  $j = 2$ . For that purpose one has to choose the initial data. This is done in the following way [7]

$$\begin{aligned}
\hat{H}^{(0)}(0) &= \frac{1}{m_0 c^2} \left( \hat{\mathcal{H}}_D + \hat{\mathcal{H}}_{rad} \right) \\
\hat{H}^{(1)}(0) &= \frac{1}{m_0 c^2} \hat{\mathcal{H}}_{\perp} \\
\hat{H}^{(2)}(0) &= \frac{1}{m_0 c^2} \left( \hat{\mathcal{V}}_{ext} + \hat{\mathcal{V}}_C \right) \\
\hat{H}^{(j)}(0) &= 0 \text{ for } j \geq 3
\end{aligned} \tag{96}$$

Note that  $\hat{H}(0) = \frac{1}{m_0 c^2} \hat{\mathcal{H}}_{QED}$ . The justification of the choice (96) is presented in the appendix in section E. There it is shown that the transversal coupling is of the order  $\alpha_{FS}$ , whereas the Coulomb interaction is of the order  $\alpha_{FS}^2$

It is very important to be clear that the energy of the radiation field  $\hat{\mathcal{H}}_{rad}$  must be put on zeroth order here. It would not be consistent to assume that it is of the order  $\alpha_{FS}^2 m_0 c^2$  of atomic physics (and hence comparable with the Coulomb energy). The reason why is that the number of occupied photon modes  $\hat{n}_{\mathbf{q},\lambda} = 0, 1, 2, 3, \dots$  can be unlimited, such that the radiation energy  $\hat{\mathcal{H}}_{rad} = \sum_{\mathbf{q},\lambda} \hbar \omega(\mathbf{q}) \left( \hat{n}_{\mathbf{q},\lambda} + \frac{1}{2} \right)$  must be put on the zeroth order next to the rest energy and the kinetic energy of the fermions. Otherwise one would assume that there are only low-energy photons in the QED soup from the beginning.

In the next step all quantities are normalized to the rest energy  $m_0 c^2$  of the fermions. Hence, the following abbreviations are introduced [7]

$$\begin{aligned}
\hat{H}^{(0)} &= \frac{1}{m_0 c^2} \left( \hat{\mathcal{H}}_D + \hat{\mathcal{H}}_{rad} \right) \equiv \hat{H}_D + \hat{H}_{rad} \\
\hat{H}_{rad} &= \frac{1}{m_0 c^2} \sum_{\mathbf{q},\lambda} \hbar \omega(\mathbf{q}) \left( \hat{a}_{\mathbf{q},\lambda}^\dagger \hat{a}_{\mathbf{q},\lambda} + \frac{1}{2} \hat{1} \right) \equiv \sum_q \tilde{\omega}_q \left( \hat{a}_q^\dagger \hat{a}_q + \frac{1}{2} \hat{1} \right) \\
\hat{H}_D &= \frac{1}{m_0 c^2} \sum_k E_k \left( c_k^\dagger c_k + b_{\bar{k}}^\dagger b_{\bar{k}} \right) = \sum_k \tilde{E}_k \left( c_k^\dagger c_k + b_{\bar{k}}^\dagger b_{\bar{k}} \right) \\
\tilde{E}_k &= \frac{E_k}{m_0 c^2} \\
\tilde{\omega}_q &= \frac{\hbar \omega(\mathbf{q})}{m_0 c^2} = \frac{\hbar c |\mathbf{q}|}{m_0 c^2} = \frac{\hbar |\mathbf{q}|}{m_0 c} = \frac{|\mathbf{q}|}{k_C}
\end{aligned} \tag{97}$$

Now for the zeroth order differential equation of (95) one finds the following nonlinear one [8, 7]

$$\frac{d}{ds}\hat{H}^{(0)}(s) = \left[ \left[ \hat{H}^{(0)}(s), \left( \left[ \hat{N}_I, \left[ \hat{N}_I, \hat{H}^{(0)}(s) \right] \right) + \left[ \hat{N}_{II}, \left[ \hat{N}_{II}, \hat{H}^{(0)}(s) \right] \right] \right) \right], \hat{H}^{(0)}(s) \right] \quad (98)$$

Since  $\left[ \hat{N}_I, \hat{H}^{(0)}(0) \right] = \hat{0} = \left[ \hat{N}_{II}, \hat{H}^{(0)}(0) \right]$  the only physical solution that to the nonlinear zeroth order differential equation (98) with respect to the initial value (96) is given by [8, 7]

$$\begin{aligned} \hat{H}^{(0)}(s) &= \hat{H}^{(0)}(0) \equiv \hat{H}^{(0)} = \frac{1}{m_0 c^2} \left( \hat{\mathcal{H}}_D + \hat{\mathcal{H}}_{rad} \right) \\ &= \hat{H}^{(0)}(\infty) \end{aligned} \quad (99)$$

Hence, it is constant for all  $s$ . This enables to find solutions for all higher orders  $j$ , because they occur as *linear* differential equations.

For the first order  $j = 1$  one finds from (95) the following linear, homogeneous differential equation [8, 7]

$$\begin{aligned} \frac{d}{ds}\hat{H}^{(1)}(s) &= - \left[ \hat{H}^{(0)}, \left[ \hat{H}^{(0)}, \left( \left[ \hat{N}_I, \left[ \hat{N}_I, \hat{H}^{(1)}(s) \right] \right) + \left[ \hat{N}_{II}, \left[ \hat{N}_{II}, \hat{H}^{(1)}(s) \right] \right] \right) \right] \right] \\ \hat{H}^{(1)}(0) &= \frac{1}{m_0 c^2} \hat{\mathcal{H}}_{\perp} \end{aligned} \quad (100)$$

And for the second order differential equation one finds from (95) [8, 7]

$$\begin{aligned} \frac{d}{ds}\hat{H}^{(2)}(s) &= \left\{ \begin{aligned} & - \left[ \hat{H}^{(0)}, \left[ \hat{H}^{(0)}, \left( \left[ \hat{N}_I, \left[ \hat{N}_I, \hat{H}^{(2)}(s) \right] \right) + \left[ \hat{N}_{II}, \left[ \hat{N}_{II}, \hat{H}^{(2)}(s) \right] \right] \right) \right] \\ & - \left[ \hat{H}^{(0)}, \left( \left[ \hat{H}^{(1)}(s), \left( \left[ \hat{N}_I, \left[ \hat{N}_I, \hat{H}^{(1)}(s) \right] \right) + \left[ \hat{N}_{II}, \left[ \hat{N}_{II}, \hat{H}^{(1)}(s) \right] \right] \right) \right] \right] \\ & - \left[ \hat{H}^{(1)}(s), \left( \left[ \hat{H}^{(0)}, \left( \left[ \hat{N}_I, \left[ \hat{N}_I, \hat{H}^{(1)}(s) \right] \right) + \left[ \hat{N}_{II}, \left[ \hat{N}_{II}, \hat{H}^{(1)}(s) \right] \right] \right) \right] \right] \right\} \\ \hat{H}^{(2)}(0) &= \frac{1}{m_0 c^2} \left( \hat{\mathcal{V}}_{ext} + \hat{\mathcal{V}}_C \right) \end{aligned} \right. \quad (101)$$

Here, several contributions drop out because  $\left[ \hat{N}_I, \hat{H}^{(0)}(0) \right] = \hat{0} = \left[ \hat{N}_{II}, \hat{H}^{(0)}(0) \right]$ .

The sought unitarily equivalent QED Hamiltonian respecting particle number conservation assumes the guise [8, 7]



$$\lim_{s \rightarrow \infty} \hat{\mathcal{H}}_U(s) = m_0 c^2 \lim_{s \rightarrow \infty} \hat{H}(s) = m_0 c^2 \left( \hat{H}^{(0)} + \hat{H}^{(1)}(\infty) + \hat{H}^{(2)}(\infty) + \dots \right) \quad (102)$$

In the following subsections the equations (100) and (101) are being solved.

#### 4.1.2 First Order Solution

For solving the first order differential equation (100) one makes the following ansatz [7]

$$\hat{H}^{(1)}(s) = \hat{H}_{<}^{(1,0)} + \hat{H}_{>}^{(1,0)}(s) + \hat{H}^{(1,+)}(s) + \hat{H}^{(1,-)}(s) \quad (103)$$

$\hat{H}_{<}^{(1,0)}$  is the contribution that comprises interactions between fermions and low energy photons (such one with wavenumber  $q$  is smaller than the Bohr wave number  $q_B = \frac{\alpha_{FS}}{\lambda_C}$  [7]:

$$\hat{H}_{<}^{(1,0)} = -\frac{1}{m_0 c^2} (c q_e) \sum_{k,k'} \sum_b \int d^3 r \sum_{\mu,\mu'} (\alpha_b)_{\mu,\mu'} \frac{1}{\sqrt{V}} \sum_{q < q_B} \mathcal{A}_b(q) \begin{pmatrix} U_\mu^*(\mathbf{r}; k) U_{\mu'}(\mathbf{r}; k') \hat{c}_k^\dagger \hat{c}_{k'} e^{i\mathbf{q}\cdot\mathbf{r}} \hat{a}_q \\ -V_\mu^*(\mathbf{r}; k) V_{\mu'}(\mathbf{r}; k') \hat{b}_{k'}^\dagger \hat{b}_k e^{i\mathbf{q}\cdot\mathbf{r}} \hat{a}_q \\ +U_\mu^*(\mathbf{r}; k) U_{\mu'}(\mathbf{r}; k') \hat{c}_k^\dagger \hat{c}_{k'} e^{-i\mathbf{q}\cdot\mathbf{r}} \hat{a}_q^\dagger \\ -V_\mu^*(\mathbf{r}; k) V_{\mu'}(\mathbf{r}; k') \hat{b}_{k'}^\dagger \hat{b}_k e^{-i\mathbf{q}\cdot\mathbf{r}} \hat{a}_q^\dagger \end{pmatrix} \quad (104)$$

This contribution is independent of the flow parameter  $s$  and therefore, these interactions are being conserved during the flow  $s \rightarrow \infty$ .

$\hat{H}_{>}^{(1,0)}(s)$  accordingly comprises interaction processes between fermions and high energy photons, such one with wavenumber  $q$  larger than  $q_B$  [7]:

$$\hat{H}_{>}^{(1,0)}(s) = -\frac{1}{m_0 c^2} (c q_e) \sum_{k,k'} \sum_b \int d^3 r \sum_{\mu,\mu'} (\alpha_b)_{\mu,\mu'} \times \frac{1}{\sqrt{V}} \sum_{q > q_B} \mathcal{A}_b(q) \begin{pmatrix} U_\mu^*(\mathbf{r}; k) U_{\mu'}(\mathbf{r}; k') e^{-s(\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)^2} \hat{c}_k^\dagger \hat{c}_{k'} e^{i\mathbf{q}\cdot\mathbf{r}} \hat{a}_q \\ -V_\mu^*(\mathbf{r}; k) V_{\mu'}(\mathbf{r}; k') e^{-s(\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q)^2} \hat{b}_{k'}^\dagger \hat{b}_k e^{i\mathbf{q}\cdot\mathbf{r}} \hat{a}_q \\ +U_\mu^*(\mathbf{r}; k) U_{\mu'}(\mathbf{r}; k') e^{-s(\tilde{E}_k - \tilde{E}_{k'} + \tilde{\omega}_q)^2} \hat{c}_k^\dagger \hat{c}_{k'} e^{-i\mathbf{q}\cdot\mathbf{r}} \hat{a}_q^\dagger \\ -V_\mu^*(\mathbf{r}; k) V_{\mu'}(\mathbf{r}; k') e^{-s(\tilde{E}_{k'} - \tilde{E}_k + \tilde{\omega}_q)^2} \hat{b}_{k'}^\dagger \hat{b}_k e^{-i\mathbf{q}\cdot\mathbf{r}} \hat{a}_q^\dagger \end{pmatrix}$$

The dependence on the flow parameter  $s$  is chosen in such a way that it reproduces the double commutator of the flow equation (100), as will be shown a few lines below.

Hence [7],

$$\hat{H}^{(1,0)}(s) = \hat{H}_{<}^{(1,0)} + \hat{H}_{>}^{(1,0)}(s) \quad (105)$$

With the definition of the step function  $\kappa_q$  according to (85) one furthermore defines [7]

$$\begin{aligned} \hat{H}^{(1,+)}(s) &= -\frac{1}{m_0 c^2} (c q_e) \sum_{k,k'} \sum_b \int d^3 r \sum_{\mu,\mu'} (\alpha_b)_{\mu,\mu'} U_\mu^*(\mathbf{r}; k) V_{\mu'}(\mathbf{r}; k') \\ &\quad \times \frac{1}{\sqrt{V}} \sum_q \mathcal{A}_b(q) \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \left( e^{-(4+\kappa_q)s(\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q)^2} e^{i\mathbf{q}\cdot\mathbf{r}} \hat{a}_q + e^{-(4+\kappa_q)s(\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q)^2} e^{-i\mathbf{q}\cdot\mathbf{r}} \hat{a}_q^\dagger \right) \end{aligned}$$

and [7]

$$\begin{aligned} \hat{H}^{(1,-)}(s) &= \left( \hat{H}^{(1,+)}(s) \right)^\dagger \\ &= -\frac{1}{m_0 c^2} (c q_e) \sum_{K,K'} \sum_{b'} \int d^3 r' \sum_{\nu,\nu'} (\alpha_{b'})_{\nu,\nu'}^* V_{\nu'}^*(\mathbf{r}'; K') U_\nu(\mathbf{r}'; K) \\ &= \times \frac{1}{\sqrt{V}} \sum_{q'} \mathcal{A}_{b'}(q') \hat{b}_{K'} \hat{c}_K \left( e^{-(4+\kappa_{q'})s(\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'})^2} e^{-i\mathbf{q}'\cdot\mathbf{r}'} \hat{a}_{q'}^\dagger + e^{-(4+\kappa_{q'})s(\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'})^2} e^{i\mathbf{q}'\cdot\mathbf{r}'} \hat{a}_{q'} \right) \end{aligned}$$

In order to show that the ansatz (103) solves the first order equation (100) it is convenient express the matrix elements in the compact Dirac bracket notation (see section A of the appendix)

$$\begin{aligned} \sum_\mu \int d^3 r U_\mu^*(\mathbf{r}, k) e^{-i\mathbf{q}\cdot\mathbf{r}} U_\mu(\mathbf{r}, k') &= \langle U_k | e^{-iq_a x_a} | U_{k'} \rangle \\ \sum_\mu \int d^3 r U_\mu^*(\mathbf{r}, k) e^{-i\mathbf{q}\cdot\mathbf{r}} V_\mu(\mathbf{r}, k') &= \langle U_k | e^{-iq_a x_a} | V_{k'} \rangle \\ \sum_\mu \int d^3 r V_\mu^*(\mathbf{r}, k) e^{-i\mathbf{q}\cdot\mathbf{r}} U_\mu(\mathbf{r}, k') &= \langle V_k | e^{-iq_a x_a} | U_{k'} \rangle \\ \sum_\mu \int d^3 r V_\mu^*(\mathbf{r}, k) e^{-i\mathbf{q}\cdot\mathbf{r}} V_\mu(\mathbf{r}, k') &= \langle V_k | e^{-iq_a x_a} | V_{k'} \rangle \end{aligned} \quad (106)$$

Note that  $x$  is an operator.

With that there holds [7]

$$\hat{H}_{<}^{(1,0)} = \left( -\frac{q_e}{m_0 c} \right) \sum_{k,k'} \frac{1}{\sqrt{V}} \sum_{q < q_B} \sum_b \mathcal{A}_b(q) \begin{pmatrix} \langle U_k | \alpha_b e^{iq_a x_a} | U_{k'} \rangle \hat{c}_k^\dagger \hat{c}_{k'} \hat{a}_q \\ - \langle V_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \hat{b}_{k'}^\dagger \hat{b}_k \hat{a}_q \\ + \langle U_k | \alpha_b e^{-iq_a x_a} | U_{k'} \rangle \hat{c}_k^\dagger \hat{c}_{k'} \hat{a}_q^\dagger \\ - \langle V_k | \alpha_b e^{-iq_a x_a} | V_{k'} \rangle \hat{b}_{k'}^\dagger \hat{b}_k \hat{a}_q^\dagger \end{pmatrix}$$

$$\hat{H}_{>}^{(1,0)}(s) = \left( -\frac{q_e}{m_0 c} \right) \sum_{k,k'} \frac{1}{\sqrt{V}} \sum_{q > q_B} \sum_b \mathcal{A}_b(q) \begin{pmatrix} \langle U_k | \alpha_b e^{iq_a x_a} | U_{k'} \rangle e^{-s(\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)^2} \hat{c}_k^\dagger \hat{c}_{k'} \hat{a}_q \\ - \langle V_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle e^{-s(\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q)^2} \hat{b}_{k'}^\dagger \hat{b}_k \hat{a}_q \\ + \langle U_k | \alpha_b e^{-iq_a x_a} | U_{k'} \rangle e^{-s(\tilde{E}_k - \tilde{E}_{k'} + \tilde{\omega}_q)^2} \hat{c}_k^\dagger \hat{c}_{k'} \hat{a}_q^\dagger \\ - \langle V_k | \alpha_b e^{-iq_a x_a} | V_{k'} \rangle e^{-s(\tilde{E}_{k'} - \tilde{E}_k + \tilde{\omega}_q)^2} \hat{b}_{k'}^\dagger \hat{b}_k \hat{a}_q^\dagger \end{pmatrix} \quad (107)$$

$$\hat{H}^{(1,+)}(s) = \left( -\frac{q_e}{m_0 c} \right) \sum_{k,k'} \frac{1}{\sqrt{V}} \sum_q \sum_b \mathcal{A}_b(q) \begin{pmatrix} \langle U_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle e^{-(4+\kappa_q)s(\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q)^2} \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q \\ + \langle U_k | \alpha_b e^{-iq_a x_a} | V_{k'} \rangle e^{-(4+\kappa_q)s(\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q)^2} \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q^\dagger \end{pmatrix}$$

$$= \hat{H}_{<}^{(1,+)}(s) + \hat{H}_{>}^{(1,+)}(s) \quad (108)$$

$$\hat{H}^{(1,-)}(s) = \left( -\frac{q_e}{m_0 c} \right) \sum_{K,K'} \frac{1}{\sqrt{V}} \sum_{q'} \sum_{b'} \mathcal{A}_{b'}(q') \begin{pmatrix} \langle V_{K'} | \alpha_{b'} e^{-iq'_a x_a} | U_K \rangle e^{-(4+\kappa_{q'})s(-\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2} \hat{b}_{K'} \hat{c}_K \hat{a}_{q'}^\dagger \\ + \langle V_{K'} | \alpha_{b'} e^{iq'_a x_a} | U_K \rangle e^{-(4+\kappa_{q'})s(-\tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_{q'})^2} \hat{b}_{K'} \hat{c}_K \hat{a}_{q'} \end{pmatrix}$$

$$= \left( \hat{H}^{(1,+)}(s) \right)^\dagger$$

$$= \hat{H}_{<}^{(1,-)}(s) + \hat{H}_{>}^{(1,-)}(s)$$

This ansatz is consistent with the chosen initial value (96) as can be seen by setting  $s \equiv 0$ .

With the given operator  $\hat{N}_I$ , see (84) one finds [7]

$$\begin{aligned} \left[ \hat{N}_I, \hat{H}^{(0)} \right] &= \hat{0} \\ \left[ \hat{N}_I, \left( \hat{H}_{<}^{(1,0)} + \hat{H}_{>}^{(1,0)}(s) \right) \right] &= \hat{0} \\ \left[ \hat{N}_I, \hat{H}^{(1,\pm)}(s) \right] &= \pm 2 \hat{H}^{(1,\pm)}(s) \end{aligned} \quad (109)$$

Hence [7],

$$\begin{aligned} \left[ \hat{N}_I, \left[ \hat{N}_I, \hat{H}^{(1)}(s) \right] \right] &= \left[ \hat{N}_I, \left[ \hat{N}_I, \left( \hat{H}^{(1,0)}(s) + \hat{H}^{(1,+)}(s) + \hat{H}^{(1,-)}(s) \right) \right] \right] \\ &= 4 \hat{H}^{(1,+)}(s) + 4 \hat{H}^{(1,-)}(s) \end{aligned} \quad (110)$$

Since the operator  $\hat{N}_{II}$  counts, according to (84) only high energy photons, there holds [7]

$$\begin{aligned} \left[ \hat{N}_{II}, \hat{H}_{<}^{(1,0)} \right] &= \hat{0} \\ \left[ \hat{N}_{II}, \hat{H}_{<}^{(1,\pm)}(s) \right] &= \hat{0} \end{aligned} \quad (111)$$

Therefore [7],

$$\left[ \hat{N}_{II}, \left[ \hat{N}_{II}, \hat{H}^{(1)}(s) \right] \right] = \hat{H}_{>}^{(1,0)}(s) + \hat{H}_{>}^{(1,+)}(s) + \hat{H}_{>}^{(1,-)}(s) \quad (112)$$

Inserting the ansatz (103) into the inner double commutators on the right hand side of the differential equation (100) one can see by the help of (110) and (112) [7]

$$\begin{aligned} &\left[ \hat{N}_I, \left[ \hat{N}_I, \hat{H}^{(1)}(s) \right] \right] + \left[ \hat{N}_{II}, \left[ \hat{N}_{II}, \hat{H}^{(1)}(s) \right] \right] \\ &= \hat{H}_{>}^{(1,0)}(s) + 4\hat{H}_{<}^{(1,+)}(s) + 5\hat{H}_{>}^{(1,+)}(s) + 4\hat{H}_{<}^{(1,-)}(s) + 5\hat{H}_{>}^{(1,-)}(s) \end{aligned} \quad (113)$$

Now for the outer double commutator of (100) one finds, with  $\hat{H}^{(0)} = \hat{H}_D + \hat{H}_{rad}$ ,  $\left[ \hat{H}_D, \hat{H}_{rad} \right] = \hat{0}$ , the definitions in (97) and the (anti-) commutator properties of the fermionic and bosonic creation and annihilation operators (15) and (27)

from [7]

$$\begin{aligned} \left[ \hat{H}_D, \hat{c}_{k'}^\dagger \hat{b}_{k''}^\dagger \right] &= \left[ \sum_k \tilde{E}_k \left( c_k^\dagger c_k + b_k^\dagger b_{\tilde{k}} \right), \hat{c}_{k'}^\dagger \hat{b}_{k''}^\dagger \right] \\ &= \sum_k \tilde{E}_k \left( \left[ c_k^\dagger c_k, \hat{c}_{k'}^\dagger \hat{b}_{k''}^\dagger \right] + \left[ b_k^\dagger b_{\tilde{k}}, \hat{c}_{k'}^\dagger \hat{b}_{k''}^\dagger \right] \right) \\ &= \sum_k \tilde{E}_k \left( c_k^\dagger \hat{b}_{k''}^\dagger \delta_{k,k'} - b_{\tilde{k}}^\dagger \hat{c}_{k'}^\dagger \delta_{k,k''} \right) \\ &= \tilde{E}_{k'} \left( c_{k'}^\dagger \hat{b}_{k''}^\dagger - b_{\tilde{k}''}^\dagger \hat{c}_{k'}^\dagger \right) \\ &= \tilde{E}_{k'} \left( c_{k'}^\dagger \hat{b}_{k''}^\dagger + \hat{c}_{k'}^\dagger b_{\tilde{k}''}^\dagger \right) \\ &= 2\tilde{E}_{k'} \hat{c}_{k'}^\dagger \hat{b}_{k''}^\dagger \end{aligned} \quad (114)$$

then [7]

$$\begin{aligned}
& \left[ \hat{H}^{(0)}, \left[ \hat{H}^{(0)}, e^{-(4+\kappa_q)s(\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q)^2} \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q \right] \right] \\
&= \left[ \left( \hat{H}_D + \hat{H}_{rad} \right), \left[ \left( \hat{H}_D + \hat{H}_{rad} \right), e^{-(4+\kappa_q)s(\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q)^2} \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q \right] \right] \\
&= \left[ \left( \hat{H}_D + \hat{H}_{rad} \right), \left( \tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q \right) e^{-(4+\kappa_q)s(\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q)^2} \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q \right] \\
&= \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \left( \tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q \right)^2 e^{-(4+\kappa_q)s(\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q)^2} \hat{a}_q \\
&= \left( -\frac{1}{4 + \kappa_q} \frac{d}{ds} \right) \hat{c}_k^\dagger \hat{b}_{k'}^\dagger e^{-(4+\kappa_q)s(\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q)^2} \hat{a}_q
\end{aligned} \tag{115}$$

or [7]

$$\begin{aligned}
& \left[ \hat{H}^{(0)}, \left[ \hat{H}^{(0)}, e^{-s(\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)^2} \hat{c}_k^\dagger \hat{c}_{k'} \hat{a}_q \right] \right] \\
&= \left[ \left( \hat{H}_D + \hat{H}_{rad} \right), \left[ \left( \hat{H}_D + \hat{H}_{rad} \right), e^{-s(\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)^2} \hat{c}_k^\dagger \hat{c}_{k'} \hat{a}_q \right] \right] \\
&= \left[ \left( \hat{H}_D + \hat{H}_{rad} \right), \left( \tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q \right) e^{-s(\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)^2} \hat{c}_k^\dagger \hat{c}_{k'} \hat{a}_q \right] \\
&= \left( \tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q \right)^2 e^{-s(\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)^2} \hat{c}_k^\dagger \hat{c}_{k'} \hat{a}_q \\
&= \left( -\frac{d}{ds} \right) e^{-s(\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)^2} \hat{c}_k^\dagger \hat{c}_{k'} \hat{a}_q
\end{aligned} \tag{116}$$

Hence, there holds [7]

$$\begin{aligned}
\left[ \hat{H}^{(0)}, \left[ \hat{H}^{(0)}, \hat{H}_{<}^{(1,\pm)}(s) \right] \right] &= -\frac{1}{4} \frac{d}{ds} \hat{H}_{<}^{(1,\pm)}(s) \\
\left[ \hat{H}^{(0)}, \left[ \hat{H}^{(0)}, \hat{H}_{>}^{(1,\pm)}(s) \right] \right] &= -\frac{1}{5} \frac{d}{ds} \hat{H}_{>}^{(1,\pm)}(s) \\
\left[ \hat{H}^{(0)}, \left[ \hat{H}^{(0)}, \hat{H}_{>}^{(1,0)}(s) \right] \right] &= -\frac{d}{ds} \hat{H}_{>}^{(1,0)}(s)
\end{aligned} \tag{117}$$

and altogether [7]

$$\begin{aligned}
& - \left[ \hat{H}^{(0)}, \left[ \hat{H}^{(0)}, \left( \left[ \hat{N}_I, \left[ \hat{N}_I, \hat{H}^{(1)}(s) \right] \right) + \left[ \hat{N}_{II}, \left[ \hat{N}_{II}, \hat{H}^{(1)}(s) \right] \right] \right) \right] \right] \\
& = - \left[ \hat{H}^{(0)}, \left[ \hat{H}^{(0)}, \left( \hat{H}_{>}^{(1,0)}(s) + 4\hat{H}_{<}^{(1,+)}(s) + 5\hat{H}_{>}^{(1,+)}(s) + 4\hat{H}_{<}^{(1,-)}(s) + 5\hat{H}_{>}^{(1,-)}(s) \right) \right] \right] \\
& = \frac{d}{ds} \left( \hat{H}_{<}^{(1,0)} + \hat{H}_{>}^{(1,0)}(s) + \hat{H}_{<}^{(1,+)}(s) + \hat{H}_{>}^{(1,+)}(s) + \hat{H}_{<}^{(1,-)}(s) + \hat{H}_{>}^{(1,-)}(s) \right) \\
& = \frac{d}{ds} \left( \hat{H}^{(1,0)} + \hat{H}^{(1,+)}(s) + \hat{H}^{(1,-)}(s) \right) \\
& = \frac{d}{ds} \hat{H}^{(1)}(s)
\end{aligned} \tag{118}$$

With that it is shown that the ansatz (103) solves the differential equation (100) for the initial value  $\hat{H}^{(1)}(0) = \frac{1}{m_0 c^2} \hat{\mathcal{H}}_{\perp}$ .

Now regarding the flow  $s \rightarrow \infty$  for the ansatz  $\hat{H}^{(1)}(s)$  one finds [7]

$$\lim_{s \rightarrow \infty} \hat{H}^{(1)}(s) = \hat{H}_{<}^{(1,0)} + \left( -\frac{q_e}{m_0 c} \right) \sum_{k,k'} \frac{1}{\sqrt{V}} \sum_q \sum_b \delta(\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q) \mathcal{A}_b(q) \left\{ \begin{array}{l} \langle U_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \times \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q \\ + \langle V_{k'} | \alpha_{b'} e^{-iq_a x_a} | U_k \rangle \hat{b}_{\tilde{k}'} \hat{c}_k \hat{a}_q^\dagger \end{array} \right. \tag{119}$$

The first term  $\hat{H}_{<}^{(1,0)}$  describes the interactions of the fermions (electrons and positrons) with low energy photons, see (104).

The second term appears here because in the summation over the mode indices  $k, k', q$  there are still high energy photons obeying to the condition  $\tilde{\omega}_q = \tilde{E}_k + \tilde{E}_{k'}$  (being of the order 1 since the energies of the fermions still contain the rest energy). This term is in fact a particle number violating term (since it is proportional to the products  $\hat{c}_k^\dagger \hat{b}_{k'}^\dagger$  and  $\hat{b}_{\tilde{k}'} \hat{c}_k$ ).

It has to be noticed, however, that if one takes the limit  $V \rightarrow \infty$ , the summation over the dense modes  $q = (\mathbf{q}, \lambda)$  is converted into the integral over the wave number  $\mathbf{q}$  (with periodic boundary conditions), and the summation  $\lambda \in \{I, II\} = 2$ . Hence, these remaining terms violating particle number are of zero measure.

Iff one agrees here and in the following to first take the limit  $V \rightarrow \infty$  and then the limit  $s \rightarrow \infty$ . In that case the second term in (119) vanishes and one finds [7]

$$\lim_{s \rightarrow \infty} \lim_{V \rightarrow \infty} \left[ \hat{N}_I, \hat{H}^{(1)}(s) \right] = \hat{0} \tag{120}$$

### 4.1.3 Second Order Solution

The differential equation (101) is a linear differential equation with an inhomogeneous term. Hence, the solution  $\hat{H}^{(2)}(s)$  is given by the superposition of the solution  $\hat{H}^{(2,h)}(s)$  to the homogeneous differential equation [7]

$$\frac{d}{ds}\hat{H}^{(2,h)}(s) = - \left[ \hat{H}^{(0)}, \left[ \hat{H}^{(0)}, \left( \left[ \hat{N}_I, \left[ \hat{N}_I, \hat{H}^{(2,h)}(s) \right] \right) + \left[ \hat{N}_{II}, \left[ \hat{N}_{II}, \hat{H}^{(2,h)}(s) \right] \right] \right] \right] \right] \quad (121)$$

with the inhomogeneous initial value  $\hat{H}^{(2,h)}(0) = \frac{1}{m_0 c^2} \left( \hat{\mathcal{V}}_{ext} + \hat{\mathcal{V}}_C \right)$ , and a special solution  $\hat{H}^{(2,i)}(s)$  to the inhomogeneous differential equation [7]

$$\begin{aligned} \frac{d}{ds}\hat{H}^{(2,i)}(s) &= \begin{cases} - \left[ \hat{H}^{(0)}, \left[ \hat{H}^{(0)}, \left( \left[ \hat{N}_I, \left[ \hat{N}_I, \hat{H}^{(2,i)}(s) \right] \right) + \left[ \hat{N}_{II}, \left[ \hat{N}_{II}, \hat{H}^{(2,i)}(s) \right] \right] \right] \right] \\ - \left[ \hat{H}^{(0)}, \left( \left[ \hat{H}^{(1)}(s), \left( \left[ \hat{N}_I, \left[ \hat{N}_I, \hat{H}^{(1)}(s) \right] \right) + \left[ \hat{N}_{II}, \left[ \hat{N}_{II}, \hat{H}^{(1)}(s) \right] \right] \right) \right] \right] \\ - \left[ \hat{H}^{(1)}(s), \left( \left[ \hat{H}^{(0)}, \left( \left[ \hat{N}_I, \left[ \hat{N}_I, \hat{H}^{(1)}(s) \right] \right) + \left[ \hat{N}_{II}, \left[ \hat{N}_{II}, \hat{H}^{(1)}(s) \right] \right] \right) \right] \right] \end{cases} \\ &\equiv \begin{cases} - \left[ \hat{H}^{(0)}, \left[ \hat{H}^{(0)}, \left( \left[ N_I, \left[ N_I, \hat{H}^{(2,i)}(s) \right] \right) + \left[ N_{II}, \left[ N_{II}, \hat{H}^{(2,i)}(s) \right] \right] \right] \right] \\ + I(s) \end{cases} \end{aligned} \quad (122)$$

with the initial value 0.

Hence, the solution is of the form  $\hat{H}^{(2)}(s) = \hat{H}^{(2,h)}(s) + \hat{H}^{(2,i)}(s)$ .

In the following two subsections the solutions to these differential equations are sketched. They rely on closed formes that are quite analagous to the ones given in (109) and (111). However, since the calculations are longish, some parts of the solution for the second order differential equation are shifted to the appendix.

### Homogeneous Differential Equation

For the solution of the homogeneous part of the second order differential equation it is convenient to decompose the the QED Coulomb interaction  $\hat{\mathcal{V}}_C$  into a sum of a part that is normally ordered,  $\mathcal{N}(\hat{\mathcal{V}}_C)$ , and a self-interaction term  $\hat{\mathcal{M}}_C$ . This decomposition can be found in the appendix chapter G.

The result is given by  $\hat{\mathcal{V}}_C = \hat{\mathcal{M}}_C(s) + \mathcal{U}(s)$ .

Having said that the ansatz for the solution to the homogeneous differential equation (121) is presented as [7]

$$\hat{H}^{(2,h)}(s) = \frac{1}{m_0 c^2} \left( \hat{\mathcal{V}}_{ext}(s) + \hat{\mathcal{M}}_C(s) + \mathcal{U}(s) \right) \quad (123)$$

which will be verified in the following.

Now, in the appendix G it is also shown how to decompose the coupling to an external Coulomb potential  $\hat{\mathcal{V}}_{ext}$  into particle number conserving and nonconserving terms. For the QED Coulomb interaction this yields an extra one-particle contribution which contributes to the renormalization of the bare mass  $m_0$  and the  $g$ -factor of the fermions as we will see in section 6.1.2.

The result of the decomposition of the QED Coulomb interaction  $\mathcal{U}(s)$  is given by [7]

$$\mathcal{U}(s) = \hat{\mathcal{U}}_C^{(0)} + \hat{\mathcal{U}}_C^{(+)}(s) + \hat{\mathcal{U}}_C^{(-)}(s) + \hat{\mathcal{U}}_C^{(+,+)}(s) + \hat{\mathcal{U}}_C^{(-,-)}(s) \quad (124)$$

Here and in the following the superscripts (+) and (−) indicate that the terms concerned raise or lower the fermion occupation number by 1, whereas the superscript (0) indicates that this term is particle number conserving. Since the Coulomb interaction is the product of two scalars  $\hat{\Psi}_\mu^\dagger(\mathbf{r})\hat{\Psi}_\mu(\mathbf{r})$  and  $\hat{\Psi}_{\mu'}^\dagger(\mathbf{r}')\hat{\Psi}_{\mu'}(\mathbf{r}')$  there occur terms that raise or lower the the fermion occupation number by 2. These terms are indicated by the superscripts (+, +) and (−, −) [7]

$$\hat{\mathcal{U}}_C^{(0)} = \mathcal{N}(\hat{\mathcal{V}}_C^{(0)})$$

$$\hat{\mathcal{U}}_C^{(+)}(s) = \frac{q_e^2}{2\varepsilon_0} \int \frac{d^3q}{(2\pi)^3} \frac{1}{|\mathbf{q}|^2} \sum_{k,k'} \sum_{K,K'} \mathcal{N} \left( \begin{array}{l} + \langle U_k | e^{-iq_a x_a} | U_{k'} \rangle \langle U_K | e^{iq_a x_a} | V_{K'} \rangle \hat{c}_k^\dagger c_{k'} \hat{c}_K^\dagger b_{K'}^\dagger e^{-4s(E_k - E_{k'} + E_K + E_{K'})^2} \\ + \langle U_k | e^{-iq_a x_a} | V_{k'} \rangle \langle U_K | e^{iq_a x_a} | U_{K'} \rangle \hat{c}_k^\dagger b_{k'}^\dagger \hat{c}_K^\dagger c_{K'} e^{-4s(E_k + E_{k'} + E_K - E_{K'})^2} \\ + \langle V_k | e^{-iq_a x_a} | V_{k'} \rangle \langle U_K | e^{iq_a x_a} | V_{K'} \rangle \hat{b}_k^\dagger b_{k'}^\dagger \hat{c}_K^\dagger b_{K'}^\dagger e^{-4s(-E_k + E_{k'} + E_K + E_{K'})^2} \\ + \langle U_k | e^{-iq_a x_a} | V_{k'} \rangle \langle V_K | e^{iq_a x_a} | V_{K'} \rangle \hat{c}_k^\dagger b_{k'}^\dagger \hat{b}_{K'}^\dagger b_{K'}^\dagger e^{-4s(E_k + E_{k'} - E_K + E_{K'})^2} \end{array} \right)$$

$$\hat{\mathcal{U}}_C^{(-)}(s) = \left( \hat{\mathcal{U}}_C^{(+)}(s) \right)^\dagger$$

$$\hat{\mathcal{U}}_C^{(+,+)}(s) = \frac{q_e^2}{2\varepsilon_0} \int \frac{d^3q}{(2\pi)^3} \frac{1}{|\mathbf{q}|^2} \sum_{k,k'} \sum_{K,K'} \mathcal{N} \left( \langle U_k | e^{-iq_a x_a} | V_{k'} \rangle \langle U_K | e^{iq_a x_a} | V_{K'} \rangle \hat{c}_k^\dagger b_{k'}^\dagger \hat{c}_K^\dagger b_{K'}^\dagger \right) e^{-16s(E_k + E_{k'} + E_K + E_{K'})^2}$$

$$\hat{\mathcal{U}}_C^{(-,-)}(s) = \left( \hat{\mathcal{U}}_C^{(+,+)}(s) \right)^\dagger$$

(125)



Accordingly, the contributions caused by the self energy  $\hat{\mathcal{M}}_C(s)$  are given as [7]

$$\begin{aligned}
\hat{\mathcal{M}}_C(s) &= \hat{\mathcal{M}}_C^{(0)} + \hat{\mathcal{M}}_C^{(+)}(s) + \hat{\mathcal{M}}_C^{(-)}(s) \\
\hat{\mathcal{M}}_C^{(0)} &= \frac{q_e^2}{2\varepsilon_0} \sum_{k,k'} \left( \langle U_k | \mathbf{M}^{(C)} | U_{k'} \rangle \hat{c}_k^\dagger c_{k'} - \langle V_k | \mathbf{M}^{(C)} | V_{k'} \rangle b_{\tilde{k}'}^\dagger \hat{b}_{\tilde{k}} \right) \\
\hat{\mathcal{M}}_C^{(+)}(s) &= \frac{q_e^2}{2\varepsilon_0} \sum_{k,k'} \langle U_k | \mathbf{M}^{(C)} | V_{k'} \rangle \hat{c}_k^\dagger b_{\tilde{k}'}^\dagger e^{-4s(\tilde{E}_k + \tilde{E}_{k'})^2} \\
\hat{\mathcal{M}}_C^{(-)}(s) &= \left( \hat{\mathcal{M}}_C^{(+)}(s) \right)^\dagger
\end{aligned} \tag{126}$$

And finally the decomposition of the interaction of the fermions with the external potential  $\hat{\mathcal{V}}_{ext}(s)$  according to [7]

$$\begin{aligned}
\hat{\mathcal{V}}_{ext}(s) &= \hat{\mathcal{V}}_{ext}^{(0)} + \hat{\mathcal{V}}_{ext}^{(+)}(s) + \hat{\mathcal{V}}_{ext}^{(-)}(s) \\
\hat{\mathcal{V}}_{ext}^{(0)} &= \int \frac{d^3q}{(2\pi)^3} \tilde{\Phi}_{ext}(\mathbf{q}) \sum_{k,k'} \left( \langle U_k | e^{-iq_a x_a} | U_{k'} \rangle \hat{c}_k^\dagger c_{k'} - \langle V_k | e^{-iq_a x_a} | V_{k'} \rangle b_{\tilde{k}'}^\dagger \hat{b}_{\tilde{k}} \right) \\
\hat{\mathcal{V}}_{ext}^{(+)}(s) &= \int \frac{d^3q}{(2\pi)^3} \tilde{\Phi}_{ext}(\mathbf{q}) \sum_{k,k'} \langle U_k | e^{-iq_a x_a} | V_{k'} \rangle \hat{c}_k^\dagger b_{\tilde{k}'}^\dagger e^{-4s(\tilde{E}_k + \tilde{E}_{k'})^2} \\
\hat{\mathcal{V}}_{ext}^{(-)}(s) &= \left( \hat{\mathcal{V}}_{ext}^{(+)}(s) \right)^\dagger
\end{aligned} \tag{127}$$

First of all, this solution (123) fulfills the initial value condition  $\hat{H}^{(2,h)}(0) = \hat{H}^{(2)}(0) = \frac{1}{m_0 c^2} \left( \hat{\mathcal{V}}_{ext} + \hat{\mathcal{M}}_C + \mathcal{N} \left( \hat{\mathcal{V}}_C \right) \right)$ .

Now one has to look at the properties of the commutators (121). Starting with the inner double commutator  $\left[ \hat{N}_I, \left[ \hat{N}_I, \hat{H}^{(2,h)}(s) \right] \right] + \left[ \hat{N}_{II}, \left[ \hat{N}_{II}, \hat{H}^{(2,h)}(s) \right] \right]$  one finds, with the anti-commutator algebra of the fermions (see also appendix section G and the commutator relations (491) ff. in section H) [7]

$$\begin{aligned}
\left[ \hat{N}_I, \hat{\mathcal{U}}_C^{(0)} \right] &= \hat{0} \\
\left[ \hat{N}_I, \hat{\mathcal{U}}_C^{(\pm)}(s) \right] &= \pm 2 \hat{\mathcal{U}}_C^{(\pm)}(s) \\
\left[ \hat{N}_I, \hat{\mathcal{U}}_C^{(\pm,\pm)}(s) \right] &= \pm 4 \hat{\mathcal{U}}_C^{(\pm,\pm)}(s)
\end{aligned} \tag{128}$$

And, of course [7],

$$\left[ \hat{N}_{II}, \left[ \hat{N}_{II}, \hat{\mathcal{U}}(s) \right] \right] = \hat{0} \quad (129)$$

since fermions and photons share no commutation relations.

Hence, for the inner double commutator in (123) regarding the Coulomb interaction contribution  $\hat{\mathcal{U}}(s)$  there holds [7]

$$\begin{aligned} & \left[ \hat{N}_I, \left[ \hat{N}_I, \hat{\mathcal{U}}(s) \right] \right] + \left[ \hat{N}_{II}, \left[ \hat{N}_{II}, \hat{\mathcal{U}}(s) \right] \right] \\ &= \left[ \hat{N}_I, \left[ \hat{N}_I, \hat{\mathcal{U}}(s) \right] \right] \\ &= \left[ \hat{N}_I, \left[ \hat{N}_I, \left( \hat{\mathcal{U}}_C^{(0)} + \hat{\mathcal{U}}_C^{(+)}(s) + \hat{\mathcal{U}}_C^{(-)}(s) + \hat{\mathcal{U}}_C^{(+,+)}(s) + \hat{\mathcal{U}}_C^{(-,-)}(s) \right) \right] \right] \\ &= 4\hat{\mathcal{U}}_C^{(+)}(s) + 4\hat{\mathcal{U}}_C^{(-)}(s) + 16\hat{\mathcal{U}}_C^{(+,+)}(s) + 16\hat{\mathcal{U}}_C^{(-,-)}(s) \end{aligned} \quad (130)$$

Furthermore, for the interaction with the external potential  $\hat{\mathcal{V}}_{ext}(s)$  and for the self energy contribution  $\hat{\mathcal{M}}_C(s)$  there holds (see also appendix section G) [7]

$$\begin{aligned} & \left[ \hat{N}_I, \hat{\mathcal{V}}_{ext}^{(0)} \right] = \hat{0} \\ & \left[ \hat{N}_I, \hat{\mathcal{V}}_{ext}^{(\pm)}(s) \right] = \pm 2\hat{\mathcal{V}}_{ext}^{(\pm)}(s) \\ & \left[ \hat{N}_I, \hat{\mathcal{M}}_C^{(0)} \right] = \hat{0} \\ & \left[ \hat{N}_I, \hat{\mathcal{M}}_C^{(\pm)}(s) \right] = \pm 2\hat{\mathcal{M}}_C^{(\pm)}(s) \end{aligned} \quad (131)$$

and again, since fermions and photons share no commutation relations, there holds [7]

$$\left[ \hat{N}_{II}, \left[ \hat{N}_{II}, \left( \hat{\mathcal{V}}_{ext}(s) + \hat{\mathcal{M}}_C(s) \right) \right] \right] = \hat{0} \quad (132)$$

So altogether one finds for the contributions  $\hat{\mathcal{V}}_{ext}(s)$  and  $\hat{\mathcal{M}}_C(s)$  of the solution (123) for the inner double commutator [7]

$$\begin{aligned}
& \left[ \hat{N}_I, \left[ \hat{N}_I, \left( \hat{\mathcal{V}}_{ext}(s) + \hat{\mathcal{M}}_C(s) \right) \right] \right] + \left[ \hat{N}_{II}, \left[ \hat{N}_{II}, \left( \hat{\mathcal{V}}_{ext}(s) + \hat{\mathcal{M}}_C(s) \right) \right] \right] \\
&= \left[ \hat{N}_I, \left[ \hat{N}_I, \left( \hat{\mathcal{V}}_{ext}(s) + \hat{\mathcal{M}}_C(s) \right) \right] \right] \\
&= \left[ \hat{N}_I, \left[ \hat{N}_I, \left( \hat{\mathcal{V}}_{ext}^{(0)} + \hat{\mathcal{V}}_{ext}^{(+)}(s) + \hat{\mathcal{V}}_{ext}^{(-)}(s) + \hat{\mathcal{M}}_C^{(0)} + \hat{\mathcal{M}}_C^{(+)}(s) + \hat{\mathcal{M}}_C^{(-)}(s) \right) \right] \right] \\
&= 4\hat{\mathcal{V}}_{ext}^{(+)}(s) + 4\hat{\mathcal{V}}_{ext}^{(-)}(s) + 4\hat{\mathcal{M}}_C^{(+)}(s) + 4\hat{\mathcal{M}}_C^{(-)}(s)
\end{aligned} \tag{133}$$

The ansatz (123) for the homogeneous differential equation (121) can now be readily confirmed by differentiating it with respect to  $s$ . On the one hand there holds [7]

$$\begin{aligned}
& \frac{d}{ds} \left( \hat{\mathcal{V}}_{ext}(s) + \hat{\mathcal{M}}_C(s) \right) \\
&= \frac{d}{ds} \left( \hat{\mathcal{V}}_{ext}^{(+)}(s) + \hat{\mathcal{V}}_{ext}^{(-)}(s) + \hat{\mathcal{M}}_C^{(+)}(s) + \hat{\mathcal{M}}_C^{(-)}(s) \right) \\
&= - \left[ \hat{H}_D, \left[ \hat{H}_D, \left( 4\hat{\mathcal{V}}_{ext}^{(+)}(s) + 4\hat{\mathcal{V}}_{ext}^{(-)}(s) + 4\hat{\mathcal{M}}_C^{(+)}(s) + 4\hat{\mathcal{M}}_C^{(-)}(s) \right) \right] \right] \\
&= \left[ \left( \hat{H}_D + \hat{H}_{rad} \right), \left[ \left( \hat{H}_D + \hat{H}_{rad} \right), \left( 4\hat{\mathcal{V}}_{ext}^{(+)}(s) + 4\hat{\mathcal{V}}_{ext}^{(-)}(s) + 4\hat{\mathcal{M}}_C^{(+)}(s) + 4\hat{\mathcal{M}}_C^{(-)}(s) \right) \right] \right]
\end{aligned} \tag{134}$$

The differentiation of the terms in the ansatz (123) with respect to  $s$  produces a factor of 4 and a factor  $(\tilde{E}_k + \tilde{E}_{k'})^2$ . The latter can be represented as a double commutator with  $\hat{H}_D$ . This principle will be verified by the help of the example  $\hat{\mathcal{V}}_{ext}^{(+)}(s)$  which can be transferred to all other contributions [7]:

$$\begin{aligned}
& \left[ \hat{H}_D, \left[ \hat{H}_D, \hat{\mathcal{V}}_{ext}^{(+)}(s) \right] \right] \\
&= \left[ \sum_k \tilde{E}_k \left( c_k^\dagger c_k + b_k^\dagger b_k \right), \left[ \sum_k \tilde{E}_k \left( c_k^\dagger c_k + b_k^\dagger b_k \right), \hat{\mathcal{V}}_{ext}^{(+)}(s) \right] \right] \\
&= \left[ \sum_k \tilde{E}_k \left( c_k^\dagger c_k + b_k^\dagger b_k \right), \left[ \sum_k \tilde{E}_k \left( c_k^\dagger c_k + b_k^\dagger b_k \right), \int \frac{d^3q}{(2\pi)^3} \tilde{\Phi}_{ext}(\mathbf{q}) \sum_{k,k'} \langle U_k | e^{iq_a x_a} | V_{k'} \rangle \hat{c}_k^\dagger \hat{b}_{k'}^\dagger e^{-4s(\tilde{E}_k + \tilde{E}_{k'})^2} \right] \right] \\
&= \left[ \sum_k \tilde{E}_k \left( c_k^\dagger c_k + b_k^\dagger b_k \right), 2(\tilde{E}_k + \tilde{E}_{k'}) \int \frac{d^3q}{(2\pi)^3} \tilde{\Phi}_{ext}(\mathbf{q}) \sum_{k,k'} \langle U_k | e^{iq_a x_a} | V_{k'} \rangle \hat{c}_k^\dagger \hat{b}_{k'}^\dagger e^{-4s(\tilde{E}_k + \tilde{E}_{k'})^2} \right] \\
&= 4(\tilde{E}_k + \tilde{E}_{k'})^2 \int \frac{d^3q}{(2\pi)^3} \tilde{\Phi}_{ext}(\mathbf{q}) \sum_{k,k'} \langle U_k | e^{iq_a x_a} | V_{k'} \rangle \hat{c}_k^\dagger \hat{b}_{k'}^\dagger e^{-4s(\tilde{E}_k + \tilde{E}_{k'})^2} \\
&= 4(\tilde{E}_k + \tilde{E}_{k'})^2 \hat{\mathcal{V}}_{ext}^{(+)}(s)
\end{aligned} \tag{135}$$

and, of course [7]

$$\begin{aligned} \frac{d}{ds} \hat{\mathcal{V}}_{ext}^{(+)}(s) &= \frac{d}{ds} \left( \int \frac{d^3q}{(2\pi)^3} \tilde{\Phi}_{ext}(\mathbf{q}) \sum_{k,k'} \langle U_k | e^{iq_a x_a} | V_{k'} \rangle \hat{c}_k^\dagger \hat{b}_{k'}^\dagger e^{-4s(\tilde{E}_k + \tilde{E}_{k'})^2} \right) \\ &= -4(\tilde{E}_k + \tilde{E}_{k'})^2 \hat{\mathcal{V}}_{ext}^{(+)}(s) \end{aligned} \quad (136)$$

As one can see from this example, one can indeed represent the differentiation with respect to  $s$  by the double commutator (multiplied by a minus sign)! This holds true for each contribution and can be traced back to the fundamental anti-commutator relations for the fermions (19).

Furthermore, in (134), use has been made of  $[\hat{H}_{rad}, (\hat{\mathcal{V}}_{ext} + \hat{\mathcal{V}}_C)] = \hat{0}$  such that it is possible to insert  $\hat{H}_{rad}$  into the outer double commutator.

Now looking at the intermediate result (133) there holds furthermore [7]

$$\begin{aligned} &\frac{d}{ds} (\hat{\mathcal{V}}_{ext}(s) + \hat{\mathcal{M}}_C(s)) \\ &= - \left[ (\hat{H}_D + \hat{H}_{rad}), \left[ (\hat{H}_D + \hat{H}_{rad}), \left( [\hat{N}_I, [\hat{N}_I, (\hat{\mathcal{V}}_{ext}(s) + \hat{\mathcal{M}}_C(s))] \right) + [\hat{N}_{II}, [\hat{N}_{II}, (\hat{\mathcal{V}}_{ext}(s) + \hat{\mathcal{M}}_C(s))] \right] \right] \right] \\ &= - \left[ \hat{H}^{(0)}, [\hat{H}^{(0)}, \left( [\hat{N}_I, [\hat{N}_I, (\hat{\mathcal{V}}_{ext}(s) + \hat{\mathcal{M}}_C(s))] \right) + [\hat{N}_{II}, [\hat{N}_{II}, (\hat{\mathcal{V}}_{ext}(s) + \hat{\mathcal{M}}_C(s))] \right] \right] \right] \end{aligned} \quad (137)$$

For the contribution of the Coulomb interaction  $\mathcal{U}(s)$  there holds, in a very analogous way [7],

$$\begin{aligned} \frac{d}{ds} \mathcal{U}(s) &= \frac{d}{ds} (\hat{\mathcal{U}}_C^{(+)}(s) + \hat{\mathcal{U}}_C^{(-)}(s) + \hat{\mathcal{U}}_C^{(+,+)}(s) + \hat{\mathcal{U}}_C^{(-,-)}(s)) \\ &= - \left[ \hat{H}_D, \left[ \hat{H}_D, \left( 4\hat{\mathcal{U}}_C^{(+)}(s) + 4\hat{\mathcal{U}}_C^{(-)}(s) + 16\hat{\mathcal{U}}_C^{(+,+)}(s) + 16\hat{\mathcal{U}}_C^{(-,-)}(s) \right) \right] \right] \\ &= - \left[ \hat{H}_D, \left[ \hat{H}_D, [\hat{N}_I, [\hat{N}_I, \hat{\mathcal{U}}(s)]] \right] \right] \\ &= - \left[ \hat{H}^{(0)}, [\hat{H}^{(0)}, \left( [\hat{N}_I, [\hat{N}_I, \hat{\mathcal{U}}(s)]] + [\hat{N}_{II}, [\hat{N}_{II}, \hat{\mathcal{U}}(s)]] \right) \right] \right] \end{aligned} \quad (138)$$

Putting the results (137) and (138) together one can verify the ansatz (123) as [7]

$$\begin{aligned}
\frac{d}{ds} \hat{H}^{(2,h)}(s) &= \frac{1}{m_0 c^2} \left( \frac{d}{ds} \hat{\mathcal{V}}_{ext}(s) + \frac{d}{ds} \hat{\mathcal{M}}_C(s) + \frac{d}{ds} \mathcal{U}(s) \right) \\
&= - \left[ \hat{H}_D, \left[ \hat{H}_D, \left[ \hat{N}_I, \left[ \hat{N}_I, \frac{1}{m_0 c^2} \left( \hat{\mathcal{V}}_{ext}(s) + \hat{\mathcal{M}}_C(s) + \mathcal{U}(s) \right) \right] \right] \right] \right] \\
&= - \left[ \hat{H}_D, \left[ \hat{H}_D, \left[ \hat{N}_I, \left[ \hat{N}_I, \hat{H}^{(2,h)}(s) \right] \right] \right] \right] \\
&= - \left[ \hat{H}^{(0)}, \left[ \hat{H}^{(0)}, \left( \left[ \hat{N}_I, \left[ \hat{N}_I, \hat{H}^{(2,h)}(s) \right] \right) + \left[ \hat{N}_{II}, \left[ \hat{N}_{II}, \hat{H}^{(2,h)}(s) \right] \right] \right) \right] \right]
\end{aligned} \tag{139}$$

End of the proof.

Now one has to take a look at the limit  $s \rightarrow \infty$  for the solution (123).

All contributions with superscripts  $(\pm)$  and  $(\pm, \pm)$  vanish in the limit  $s \rightarrow \infty$  iff one first take the limit  $V \rightarrow \infty$  such that the mode indices  $k, k', K, K', q, q'$  can be converted to an integral (see discussion for the solution (119)) [7]:

$$\begin{aligned}
\lim_{s \rightarrow \infty} \lim_{V \rightarrow \infty} \hat{\mathcal{V}}_{ext}^{(\pm)}(s) &= \hat{0} \\
\lim_{s \rightarrow \infty} \lim_{V \rightarrow \infty} \hat{\mathcal{M}}_C^{(\pm)}(s) &= \hat{0} \\
\lim_{s \rightarrow \infty} \lim_{V \rightarrow \infty} \mathcal{U}_C^{(\pm)}(s) &= \hat{0} \\
\lim_{s \rightarrow \infty} \lim_{V \rightarrow \infty} \mathcal{U}^{(\pm, \pm)}(s) &= \hat{0}
\end{aligned} \tag{140}$$

Therefore, the solution of the homogeneous part of the second order differential equation is given by [7]

$$\lim_{s \rightarrow \infty} \lim_{V \rightarrow \infty} \hat{H}^{(2,h)}(s) = \frac{1}{m_0 c^2} \left( \hat{\mathcal{V}}_{ext}^{(0)} + \hat{\mathcal{M}}_C^{(0)} + \mathcal{U}_C^{(0)} \right) \tag{141}$$

with  $\hat{\mathcal{V}}_{ext}^{(0)}$  as given in (127),  $\hat{\mathcal{M}}_C^{(0)}$  as given in (126), and  $\mathcal{U}_C^{(0)}$  as given in (125).

In the appendix section G it is shown that the normal ordered QED Coulomb interaction part which conserves the particle number is given by [7]

$$\begin{aligned}
\mathcal{N}(\hat{\mathcal{Y}}_C^{(0)}) &= \left(\frac{q_e^2}{2\varepsilon_0}\right) \int \frac{d^3q}{(2\pi)^3} \frac{1}{|\mathbf{q}|^2} \sum_{K,k} \sum_{K',k'} \left( \begin{aligned} &\langle U_K | e^{-iq_a x_a} | U_k \rangle \langle U_{K'} | e^{iq_a x_a} | U_{k'} \rangle \hat{c}_K^\dagger \hat{c}_{K'}^\dagger \hat{c}_{k'} \hat{c}_k \\ &+ \langle V_k | e^{-iq_a x_a} | V_{K'} \rangle \langle V_{k'} | e^{iq_a x_a} | V_K \rangle \hat{b}_K^\dagger \hat{b}_{K'}^\dagger \hat{b}_{k'} \hat{b}_k \\ &- 2 \langle U_K | e^{-iq_a x_a} | U_k \rangle \langle V_{k'} | e^{iq_a x_a} | V_{K'} \rangle \hat{c}_K^\dagger \hat{c}_k \hat{b}_{K'}^\dagger \hat{b}_{k'} \\ &+ 2 \langle U_K | e^{-iq_a x_a} | V_k \rangle \langle V_{k'} | e^{iq_a x_a} | U_{K'} \rangle \hat{c}_K^\dagger \hat{b}_k \hat{b}_{k'}^\dagger \hat{c}_{K'} \end{aligned} \right) \\
&= \hat{\mathcal{U}}_C^{(0)}
\end{aligned} \tag{142}$$

There, also the deductions of the expressions (126) and (127) can be found.

### Inhomogeneous Differential Equation

The construction of the special solution  $\hat{H}^{(2,i)}(s)$  to the inhomogeneous differential equation (122) is long, but is based on the same approach as before: the multiple commutators of quadratic forms on one side of the differential equation can be represented by derivatives of exponential functions on the other side of the differential equation. Hence, for the sake of readability, the construction is placed in the appendix, see section H. Here, only the solution  $\lim_{s \rightarrow \infty} \hat{H}^{(2,i)}(s)$  is presented.

The result is given as follows [7]

$$\begin{aligned}
&m_0 c^2 \lim_{s \rightarrow \infty} \lim_{V \rightarrow \infty} \hat{H}^{(2,i)}(s) \\
&= \mathcal{C}_\perp \hat{1} + \hat{\mathcal{M}}_{\perp,e} + \hat{\mathcal{M}}_{\perp,p} + \hat{\mathcal{V}}_{\perp,ee} + \hat{\mathcal{V}}_{\perp,pp} + \hat{\mathcal{V}}_{\perp,ep} + \hat{\mathcal{H}}_{e,ph} + \hat{\mathcal{H}}_{p,ph} + \hat{\mathcal{Q}}_{\perp,ph}
\end{aligned} \tag{143}$$

All contributions are caused by the normal ordering rule in the particle number conserving parts of the solution  $\hat{H}^{(2,i)}(\infty)$ , see also section H of the appendix.

The first term  $\mathcal{C}_\perp \hat{1}$  is a constant spectral shift [7]

$$\begin{aligned}
\mathcal{C}_\perp \hat{1} &= -m_0 c^2 \left(\frac{q_e}{m_0 c}\right)^2 \frac{1}{V} \sum_{\mathbf{q}} \frac{\hbar}{2\varepsilon_0 \omega(\mathbf{q})} \sum_{b,b'} \left( \delta_{b,b'} - \frac{q_b q_{b'}}{|\mathbf{q}|^2} \right) \\
&\times \sum_{K,K'} \langle U_K | \alpha_b e^{-iq_a x_a} | V_{K'} \rangle \langle V_{K'} | \alpha_{b'} e^{iq_a x_a} | U_K \rangle \frac{(\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_q) + (\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_q)}{(\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_q)^2 + (\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_q)^2} \hat{1}
\end{aligned} \tag{144}$$

The second term  $\hat{\mathcal{M}}_{\perp}^{(0)} = \hat{\mathcal{M}}_{\perp}^{(e)} + \hat{\mathcal{M}}_{\perp}^{(p)}$  describes the renormalization of the fermion attributes mass  $m_0$  and g-factor due to the interaction with the high energy photons [7]:

$$\begin{aligned} \hat{\mathcal{M}}_{\perp}^{(e)} &= m_0 c^2 \sum_{k,K} \hat{c}_k^\dagger \hat{c}_K \left( \frac{q_e}{m_0 c} \right)^2 \frac{1}{V} \sum_{\mathbf{q}} \frac{\hbar}{2\varepsilon_0 \omega(\mathbf{q})} \sum_{b,b'} \left( \delta_{b,b'} - \frac{q_b q_{b'}}{|\mathbf{q}|^2} \right) \\ &\times \left\{ \begin{aligned} &\kappa_q \times \sum_{K'} \langle U_k | \alpha_b e^{i q_a x_a} | U_{K'} \rangle \langle U_{K'} | \alpha_{b'} e^{-i q_a x_a} | U_K \rangle \frac{(\tilde{E}_k - \tilde{E}_{K'} - \tilde{\omega}_q) - (\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_q)}{(\tilde{E}_k - \tilde{E}_{K'} - \tilde{\omega}_q)^2 + (\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_q)^2} \\ &+ \sum_{K'} \langle U_k | \alpha_b e^{-i q_a x_a} | V_{K'} \rangle \langle V_{K'} | \alpha_{b'} e^{+i q_a x_a} | U_K \rangle \frac{(\tilde{E}_k + \tilde{E}_{K'} + \tilde{\omega}_q) + (\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_q)}{(\tilde{E}_k + \tilde{E}_{K'} + \tilde{\omega}_q)^2 + (\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_q)^2} \end{aligned} \right. \end{aligned} \quad (145)$$

$$\begin{aligned} \hat{\mathcal{M}}_{\perp}^{(p)} &= m_0 c^2 \sum_{k',K'} \hat{b}_{k'}^\dagger \hat{b}_{K'} \left( \frac{q_e}{m_0 c} \right)^2 \frac{1}{V} \sum_{\mathbf{q}} \frac{\hbar}{2\varepsilon_0 \omega(\mathbf{q})} \sum_{b,b'} \left( \delta_{b,b'} - \frac{q_b q_{b'}}{|\mathbf{q}|^2} \right) \\ &\times \left\{ \begin{aligned} &\kappa_q \times \sum_K \langle V_K | \alpha_b e^{i q_a x_a} | V_{k'} \rangle \langle V_{k'} | \alpha_{b'} e^{-i q_a x_a} | V_K \rangle \frac{(\tilde{E}_{k'} - \tilde{E}_K - \tilde{\omega}_q) - (\tilde{E}_K - \tilde{E}_{k'} + \tilde{\omega}_q)}{(\tilde{E}_{k'} - \tilde{E}_K - \tilde{\omega}_q)^2 + (\tilde{E}_K - \tilde{E}_{k'} + \tilde{\omega}_q)^2} \\ &+ \sum_K \langle U_K | \alpha_b e^{-i q_a x_a} | V_{k'} \rangle \langle V_{k'} | \alpha_{b'} e^{+i q_a x_a} | U_K \rangle \frac{(\tilde{E}_K + \tilde{E}_{k'} + \tilde{\omega}_q) + (\tilde{E}_K + \tilde{E}_{k'} + \tilde{\omega}_q)}{(\tilde{E}_K + \tilde{E}_{k'} + \tilde{\omega}_q)^2 + (\tilde{E}_K + \tilde{E}_{k'} + \tilde{\omega}_q)^2} \end{aligned} \right. \end{aligned} \quad (146)$$

The appearance of  $\kappa_q$  in all effective terms indicates that the respective term originates from the interaction with high energy photons and/or high energy (anti-)matter modes.

The following three terms decompose into three normal ordered, effective two-particle interactions: an effective electron-electron interaction  $\hat{\mathcal{V}}_{\perp,ee}$ , an effective positron-positron interaction  $\hat{\mathcal{V}}_{\perp,pp}$ , and an effective electron-positron interaction  $\hat{\mathcal{V}}_{\perp,ep}$  [7]:

$$\begin{aligned} \hat{\mathcal{V}}_{\perp,ee} &= m_0 c^2 \left( \frac{q_e}{m_0 c} \right)^2 \sum_{k,k'} \sum_{K,K'} \hat{c}_k^\dagger \hat{c}_{K'}^\dagger \hat{c}_K \hat{c}_{k'} \\ &\times \left\{ \begin{aligned} &\frac{1}{V} \sum_{\mathbf{q}} \kappa_q \frac{\hbar}{2\varepsilon_0 \omega(\mathbf{q})} \sum_{b,b'} \left( \delta_{b,b'} - \frac{q_b q_{b'}}{|\mathbf{q}|^2} \right) \times \\ &\times \langle U_k | \alpha_b e^{i q_a x_a} | U_{k'} \rangle \langle U_{K'} | \alpha_{b'} e^{-i q_a x_a} | U_K \rangle \frac{(\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q) - (\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_q)}{(\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)^2 + (\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_q)^2} \end{aligned} \right. \end{aligned} \quad (147)$$

$$\begin{aligned}
\hat{\mathcal{V}}_{\perp,pp} &= m_0 c^2 \left( \frac{q_e}{m_0 c} \right)^2 \sum_{k,k'} \sum_{K,K'} \hat{b}_{\tilde{k}'}^\dagger \hat{b}_{\tilde{K}}^\dagger \hat{b}_{\tilde{K}'} \hat{b}_{\tilde{k}} \\
&\times \left\{ \frac{1}{V} \sum_{\mathbf{q}} \kappa_q \frac{\hbar}{2\varepsilon_0 \omega(\mathbf{q})} \sum_{b,b'} \left( \delta_{b,b'} - \frac{q_b q_{b'}}{|\mathbf{q}|^2} \right) \times \right. \\
&\times \langle V_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{-iq_a x_a} | V_K \rangle \frac{(\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q) - (\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_q)}{(\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q)^2 + (\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_q)^2} \\
&\left. \right\} \quad (148)
\end{aligned}$$

$$\begin{aligned}
\hat{\mathcal{V}}_{\perp,ep} &= m_0 c^2 \left( \frac{q_e}{m_0 c} \right)^2 \sum_{k,k'} \sum_{K,K'} \frac{1}{V} \sum_{\mathbf{q}} \frac{\hbar}{2\varepsilon_0 \omega(\mathbf{q})} \sum_{b,b'} \left( \delta_{b,b'} - \frac{q_b q_{b'}}{|\mathbf{q}|^2} \right) \times \\
&\times \left\{ +\kappa_q \langle U_k | \alpha_b e^{iq_a x_a} | U_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{-iq_a x_a} | V_K \rangle \hat{c}_k^\dagger \hat{c}_{k'} \hat{b}_{\tilde{K}}^\dagger \hat{b}_{\tilde{K}'} \times \right. \\
&\times \left( \frac{(\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_q) - (\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)}{(\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)^2 + (\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_q)^2} + \frac{(\tilde{E}_k - \tilde{E}_{k'} + \tilde{\omega}_q) - (\tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_q)}{(\tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_q)^2 + (\tilde{E}_k - \tilde{E}_{k'} + \tilde{\omega}_q)^2} \right) \\
&\times \left\{ +\langle U_k | \alpha_b e^{-iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{iq_a x_a} | U_K \rangle \hat{c}_k^\dagger \hat{c}_K \hat{b}_{\tilde{k}'}^\dagger \hat{b}_{\tilde{K}'} \times \right. \\
&\times \left( \frac{(\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q) + (\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_q)}{(\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q)^2 + (\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_q)^2} - \frac{(\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q) + (\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_q)}{(\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q)^2 + (\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_q)^2} \right) \\
&\left. \right\} \quad (149)
\end{aligned}$$

The term  $\hat{\mathcal{V}}_{\perp,ep}$  describes positronium. It would be very interesting to retranslate it to first quantization and check whether it coincides with the term found for example by Landau et. al [37]. A similar term, indeed describing the positronium system, is derived and evaluated in [8].



The terms  $\hat{\mathcal{H}}_{e,ph} + \hat{\mathcal{H}}_{p,ph}$  describe interactions between Dirac fermions and photons. Their explicit form is given as [7]

$$\begin{aligned}
\hat{\mathcal{H}}_{e,ph} = & +m_0c^2 \left( \frac{q_0}{m_0c} \right)^2 \sum_{k,k'} \sum_{K,K'} \lim_{V \rightarrow \infty} \frac{1}{V} \sum_{q,q'} \sum_{b,b'} \mathcal{A}_b(q) \mathcal{A}_{b'}(q') \times \\
& \left\{ \begin{aligned}
& \kappa_q \kappa_{q'} \langle U_k | \alpha_b e^{iq_a x_a} | U_{k'} \rangle \langle U_{K'} | \alpha_{b'} e^{-iq'_a x_a} | U_K \rangle \times \\
& \times \frac{(\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q) - (\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})}{(\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)^2 + (\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2} \left( \delta_{k',K'} \hat{c}_k^\dagger \hat{c}_K - \delta_{k,K} \hat{c}_{K'}^\dagger \hat{c}_{k'} \right) \hat{a}_{q'}^\dagger \hat{a}_q \\
& + ((1 - \kappa_q)(1 - \kappa_{q'}) + \kappa_q \kappa_{q'}) \langle U_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{-iq'_a x_a} | U_K \rangle \times \\
& \times \frac{(\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q) + (\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'})}{(\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q)^2 + (\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'})^2} \delta_{k',K'} \hat{c}_k^\dagger \hat{c}_K \hat{a}_{q'}^\dagger \hat{a}_q \\
& + ((1 - \kappa_q)(1 - \kappa_{q'}) + \kappa_q \kappa_{q'}) \langle U_k | \alpha_b e^{-iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{+iq'_a x_a} | U_K \rangle \times \\
& \times \frac{(\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q) + (\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'})}{(\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q)^2 + (\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'})^2} \delta_{K',k'} \hat{c}_k^\dagger \hat{c}_K \hat{a}_{q'}^\dagger \hat{a}_q \\
& + (1 - \kappa_q)(1 - \kappa_{q'}) \langle U_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{+iq'_a x_a} | U_K \rangle \times \\
& \times \frac{(\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'}) + (\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q)}{(\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'})^2 + (\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q)^2} \delta_{K',k'} \hat{c}_k^\dagger \hat{c}_K \hat{a}_{q'}^\dagger \hat{a}_q \\
& + (1 - \kappa_q)(1 - \kappa_{q'}) \langle V_{K'} | \alpha_{b'} e^{-iq'_a x_a} | U_K \rangle \langle U_k | \alpha_b e^{-iq_a x_a} | V_{k'} \rangle \times \\
& \times \frac{(\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'}) + (\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q)}{(\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'})^2 + (\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q)^2} \delta_{K',k'} \hat{c}_k^\dagger \hat{c}_K \hat{a}_{q'}^\dagger \hat{a}_q
\end{aligned} \right. \quad (150)
\end{aligned}$$



Finally, the term that seems like renormalizing the dispersion relation of the photons is given by [7]

$$\begin{aligned}
\hat{Q}_{\perp,ph} = & -m_0 c^2 \left( \frac{q_e}{m_0 c} \right)^2 \frac{1}{V} \sum_{q,q'} \sum_{b,b'} \mathcal{A}_b(q) \mathcal{A}_{b'}(q') \times \\
& \left( \kappa_q \kappa_{q'} \hat{a}_q^\dagger \hat{a}_q \sum_{K,K'} \left( \begin{aligned} & \langle U_K | \alpha_b e^{iq_a x_a} | V_{K'} \rangle \langle V_{K'} | \alpha_{b'} e^{-iq'_a x_a} | U_K \rangle \times \\ & \times \frac{(\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_q) + (\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'})}{(\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_q)^2 + (\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'})^2} \\ & + \langle V_{K'} | \alpha_b e^{+iq_a x_a} | U_K \rangle \langle U_K | \alpha_{b'} e^{-iq'_a x_a} | V_{K'} \rangle \times \\ & \times \frac{(\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'}) + (\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_q)}{(\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'})^2 + (\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_q)^2} \end{aligned} \right) \right. \\
& \times \left. \begin{aligned} & + (1 - \kappa_q) (1 - \kappa_{q'}) \hat{a}_{q'} \hat{a}_q \sum_{K,K'} \langle U_K | \alpha_b e^{iq_a x_a} | V_{K'} \rangle \langle V_{K'} | \alpha_{b'} e^{+iq'_a x_a} | U_K \rangle \times \\ & \times \frac{(\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'}) + (\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_q)}{(\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'})^2 + (\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_q)^2} \\ & + (1 - \kappa_q) (1 - \kappa_{q'}) \hat{a}_{q'}^\dagger \hat{a}_q^\dagger \sum_{K,K'} \langle V_{K'} | \alpha_{b'} e^{-iq'_a x_a} | U_K \rangle \langle U_K | \alpha_b e^{-iq_a x_a} | V_{K'} \rangle \times \\ & \times \frac{(\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'}) + (\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_q)}{(\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'})^2 + (\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_q)^2} \end{aligned} \right) \tag{152}
\end{aligned}$$

If true, this term would be very interesting, because it points out that for very high energies  $\hbar q \gg \hbar q_B$  the dispersion relation of the photons is altered which can be seen from the operator valued wave equation derived in section J of the appendix. It adds to the vacuum velocity of light  $c$  which can be seen from the homogeneous wave equation (656). However, the dealing with this term is a project that stands for its own. Dirac counted the modification of the photon's properties among the last fundamental problems of QED [46], but requiring to treat all constituents of QED on equal footing, it does not seem unreasonable that there arises a term which describes the modification of the photons properties. This would then mean that the photons being part of the QED soup have different properties than the photons acting in our nonrelativistic world, just as it is the case for the fermions.

It has to be emphasized that in the solution  $\hat{H}^{(2,i)}(\infty)$  all denominators containing the energies of the particles are manifestly positive (due to the square). Hence, it comprises no further singularities. This

shows that applying the flow equation as a tool for unitarily transforming Hamiltonians once again leads to a non-singular result like in the case of Peter Lenz and Franz Wegner who also achieved a manifestly positive denominator by applying the flow equation to BCS Hamiltonian [47].

## 4.2 Interim Summary

The flow equation for generating particle number conservation yields a field theory Hamiltonian  $\mathcal{H}_U$  which is unitarily equivalent to the order  $\alpha_{FS}^2$  to the Hamiltonian of QED (8) by the help of the generator  $\hat{\eta}^{(LM)}(s)$ .

The Hamiltonian  $\mathcal{H}_U$  assumes the following guise [7, 8]

$$\begin{aligned}
\mathcal{H}_U &= m_0 c^2 \lim_{s \rightarrow \infty} \lim_{V \rightarrow \infty} \left( \hat{H}^{(0)} + \hat{H}^{(1)}(s) + \hat{H}^{(2,h)}(s) + \hat{H}^{(2,i)}(s) + \dots \right) \\
&= \begin{cases} m_0 c^2 \left( \hat{H}_D + \hat{H}_{rad} \right) + m_0 c^2 \hat{H}_{<}^{(1,0)} \\ + \hat{\mathcal{V}}_{ext}^{(0)} + \hat{\mathcal{M}}_C^{(0)} + \mathcal{U}_C^{(0)} \\ + \hat{\mathcal{M}}_{\perp,e} + \hat{\mathcal{M}}_{\perp,p} + \hat{\mathcal{V}}_{\perp,ee} + \hat{\mathcal{V}}_{\perp,pp} + \hat{\mathcal{V}}_{\perp,ep} \\ + \hat{\mathcal{H}}_{e,ph} + \hat{\mathcal{H}}_{p,ph} + \hat{\mathcal{Q}}_{\perp,ph} + \mathcal{C}_{\perp} \hat{1} \end{cases} \\
&= \begin{cases} \hat{\mathcal{H}}_D + \hat{\mathcal{M}}_C^{(e)} + \hat{\mathcal{M}}_C^{(p)} + \hat{\mathcal{M}}_{\perp}^{(e)} + \hat{\mathcal{M}}_{\perp}^{(p)} \\ + \hat{\mathcal{H}}_{\perp}^{(low,0)} \\ + \mathcal{U}_C^{(0)} + \hat{\mathcal{V}}_{ext}^{(0)} \\ + \mathcal{C}_{\perp} \hat{1} + \hat{\mathcal{V}}_{\perp,ee} + \hat{\mathcal{V}}_{\perp,pp} + \hat{\mathcal{V}}_{\perp,ep} \\ + \hat{\mathcal{H}}_{p,ph} + \hat{\mathcal{H}}_{e,ph} + \hat{\mathcal{Q}}_{\perp,ph} \end{cases} \tag{153}
\end{aligned}$$

Here the zeroth order solution (99), the first order solution (119) (the berry colored term) and the second order solution (143) (the orange colored term of the homogeneous solution and the emerald colored term of the inhomogeneous solution) have been inserted.

$\mathcal{H}_U$  has the utmost important property of conserving the particle number, hence [7]

$$\begin{aligned} \left[ \mathcal{H}_U, \hat{N}_I \right] &= \hat{0} \\ \left[ \mathcal{H}_U, \hat{N}_{II} \right] &= \hat{0} \end{aligned} \tag{154}$$

This Hamiltonian  $\mathcal{H}_U$  is given in the Dirac representation, which means that it is expressed by the Dirac field operators (14). Therefore it is a many-body Hamiltonian of superposed matter and antimatter modes interacting with low-energy photons. It can now be transformed by the help of the Eriksen transformation  $\mathbb{T}$  to the Newton-Wigner representation in which it decomposes into subspaces for electrons and positrons *separately*. This is done in the second part of the solution to the nonrelativistic limit problem of QED.

As will be shown, the parts  $\hat{\mathcal{M}}_C^{(e)} + \hat{\mathcal{M}}_C^{(p)} + \hat{\mathcal{M}}_{\perp}^{(e)} + \hat{\mathcal{M}}_{\perp}^{(p)}$  of the solution generated by the flow equation aiming at particle number conservation are those that renormalize the bare mass  $m_0$  of the fermions and their  $g$ -factor. The orange ones with the subscript  $C$  are attributable to the (longitudinal) high-energy QED Coulomb interaction between the matter fields, whereas the emerald ones with the subscript  $\perp$  are attributable to the (transversal) interactions of the (anti-)matter fields with the high energy photons. These terms represent integrals over the wavenumber  $q$  of the photons. For these divergent integrals one has to choose a physical cut-off which can be done by truncating not only the energy of the photons, but also the kinetic energy of the fermions.

By retranslating these terms to first quantization it becomes obvious that they add to the terms of the effective single-particle Schrödinger-Pauli Hamiltonian. In that way one gets a *consistent* renormalization of the bare mass  $m_0$  the anomalous magnetic moment.

Hence, in the following section the Eriksen transformation  $\mathbb{T}$  is introduced which allows to express the single-particle Dirac Hamiltonian in the Newton-Wigner representation, and in which matter and antimatter degrees of freedom are described separately. Thereby the Newton-Wigner representation of the single-particle Dirac Hamiltonian is discussed.

## 5 The Eriksen Transformation and the Newton–Wigner Representation of the Single–Particle Dirac Hamiltonian

The Eriksen transformation  $\mathbb{T}$  [20, 21, 22, 23, 24, 25, 11, 26, 27, 28, 29] makes it possible to transform the single–particle Dirac Hamiltonian  $\hat{\mathbf{H}}^{(D)}$  to the Newton–Wigner representation  $\hat{\mathbf{H}}^{(NW)}$ . For a recent discussion of the Eriksen transformation see [10]. It is in this representation where the Hamiltonian, as well as other observables like the velocity and the angular momentum, resemble their classical expressions the most [9].

The Eriksen transformation  $\mathbb{T}$  is given by [10, 7]

$$\mathbb{T} = \sqrt{\frac{1}{2} \left( \mathbf{1}_{4 \times 4} + \frac{m_e c^2}{\mathbf{E}(\infty)} \right)} + \beta D_A \sqrt{\frac{1}{2} \left( \mathbf{1}_{4 \times 4} - \frac{m_e c^2}{\mathbf{E}(\infty)} \right)} \quad (155)$$

or [10, 7]

$$\mathbb{T}^\dagger = \sqrt{\frac{1}{2} \left( \mathbf{1}_{4 \times 4} + \frac{m_e c^2}{\mathbf{E}(\infty)} \right)} - \beta D_A \sqrt{\frac{1}{2} \left( \mathbf{1}_{4 \times 4} - \frac{m_e c^2}{\mathbf{E}(\infty)} \right)} \quad (156)$$

where [10, 7]

$$\mathbf{E}(\infty) = m_0 c^2 \sqrt{\mathbf{1}_{4 \times 4} + \frac{2}{m_0 c^2} \mathbf{H}_{4 \times 4}^{(P,0)}} \quad (157)$$

and [10, 7]

$$\begin{aligned} \mathbf{H}_{4 \times 4}^{(P,0)} &= \frac{\Pi_b \Pi_b}{2m_0} \mathbf{1}_{4 \times 4} - \frac{q_e \hbar}{2m_0} B_b^{(ext)} \sigma_b \\ \sigma_b &= \sigma_x \otimes \sigma_b^{(P)} \end{aligned} \quad (158)$$

This transformation is defined by two properties: first it enables to blockdiagonalize the single particle Dirac Hamilton  $\hat{\mathbf{H}}^{(D)}$ , and second, it decouples the matter and antimatter degrees of freedom in the amplitudes  $U_{\mu'}^{(D)}(\mathbf{r}, k)$  and  $V_{\mu'}^{(D)}(\mathbf{r}, k)$ . It is important to emphasize that both requirements must be met, it is not sufficient to only

blockdiagonalize the Dirac Hamiltonian. The latter required property of the Eriksen transformation is also called *energy-separating*.

In the appendix B it is shown how the Eriksen transformation  $\mathsf{T}$  can be derived by a Brockett type of flow equation which can indeed be solved exactly.

The Newton–Wigner representation of the Dirac Hamiltonian follows as [10, 8]

$$\begin{aligned}
\mathsf{H}^{(NW)} &= \mathsf{T} \circ \mathsf{H}^{(D)} \circ \mathsf{T}^\dagger \\
&= \beta \circ \sqrt{\mathsf{H}^{(D)} \circ \mathsf{H}^{(D)}} \\
&= \beta \circ \mathsf{E}(\infty) \\
&= m_0 c^2 \beta \circ \sqrt{\mathbf{1}_{4 \times 4} + \frac{2}{m_0 c^2} \mathsf{H}_{4 \times 4}^{(P,0)}}
\end{aligned} \tag{159}$$

Please recognize the operator  $\beta = \sigma_z^{(P)} \otimes \mathbf{1}_{2 \times 2}$ ! The Newton–Wigner Hamiltonian is, indeed, blockdiagonal.

Furthermore [10, 7],

$$\mathsf{H}_{4 \times 4}^{(P,0)} = \sqrt{\mathbf{1}_{2 \times 2} \otimes \mathsf{H}_{2 \times 2}^{(SP,0)}} \tag{160}$$

is the relativistic Schrödinger–Pauli Hamiltonian being related to the nonrelativistic Schrödinger–Pauli Hamiltonian  $\mathsf{H}_{2 \times 2}^{(SP,0)}$  given by [10, 7]

$$\mathsf{H}_{2 \times 2}^{(SP,0)} = \frac{\Pi_b \Pi_b}{2m_0} \mathbf{1}_{2 \times 2} - \frac{q_e \hbar}{2m_0} B_b^{(ext)} \sigma_b^{(P)} \tag{161}$$

With that one finds [10, 7]

$$\begin{aligned}
\mathsf{H}^{(NW)} &= m_0 c^2 \left( \sigma_z^{(P)} \otimes \mathbf{1}_{2 \times 2} \right) \circ \left( \mathbf{1}_{2 \times 2} \otimes \sqrt{\mathbf{1}_{2 \times 2} + \frac{2}{m_0 c^2} \mathsf{H}_{2 \times 2}^{(SP,0)}} \right) \\
&= m_0 c^2 \sigma_z^{(P)} \otimes \sqrt{\mathbf{1}_{2 \times 2} + \frac{2}{m_0 c^2} \mathsf{H}_{2 \times 2}^{(SP,0)}}
\end{aligned} \tag{162}$$

The property of being energy separating can formally be expressed by [10]

$$\begin{aligned}
\mathbf{H}^{(NW)} &= \beta \sqrt{\mathbf{H}^{(NW)}\mathbf{H}^{(NW)}} \\
(\mathbf{0}_{4 \times 1})_\mu &= \left( \mathbf{H}^{(NW)} - \beta \sqrt{\mathbf{H}^{(NW)}\mathbf{H}^{(NW)}} \right)_{\mu, \mu'} U_{\mu'}^{(NW)}(\mathbf{r}, k) \\
&= E_k (\hat{\mathbf{1}}_{4 \times 4} - \beta)_{\mu, \mu'} U_{\mu'}^{(NW)}(\mathbf{r}, k) \\
(\mathbf{0}_{4 \times 1})_\mu &= \left( \mathbf{H}^{(NW)} - \beta \sqrt{\mathbf{H}^{(NW)}\mathbf{H}^{(NW)}} \right)_{\mu, \mu'} V_{\mu'}^{(NW)}(\mathbf{r}, \tilde{k}) \\
&= (-E_{\tilde{k}}) (\hat{\mathbf{1}}_{4 \times 4} + \beta)_{\mu, \mu'} V_{\mu'}^{(NW)}(\mathbf{r}, \tilde{k})
\end{aligned} \tag{163}$$

These relations are only fulfilled iff the eigenfunctions  $U_{\mu'}^{(NW)}(\mathbf{r}, k)$  are of the form [10, 8]

$$\begin{pmatrix} U_1(\mathbf{r}, k) \\ U_2(\mathbf{r}, k) \\ 0 \\ 0 \end{pmatrix}_{\mu'} \tag{164}$$

and  $V_{\mu'}^{(NW)}(\mathbf{r}, \tilde{k})$  are of the form [10, 8]

$$\begin{pmatrix} 0 \\ 0 \\ V_3(\mathbf{r}, \tilde{k}) \\ V_4(\mathbf{r}, \tilde{k}) \end{pmatrix}_{\mu'} \tag{165}$$

because

$$(\hat{\mathbf{1}}_{4 \times 4} - \beta) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -2 & 0 \\ 0 & 0 & 0 & -2 \end{pmatrix}, \quad (\hat{\mathbf{1}}_{4 \times 4} + \beta) = \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{166}$$

The solution to a flow equation which blockdiagonalizes the single-particle Dirac Hamiltonian does not automatically fulfill the condition (163). In case of an additional external electric field the derivation of the Newton–Wigner Hamiltonian is much more intricate because  $\mathbf{H}^{(NW)} \circ \mathbf{H}^{(NW)} \neq \mathbf{H}^{(D)} \circ \mathbf{H}^{(D)}$ . For a recent in-depth discussion see



[10]. However, since here, only a static magnetic induction field is considered, there holds  $\mathbf{H}^{(NW)} \circ \mathbf{H}^{(NW)} = \mathbf{H}^{(D)} \circ \mathbf{H}^{(D)}$ , and therefore the energy separation condition (163) is valid.

Now since indeed

$$\left[ \beta, \mathbf{H}_{4 \times 4}^{(P,0)} \right] = \mathbf{0}_{4 \times 4} \quad (167)$$

the Eriksen transformation  $\mathbb{T}$  transforms eigenfunctions  $U_\mu(\mathbf{r}, k)$  of the Dirac Hamiltonian  $\hat{H}^{(D)}$  belonging to positive energy eigenvalues  $E_k > 0$  to the eigenfunctions  $U_\mu^{(NW)}(\mathbf{r}, k)$  of the bare relativistic Pauli Hamiltonian  $\mathbf{H}_{4 \times 4}^{(P,0)}$ , see equation (160), which are *simultanouesly* the eigenfunctions of the Dirac  $\beta$  matrix belonging to the eigenvalue +1!

Therefore [10, 8]

$$\begin{aligned} U_{\mu'}(\mathbf{r}, k) &= (\mathbb{T}^\dagger \circ \mathbb{T}) U_{\mu'}(\mathbf{r}, k) \\ &= \mathbb{T}^\dagger U_{\mu'}^{(NW)}(\mathbf{r}, k) \\ \beta U_{\mu'}^{(NW)}(\mathbf{r}, k) &= +U_{\mu'}^{(NW)}(\mathbf{r}, k) \end{aligned} \quad (168)$$

In addition, the eigenfunctions  $V_\mu(\mathbf{r}, k)$  of the Dirac Hamiltonian  $\hat{H}^{(D)}$  belonging to the negative energy eigenvalue  $E_k < 0$  are transformed to the eigenfunctions  $V_\mu^{(NW)}(\mathbf{r}, k)$  of the bare relativistic Pauli Hamiltonian  $\mathbf{H}_{4 \times 4}^{(P,0)}$  which are *simultanouesly* the eigenfunctions of the Dirac  $\beta$  matrix belonging to the eigenvalue  $-1$  [10, 8]:

$$\begin{aligned} V_{\mu'}(\mathbf{r}, \tilde{k}) &= (\mathbb{T}^\dagger \circ \mathbb{T}) V_{\mu'}(\mathbf{r}, \tilde{k}) \\ &= \mathbb{T}^\dagger V_{\mu'}^{(NW)}(\mathbf{r}, \tilde{k}) \\ \beta V_{\mu'}^{(NW)}(\mathbf{r}, \tilde{k}) &= -V_{\mu'}^{(NW)}(\mathbf{r}, \tilde{k}) \end{aligned} \quad (169)$$

The related eigenvalue problem assumes the following guise [10]:

$$\begin{aligned} \sum_{\mu'} \left( \mathbf{H}^{(NW)} \right)_{\mu, \mu'} U_{\mu'}^{(NW)}(\mathbf{r}, k) &= E_k U_\mu^{(NW)}(\mathbf{r}, k) \\ \sum_{\mu'} \left( \mathbf{H}^{(NW)} \right)_{\mu, \mu'} V_{\mu'}^{(NW)}(\mathbf{r}, k) &= -E_k V_\mu^{(NW)}(\mathbf{r}, k) \end{aligned} \quad (170)$$

Since(!)  $\mathbf{H}_{4 \times 4}^{(P,0)} \equiv \mathbf{1}_{2 \times 2} \otimes \mathbf{H}_{2 \times 2}^{(SP,0)}$  the eigenvalues and eigenfunctions of  $\mathbf{H}^{(NW)}$  can now be related to the well-known eigenvalues and eigenfunctions of the Schrödinger–Pauli Hamiltonian  $\mathbf{H}_{2 \times 2}^{(SP,0)}$ ! Therefore, the Newton–Wigner eigenfunctions  $U_{\mu}^{(NW)}(\mathbf{r}, k)$  and  $V_{\mu}^{(NW)}(\mathbf{r}, k)$  are four–spinors with two empty arguments, while the other two arguments can be related to the eigenfunctions of the Schrödinger–Pauli Hamiltonian  $\mathbf{H}_{2 \times 2}^{(SP,0)}$ !

For the bare nonrelativistic Schrödinger–Pauli Hamiltonian the following eigenvalue problem is valid [10]:

$$\sum_{\sigma'} \left( \mathbf{H}_{2 \times 2}^{(SP,0)} \right)_{\sigma, \sigma'} u_{\sigma'}^{(SP)}(\mathbf{r}, k) = E_k^{(SP)} u_{\sigma}^{(SP)}(\mathbf{r}, k) \quad (171)$$

$$\sigma, \sigma' \in \{+, -\}$$

$$k = (k_z, n, \zeta)$$

The eigenfunctions  $u_{\sigma}^{(SP)}(\mathbf{r}, k)$  build a complete orthonormal basis of the hermitean operator  $\mathbf{H}_{2 \times 2}^{(SP,0)}$  such that [7]

$$\int d^3r \sum_{\sigma \in \{+, -\}} u_{\sigma}^{\star(SP)}(\mathbf{r}, k) u_{\sigma}^{(SP)}(\mathbf{r}, k') = \delta_{k, k'} \quad (172)$$

$$\sum_k u_{\sigma}^{(SP)}(\mathbf{r}, k) u_{\sigma'}^{\star(SP)}(\mathbf{r}', k) = \delta_{\sigma, \sigma'} \delta^{(3)}(\mathbf{r} - \mathbf{r}')$$

Hence, the Newton–Wigner eigenfunctions of the relativistic Pauli Hamiltonian have the following structure [10]:

$$U_{\mu}^{(NW)}(\mathbf{r}, k) = \begin{pmatrix} u_{+}^{(SP)}(\mathbf{r}, k) \\ u_{-}^{(SP)}(\mathbf{r}, k) \\ 0 \\ 0 \end{pmatrix}_{\mu} \quad (173)$$

and [10]

$$V_{\mu}^{(NW)}(\mathbf{r}, k) = \begin{pmatrix} 0 \\ 0 \\ u_{+}^{(SP)}(\mathbf{r}, k) \\ u_{-}^{(SP)}(\mathbf{r}, k) \end{pmatrix}_{\mu} \quad (174)$$

and the relativistic energy is given by  $E_k = m_0 c^2 \sqrt{\mathbf{1}_{2 \times 2} + \frac{2}{m_0 c^2} E_k^{(SP)}}$ .

From  $(\beta)_{\mu, \mu'} U_{\mu'}^{(NW)}(\mathbf{r}, k) = +U_{\mu'}^{(NW)}(\mathbf{r}, k)$  and  $(\beta)_{\mu, \mu'} V_{\mu'}^{(NW)}(\mathbf{r}, k) = -V_{\mu'}^{(NW)}(\mathbf{r}, k)$  one readily confirms [7]

$$\begin{aligned}
\sum_{\mu'} (\mathbf{H}^{(NW)})_{\mu, \mu'} U_{\mu'}^{(NW)}(\mathbf{r}, k) &= \sum_{\mu'} m_0 c^2 \left( \sigma_z^{(P)} \otimes \sqrt{\mathbf{1}_{2 \times 2} + \frac{2}{m_0 c^2} \mathbf{H}_{2 \times 2}^{(SP, 0)}} \right)_{\mu, \mu'} \begin{pmatrix} u_+^{(SP)}(\mathbf{r}, k) \\ u_-^{(SP)}(\mathbf{r}, k) \\ 0 \\ 0 \end{pmatrix}_{\mu'} \\
&= m_0 c^2 \begin{pmatrix} \sum_{\sigma'} \left( \sqrt{\mathbf{1}_{2 \times 2} + \frac{2}{m_0 c^2} \mathbf{H}_{2 \times 2}^{(SP, 0)}} \right)_{+, \sigma'} u_{\sigma'}^{(SP)}(\mathbf{r}, k) \\ \sum_{\sigma'} \left( \sqrt{\mathbf{1}_{2 \times 2} + \frac{2}{m_0 c^2} \mathbf{H}_{2 \times 2}^{(SP, 0)}} \right)_{-, \sigma'} u_{\sigma'}^{(SP)}(\mathbf{r}, k) \\ 0 \\ 0 \end{pmatrix}_{\mu} \\
&= m_0 c^2 \sqrt{\mathbf{1}_{2 \times 2} + \frac{2}{m_0 c^2} E_k^{(SP)}} \begin{pmatrix} u_+^{(SP)}(\mathbf{r}, k) \\ u_-^{(SP)}(\mathbf{r}, k) \\ 0 \\ 0 \end{pmatrix}_{\mu} \\
&= E_k U_{\mu}^{(NW)}(\mathbf{r}, k)
\end{aligned} \tag{175}$$

and [7]

$$\begin{aligned}
\sum_{\mu'} (\mathbf{H}^{(NW)})_{\mu, \mu'} V_{\mu'}^{(NW)}(\mathbf{r}, k) &= \sum_{\mu'} m_0 c^2 \left( \sigma_z^{(P)} \otimes \sqrt{\mathbf{1}_{2 \times 2} + \frac{2}{m_0 c^2} \mathbf{H}_{2 \times 2}^{(SP, 0)}} \right)_{\mu, \mu'} \begin{pmatrix} 0 \\ 0 \\ u_+^{(SP)}(\mathbf{r}, k) \\ u_-^{(SP)}(\mathbf{r}, k) \end{pmatrix}_{\mu'} \\
&= m_0 c^2 \begin{pmatrix} 0 \\ 0 \\ -\sum_{\sigma'} \left( \sqrt{\mathbf{1}_{2 \times 2} + \frac{2}{m_0 c^2} \mathbf{H}_{2 \times 2}^{(SP, 0)}} \right)_{+, \sigma'} u_{\sigma'}^{(SP)}(\mathbf{r}, k) \\ -\sum_{\sigma'} \left( \sqrt{\mathbf{1}_{2 \times 2} + \frac{2}{m_0 c^2} \mathbf{H}_{2 \times 2}^{(SP, 0)}} \right)_{-, \sigma'} u_{\sigma'}^{(SP)}(\mathbf{r}, k) \end{pmatrix}_{\mu} \\
&= -m_0 c^2 \sqrt{\mathbf{1}_{2 \times 2} + \frac{2}{m_0 c^2} E_k^{(SP)}} \begin{pmatrix} 0 \\ 0 \\ u_+^{(SP)}(\mathbf{r}, k) \\ u_-^{(SP)}(\mathbf{r}, k) \end{pmatrix}_{\mu} \\
&= -E_k V_{\mu}^{(NW)}(\mathbf{r}, k)
\end{aligned} \tag{176}$$

Hence, the relations [10]

$$\begin{aligned}
\sum_{\mu'} (\mathbb{T})_{\mu,\mu'} U_{\mu'}(\mathbf{r}, k) &\equiv U_{\mu}^{(NW)}(\mathbf{r}, k) \equiv 0 \text{ for } \mu = 3, 4 \\
\sum_{\mu'} (\mathbb{T})_{\mu,\mu'} V_{\mu'}(\mathbf{r}, k) &\equiv V_{\mu}^{(NW)}(\mathbf{r}, k) \equiv 0 \text{ for } \mu = 1, 2
\end{aligned} \tag{177}$$

between the Dirac amplitudes  $U_{\mu'}(\mathbf{r}, k)$  and  $V_{\mu'}(\mathbf{r}, k)$ , and the Newton–Wigner amplitudes  $U_{\mu}^{(NW)}(\mathbf{r}, k)$  and  $V_{\mu}^{(NW)}(\mathbf{r}, k)$  are valid.

With the transformation  $\mathbb{T}$  there is a unitary transformation which has two important properties: it blockdiagonalizes the Dirac Hamiltonian according to (159), and it separates the modes of positive energy and negative energy states according to (177). This will be the key to the aim of reexpressing the particle number conserving QED Hamiltonian  $\hat{\mathcal{H}}_U$  in first quantization. As will be shown in the next section 6, from  $\mathbb{T}$  indeed follows the nonrelativistic light–matter interaction Hamiltonian  $\mathbf{H}_{LM}^{(el)}$  of electrons interacting with low–energy photons.

An important aspect of the Newton–Wigner amplitudes (173) and (174) is that matrix elements of the form [8, 7]

$$\int d^3r \sum_{k,k'} U_{\mu}^{*(NW)}(\mathbf{r}, k) (\alpha_a)_{\mu,\mu'} U_{\mu'}^{(NW)}(\mathbf{r}, k') = 0_{4 \times 4} \tag{178}$$

vanish identically, because the Dirac  $\alpha_a$  matrix is nondiagonal while the Newton–Wigner amplitudes are “diagonal”.

As an example the Dirac  $\alpha_a$  assumes the following guise in the Newton–Wigner representation (see section B of the appendix) [7]:

$$\begin{aligned}
\mathbb{T} \alpha_a \mathbb{T}^\dagger &= \mathbb{T} (\Pi) \alpha_a \mathbb{T}^\dagger (\Pi) \\
&= \alpha_a + \frac{\Pi_a}{m_0 c} \beta - \frac{1}{4} \frac{\Pi_b}{m_0 c} \frac{\Pi_{b'}}{m_0 c} \left( \alpha_b \alpha_{b'} \alpha_a + \underbrace{\left( \alpha_b \alpha_a + \alpha_a \alpha_b \right)}_{2\delta_{a,b}} \alpha_{b'} \right)
\end{aligned} \tag{179}$$

It is well known that in the Heisenberg picture the velocity of the Dirac particle is  $v_a = c \alpha_a$ , see for example [18, 9]. Interestingly, in the Newton–Wigner representation the nondiagonality of the Newton–Wigner particles velocity associated with (179) is still there, however,

by evaluation matrix elements, for which one has to make use of the Newton–Wigner eigenfunctions (173) and (174), the contribution due to the nondiagonal  $\alpha_a$  matrices in (179) vanish exactly. Hence, on the operator level the velocity of the Newton–Wigner particle comprises also nondiagonal parts, but these are not visible by evaluating matrix elements (see also the discussion in the beginning of section 6.4).

It should be mentioned that one can show that in the Newton–Wigner representation of the Dirac Hamiltonian there does not exist any paradox like the so-called Zitterbewegung [10, 7].

## 6 Solution to the Classical Limit Problem of QED Part II: Applying the Eriksen Transformation

In section 4 the particle number conserving Hamiltonian  $\hat{\mathcal{H}}_U$  has been derived up to the order  $\alpha_{FS}^2$  of the finestructure constant  $\alpha_{FS}$  by solving the flow equation perturbatively. The result was given by [7, 8]

$$\begin{aligned}
\lim_{s \rightarrow \infty} \hat{\mathcal{H}}_U(s) &= m_0 c^2 \left( \hat{H}^{(0)} + \hat{H}^{(1)}(\infty) + \hat{H}^{(2,h)}(\infty) + \hat{H}^{(2,i)}(\infty) \dots \right) \\
&= \hat{\mathcal{H}}_D + \hat{\mathcal{M}}_C^{(e)} + \hat{\mathcal{M}}_C^{(p)} + \hat{\mathcal{M}}_{\perp}^{(e)} + \hat{\mathcal{M}}_{\perp}^{(p)} \\
&+ \hat{\mathcal{H}}_{rad} + \hat{\mathcal{H}}_{\perp}^{(low,0)} + \hat{\mathcal{H}}_{p,ph} + \hat{\mathcal{H}}_{e,ph} + \hat{\mathcal{Q}}_{\perp,ph} \\
&+ \mathcal{U}_C^{(0)} + \hat{\mathcal{V}}_{ext}^{(0)} + \mathcal{C}_{\perp} \hat{1} + \hat{\mathcal{V}}_{\perp,ee} + \hat{\mathcal{V}}_{\perp,pp} + \hat{\mathcal{V}}_{\perp,ep}
\end{aligned} \tag{180}$$

This unitarily equivalent QED Hamiltonian describes the interaction between matter and antimatter fields moving at arbitrary speed, and low energy photons.

Then in section 5 the Eriksen transformation  $\mathbb{T}$  has been introduced which makes it possible to decouple the matter and antimatter degrees of freedom.

This part is dedicated to the goal of now putting the results together in such a way that one gets a Hamiltonian  $\hat{\mathbf{H}}^{(LM)}$  from  $\hat{\mathcal{H}}_U$  by applying the Eriksen transformation.  $\hat{\mathbf{H}}^{(LM)}$  then describes the interaction of nonrelativistic electrons as point particles with low-energy photons. It is thus a nonrelativistic, classical light-matter interaction Hamiltonian for the electrons. Several steps are necessary for doing this.

First of all, in the following, the interaction terms  $\hat{\mathcal{H}}_{p,ph} + \hat{\mathcal{H}}_{e,ph} + \hat{\mathcal{V}}_{\perp,ep}$ , and the terms  $\hat{\mathcal{Q}}_{\perp,ph} + \mathcal{C}_{\perp} \hat{1} + \hat{\mathcal{V}}_{\perp,pp}$  in the Hamiltonian (180) will not be considered further. The study of these would be very interesting, but for the time being they do not play a role in the derivation of the nonrelativistic many-electron Hamiltonian of light-matter interaction.

The remaining contributions in (180) decompose into matter and antimatter parts once the Eriksen transformation has been applied. However, the parts describing interactions of positrons with photons

will also not be evaluated. The evaluation is analogous as for the electrons and as I have outlined in (238) there is a shorter way for receiving the nonrelativistic positron Hamiltonian.  $\hat{\mathcal{H}}_{LM}^{(pos)}$  principally results from the charge conjugation symmetry operation  $\mathcal{C}_F$ .

Hence, first, the Hamiltonian [7, 8]

$$\begin{aligned} \hat{\mathcal{H}}_{LM}^{(el)} = & \hat{\mathcal{H}}_D^{(el)} + \hat{\mathcal{M}}_C^{(e)} + \hat{\mathcal{M}}_{\perp}^{(e)} + \hat{\mathcal{H}}_{rad} + \hat{\mathcal{H}}_{\perp}^{(low,el)} \\ & + \hat{\mathcal{V}}_{C,ee} + \hat{\mathcal{V}}_{ext}^{(el)} + \hat{\mathcal{V}}_{\perp,ee} \end{aligned} \quad (181)$$

is derived from the the respective parts of the Hamiltonian (180) by applying the Eriksen transformation. Here,  $\hat{\mathcal{V}}_{C,ee}$  is the matter part of the particle number conserving Coulomb interaction, and  $\hat{\mathcal{H}}_{\perp}^{(low,el)}$  is the matter part of the coupling of the matter fields to the low energy photons.

The reexpression of the Hamiltonian  $\hat{\mathcal{H}}_{LM}^{(el)}$  in the Newton–Wigner representation is in large parts a discussion about orders of magnitude that must be considered or can be neglected (regarding the finestructure constant). Here, one must be guided by the physics. For that it is very important to know that the Newton–Wigner field operators are proportional to the nonrelativistic Schrödinger–Pauli amplitudes (for electrons and positrons separately). The latter are slowly varying functions on the Bohr length scale (compared to the length scale of pair creation defined by the Compton wavelength  $\lambda_C$ ). Therefore, the operators occurring between the Newton–Wigner amplitudes, or the respective matrix elements, can be evaluated as a gradient expansion with respect to the gauge invariant momentum operator  $\hat{\Pi}_b$ . Thereby all contributions higher than the order  $\alpha_{FS}^2$  will be neglected, which is consistent with the solution of the perturbation expansion applied in section 4.

First the renormalization terms for the electrons  $\hat{\mathcal{M}}_C^{(e)} + \hat{\mathcal{M}}_{\perp}^{(e)}$  are evaluated. These calculations are extensive and have therefore been shifted in large parts to the appendix.

Then the matter part  $\hat{\mathcal{H}}_D^{(el)}$  of the Dirac quantum field is evaluated, such that one can find from  $\hat{\mathcal{H}}_D^{(el)} + \hat{\mathcal{M}}_C^{(e)} + \hat{\mathcal{M}}_{\perp}^{(e)} \equiv \hat{\mathcal{H}}_{SP}^{(el)}$  the effective Schrödinger–Pauli Hamilton. In this context the physical cut-off is introduced and the renormalization integrals are evaluated. It

will then become obvious how the bare mass  $m_0$  of the electrons is renormalized and with that, accordingly, the  $g$ -factor.

Finally, the effective interaction terms are evaluated. For this one has to calculate matrix elements in the Newton–Wigner representation, which give the corrections to the Dirac representation. In this context the first order effective transversal interaction  $\hat{\mathcal{H}}_{\perp}^{(low,0)}$  and the second order transversal interaction  $\hat{\mathcal{V}}_{\perp,ee}$  are evaluated, then the second order longitudinal interactions  $\hat{\mathcal{V}}_{C,ee}$  and  $\hat{\mathcal{V}}_{ext}^{(el)}$  are evaluated.

Then, when one has succeeded in deriving the Hamiltonian  $\hat{\mathcal{H}}_{LM}^{(el)}$  from  $\hat{\mathcal{H}}_{\mathcal{U}}$ , it will be possible to express it in first quantization. In that guise the light–matter Hamiltonian for electrons  $\hat{\mathbf{H}}_{LM}^{(el)}$  arises from  $\hat{\mathcal{H}}_{LM}^{(el)}$ , derived by full QED.



## 6.1 Evaluation of the Renormalization Terms

The terms that renormalize the bare mass  $m_0$  and the  $g$ -factor of the fermions have been deduced in section 4.1.3. They are given by  $\hat{\mathcal{M}}^{(0)} = \hat{\mathcal{M}}_C^{(0)} + \hat{\mathcal{M}}_\perp^{(0)}$ , where  $\hat{\mathcal{M}}_C^{(0)}$  renormalizes the fermionic attributes due to the high-energy Coulomb-interaction between the (anti-)matter fields, and  $\hat{\mathcal{M}}_\perp^{(0)}$  renormalizes the fermionic attributes due to the interaction of the (anti-)matter fields with the high-energy photons.

These terms decompose into renormalization terms for matter (e) and antimatter (p) separately according to [7, 8]

$$\begin{aligned}\hat{\mathcal{M}}_C^{(0)} &= \hat{\mathcal{M}}_C^{(e)} + \hat{\mathcal{M}}_C^{(p)} \\ \hat{\mathcal{M}}_\perp^{(0)} &= \hat{\mathcal{M}}_\perp^{(e)} + \hat{\mathcal{M}}_\perp^{(p)}\end{aligned}$$

In the following it will be concentrated on the evaluation matter parts  $\hat{\mathcal{M}}_C^{(e)}$  and  $\hat{\mathcal{M}}_\perp^{(e)}$  of the renormalization. These are given by [7]

$$\begin{aligned}\hat{\mathcal{M}}_C^{(e)} &= \sum_{K,k} \left( \frac{q_e^2}{2\varepsilon_0} \right) \int \frac{d^3q}{(2\pi)^3} \frac{1}{|\mathbf{q}|^2} \langle U_k | e^{-iq_a \hat{x}_a} (\mathbf{P}^{(+)} - \mathbf{P}^{(-)}) \circ e^{iq_a \hat{x}_a} | U_K \rangle \hat{c}_k^\dagger \hat{c}_K \\ \hat{\mathcal{M}}_\perp^{(e)} &= m_0 c^2 \sum_{k,K} \hat{c}_k^\dagger \hat{c}_K \left( \frac{q_e}{m_0 c} \right)^2 \frac{1}{V} \sum_{\mathbf{q}} \frac{\hbar}{2\varepsilon_0 \omega(\mathbf{q})} \sum_{b,b'} \left( \delta_{b,b'} - \frac{q_b q_{b'}}{|\mathbf{q}|^2} \right) \\ &\quad \times \begin{cases} \kappa_q \times \sum_{K'} \langle U_k | \alpha_b e^{iq_a \hat{x}_a} | U_{K'} \rangle \langle U_{K'} | \alpha_{b'} e^{-iq_{a'} \hat{x}_{a'}} | U_K \rangle \frac{(\tilde{E}_k - \tilde{E}_{K'} - \tilde{\omega}_q) + (\tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_q)}{(\tilde{E}_k - \tilde{E}_{K'} - \tilde{\omega}_q)^2 + (\tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_q)^2} \\ + \sum_{K'} \langle U_k | \alpha_b e^{-iq_a \hat{x}_a} | V_{K'} \rangle \langle V_{K'} | \alpha_{b'} e^{+iq_{a'} \hat{x}_{a'}} | U_K \rangle \frac{(\tilde{E}_k + \tilde{E}_{K'} + \tilde{\omega}_q) + (\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_q)}{(\tilde{E}_k + \tilde{E}_{K'} + \tilde{\omega}_q)^2 + (\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_q)^2} \end{cases} \quad (182)\end{aligned}$$

With the abbreviations [7]

$$\begin{aligned}\hat{\mathcal{M}}_C^{(e)} &= \sum_{k,K} \tilde{\mathcal{M}}_{k,K}^{(C,e)} \hat{c}_k^\dagger \hat{c}_K \\ \hat{\mathcal{M}}_\perp^{(e)} &= \sum_{k,K} \tilde{\mathcal{M}}_{k,K}^{(\perp,e)} \hat{c}_k^\dagger \hat{c}_K\end{aligned} \quad (183)$$

there holds [7]

$$\hat{\mathcal{M}}^{(e)} = \hat{\mathcal{M}}_C^{(e)} + \hat{\mathcal{M}}_\perp^{(e)} = \sum_{k,K} \left( \tilde{\mathcal{M}}_{k,K}^{(C,e)} + \tilde{\mathcal{M}}_{k,K}^{(\perp,e)} \right) \hat{c}_k^\dagger \hat{c}_K \quad (184)$$

In section 6.3 it will become clear how the terms (184) add up to the bare rest energy, the bare kinetic energy and the bare Zeeman energy of the single-particle Dirac Hamiltonian: they numerically alter the bare mass  $m_0$  and the  $g$ -factor of the electron.

### 6.1.1 Evaluation of the Transversal Contribution to the Renormalization

For the following it is convenient to introduce [7]

$$\tilde{\omega}_q = \frac{|\mathbf{q}|}{k_C} \quad (185)$$

$$m_0 c^2 \left( \frac{q_e}{m_0 c} \right)^2 \frac{\hbar}{2\varepsilon_0 \omega(\mathbf{q})} = \left( \frac{q_e^2}{2\varepsilon_0} \right) \left( \frac{\hbar}{m_0 c} \right)^2 \frac{1}{\tilde{\omega}_q}$$

From that follows for the transversal matrix element in (182) [7]

$$\tilde{M}_{k,K}^{(\perp,e)} = \left( \frac{q_e^2}{2\varepsilon_0} \right) \left( \frac{\hbar}{m_0 c} \right)^2 \frac{1}{V} \sum_{\mathbf{q}} \frac{1}{\tilde{\omega}_q} \sum_{b,b'} \left( \delta_{b,b'} - \frac{q_b q_{b'}}{|\mathbf{q}|^2} \right)$$

$$\times \begin{cases} \kappa_q \sum_{K'} \langle U_k | \alpha_b e^{iq_a \hat{x}_a} \frac{(\tilde{E}_k - \tilde{E}_{K'} - \tilde{\omega}_q) + (\tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_q)}{(\tilde{E}_k - \tilde{E}_{K'} - \tilde{\omega}_q)^2 + (\tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_q)^2} | U_{K'} \rangle \langle U_{K'} | \alpha_{b'} e^{-iq_{a'} \hat{x}_{a'}} | U_K \rangle \\ + \sum_{K'} \langle U_k | \alpha_b e^{-iq_a \hat{x}_a} \frac{(\tilde{E}_k + \tilde{E}_{K'} + \tilde{\omega}_q) + (\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_q)}{(\tilde{E}_k + \tilde{E}_{K'} + \tilde{\omega}_q)^2 + (\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_q)^2} | V_{K'} \rangle \langle V_{K'} | \alpha_{b'} e^{+iq_{a'} \hat{x}_{a'}} | U_K \rangle \end{cases} \quad (186)$$

Obviously, due to the summation over all photon wavenumbers  $\mathbf{q}$ , this expression is divergent. Hence, one has to introduce a cut-off. At this point there are several possibilities for choosing such a cut-off [32]: one could truncate the photon energy only, or one could truncate both the photon energy and the kinetic energy of the fermions. One could also consider the potential energy of the photons in the cut-off. However, it turns out that the correct physical cut-off is the one where one truncates the energy  $\tilde{\omega}_q$  of the photons **and** the kinetic energy  $\tilde{E}_{K'}$  of the fermions. From a general point of view there is no reason to assume that the photon energy should be limited, whereas the fermions can move at any speed. It will be shown in subsection 6.3 that such a choice of the cut-off leads to a consistent renormalization of the bare electron mass  $m_e$ .

For now it will be assumed that the cut-off  $\tilde{\Omega}_{max}$  is given by [7]

$$\begin{aligned}\tilde{\omega}_q + \tilde{E}_{K'} &< 2\tilde{\Omega}_{max} \\ \tilde{\Omega}_{max} &\gg 1\end{aligned}\tag{187}$$

The setting that  $\tilde{\Omega}_{max} \gg 1$  will be justified in subsection 6.3, where it is shown that the sum or the integral in (186) is of logarithmic nature, such that  $\frac{\alpha_{FS}}{\pi} \ln \tilde{\Omega}_{max}$  is a small number leading to the fact that there is no big difference between the bare mass  $m_0$  and the true electron mass  $m_e$ . The fact that it is possible to choose the cutoff  $\tilde{\Omega}_{max} \gg 1$  in this way implies, moreover, that one is able to account for a wide range of photon modes.

Formally, the cut-off (187) can be introduced by the Heaviside stepfunction  $\Theta_H(x)$ :

$$\Theta_H(x) = \frac{1}{2} \left( 1 + \frac{x}{|x|} \right) = \begin{cases} 1 & \text{für } x > 0 \\ 0 & \text{für } x < 0 \end{cases}\tag{188}$$

according to [7]

$$\Theta_H(2\tilde{\Omega}_{max} - x) = \begin{cases} 1 & \text{für } x < 2\tilde{\Omega}_{max} \\ 0 & \text{für } x > 2\tilde{\Omega}_{max} \end{cases}\tag{189}$$

With this one can express (186) as [7]

$$\begin{aligned}\tilde{M}_{k,K}^{(\perp,e)} &= \left( \frac{q_e^2}{2\varepsilon_0} \right) \left( \frac{\hbar}{m_0 c} \right)^2 \frac{1}{V} \sum_{\mathbf{q}} \frac{1}{\tilde{\omega}_q} \sum_{b,b'} \left( \delta_{b,b'} - \frac{q_b q_{b'}}{|\mathbf{q}|^2} \right) \\ &\times \left\{ \begin{aligned} &\kappa_q \sum_{K'} \langle U_k | \alpha_b e^{iq_a \hat{x}_a} \frac{(\tilde{E}_k - \tilde{E}_{K'} - \tilde{\omega}_q) + (\tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_q)}{(\tilde{E}_k - \tilde{E}_{K'} - \tilde{\omega}_q)^2 + (\tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_q)^2} \Theta_H(2\tilde{\Omega}_{max} - \tilde{\omega}_q - \tilde{E}_{K'}) |U_{K'}\rangle \langle U_{K'} | \alpha_{b'} e^{-iq_{a'} \hat{x}_{a'}} |U_K\rangle \\ &+ \sum_{K'} \langle U_k | \alpha_b e^{-iq_a \hat{x}_a} \frac{(\tilde{E}_k + \tilde{E}_{K'} + \tilde{\omega}_q) + (\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_q)}{(\tilde{E}_k + \tilde{E}_{K'} + \tilde{\omega}_q)^2 + (\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_q)^2} \Theta_H(2\tilde{\Omega}_{max} - \tilde{\omega}_q - \tilde{E}_{K'}) |V_{K'}\rangle \langle V_{K'} | \alpha_{b'} e^{iq_{a'} \hat{x}_{a'}} |U_K\rangle \end{aligned} \right.\end{aligned}\tag{190}$$

Using the Dirac eigenvalue relation

$$\begin{aligned}\tilde{H}^{(D)} |U_k\rangle &= \tilde{E}_k |U_k\rangle \\ \tilde{H}^{(D)} |V_{k'}\rangle &= -\tilde{E}_{k'} |V_{k'}\rangle\end{aligned}\tag{191}$$

implying for any analytical function  $F(z)$  [7]

$$F\left(\tilde{\mathbf{H}}^{(D)}\right)|U_k\rangle = F\left(\tilde{E}_k\right)|U_k\rangle F\left(\tilde{\mathbf{H}}^{(D)}\right)|V_{k'}\rangle = F\left(-\tilde{E}_{k'}\right)|V_{k'}\rangle \quad (192)$$

for introducing the *Operator*  $\mathbf{C}_q$  [7]

$$\begin{aligned} \mathbf{C}_q &\equiv \Theta_H \left[ \left( 2\tilde{\Omega}_{max} - \tilde{\omega}_q \right) \mathbf{1}_{4 \times 4} - \sqrt{\tilde{\mathbf{H}}^{(D)}\tilde{\mathbf{H}}^{(D)}} \right] \\ \mathbf{C}_q |U_{K'}\rangle &= \Theta_H \left( 2\tilde{\Omega}_{max} - \tilde{\omega}_q - \tilde{E}_{K'} \right) |U_{K'}\rangle \\ \mathbf{C}_q |V_{K'}\rangle &= \Theta_H \left( 2\tilde{\Omega}_{max} - \tilde{\omega}_q - \tilde{E}_{K'} \right) |V_{K'}\rangle \end{aligned} \quad (193)$$

Inserting this into the transversal matrix element (190) one finds [7]

$$\begin{aligned} \tilde{\mathbf{M}}_{k,K}^{(\perp,e)} &= \left( \frac{q_e^2}{2\varepsilon_0} \right) \left( \frac{\hbar}{m_0c} \right)^2 \frac{1}{V} \sum_{\mathbf{q}} \frac{1}{\tilde{\omega}_q} \sum_{b,b'} \left( \delta_{b,b'} - \frac{q_b q_{b'}}{|\mathbf{q}|^2} \right) \\ &\times \left\{ \begin{aligned} &\kappa_q \langle U_k | \alpha_b e^{iq_a \hat{x}_a} \circ \frac{(\tilde{E}_k - \tilde{\mathbf{H}}^{(D)} - \tilde{\omega}_q) + (\tilde{E}_K - \tilde{\mathbf{H}}^{(D)} - \tilde{\omega}_q)}{(\tilde{E}_k - \tilde{\mathbf{H}}^{(D)} - \tilde{\omega}_q)^2 + (\tilde{E}_K - \tilde{\mathbf{H}}^{(D)} - \tilde{\omega}_q)^2} \circ \mathbf{C}_q \circ (\sum_{K'} |U_{K'}\rangle \langle U_{K'}|) \circ e^{-iq_a \hat{x}_a} \alpha_{b'} |U_K\rangle \\ &+ \langle U_k | \alpha_b e^{-iq_a \hat{x}_a} \circ \frac{(\tilde{E}_k - \tilde{\mathbf{H}}^{(D)} + \tilde{\omega}_q) + (\tilde{E}_K - \tilde{\mathbf{H}}^{(D)} + \tilde{\omega}_q)}{(\tilde{E}_k - \tilde{\mathbf{H}}^{(D)} + \tilde{\omega}_q)^2 + (\tilde{E}_K - \tilde{\mathbf{H}}^{(D)} + \tilde{\omega}_q)^2} \circ \mathbf{C}_q \circ (\sum_{K'} |V_{K'}\rangle \langle V_{K'}|) \circ e^{+iq_a \hat{x}_a} \alpha_{b'} |U_K\rangle \end{aligned} \right. \\ &= \left( \frac{q_e^2}{2\varepsilon_0} \right) \left( \frac{\hbar}{m_0c} \right)^2 \frac{1}{V} \sum_{\mathbf{q}} \frac{1}{\tilde{\omega}_q} \sum_{b,b'} \left( \delta_{b,b'} - \frac{q_b q_{b'}}{|\mathbf{q}|^2} \right) \\ &\times \left\{ \begin{aligned} &\kappa_q \langle U_k | \alpha_b e^{iq_a \hat{x}_a} \circ \frac{(\tilde{E}_k - \tilde{\mathbf{H}}^{(D)} - \tilde{\omega}_q) + (\tilde{E}_K - \tilde{\mathbf{H}}^{(D)} - \tilde{\omega}_q)}{(\tilde{E}_k - \tilde{\mathbf{H}}^{(D)} - \tilde{\omega}_q)^2 + (\tilde{E}_K - \tilde{\mathbf{H}}^{(D)} - \tilde{\omega}_q)^2} \circ \mathbf{C}_q \circ \mathbf{P}^{(+)} \alpha_{b'} e^{-iq_a \hat{x}_a} |U_K\rangle \\ &+ \langle U_k | \alpha_b e^{-iq_a \hat{x}_a} \circ \frac{(\tilde{E}_k - \tilde{\mathbf{H}}^{(D)} + \tilde{\omega}_q) + (\tilde{E}_K - \tilde{\mathbf{H}}^{(D)} + \tilde{\omega}_q)}{(\tilde{E}_k - \tilde{\mathbf{H}}^{(D)} + \tilde{\omega}_q)^2 + (\tilde{E}_K - \tilde{\mathbf{H}}^{(D)} + \tilde{\omega}_q)^2} \circ \mathbf{C}_q \circ \mathbf{P}^{(-)} \circ e^{+iq_a \hat{x}_a} \alpha_{b'} |U_K\rangle \end{aligned} \right. \end{aligned} \quad (194)$$

Here, use has been made of the definition (307) of the projection operators  $\mathbf{P}^{(+)}$  and  $\mathbf{P}^{(-)}$ .

The expression (194) can be further transformed by using that the sum is not altered if one substitutes  $q_a \rightarrow -q_a$  in the first line [7]:

$$\begin{aligned} \tilde{\mathbf{M}}_{k,K}^{(\perp,e)} &= \left( \frac{q_e^2}{2\varepsilon_0} \right) \left( \frac{\hbar}{m_0c} \right)^2 \frac{1}{V} \sum_{\mathbf{q}} \frac{1}{\tilde{\omega}_q} \sum_{b,b'} \left( \delta_{b,b'} - \frac{q_b q_{b'}}{|\mathbf{q}|^2} \right) \\ &= \times \left\{ \begin{aligned} &\langle U_k | \alpha_b e^{-iq_a \hat{x}_a} \circ \mathbf{C}_q \circ \left( \begin{aligned} &\frac{(\tilde{E}_k - \tilde{\mathbf{H}}^{(D)} - \tilde{\omega}_q) + (\tilde{E}_K - \tilde{\mathbf{H}}^{(D)} - \tilde{\omega}_q)}{(\tilde{E}_k - \tilde{\mathbf{H}}^{(D)} - \tilde{\omega}_q)^2 + (\tilde{E}_K - \tilde{\mathbf{H}}^{(D)} - \tilde{\omega}_q)^2} \mathbf{P}^{(+)} \\ &+ \frac{(\tilde{E}_k - \tilde{\mathbf{H}}^{(D)} + \tilde{\omega}_q) + (\tilde{E}_K - \tilde{\mathbf{H}}^{(D)} + \tilde{\omega}_q)}{(\tilde{E}_k - \tilde{\mathbf{H}}^{(D)} + \tilde{\omega}_q)^2 + (\tilde{E}_K - \tilde{\mathbf{H}}^{(D)} + \tilde{\omega}_q)^2} \mathbf{P}^{(-)} \end{aligned} \right) \circ e^{+iq_a \hat{x}_a} \alpha_{b'} |U_K\rangle \\ &-(1 - \kappa_q) \langle U_k | \alpha_b e^{-iq_a \hat{x}_a} \circ \mathbf{C}_q \circ \frac{(\tilde{E}_k - \tilde{\mathbf{H}}^{(D)} - \tilde{\omega}_q) + (\tilde{E}_K - \tilde{\mathbf{H}}^{(D)} - \tilde{\omega}_q)}{(\tilde{E}_k - \tilde{\mathbf{H}}^{(D)} - \tilde{\omega}_q)^2 + (\tilde{E}_K - \tilde{\mathbf{H}}^{(D)} - \tilde{\omega}_q)^2} \circ \mathbf{P}^{(+)} \circ e^{iq_a \hat{x}_a} \alpha_{b'} |U_K\rangle \end{aligned} \right. \end{aligned} \quad (195)$$

The contribution of the first line is independent of the photon, since the sum runs over all wavenumbers  $\mathbf{q}$ . It describes the renormalization due to the presence of the high energy photons in the QED soup. This contribution is always present, even if one would eliminate all photons. Eliminating all photons, including the high energy photons, formally means that  $\kappa_q \equiv 1$  (see (85)), and the contribution of the second line vanishes.

The following identity will be useful [7]:

$$\mathbf{F}(z) \mathbf{P}^{(+)} + \mathbf{F}(-z) \mathbf{P}^{(-)} = \mathbf{F} \left[ z \left( \mathbf{P}^{(+)} - \mathbf{P}^{(-)} \right) \right] \quad (196)$$

This is valid for a power series  $\mathbf{F}(w) = \sum_{n=0}^{\infty} \mathbf{F}_n \cdot w^n$  with matrix coefficients  $\mathbf{F}_n$ . The identity (196) is proven in the appendix I.

It leads to [7]

$$\begin{aligned} & \frac{(\tilde{E}_k - \tilde{\mathbf{H}}^{(D)} - \tilde{\omega}_q) + (\tilde{E}_K - \tilde{\mathbf{H}}^{(D)} - \tilde{\omega}_q)}{(\tilde{E}_k - \tilde{\mathbf{H}}^{(D)} - \tilde{\omega}_q)^2 + (\tilde{E}_K - \tilde{\mathbf{H}}^{(D)} - \tilde{\omega}_q)^2} \circ \mathbf{P}^{(+)} + \frac{(\tilde{E}_k - \tilde{\mathbf{H}}^{(D)} + \tilde{\omega}_q) + (\tilde{E}_K - \tilde{\mathbf{H}}^{(D)} + \tilde{\omega}_q)}{(\tilde{E}_k - \tilde{\mathbf{H}}^{(D)} + \tilde{\omega}_q)^2 + (\tilde{E}_K - \tilde{\mathbf{H}}^{(D)} + \tilde{\omega}_q)^2} \circ \mathbf{P}^{(-)} \\ &= \frac{(\tilde{E}_k - \tilde{\mathbf{H}}^{(D)} - \tilde{\omega}_q (\mathbf{P}^{(+)} - \mathbf{P}^{(-)})) + (\tilde{E}_K - \tilde{\mathbf{H}}^{(D)} - \tilde{\omega}_q (\mathbf{P}^{(+)} - \mathbf{P}^{(-)}))}{(\tilde{E}_k - \tilde{\mathbf{H}}^{(D)} - \tilde{\omega}_q (\mathbf{P}^{(+)} - \mathbf{P}^{(-)}))^2 + (\tilde{E}_K - \tilde{\mathbf{H}}^{(D)} - \tilde{\omega}_q (\mathbf{P}^{(+)} - \mathbf{P}^{(-)}))^2} \\ &= \frac{\left( \tilde{E}_k - \tilde{\mathbf{H}}^{(D)} - \tilde{\omega}_q \frac{\tilde{\mathbf{H}}^{(D)}}{\sqrt{\tilde{\mathbf{H}}^{(D)} \circ \tilde{\mathbf{H}}^{(D)}}} \right) + \left( \tilde{E}_K - \tilde{\mathbf{H}}^{(D)} - \tilde{\omega}_q \frac{\tilde{\mathbf{H}}^{(D)}}{\sqrt{\tilde{\mathbf{H}}^{(D)} \circ \tilde{\mathbf{H}}^{(D)}}} \right)}{\left( \tilde{E}_k - \tilde{\mathbf{H}}^{(D)} - \tilde{\omega}_q \frac{\tilde{\mathbf{H}}^{(D)}}{\sqrt{\tilde{\mathbf{H}}^{(D)} \circ \tilde{\mathbf{H}}^{(D)}}} \right)^2 + \left( \tilde{E}_K - \tilde{\mathbf{H}}^{(D)} - \tilde{\omega}_q \frac{\tilde{\mathbf{H}}^{(D)}}{\sqrt{\tilde{\mathbf{H}}^{(D)} \circ \tilde{\mathbf{H}}^{(D)}}} \right)^2} \end{aligned}$$

and with that one finds [7]

$$\begin{aligned} \tilde{\mathbf{M}}_{k,K}^{(\perp,e)} &= \left( \frac{q_e^2}{2\varepsilon_0} \right) \left( \frac{\hbar}{m_0 c} \right)^2 \frac{1}{V} \sum_{\mathbf{q}} \frac{1}{\tilde{\omega}_q} \sum_{b,b'} \left( \delta_{b,b'} - \frac{q_b q_{b'}}{|\mathbf{q}|^2} \right) \\ &\times \left( \begin{aligned} & \langle U_k | \alpha_b e^{-iq_a \hat{x}_a} \circ \mathbf{C}_q \circ \frac{(\tilde{E}_k - \tilde{\mathbf{H}}^{(D)} - \tilde{\omega}_q \frac{\tilde{\mathbf{H}}^{(D)}}{\sqrt{\tilde{\mathbf{H}}^{(D)} \circ \tilde{\mathbf{H}}^{(D)}}}) + (\tilde{E}_K - \tilde{\mathbf{H}}^{(D)} - \tilde{\omega}_q \frac{\tilde{\mathbf{H}}^{(D)}}{\sqrt{\tilde{\mathbf{H}}^{(D)} \circ \tilde{\mathbf{H}}^{(D)}}})}{(\tilde{E}_k - \tilde{\mathbf{H}}^{(D)} - \tilde{\omega}_q \frac{\tilde{\mathbf{H}}^{(D)}}{\sqrt{\tilde{\mathbf{H}}^{(D)} \circ \tilde{\mathbf{H}}^{(D)}}})^2 + (\tilde{E}_K - \tilde{\mathbf{H}}^{(D)} - \tilde{\omega}_q \frac{\tilde{\mathbf{H}}^{(D)}}{\sqrt{\tilde{\mathbf{H}}^{(D)} \circ \tilde{\mathbf{H}}^{(D)}}})^2} \circ e^{iq_{a'} \hat{x}_{a'}} \alpha_{b'} | U_K \rangle \\ & - (1 - \kappa_q) \langle U_k | \alpha_b e^{-iq_a \hat{x}_a} \circ \mathbf{C}_q \circ \frac{(\tilde{E}_k - \tilde{\mathbf{H}}^{(D)} - \tilde{\omega}_q) + (\tilde{E}_K - \tilde{\mathbf{H}}^{(D)} - \tilde{\omega}_q)}{(\tilde{E}_k - \tilde{\mathbf{H}}^{(D)} - \tilde{\omega}_q)^2 + (\tilde{E}_K - \tilde{\mathbf{H}}^{(D)} - \tilde{\omega}_q)^2} \circ \mathbf{P}^{(+)} \circ e^{iq_{a'} \hat{x}_{a'}} \alpha_{b'} | U_K \rangle \end{aligned} \right) \quad (197) \end{aligned}$$

The fractions are of the form  $R(x) = \frac{(x+a)+(x+b)}{(x+a)^2+(x+b)^2}$  which can be transformed with the help of elementary algebra to  $R(x) =$

$$\frac{x + \frac{a+b}{2}}{\left(x + \frac{a+b}{2}\right)^2 + \frac{(a-b)^2}{4}} .$$

Together with the abbreviation  $\mathbf{Z} = \tilde{\mathbf{H}}^{(D)} \circ \left( \mathbf{1}_{4 \times 4} + \frac{\tilde{\omega}_q}{\sqrt{\tilde{\mathbf{H}}^{(D)} \circ \tilde{\mathbf{H}}^{(D)}}} \right)$  one can rewrite (197) according to [7]

$$\begin{aligned} \tilde{\mathbf{M}}_{k,K}^{(1,e)} &= \left( \frac{q_e^2}{2\varepsilon_0} \right) \left( \frac{\hbar}{m_0 c} \right)^2 \frac{1}{V} \sum_{\mathbf{q}} \frac{1}{\tilde{\omega}_q} \sum_{b,b'} \left( \delta_{b,b'} - \frac{q_b q_{b'}}{|\mathbf{q}|^2} \right) \\ &\times \left( \begin{aligned} &\langle U_k | \alpha_b e^{-iq_a \hat{x}_a} \circ \mathbf{C}_q \circ \frac{-Z + \frac{\tilde{E}_k + \tilde{E}_K}{2} \mathbf{1}_{4 \times 4}}{\left( -Z + \frac{\tilde{E}_k + \tilde{E}_K}{2} \mathbf{1}_{4 \times 4} \right)^2 + \frac{(\tilde{E}_k - \tilde{E}_K)^2}{4} \mathbf{1}_{4 \times 4}} \circ e^{+iq_{a'} \hat{x}_{a'}} \alpha_{b'} | U_K \rangle \\ &- (1 - \kappa_q) \langle U_k | \alpha_b e^{-iq_a \hat{x}_a} \circ \mathbf{C}_q \circ \frac{-\tilde{\mathbf{H}}^{(D)} + \left( \tilde{\omega}_q + \frac{\tilde{E}_k + \tilde{E}_K}{2} \right) \mathbf{1}_{4 \times 4}}{\left( -\tilde{\mathbf{H}}^{(D)} + \left( \tilde{\omega}_q + \frac{\tilde{E}_k + \tilde{E}_K}{2} \right) \mathbf{1}_{4 \times 4} \right)^2 + \frac{(\tilde{E}_k - \tilde{E}_K)^2}{4} \mathbf{1}_{4 \times 4}} \circ \mathbf{P}^{(+)} \circ e^{iq_{a'} \hat{x}_{a'}} \alpha_{b'} | U_K \rangle \end{aligned} \right) \end{aligned} \quad (198)$$

One now has to think about the orders of magnitude. The goal is to limit oneself to the nonrelativistic sector of QED, and therefore, for being consistent with the perturbative solution of the flow equation (102), this means that one has to keep corrections up to order  $\alpha_{FS}^2$  regarding the energies  $\tilde{E}_k$  and  $\tilde{E}_K$ .

In the appendix section E there is a discussion about the orders of magnitude relevant for atomic and molecular physics. There one can see that the kinetic energy  $\tilde{E}_{kin}$  and the Zeeman energy  $\tilde{E}_{Zee}$  are already of second order in the finestructure constant  $\alpha_{FS}$  compared to the rest energy of the electron.

From this follows that (dimensionless) differences like  $\tilde{E}_k^2 - 1$  are comparable to  $\frac{H_{4 \times 4}^{(P,0)}}{m_0 c^2} \sim \alpha_{FS}^2$ . This is because the rest energy  $\tilde{E}_0$  is of order  $\alpha_{FS}^0 = 1$ . Subtracting the  $1 = \tilde{E}_0$  from the total energy  $\tilde{E}_k = \tilde{E}_0 + \tilde{E}_{kin} + \tilde{E}_{Zee}$  then there remains the kinetic energy and the Zeeman energy. Hence, such contributions in (198) are of the order  $\alpha_{FS}^2$  like the Pauli term  $\frac{H_{4 \times 4}^{(P,0)}}{m_0 c^2}$ .

It follows immediately that differences like  $\left( \tilde{E}_k - \tilde{E}_K \right)^2$  are of the order  $\alpha_{FS}^4$ . These can thus be neglected in (198).

Having said that there follows for (198) [7]

$$\frac{-Z + \frac{\tilde{E}_k + \tilde{E}_K}{2} \mathbf{1}_{4 \times 4}}{\left( -Z + \frac{\tilde{E}_k + \tilde{E}_K}{2} \mathbf{1}_{4 \times 4} \right)^2 + \frac{(\tilde{E}_k - \tilde{E}_K)^2}{4} \mathbf{1}_{4 \times 4}} = - \frac{Z + \frac{\tilde{E}_k + \tilde{E}_K}{2} \mathbf{1}_{4 \times 4}}{Z^2 - \left( \frac{\tilde{E}_k + \tilde{E}_K}{2} \right)^2 \mathbf{1}_{4 \times 4}} + O(\alpha_{FS}^4) \quad (199)$$

and [7]

$$\frac{-\check{H}^{(D)} + \left(\tilde{\omega}_q + \frac{\tilde{E}_k + \tilde{E}_K}{2}\right) \mathbf{1}_{4 \times 4}}{\left(-\check{H}^{(D)} + \left(\tilde{\omega}_q + \frac{\tilde{E}_k + \tilde{E}_K}{2}\right) \mathbf{1}_{4 \times 4}\right)^2 + \frac{(\tilde{E}_k - \tilde{E}_K)^2}{4} \mathbf{1}_{4 \times 4}} = - \frac{\check{H}^{(D)} + \left(\tilde{\omega}_q + \frac{\tilde{E}_k + \tilde{E}_K}{2}\right) \mathbf{1}_{4 \times 4}}{\check{H}^{(D)} \check{H}^{(D)} - \left(\tilde{\omega}_q + \frac{\tilde{E}_k + \tilde{E}_K}{2}\right)^2 \mathbf{1}_{4 \times 4}} + O(\alpha_{FS}^4) \quad (200)$$

yielding [7]

$$\begin{aligned} \tilde{M}_{k,K}^{(\perp,e)} &= \left(\frac{q_e^2}{2\varepsilon_0}\right) \left(\frac{\hbar}{m_0 c}\right)^2 \frac{1}{V} \sum_{\mathbf{q}} \frac{1}{\tilde{\omega}_q} \sum_{b,b'} \left(\delta_{b,b'} - \frac{q_b q_{b'}}{|\mathbf{q}|^2}\right) \\ &\times \begin{cases} - \langle U_k | \alpha_b (e^{-iq_a \hat{x}_a} \circ \mathbf{C}_q \circ e^{iq_a x_a}) \circ e^{-iq_a x_a} \circ \frac{Z + \frac{\tilde{E}_k + \tilde{E}_K}{2} \mathbf{1}_{4 \times 4}}{Z^2 - \left(\frac{\tilde{E}_k + \tilde{E}_K}{2}\right)^2 \mathbf{1}_{4 \times 4}} \circ e^{iq_{a'} \hat{x}_{a'}} \alpha_{b'} | U_K \rangle \\ + (1 - \kappa_q) \langle U_k | \alpha_b e^{-iq_a \hat{x}_a} \circ \mathbf{C}_q \circ \frac{\check{H}^{(D)} + \left(\tilde{\omega}_q + \frac{\tilde{E}_k + \tilde{E}_K}{2}\right) \mathbf{1}_{4 \times 4}}{\check{H}^{(D)} \check{H}^{(D)} - \left(\tilde{\omega}_q + \frac{\tilde{E}_k + \tilde{E}_K}{2}\right)^2 \mathbf{1}_{4 \times 4}} \circ \mathbf{P}^{(+)} \circ e^{iq_{a'} \hat{x}_{a'}} \alpha_{b'} | U_K \rangle \end{cases} \quad (201) \end{aligned}$$

Yet another simplification is possible. In the second line being proportional to  $(1 - \kappa_q)$  the corrections are of the order  $O(\alpha_{FS}^3)$ . This is because the term with  $1 - \kappa_q$  describes the renormalization contribution due to the low energy photons. It is therefore small. Additionally, for the low energy photons one can make use of the dipole approximation, meaning that we one set  $e^{iq_a x_a} \simeq 1$  and  $\mathbf{C}_q \equiv 1$ , because this is far below the cut-off regime (189). The remaining corrections are then of the order  $O(\alpha_{FS}^3)$ .

Altogether one can set [7]

$$\begin{aligned} \tilde{M}_{k,K}^{(\perp,e,high)} &= - \left(\frac{q_e^2}{2\varepsilon_0}\right) \left(\frac{\hbar}{m_0 c}\right)^2 \frac{1}{V} \sum_{\mathbf{q}} \frac{1}{\tilde{\omega}_q} \sum_{b,b'} \left(\delta_{b,b'} - \frac{q_b q_{b'}}{|\mathbf{q}|^2}\right) \\ &\times \langle U_k | \alpha_b \left(e^{-iq_a \hat{x}_a} \circ \mathbf{C}_q \circ e^{iq_a x_a}\right) \circ e^{-iq_a \hat{x}_a} \circ \frac{Z + \frac{\tilde{E}_k + \tilde{E}_K}{2} \mathbf{1}_{4 \times 4}}{Z^2 - \left(\frac{\tilde{E}_k + \tilde{E}_K}{2}\right)^2 \mathbf{1}_{4 \times 4}} \circ e^{iq_{a'} x_{a'}} \alpha_{b'} | U_K \rangle \end{aligned} \quad (202)$$

which provides corrections up to the order  $\alpha_{FS}^2$ .

The evaluation of the operators  $e^{-iq_a \hat{x}_a} \circ \frac{Z - \frac{\tilde{E}_{k'} + \tilde{E}_{K'}}{2} \mathbf{1}_{4 \times 4}}{Z^2 - \left(\frac{\tilde{E}_{k'} + \tilde{E}_{K'}}{2}\right)^2 \mathbf{1}_{4 \times 4}} \circ e^{iq_a \hat{x}_a}$  and  $e^{-iq_a \hat{x}_a} \circ \mathbf{C}_q \circ e^{iq_a \hat{x}_a}$  is shifted to the appendix section I. The final result is given by [7]

$$\begin{aligned}
\tilde{M}_{k,K}^{(l,e,high)} &= -m_0 c^2 \frac{\alpha_{FS}}{\pi} \times \\
&\times \left( \langle U_k | \int_0^{\tilde{\Omega}_{max}} d\xi \xi \left( \begin{aligned} & \left( \frac{\xi}{w} - 1 \right) \beta \\ & \left( -\frac{1}{3} \left( \left( \frac{w}{\xi} - \frac{\xi}{w} \right) + \left( -1 + \frac{\xi^3}{w^3} \right) \right) \right) \frac{\Pi_a}{m_0 c} \alpha_a \right. \\ & \left. + \left( -\frac{1}{2\xi^2} - \frac{\xi}{2w} + \frac{w}{2\xi} \right) \right. \\ & \left. + \frac{1}{m_0 c^2} \left( -\frac{1}{\xi^2} + \frac{\xi}{w^3} \right) \frac{1}{3} \tilde{\mathcal{H}}_{4 \times 4}^{(P)} \beta \right. \\ & \left. - \frac{1}{m_0 c^2} \left( 2 \left( -\frac{1}{\xi^2} + \frac{\xi}{w^3} \right) + \frac{2+5\xi^2}{2\xi w^5} \right) \frac{2}{3} \frac{\Pi_a \Pi_a}{2m_0} \beta \right. \\ & \left. + \frac{1}{m_0 c^2} \left( \left( \left( -1 + \frac{w}{\xi} - \frac{\xi}{2w^3} \right) + 2 \left( \frac{w}{\xi} - \frac{\xi}{w} - \frac{1}{\xi^2} \right) \right) \frac{2}{3} \left( \frac{\Pi_a \Pi_a}{2m_0} \frac{\tilde{\mathcal{H}}^{(D)}}{2} + \frac{\tilde{\mathcal{H}}^{(D)}}{2} \frac{\Pi_a \Pi_a}{2m_0} \right) \right. \right. \\ & \left. \left. - \left( \frac{w}{\xi} - \frac{\xi}{w} - \frac{1}{\xi^2} \right) \frac{1}{3} \left( \tilde{\mathcal{H}}_{4 \times 4}^{(P)} \frac{\tilde{\mathcal{H}}^{(D)}}{2} + \frac{\tilde{\mathcal{H}}^{(D)}}{2} \tilde{\mathcal{H}}_{4 \times 4}^{(P)} \right) \right. \right. \\ & \left. \left. + \left( \frac{w}{\xi} - 1 - \frac{1}{2\xi^2} \right) \left( -\frac{2}{m_0 c^2} \tilde{\mathcal{H}}_{4 \times 4}^{(P)} \right) \tilde{\mathcal{H}}^{(D)} \right. \right. \\ & \left. \left. + O(\alpha_{FS}^3) \right) \right) |U_K\rangle \\
&+ \langle U_k | \frac{1}{6} \frac{\Pi_b}{m_0 c} \alpha_b |U_K\rangle
\end{aligned} \tag{203}$$

where the abbreviations  $\xi = \tilde{\omega}_q = \frac{q}{k_C}$  and  $w = \sqrt{1 + \xi^2}$  have been introduced for convenience.

The small correction term in the last line is very important. As will be shown in section 6.3, a consistent renormalization of the bare electron  $m_0$  can only be achieved with this term.

Furthermore, in the derivation of (203), regarding the radial integration variable  $\xi$ , all terms which yield corrections of the order  $O(\tilde{\Omega}_{max}^{-2})$  have been neglected. This will become clear when the integrals are finally evaluated, see (248).

The representation (203) is the final result which can be evaluated as a gradient expansion. For this purpose one first has to replace the Dirac amplitudes  $|U_K\rangle$  by the Newton–Wigner amplitudes  $|U_K^{(NW)}\rangle$  according to (173).

Now first there holds  $\langle U_k^{(NW)} | \alpha_b | U_K^{(NW)} \rangle = 0_{4 \times 4}$ , see (178).

Next, for a constant magnetic induction field there holds  $\left[ \frac{\Pi_a \Pi_a}{2m_0}, \tilde{\mathcal{H}}_{4 \times 4}^{(P,0)} \right] = 0_{4 \times 4}$ . Therefore one finds [7]

$$\mathbb{T} \left( \frac{\Pi_a \Pi_a}{2m_0} \right) \mathbb{T}^\dagger = \frac{\Pi_a \Pi_a}{2m_0} \mathbf{1}_{4 \times 4} + O(\alpha_{FS}^3) \tag{204}$$

Furthermore there holds [7]



$$\mathbb{T} \left( \frac{2}{m_0 c^2} \mathbf{H}_{4 \times 4}^{(P,0)} \right) \mathbb{T}^\dagger = \frac{2}{m_0 c^2} \mathbf{H}_{4 \times 4}^{(P,0)} \quad (205)$$

$$\mathbb{T} \left( \alpha_b \frac{\Pi_b}{m_0 c} \right) \mathbb{T}^\dagger = \frac{\frac{2}{m_0 c^2} \mathbf{H}_{4 \times 4}^{(P,0)} \beta}{\sqrt{\mathbf{1}_{4 \times 4} + \frac{2}{m_0 c^2} \mathbf{H}_{4 \times 4}^{(P,0)}}} \quad (206)$$

and [7]

$$\mathbb{T} \beta \mathbb{T}^\dagger = \frac{1}{\sqrt{\mathbf{1}_{4 \times 4} + \frac{2}{m_0 c^2} \mathbf{H}_{4 \times 4}^{(P,0)}}} \beta \quad (207)$$

The relations (205), (206) and (207) are derived in the end of section B of the appendix.

Putting this together one finally finds for (203) after dropping contributions of the order  $O(\alpha_{FS}^3)$ , [7]

$$\tilde{\mathbb{M}}_{k,K}^{(\perp, e, high)} = \frac{\alpha_{FS}}{\pi} \left( \begin{array}{c} \left\langle U_k^{(NW)} \right| \int_0^{\tilde{\Omega}_{max}} d\xi \left( \begin{array}{c} m_0 c^2 \left( \xi - w + \frac{1}{w} \right) \beta \\ \left( \frac{5}{3} w - \frac{5}{3} \xi - \frac{8}{3w} + \frac{1}{w^3} \right) \mathbf{H}_{4 \times 4}^{(P,0)} \beta \\ + \left( \frac{2}{3} \xi - \frac{2}{3} w + \frac{1}{3w} - \frac{1}{w^5} \right) \frac{\Pi_a \Pi_a}{2m_0} \beta \end{array} \right) \left| U_K^{(NW)} \right\rangle \\ - \left\langle U_k^{(NW)} \right| \frac{1}{3} \mathbf{H}_{4 \times 4}^{(P,0)} \beta \left| U_K^{(NW)} \right\rangle \\ + O(\alpha_{FS}^3) \end{array} \right) \quad (208)$$

In the following subsection the longitudinal part of the renormalization is evaluated.

### 6.1.2 Evaluation of the Longitudinal Contribution to the Renormalization

Recall the form of the longitudinal contribution to the renormalization of the bare mass  $m_0$  and the  $g$ -factor of the fermions (182).

With the definition of the projection operators (307) and the relation  $\mathbf{P}^{(+)} - \mathbf{P}^{(-)} = \frac{\tilde{\mathbf{H}}^{(D)}}{\sqrt{\tilde{\mathbf{H}}^{(D)} \circ \tilde{\mathbf{H}}^{(D)}}}$  derived in section A of the appendix, the definition (193) for the operator valued step function  $\mathbf{C}_q$  one finds [7]

$$\begin{aligned}
\tilde{M}_{k,K}^{(C,e)} &= \left( \frac{q_e^2}{2\varepsilon_0} \right) \int \frac{d^3q}{(2\pi)^3} \frac{1}{|\mathbf{q}|^2} \langle U_k | e^{-iq_a \cdot \hat{x}_a} \circ \mathbf{C}_q \circ \frac{\tilde{\mathbf{H}}^{(D)}}{\sqrt{\tilde{\mathbf{H}}^{(D)} \circ \tilde{\mathbf{H}}^{(D)}}} \circ e^{iq_a \cdot \hat{x}_a} | U_K \rangle \\
&= \left( \frac{q_e^2}{2\varepsilon_0} \right) \int \frac{d^3q}{(2\pi)^3} \frac{1}{|\mathbf{q}|^2} \langle U_k | \mathbf{K}_q \circ \mathbf{R}_q | U_K \rangle
\end{aligned} \tag{209}$$

Here, the abbreviations  $\mathbf{R}_q = e^{-iq_a \cdot \hat{x}_a} \circ \frac{\tilde{\mathbf{H}}^{(D)}}{\sqrt{\tilde{\mathbf{H}}^{(D)} \circ \tilde{\mathbf{H}}^{(D)}}} \circ e^{iq_a \cdot \hat{x}_a}$  and  $\mathbf{K}_q = e^{-iq_a \cdot \hat{x}_a} \circ \mathbf{C}_q \circ e^{iq_a \cdot \hat{x}_a}$  as defined in (594) and (601) have been used. If one symmetrizes (209) with respect to the substitution  $q_b \rightarrow -q_b$  one finds [7]

$$\tilde{M}_{k,K}^{(C,e)} = \left( \frac{q_e^2}{2\varepsilon_0} \right) \int \frac{d^3q}{(2\pi)^3} \frac{1}{|\mathbf{q}|^2} \langle U_k | \left( \frac{\mathbf{K}_q + \mathbf{K}_{-q}}{2} \frac{\mathbf{R}_q + \mathbf{R}_{-q}}{2} + \frac{\mathbf{K}_q - \mathbf{K}_{-q}}{2} \frac{\mathbf{R}_q - \mathbf{R}_{-q}}{2} \right) | U_K \rangle \tag{210}$$

Introducing spheric coordinates according to

$$\left( \frac{q_e^2}{2\varepsilon_0} \right) \int \frac{d^3q}{(2\pi)^3} \frac{1}{|\mathbf{q}|^2} f \left( \frac{q}{k_C} \hat{\mathbf{q}} \right) = m_0 c^2 \frac{\alpha_{FS}}{\pi} \int_0^\infty d\xi \int \frac{d\Omega_{\hat{\mathbf{q}}}}{4\pi} f(\xi \hat{\mathbf{q}}) \tag{211}$$

one can rewrite (210) as [7]

$$\tilde{M}_{k,K}^{(C,e)} = m_0 c^2 \frac{\alpha_{FS}}{\pi} \int_0^{\tilde{\Omega}_{max}} d\xi \langle U_k | \int \frac{d\Omega_{\hat{\mathbf{q}}}}{4\pi} \left( \frac{\mathbf{K}_q + \mathbf{K}_{-q}}{2} \frac{\mathbf{R}_q + \mathbf{R}_{-q}}{2} + \frac{\mathbf{K}_q - \mathbf{K}_{-q}}{2} \frac{\mathbf{R}_q - \mathbf{R}_{-q}}{2} \right) | U_K \rangle \tag{212}$$

Here the integral measure does not depend on the variable  $\xi$  because the introduction of spheric coordinates cancels it. (This is in distinction to the transversal renormalization term, where there is the transversal projector carrying  $\frac{1}{|\mathbf{q}|^2}$ , see (617))

In the appendix section I it is explained in great detail that the symmetric part  $\frac{\mathbf{K}_q + \mathbf{K}_{-q}}{2} \frac{\mathbf{R}_q + \mathbf{R}_{-q}}{2}$  yields the main contribution to the integral, whereas the antisymmetric part  $\frac{\mathbf{K}_q - \mathbf{K}_{-q}}{2} \frac{\mathbf{R}_q - \mathbf{R}_{-q}}{2}$  yields a tiny correction. Therefore, for the symmetric  $\frac{\mathbf{K}_q + \mathbf{K}_{-q}}{2} \frac{\mathbf{R}_q + \mathbf{R}_{-q}}{2}$  one can set  $\frac{\mathbf{K}_q + \mathbf{K}_{-q}}{2} = \Theta_H(\Omega_{max} - \xi)$ , see (605).

With the expansion (599) of  $R_q$ , and with  $\frac{\hbar q_a}{m_0 c} = \xi \hat{q}_a$ , one finds [7]

$$\frac{R_q + R_{-q}}{2} = \begin{cases} \beta \frac{1}{w} \\ + \alpha_a \frac{\Pi_{a'}}{m_0 c} \left( \frac{1}{w} \delta_{a,a'} - \frac{\xi^2}{w^3} \hat{q}_a \hat{q}_{a'} \right) \\ + \beta \frac{3\xi^2}{2w^5} \hat{q}_a \hat{q}_{a'} \frac{\Pi_a \Pi_{a'}}{m_0 c m_0 c} \\ - \frac{1}{w^3} \beta \frac{H_{4 \times 4}^{(P,0)}}{m_0 c^2} \\ + O(\alpha_{FS}^3) \end{cases} \quad (213)$$

Evaluating the angle integrals then [7]

$$\int \frac{d\Omega_{\hat{q}}}{4\pi} \frac{R_q + R_{-q}}{2} = \begin{cases} \beta \frac{1}{w} \\ + \alpha_a \frac{\Pi_a}{m_0 c} \left( \frac{1}{w} - \frac{1}{3} \frac{\xi^2}{w^3} \right) \\ + \frac{1}{m_0 c^2} \frac{\xi^2}{w^5} \frac{\Pi_a \Pi_a}{2m_0} \beta \\ - \frac{1}{w^3} \beta \frac{H_{4 \times 4}^{(P,0)}}{m_0 c^2} \\ + O(\alpha_{FS}^3) \end{cases} \quad (214)$$

Now since  $\frac{1}{w} - \frac{1}{3} \frac{\xi^2}{w^3} = \frac{1}{3w^3} + \frac{2}{3w}$  and  $w = \sqrt{1 + \xi^2}$  one can finally express (212) as [7]

$$\tilde{M}_{k,K}^{(C,e)} = m_0 c^2 \frac{\alpha_{FS}}{\pi} \int_0^{\tilde{\Omega}_{max}} d\xi \langle U_k | \begin{pmatrix} \beta \frac{1}{w} \\ + \left( \frac{1}{3w^3} + \frac{2}{3w} \right) \frac{\Pi_a}{m_0 c} \alpha_a \\ + \frac{1}{m_0 c^2} \frac{\xi^2}{w^5} \frac{\Pi_a \Pi_a}{2m_0} \beta \\ - \frac{1}{w^3} \frac{1}{m_0 c^2} H_{4 \times 4}^{(P,0)} \beta \\ + O(\alpha_{FS}^3) \end{pmatrix} | U_K \rangle \quad (215)$$

This result can now be evaluated as a gradient expansion once the Dirac amplitudes have been replaced for the Newton–Wigner amplitudes according to (173). Then, by again using the relations (205), (206) and (207), and by dropping corrections of the order  $O(\alpha_{FS}^3)$ , one finally finds [7]

$$\tilde{M}_{k,K}^{(C,e)} = \frac{\alpha_{FS}}{\pi} \int_0^{\tilde{\Omega}_{max}} d\xi \langle U_k^{(NW)} | \begin{pmatrix} m_0 c^2 \frac{1}{w} \beta \\ + \frac{\xi^2}{w^5} \frac{\Pi_a \Pi_a}{2m_0} \beta \\ + \left( -\frac{1}{w} + \frac{4}{3w} + \frac{2}{3w^3} - \frac{1}{w^3} \right) H_{4 \times 4}^{(P,0)} \beta \\ + O(\alpha_{FS}^3) \end{pmatrix} | U_K^{(NW)} \rangle \quad (216)$$

Collecting the results for the longitudinal contribution  $\hat{\mathcal{M}}_C^{(e)}$  and the transversal contribution  $\hat{\mathcal{M}}_\perp^{(e)}$  (mainly given by  $\hat{\mathcal{M}}_\perp^{((e),high)}$ , see (208)) one finds for (184) [7]

$$\begin{aligned}\hat{\mathcal{M}}^{(e)} &= \hat{\mathcal{M}}_C^{(e)} + \hat{\mathcal{M}}_\perp^{(e)} = \sum_{k,K} \left( \tilde{\mathcal{M}}_{k,K}^{(C,e)} + \tilde{\mathcal{M}}_{k,K}^{(\perp,e)} \right) \hat{c}_k^\dagger \hat{c}_K \\ &= \sum_{k,K} \left( \tilde{\mathcal{M}}_{k,K}^{(C,e)} + \tilde{\mathcal{M}}_{k,K}^{(\perp,e,high)} \right) \hat{c}_k^\dagger \hat{c}_K\end{aligned}\quad (217)$$

where, by using (208) and (216) [7]

$$\tilde{\mathcal{M}}_{k,K}^{(C,e)} + \tilde{\mathcal{M}}_{k,K}^{(\perp,e,high)} = \frac{\alpha_{FS}}{\pi} \left\langle U_k^{(NW)} \right| \left( \int_0^{\tilde{\Omega}_{max}} d\xi \begin{pmatrix} m_0 c^2 \frac{1}{w} \beta \\ + \frac{\xi^2}{w^5} \frac{\Pi_a \Pi_a}{2m_0} \beta \\ + \left( -\frac{1}{w} + \frac{4}{3w} + \frac{2}{3w^3} - \frac{1}{w^3} \right) \mathbf{H}_{4 \times 4}^{(P,0)} \beta \\ + m_0 c^2 \left( \xi - w + \frac{1}{w} \right) \beta \\ + \left( \frac{5}{3}w - \frac{5}{3}\xi - \frac{8}{3w} + \frac{1}{w^3} \right) \mathbf{H}_{4 \times 4}^{(P,0)} \beta \\ + \left( \frac{2}{3}\xi - \frac{2}{3}w + \frac{1}{3w} - \frac{1}{w^5} \right) \frac{\Pi_a \Pi_a}{2m_0} \beta \end{pmatrix} \right| U_K^{(NW)} \rangle - \left\langle U_k^{(NW)} \right| \frac{1}{3} \mathbf{H}_{4 \times 4}^{(P,0)} \beta \left| U_K^{(NW)} \right\rangle + O(\alpha_{FS}^3)\quad (218)$$

Elementary algebra and the eigenvalue relation  $\beta \left| U_K^{(NW)} \right\rangle = \left| U_K^{(NW)} \right\rangle$  yields [7]

$$\begin{aligned}\tilde{\mathcal{M}}_{k,K}^{(C,e,high)} + \tilde{\mathcal{M}}_{k,K}^{(\perp,e,high)} &= \frac{\alpha_{FS}}{\pi} \left\langle U_k^{(NW)} \right| \left( \begin{aligned} & m_0 c^2 \int_0^{\tilde{\Omega}_{max}} d\xi \left( \frac{1}{w} + \left( \xi - w + \frac{1}{w} \right) \right) \\ & + \left( -\frac{1}{3} + \int_0^{\tilde{\Omega}_{max}} d\xi \left( \begin{aligned} & \frac{\xi^2}{w^5} + \left( \frac{2}{3}\xi - \frac{2}{3}w + \frac{1}{3w} - \frac{1}{w^5} \right) \\ & - \frac{1}{w} + \frac{4}{3w} + \frac{2}{3w^3} - \frac{1}{w^3} \\ & + \frac{5}{3}w - \frac{5}{3}\xi - \frac{8}{3w} + \frac{1}{w^3} \end{aligned} \right) \right) \frac{\Pi_a \Pi_a}{2m_0} \\ & + \left( -\frac{1}{3} + \int_0^{\tilde{\Omega}_{max}} d\xi \left( \begin{aligned} & -\frac{1}{w} + \frac{4}{3w} + \frac{2}{3w^3} - \frac{1}{w^3} \\ & + \frac{5}{3}w - \frac{5}{3}\xi - \frac{2\xi}{w^2} - \frac{8}{3w} + \frac{1}{w^3} \end{aligned} \right) \right) \left( -\frac{g_e \hbar}{2m_0} B_b^{(ext)} \sigma_b \right) \\ & + O(\alpha_{FS}^3) \end{aligned} \right) \beta \left| U_K^{(NW)} \right\rangle\end{aligned}\quad (219)$$

Recalling  $w = \sqrt{1 + \xi^2}$  one can reexpress (219) as [7]

$$\tilde{M}_{k,K}^{(C,e)} + \tilde{M}_{k,K}^{(\perp,e,high)} = \frac{\alpha_{FS}}{\pi} \langle U_k^{(NW)} | \left( \begin{array}{c} m_0 c^2 \int_0^{\tilde{\Omega}_{max}} d\xi F_1(\xi) \\ - \left( \frac{1}{3} + \int_0^{\tilde{\Omega}_{max}} d\xi F_2(\xi) \right) \frac{\Pi_a \Pi_a}{2m_0} \\ + \left( \frac{1}{3} + \int_0^{\tilde{\Omega}_{max}} d\xi F_3(\xi) \right) \frac{q_e \hbar}{2m_0} B_b^{(ext)} \sigma_b \\ + O(\alpha_{FS}^3) \end{array} \right) | U_K^{(NW)} \rangle \quad (220)$$

Where the functions  $F_1(\xi)$ ,  $F_2(\xi)$  and  $F_3(\xi)$ , expressed by the variable  $\xi$  only, are given by [7]

$$\begin{aligned} F_1(\xi) &= \xi - \sqrt{1 + \xi^2} + \frac{2}{\sqrt{1 + \xi^2}} \\ F_2(\xi) &= \xi - \sqrt{1 + \xi^2} + \frac{2}{\sqrt{1 + \xi^2}} - \frac{5}{3(\sqrt{1 + \xi^2})^3} + \frac{2}{(\sqrt{1 + \xi^2})^5} \\ F_3(\xi) &= \frac{5}{3} \left( \xi - \sqrt{1 + \xi^2} \right) + \frac{7}{3\sqrt{1 + \xi^2}} - \frac{2}{3(\sqrt{1 + \xi^2})^3} \end{aligned} \quad (221)$$

As will be shown in the following subsection, if one transforms the Dirac (anti-)matter field  $\hat{\mathcal{H}}_D$  to the Newton–Wigner representation, the bare relativistic Pauli Hamiltonian  $\mathbf{H}_{4 \times 4}^{(P,0)} = \frac{\Pi_b \Pi_b}{2m_0} \mathbf{1}_{4 \times 4} - \frac{q_e \hbar}{2m_0} B_b^{(ext)} \sigma_b$  arises.

It will then become obvious how the renormalization terms  $\tilde{M}_{k,K}^{(C,e)} + \tilde{M}_{k,K}^{(\perp,e,high)}$  match the bare Pauli–Hamiltonian: the first line in (220) matches the rest energy, the second line matches the kinetic energy and the third line matches the Zeeman energy. However, all these terms are weighted by the numerical integrals defined by the functions (221).

In that way the ”true” electron mass  $m_e$  and the “true”, the anomalous  $g$ -factor, arise.

## 6.2 The Dirac (Anti-)Matter Field in the Newton–Wigner Representation

The Dirac (anti-)matter field operator has been introduced in (8) according to

$$\hat{\mathcal{H}}_D = \int d^3r \sum_{\mu, \mu' \in \{1,2,3,4\}} \mathcal{N} \left( \hat{\Psi}_\mu^\dagger(\mathbf{r}) \mathbf{H}_{\mu, \mu'}^{(D)} \hat{\Psi}_{\mu'}(\mathbf{r}) \right) \quad (222)$$

where the Dirac field operators are given by

$$\begin{aligned} \hat{\Psi}_\mu^\dagger(\mathbf{r}) &= \sum_k \left( U_\mu^*(\mathbf{r}; k) \hat{c}_k^\dagger + V_\mu^*(\mathbf{r}; k) \hat{b}_{\tilde{k}} \right) \\ \hat{\Psi}_\mu(\mathbf{r}) &= \sum_k \left( U_\mu(\mathbf{r}; k) \hat{c}_k + V_\mu(\mathbf{r}; k) \hat{b}_{\tilde{k}}^\dagger \right) \end{aligned} \quad (223)$$

Now in section 5 it has been shown that in the Newton–Wigner representation of the Dirac Hamiltonian the amplitudes  $U_\mu(\mathbf{r}; k)$  and  $V_\mu(\mathbf{r}; k)$  can be related to the Schrödinger–Pauli eigenfunctions  $u_\pm^{(SP)}(\mathbf{r}, k)$  describing physics on the atomic length scale [10, 8, 7]

$$\begin{aligned} U_\mu(\mathbf{r}; k) &= \mathbb{T}^\dagger U_\mu^{(NW)}(\mathbf{r}; k) \\ V_\mu(\mathbf{r}; k) &= \mathbb{T}^\dagger V_\mu^{(NW)}(\mathbf{r}; k) \end{aligned} \quad (224)$$

with

$$\begin{aligned} U_\mu^{(NW)}(\mathbf{r}; k) &= \begin{pmatrix} u_+^{(SP)}(\mathbf{r}, k) \\ u_-^{(SP)}(\mathbf{r}, k) \\ 0 \\ 0 \end{pmatrix}_\mu \\ V_\mu^{(NW)}(\mathbf{r}; k) &= \begin{pmatrix} 0 \\ 0 \\ u_+^{(SP)}(\mathbf{r}, k) \\ u_-^{(SP)}(\mathbf{r}, k) \end{pmatrix}_\mu \end{aligned} \quad (225)$$

For the goal of deducing the nonrelativistic Hamiltonian of light–matter interaction from the QED Hamiltonian this is *absolutely essential*, because one can now express the Dirac amplitudes in (222) in the Newton–Wigner representation according to (224).

Therefore, the Newton–Wigner field operators  $\Phi_\mu(\mathbf{r})$  can be defined with the help of the Eriksen transformation  $\mathbb{T}$  according to [10, 8, 7]

$$\Phi_\mu(\mathbf{r}) = (\mathbb{T})_{\nu,\mu} \hat{\Psi}_\mu(\mathbf{r}) = \begin{pmatrix} \hat{\psi}_+(\mathbf{r}) \\ \hat{\psi}_-(\mathbf{r}) \\ \hat{\chi}_+(\mathbf{r}) \\ \hat{\chi}_-(\mathbf{r}) \end{pmatrix}_\mu \quad (226)$$

and [10, 8, 7]

$$\Phi_\mu^\dagger(\mathbf{r}) = \left( \hat{\psi}_+^\dagger(\mathbf{r}), \hat{\psi}_-^\dagger(\mathbf{r}), \hat{\chi}_+(\mathbf{r}), \hat{\chi}_-(\mathbf{r}) \right)_\mu \quad (227)$$

Now the relation between the Schrödinger–Pauli amplitudes  $u_\pm^{(SP)}(\mathbf{r}, k)$  and the field operator  $\hat{\psi}_s(\mathbf{r})$  and  $\hat{\chi}_s(\mathbf{r})$  of many–body physics for electrons and positrons separately is as follows:

$$\begin{aligned} \hat{\psi}_s(\mathbf{r}) &= \sum_k u_s^{(SP)}(\mathbf{r}, k) \hat{c}_k \\ \hat{\psi}_s^\dagger(\mathbf{r}) &= \sum_k u_s^{*(SP)}(\mathbf{r}, k) \hat{c}_k^\dagger \end{aligned} \quad (228)$$

$$\begin{aligned} \hat{\chi}_s^\dagger(\mathbf{r}) &= \sum_k u_s^{(SP)}(\mathbf{r}, \tilde{k}) \hat{b}_{\tilde{k}}^\dagger \\ \hat{\chi}_s(\mathbf{r}) &= \sum_{\tilde{k}} u_s^{*(SP)}(\mathbf{r}, \tilde{k}) \hat{b}_{\tilde{k}} \end{aligned} \quad (229)$$

Using the properties (172) of the VONS  $u_\pm^{(SP)}(\mathbf{r}, k)$  there readily follows

$$\begin{aligned} \left\{ \hat{\psi}_s(\mathbf{r}), \hat{\psi}_{s'}(\mathbf{r}') \right\} &= \hat{0} = \left\{ \hat{\psi}_s^\dagger(\mathbf{r}), \hat{\psi}_{s'}^\dagger(\mathbf{r}') \right\} \\ \left\{ \hat{\psi}_s(\mathbf{r}), \hat{\psi}_{s'}^\dagger(\mathbf{r}') \right\} &= \sum_k u_s^{(SP)}(\mathbf{r}, k) u_{s'}^{*(SP)}(\mathbf{r}', k) \\ &= \delta_{s,s'} \delta^{(3)}(\mathbf{r} - \mathbf{r}') \hat{1} \end{aligned} \quad (230)$$

As well as for the positron field operators  $\hat{\chi}_s(\mathbf{r})$ .

With the Eriksen transformation  $\mathbb{T}$ , the Newton–Wigner amplitudes (226) and (227), and the properties (230) one can readily write for (222)

$$\begin{aligned}
\hat{\mathcal{H}}_D &\stackrel{NW}{=} \int d^3r \sum_{\mu, \mu' \in \{1,2,3,4\}} \mathcal{N} \left( \hat{\Psi}_{\mu'}^\dagger(\mathbf{r}) \left( (\mathbb{T})_{\mu', \mu''}^\dagger \right) (\mathbb{T})_{\mu'', \mu} \mathbf{H}_{\mu, \mu'}^{(D)} \left( \left( (\mathbb{T})_{\mu', \nu'}^\dagger \right) (\mathbb{T})_{\nu', \nu} \right) \hat{\Psi}_\nu(\mathbf{r}) \right) \\
&= \int d^3r \mathcal{N} \left( \Phi_{\mu''}^\dagger(\mathbf{r}) \left( (\mathbb{T})_{\mu'', \mu} \mathbf{H}_{\mu, \mu'}^{(D)} \left( (\mathbb{T})_{\mu', \nu'}^\dagger \right) \right) \Phi_{\nu'}(\mathbf{r}) \right) \\
&= \int d^3r \mathcal{N} \left( \Phi_{\mu''}^\dagger(\mathbf{r}) \mathbf{H}_{\mu'', \nu'}^{(NW)} \Phi_{\nu'}(\mathbf{r}) \right) \\
&= \int d^3r \mathcal{N} \left( \Phi_{\mu''}^\dagger(\mathbf{r}) \left( m_0 c^2 \beta \circ \sqrt{\mathbf{1}_{4 \times 4} + \frac{2}{m_0 c^2} \mathbf{H}_{4 \times 4}^{(P,0)}} \right)_{\mu'', \nu'} \Phi_{\nu'}(\mathbf{r}) \right)
\end{aligned} \tag{231}$$

Since  $\beta$  and  $\mathbf{H}_{4 \times 4}^{(P,0)}$  commute there follows for electrons and positrons separately

$$\hat{\mathcal{H}}_D = m_0 c^2 \int d^3r \mathcal{N} \left( \begin{array}{c} \hat{\psi}_s^\dagger(\mathbf{r}) \left( \sqrt{\mathbf{1}_{4 \times 4} + \frac{2}{m_0 c^2} \mathbf{H}_{4 \times 4}^{(P,0)}} \right)_{s, s'} \hat{\psi}_{s'}(\mathbf{r}) \\ - \hat{\chi}_s(\mathbf{r}) \left( \sqrt{\mathbf{1}_{4 \times 4} + \frac{2}{m_0 c^2} \mathbf{H}_{4 \times 4}^{(P,0)}} \right)_{s, s'} \hat{\chi}_{s'}^\dagger(\mathbf{r}) \end{array} \right) \tag{232}$$

Partial integration in the second line yields

$$\hat{\mathcal{H}}_D = m_0 c^2 \int d^3r \mathcal{N} \left( \begin{array}{c} \hat{\psi}_s^\dagger(\mathbf{r}) \left( \sqrt{\mathbf{1}_{4 \times 4} + \frac{2}{m_0 c^2} \mathbf{H}_{4 \times 4}^{(P,0)}} \right)_{s, s'} \hat{\psi}_{s'}(\mathbf{r}) \\ - \left( \left( \sqrt{\mathbf{1}_{4 \times 4} + \frac{2}{m_0 c^2} \left( \mathbf{H}_{4 \times 4}^{(P,0)} \right)^\star} \right)_{s, s'} \hat{\chi}_s(\mathbf{r}) \right) \hat{\chi}_{s'}^\dagger(\mathbf{r}) \end{array} \right) \tag{233}$$

And using the normal ordering rule then

$$\begin{aligned}
\hat{\mathcal{H}}_D &= m_0 c^2 \int d^3r \left( \begin{array}{c} \hat{\psi}_s^\dagger(\mathbf{r}) \left( \sqrt{\mathbf{1}_{4 \times 4} + \frac{2}{m_0 c^2} \mathbf{H}_{4 \times 4}^{(P,0)}} \right)_{s, s'} \hat{\psi}_{s'}(\mathbf{r}) \\ + \hat{\chi}_{s'}^\dagger(\mathbf{r}) \left( \sqrt{\mathbf{1}_{4 \times 4} + \frac{2}{m_0 c^2} \left( \mathbf{H}_{4 \times 4}^{(P,0)} \right)^\star} \right)_{s, s'} \hat{\chi}_s(\mathbf{r}) \end{array} \right) \\
&\equiv \hat{\mathcal{H}}_D^{(el)} + \hat{\mathcal{H}}_D^{(p)}
\end{aligned} \tag{234}$$

where



$$\begin{aligned}\hat{\psi}_\sigma^\dagger(\mathbf{r}) &= \left( \hat{\psi}_+^\dagger(\mathbf{r}), \hat{\psi}_-^\dagger(\mathbf{r}), 0, 0 \right)_\sigma \\ \hat{\chi}_{\sigma'}^\dagger(\mathbf{r}) &= \left( 0, 0, \hat{\chi}_+^\dagger(\mathbf{r}), \hat{\chi}_-^\dagger(\mathbf{r}) \right)_{\sigma'}\end{aligned}\quad (235)$$

Furthermore, there holds

$$\Pi_b^* = - \left( \frac{\hbar}{i} \nabla_b + q_e A_b(\mathbf{r}) \right) \quad (236)$$

And for the positron contribution please recognize  $(\sigma_b)_{s,s'} = -(\sigma_y \sigma_b \sigma_y)_{s',s}$

However, in the following, only the electron part is discussed.

$$\hat{\mathcal{H}}_D^{(el)} = m_0 c^2 \int d^3r \left( \hat{\psi}_s^\dagger(\mathbf{r}) \left( \sqrt{\mathbf{1}_{2 \times 2} + \frac{2}{m_0 c^2} \mathbf{H}_{2 \times 2}^{(P,0)}} \right)_{s,s'} \hat{\psi}_{s'}(\mathbf{r}) \right) \quad (237)$$

The positron Hamiltonian  $\hat{\mathcal{H}}_{LM}^{(pos)}$  principally results from the charge conjugation symmetry operation  $\hat{\mathcal{C}}_F$  introduced in [F](#).

$$\hat{\mathcal{H}}_{LM}^{(pos)} = \hat{\mathcal{C}}_F \circ \left( \hat{\mathcal{H}}_{LM}^{(el)} \right) \circ \hat{\mathcal{C}}_F^\dagger \quad (238)$$

For gaining all the finestructure corrections one has to expand the square root according to

$$m_0 c^2 \sqrt{\mathbf{1}_{4 \times 4} + \frac{2}{m_0 c^2} \mathbf{H}_{4 \times 4}^{(P,0)}} = m_0 c^2 \mathbf{1}_{4 \times 4} + \mathbf{H}_{4 \times 4}^{(P,0)} - \frac{1}{2} \frac{1}{m_0 c^2} (\mathbf{H}_{4 \times 4}^{(P,0)})^2 + \dots \quad (239)$$

The third term in [\(239\)](#) contains the first relativistic correction to the kinetic energy of the electron, the famous finestructure correction  $-\frac{1}{2} \frac{\Pi_a^4}{(2m_0 c)^2}$ . The other terms contained in  $(\mathbf{H}_{4 \times 4}^{(P,0)})^2$  can be neglected since the one being proportional to  $\hat{\Pi}_a B_b^{(ext)}$  is a (small) gradient term, and the square of the Zeeman-Term is even smaller than this gradient term.

Hence, the nonrelativistic second quantized Hamiltonian  $\hat{\mathcal{H}}_D^{(el)}$  for the electrons (matter) is given by

$$\hat{\mathcal{H}}_D^{(el)} = \begin{cases} \hat{\psi}_s^\dagger(\mathbf{r}) m_0 c^2 \hat{\psi}_s(\mathbf{r}) + \hat{\psi}_s^\dagger(\mathbf{r}) \left( \mathbf{H}_{4 \times 4}^{(P,0)} \right)_{s,s'} \hat{\psi}_{s'}(\mathbf{r}) \\ -\hat{\psi}_s^\dagger(\mathbf{r}) \left( \frac{1}{8} \frac{1}{m_0^3 c^2} \left( \hat{\Pi}_b \right)^4 \right) \hat{\psi}_s(\mathbf{r}) \end{cases} \quad (240)$$

The relativistic bare Pauli Hamiltonian  $\mathbf{H}_{4 \times 4}^{(P,0)}$  is given by

$$\mathbf{H}_{4 \times 4}^{(P,0)} = \frac{\Pi_a \Pi_a}{2m_0} \hat{1} 4 \times 4 - \frac{q_e \hbar}{2m_0} \frac{1}{2} \sigma_b B_b^{(ext)} \quad (241)$$

(see (158)). From this one finally finds

$$\hat{\mathcal{H}}_D^{(el)} = \begin{cases} \hat{\psi}_s^\dagger(\mathbf{r}) m_0 c^2 \hat{\psi}_s(\mathbf{r}) + \hat{\psi}_s^\dagger(\mathbf{r}) \left( \frac{\Pi_b \Pi_b}{2m_0} - \frac{1}{8} \frac{1}{m_0^3 c^2} \left( \hat{\Pi}_b \right)^4 \right)_{s,s'} \hat{\psi}_{s'}(\mathbf{r}) \\ -\hat{\psi}_s^\dagger(\mathbf{r}) \left( \frac{q_e \hbar}{2m_0} B_b^{(ext)} \sigma_b \right)_{s,s'} \hat{\psi}_{s'}(\mathbf{r}) \end{cases} \quad (242)$$

This is a  $4 \times 4$  matrix operator with only one entry in the upper block, whereas all other blocks are empty. The total Hamiltonian  $\hat{\mathcal{H}}_D = \hat{\mathcal{H}}_D^{(el)} + \hat{\mathcal{H}}_D^{(p)}$ , see (234), comprises  $\hat{\mathcal{H}}_D^{(el)}$  in the first component, and  $\hat{\mathcal{H}}_D^{(pos)}$  in the fourth component, hence  $\hat{\mathcal{H}}_D$  is blockdiagonal.

In the following subsection the effective Schrödinger–Pauli Hamiltonian for a plurality of electrons is derived by putting the results for the renormalization terms (220) and the bare electron Hamiltonian (242) together.

### 6.3 The Effective Schrödinger–Pauli Hamiltonian and the Justification of the Physical Cut–Off

T. Welton estimated in 1948 the anomalous  $g$ –factor by considerations regarding the nonrelativistic equation of motion of the angular momentum operator. He calculated the expectation value of its dynamics with respect to the electromagnetic vacuum. The latter is well–known to fluctuate, meaning that the square of the electric field component  $E$  and the magnetic field component  $B$  of the radiation field do not vanish in the vacuum state,  $\langle 0 | E^2 | 0 \rangle \neq 0$ . Associating these “fluctuation corrections” to the intrinsic magnetic moment of

the electron he found that their order of magnitude is “nearly correct” with respect to the Schwinger result  $g - 2 = \frac{\alpha_{FS}}{\pi}$  (the anomalous magnetic moment). Unfortunately, however, proceeding in this way, Welton received the wrong sign, he found that  $g - 2 < 0$  is negative [48].

As will be shown in this subsection, the derivation of the anomalous magnetic moment  $g$  on the basis of the flow equation unitarily transforming the QED Hamiltonian makes it clear that it is the mass renormalization which causes the anomalous magnetic moment of the fermions. The mass renormalization, on the other side, is caused by elimination of the transversal QED interaction (the interaction of matter and antimatter fields with high energy photons) and additionally by the elimination of the pair terms in the longitudinal interaction (the QED Coulomb interaction).

In the sections 6.1.1 and 6.1.2 the renormalization terms  $\tilde{M}_{k,K}^{(\perp,e)}$  and  $\tilde{M}_{k,K}^{(C,e)}$  were evaluated in such a way that only terms in agreement with the order of the solution of the flow equation were considered or retained. Therefore, the results for the renormalization terms include terms up to order  $\alpha_{FS}^2$ , see (220).

The resulting renormalization contributions (220) comprise the functions

$F_1(\xi)$ ,  $F_2(\xi)$ ,  $F_3(\xi)$  defined in (221). These functions, once the radial integral  $d\xi$  has been evaluated, give numerical weights to the rest energy, the kinetic energy and the Zeeman energy.

For the evaluation of the renormalization terms the assumption has been made that the cut-off  $\tilde{\Omega}_{max}$  is large,  $\tilde{\Omega}_{max} \gg 1$  (see (187)), implying that one can consider a wide range of photon modes. As will be justified in this subsection, assuming  $\tilde{\Omega}_{max} \gg 1$  is only possible because the integrals of the functions  $F_1(\xi)$ ,  $F_2(\xi)$ ,  $F_3(\xi)$  give

**logarithmic** results for the renormalization. This means that  $\ln \tilde{\Omega}_{max}$  is a small number, especially if it is again multiplied by the finestructure constant  $\alpha_{FS}$ . From equation (244) one can thus see that the difference between the bare mass  $m_0$  and the “true” electron mass  $m_e$  is small, of the order  $\alpha_{FS} \sim \frac{1}{137}$ , and also the difference between the bare  $g$ -factor and the “true”, anomalous  $g$ -factor.

Now, as has been shown in subsection 6.2, the bare Schrödinger–Pauli Hamiltonian  $\hat{\mathcal{H}}_D^{(el)}$  for a many–electron system interacting with

an external magnetic induction field is given by

$$\hat{\mathcal{H}}_D^{(el)} = \begin{cases} \hat{\psi}_s^\dagger(\mathbf{r}) m_0 c^2 \hat{\psi}_s(\mathbf{r}) + \hat{\psi}_s^\dagger(\mathbf{r}) \left( \frac{\Pi_b \Pi_b}{2m_0} - \frac{1}{8} \frac{1}{m_0^3 c^2} \left( \hat{\Pi}_b \right)^4 \right) \hat{\psi}_{s'}(\mathbf{r}) \\ - \hat{\psi}_s^\dagger(\mathbf{r}) \left( \frac{q_e \hbar}{2m_0} B_b^{(ext)} \sigma_b \right) \hat{\psi}_{s'}(\mathbf{r}) \end{cases}_{s,s'} \quad (243)$$

Adding the renormalization terms (220) to (243) one finds the effective Schrödinger–Pauli Hamiltonian in second quantization as

$$\hat{\mathcal{H}}_{SP}^{(el)} \equiv \hat{\mathcal{H}}_D^{(el)} + \tilde{\mathcal{M}}_{k,K}^{(C,e)} + \tilde{\mathcal{M}}_{k,K}^{(\perp,e)}$$

$$= \int d^3 r \hat{\psi}_s^\dagger(\mathbf{r}) \begin{pmatrix} \left( 1 + \frac{\alpha_{FS}}{\pi} \int_0^{\tilde{\Omega}_{max}} d\xi F_1(\xi) \right) \delta_{s,s'} m_0 c^2 \\ + \left( 1 - \frac{\alpha_{FS}}{\pi} \left( \frac{1}{3} + \int_0^{\tilde{\Omega}_{max}} d\xi F_2(\xi) \right) \right) \delta_{s,s'} \left( \frac{\Pi_b \Pi_b}{2m_0} \right) \\ - \left( 1 - \frac{\alpha_{FS}}{\pi} \left( \frac{1}{3} + \int_0^{\tilde{\Omega}_{max}} d\xi F_3(\xi) \right) \right) \left( \frac{q_e \hbar}{2m_0} B_b^{(ext)} \sigma_b \right)_{s,s'} \\ - \frac{1}{8} \frac{1}{m_0^3 c^2} \left( \hat{\Pi}_b \right)^4 \delta_{s,s'} \\ + O(\alpha_{FS}^3) \end{pmatrix} \hat{\psi}_{s'}(\mathbf{r}) \quad (244)$$

First, for the Zeeman term in the third line there has to hold [7, 8]

$$\frac{m_e}{m_0} \left( 1 - \frac{\alpha_{FS}}{\pi} \left( \frac{1}{3} + \int_0^{\tilde{\Omega}_{max}} d\xi F_3(\xi) \right) \right) \equiv \frac{g}{2} \quad (245)$$

such that the mass renormalization corrects the result  $g = 2$  following from the Dirac theory of the electron.

Second, for a physically coherent picture it is required that the bare rest mass term and the bare kinetic mass term are renormalized consistently. This means that the constant  $C_1$  belonging to the integral of the function  $F_1(\xi)$  and the constant  $C_2$  belonging to the integral of the function  $F_2(\xi)$  are equal. The physical cut-off (187) indeed yields such a consistent renormalization: for the renormalization of the bare rest mass  $m_0$  term one finds [7]

$$m_e c^2 = m_0 c^2 \left( 1 + \frac{\alpha_{FS}}{\pi} \int_0^{\tilde{\Omega}_{max}} d\xi F_1(\xi) \right) \quad (246)$$

And for the kinetic mass term [7]

$$\frac{1}{m_e} = \frac{1}{m_0} \left( 1 - \frac{\alpha_{FS}}{\pi} \left( \frac{1}{3} + \int_0^{\tilde{\Omega}_{max}} d\xi F_2(\xi) \right) \right) \quad (247)$$

Evaluating the integrals yields [7]

$$\begin{aligned} \int_0^{\tilde{\Omega}_{max}} d\xi F_1(\xi) &= \frac{3}{2} \ln \tilde{\Omega}_{max} + C_1 + O\left(\frac{1}{\Omega_{max}^2}\right) \\ \frac{1}{3} + \int_0^{\tilde{\Omega}_{max}} d\xi F_2(\xi) &= \frac{3}{2} \ln \tilde{\Omega}_{max} + C_2 + O\left(\frac{1}{\Omega_{max}^2}\right) \\ \frac{1}{3} + \int_0^{\tilde{\Omega}_{max}} d\xi F_3(\xi) &= \frac{3}{2} \ln \tilde{\Omega}_{max} + C_3 + O\left(\frac{1}{\Omega_{max}^2}\right) \end{aligned} \quad (248)$$

where the constants are given by [7]

$$\begin{aligned} C_1 &= -\frac{1}{4} + \frac{3}{2} \ln(2) \\ C_2 &= \frac{1}{3} - \frac{7}{12} + \frac{3}{2} \ln(2) = -\frac{1}{4} + \frac{3}{2} \ln 2 \equiv C_1 \\ C_3 &= \frac{1}{3} - \frac{13}{12} + \frac{3}{2} \ln(2) = -\frac{3}{4} + \frac{3}{2} \ln 2 \end{aligned} \quad (249)$$

Now using (246) and (247) one finds for the anomalous  $g$ -factor [7]

$$\begin{aligned} g &= 2 \frac{m_e}{m_0} \left( 1 - \frac{\alpha_{FS}}{\pi} \left( \frac{1}{3} + \int_0^{\tilde{\Omega}_{max}} d\xi F_3(\xi) \right) \right) \\ &= 2 \frac{1 - \frac{\alpha_{FS}}{\pi} \left( \frac{1}{3} + \int_0^{\tilde{\Omega}_{max}} d\xi F_3(\xi) \right)}{1 - \frac{\alpha_{FS}}{\pi} \left( \frac{1}{3} + \int_0^{\tilde{\Omega}_{max}} d\xi F_2(\xi) \right)} \\ &= 2 \left( 1 + \frac{\alpha_{FS}}{\pi} \int_0^{\tilde{\Omega}_{max}} d\xi (F_2(\xi) - F_3(\xi)) + O\left(\frac{\alpha_{FS}}{\pi}\right)^2 \right) \\ &= 2 + \frac{\alpha_{FS}}{\pi} + O\left(\frac{\alpha_{FS}}{\pi}\right)^2 \end{aligned} \quad (250)$$

This is the Schwinger result [17, 49] (“trumpets please” [35]).

Similar calculations of Cohen–Tannoudji et al. [50] also yield the Schwinger result of  $g$ . In their work they evaluate matrix elements considering effectively a one–electron problem. They derive the following numerical values for the constants (249)

$$\begin{aligned} C_1^* &= \frac{3}{2} \ln(2) - \frac{1}{4} \\ C_2^* &= \frac{3}{2} \ln(2) - \frac{7}{12} \\ C_3^* &= \frac{3}{2} \ln(2) - \frac{13}{12} \end{aligned} \quad (251)$$

As can be seen,  $C_1^* \neq C_2^*$ . However, since the anomalous magnetic moment is given by the difference  $C_2^* - C_3^*$  from the difference of the integrals  $\int d\xi (F_2(\xi(q)) - F_3(\xi(q)))$ , they also derive the Schwinger result for  $g$ :

$$C_2^* - C_3^* = \frac{1}{2} = C_2 - C_3 \quad (252)$$

The constants  $C_2^*$  and  $C_2$ , and  $C_3^*$  and  $C_3$  differ by the factor  $\frac{1}{3}$ . It is this small correction which yields  $C_1 \equiv C_2$ ! Regarding the calculations presented here, the constants  $C_2$  and  $C_3$  contain the factor  $\frac{1}{3}$  because of a different choice for the cut-off. Here, both the photon energy and the fermion energy have been truncated, which leads to the small correction term  $-\left\langle U_k^{(NW)} \left| \frac{1}{3} \mathbf{H}_{4 \times 4}^{(P,0)} \beta \right| U_K^{(NW)} \right\rangle$  in the high–energy photon renormalization contribution (208)! This is in sharp contradistinction the the cut-off chosen by Cohent–Tannoudji et. al. who truncate the photons energy only. This also yields the correct Schwinger result, however, the renormalization of the bare electron mass  $m_0$  is not consistent because  $C_1^* \neq C_2^*$ .

Cohen–Tannoudji et. al argue that such a consistent renormalization of the bare electron mass  $m_0$  can only be achieved by a covariant cut-off procedure. Here it has been shown that the physical cut-off (187) which truncates both the photons energy and the fermions kinetic energy gives both the renormalization of the  $g$ –factor (250) and a consistent renormalization of the rest mass term and the kinetic energy mass term. It has to be emphasized that, if one only truncates the photon energy  $\tilde{\omega}_q$  and lets the fermions move arbitrarily fast, such

that their kinetic energy  $\tilde{E}_k$  is arbitrarily high, this is physically inconsistent. It is important to treat all constituents of the QED soup on equal footing. This inconsistency is reflected by the fact that with such a calculation the mass occurring in the rest energy term and the mass occurring in the kinetic energy term are being renormalized differently, meaning that the constants  $C_1^*$  and  $C_2^*$  are different. The physical (not covariant) cut-off (253) provides a small correction  $\frac{1}{3}$  such that  $C_1 = C_2$  holds true!

From graph 2 one can see that it is the photons beneath the Compton wavelength  $\lambda_C$  which contribute to the renormalization of the  $g$ -factor: the main contribution comes from photons with wave numbers between  $\frac{q\lambda_C}{2\pi} \approx 0.05$  and  $\frac{q\lambda_C}{2\pi} \approx 1$ . Hence, it is not the ultrarelativistic photons which cause the correct sign of the anomalous magnetic moment [50]. Please recognize that only the photons with wave numbers  $q > q_B = \frac{2\pi}{a_B}$  have been eliminated, but *all* photons from  $q\lambda_C = 0$  to  $q\lambda_C \gg 1$  contribute to the renormalization of  $g$ . However, the photons relevant for light-matter interactions, those with  $q \sim q_B$  and lower provide a relatively small weight in the integral shown in 2 (the red arrow and below). Please recognize that the contribution to the renormalization from photons with wave numbers  $q \gtrsim \frac{1}{\lambda_C}$  is even negative, hence, UV photons and X-ray photons *reduce* the  $g$ -factor.

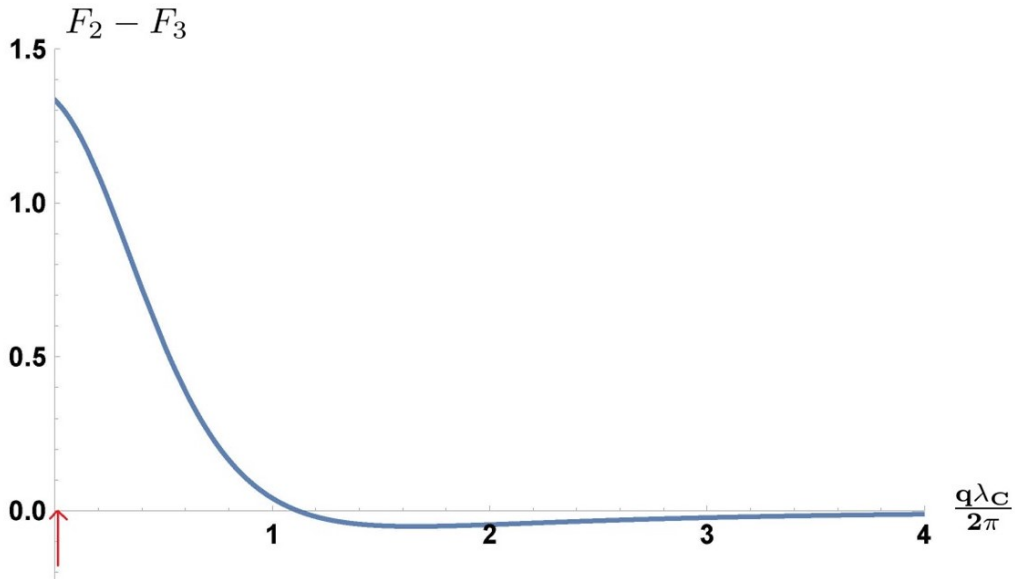


Figure 2: Photons contributing to  $\frac{g-2}{2} = \frac{\alpha_{FS}}{2\pi}$ . The red arrow indicates the starting point of the wave number range  $q > q_B = \frac{1}{a_B}$  of the photons which have been eliminated by the generator  $\hat{\eta}^{(LM)}(s)$ . This corresponds to a numerical value  $\frac{q_B\lambda_C}{2\pi} = \frac{\lambda_C}{2\pi a_B} = \frac{2.4 \cdot 10^{-12} \text{m}}{2\pi \cdot 5.3 \cdot 10^{-11} \text{m}} \approx 0.01$ . Adapted from [7].

Having discussed these aspects the choice of the cut-off (187) according to [7]

$$\begin{aligned}\tilde{\omega}_q + \tilde{E}_k &< 2\tilde{\Omega}_{max} \\ \tilde{\Omega}_{max} &\gg 1 \\ 1 &\ll \tilde{\Omega}_{max} \ll e^{137}\end{aligned}\tag{253}$$

is now justified. The choice  $\tilde{\omega}_q + \tilde{E}_k < 2\tilde{\Omega}_{max}$  gives a consistent renormalization of the bare mass  $m_0$ , and the choice  $\tilde{\Omega}_{max} \gg 1$ , which guarantees that the main contribution to the renormalization in 2 is included, is possible because of the logarithmic nature of the integrals.

For example, the cut-off  $\tilde{\Omega}_{max} = e^{137}$  is “a huge number” [50] which sets up a large range for photon wave numbers for which the renormalization procedure is still physically sensible, because in that case  $\frac{\alpha_{FS}}{\pi} \ln \tilde{\Omega}_{max} < 1$ . On the other hand, for  $\tilde{\Omega}_{max} = 1$  corresponding to  $q = \frac{2\pi}{\lambda_C}$  in figure 2 the renormalization of the bare fermion mass is still mostly included.

Altogether, the effective Schrödinger–Pauli Hamiltonian  $\hat{\mathcal{H}}_{SP}^{(el)}$  in (244) is given by inserting the numerical results (248) and (249) for the integrals. This yields [7]

$$\hat{\mathcal{H}}_{SP}^{(el)} = \int d^3r \hat{\psi}_s^\dagger(\mathbf{r}) \begin{pmatrix} m_e c^2 + \frac{\Pi_b \Pi_b}{2m_e} - \frac{1}{8} \frac{1}{m_e^3 c^2} \left( \hat{\Pi}_b \right)^4 \\ - \left( 2 + \frac{\alpha_{FS}}{\pi} \right) \left( \frac{q_e \hbar}{2m_e} B_b^{(ext)} \sigma_b \right)_{s,s'} \\ + O(\alpha_{FS}^3) \end{pmatrix} \hat{\psi}_{s'}(\mathbf{r}) \tag{254}$$

Here, in the term of the relativistic correction to the kinetic energy,  $m_0$  has been replaced by  $m_e$ , because a correction to this term occurs only in higher order perturbation theory. However, the error is of order  $\alpha_{FS}^3$ , as can be seen from equation (247).



## 6.4 The Effective Interaction Terms

In this section the effective interactions are evaluated. For doing this one has to calculate matrix elements as a gradient expansion once the Dirac amplitudes have been replaced by the Newton–Wigner amplitudes. This is possible because the Newton–Wigner amplitudes are slowly varying functions on the length scale of the Bohr radius. For the evaluation of the first order effective interaction  $\hat{\mathcal{H}}_{\perp}^{(low,0)}$ , the coupling of the matter fields to the low–energy photons, as well as for the second order effective transversal interaction  $\hat{\mathcal{V}}_{\perp,ee}$  it is necessary to evaluate matrix elements of the form  $\langle U_k^{(NW)} | \mathbb{T} \circ \alpha_b \circ e^{\pm i q_a x_a} \mathbb{T}^\dagger | U_{k'}^{(NW)} \rangle$ . For the second order effective longitudinal interactions, the effective Coulomb interaction  $\hat{\mathcal{U}}_C^{(0)}$  between the matter fields and the coupling of the matter fields an external source  $\hat{\mathcal{V}}_{ext}^{(0)}$ , it is necessary to evaluate matrix elements  $\langle U_k^{(NW)} | \mathbb{T} e^{\pm i q_a x_a} \mathbb{T}^\dagger | U_{k'}^{(NW)} \rangle$ . Proceeding in this way one has to be careful to keep all orders  $\alpha_{FS}^2$  and neglect higher order corrections.

The matrix elements of a functional  $F_{\mu',\mu}(\mathbf{x}, \mathbf{p})$  depending on the abstract operators  $\mathbf{x}_a$  and  $\mathbf{p}_b$  with the commutator  $[\mathbf{p}_b, \mathbf{x}_a] = \frac{\hbar}{i} \delta_{a,b} \mathbf{1}$  are given by

$$\begin{aligned} & \langle U_K^{(NW)} | F_{4 \times 4}(\mathbf{x}, \mathbf{p}) | U_k^{(NW)} \rangle \\ &= \sum_{\mu} \int d^3 r \left( U_{\mu}^{(NW)}(\mathbf{r}, K) \right)^* \left( F_{\mu,\mu'} \left( \mathbf{r}, \frac{\hbar}{i} \nabla \right) U_{\mu'}^{(NW)}(\mathbf{r}, k) \right) \end{aligned} \quad (255)$$

see [7, 51]. In the last line the agreement has been made that the gradient  $\nabla$  shall operator on the function  $U_{\mu'}^{(NW)}(\mathbf{r}, k)$  to the right. A deeper justification can be found in the appendix C.

As has been shown in section 5, the Eriksen transformation  $\mathbb{T}$  is a functional of the operator  $\Pi$ , hence  $\mathbb{T} = \mathbb{T}(\Pi)$ , see (155). Therefore there holds for the operator  $\mathbb{T} \circ e^{\pm i q_a x_a} \circ \mathbb{T}^\dagger$  [7]

$$\begin{aligned} \mathbb{T} \circ e^{\pm i q_a x_a} \circ \mathbb{T}^\dagger &= e^{\pm i q_a \hat{x}_a} \circ \left( e^{\mp i q_a \hat{x}_a} \circ \mathbb{T}(\Pi) \circ e^{\pm i q_a \hat{x}_a} \right) \circ \mathbb{T}^\dagger(\Pi) \\ &= e^{\pm i q_a \hat{x}_a} \circ \mathbb{T}(\Pi \pm \hbar \mathbf{q}) \circ \mathbb{T}^\dagger(\Pi) \end{aligned} \quad (256)$$

Since the operators  $\mathbb{T}^\dagger(\Pi)$  and  $\mathbb{T}(\Pi \pm \hbar \mathbf{q})$  act on the slowly varying functions  $U_\mu^{(NW)}(\mathbf{r}, k)$  of  $\mathbf{H}_{4 \times 4}^{(P,0)}$ , see (173) and (174), one can evaluate (256) by expanding it with respect to the gauge invariant momentum operator  $\Pi_b$ . Up to the order  $\alpha_{FS}^2$  there follows [7]

$$\begin{aligned}
\mathbb{T}(\Pi) &= \mathbf{1}_{4 \times 4} - \frac{1}{4} \frac{\frac{\Pi_b \Pi_b}{2m_0} \mathbf{1}_{4 \times 4} - \frac{q_e \hbar}{2m_0} B_b^{(ext)} \sigma_b}{m_0 c^2} + \frac{\beta}{2} \alpha_b \frac{\Pi_b}{m_0 c} + O(\alpha_{FS}^3) \\
\mathbb{T}^\dagger(\Pi) &= \mathbf{1}_{4 \times 4} - \frac{1}{4} \frac{\frac{\Pi_b \Pi_b}{2m_0} \mathbf{1}_{4 \times 4} - \frac{q_e \hbar}{2m_0} B_b^{(ext)} \sigma_b}{m_0 c^2} - \frac{\beta}{2} \alpha_b \frac{\Pi_b}{m_0 c} + O(\alpha_{FS}^3) \\
\mathbb{T}(\Pi \pm \hbar \mathbf{q}) &= \mathbf{1}_{4 \times 4} - \frac{1}{4} \frac{\frac{(\Pi_b \pm \hbar q_b)(\Pi_b \pm \hbar q_b)}{2m_0} \mathbf{1}_{4 \times 4} - \frac{q_e \hbar}{2m_0} B_b^{(ext)} \sigma_b}{m_0 c^2} + \frac{\beta}{2} \alpha_b \frac{(\Pi_b \pm \hbar q_b)}{m_0 c} \\
&\quad + O(\alpha_{FS}^3)
\end{aligned} \tag{257}$$

Hence, for the operator (256) there holds [7]

$$\begin{aligned}
\mathbb{T} \circ e^{\pm i q_a x_a} \circ \mathbb{T}^\dagger &= e^{\pm i q_a \hat{x}_a} \circ \mathbb{T}(\Pi \pm \hbar \mathbf{q}) \circ \mathbb{T}^\dagger(\Pi) \\
&= e^{\pm i q_{a'} \hat{x}_{a'}} \circ \begin{pmatrix} \left( 1 - \frac{1}{8} \frac{\hbar q_b}{m_0 c} \frac{\hbar q_b}{m_0 c} \right) \mathbf{1}_{4 \times 4} \\ \pm \frac{\beta}{2} \alpha_b \frac{\hbar q_b}{m_0 c} \\ \pm \frac{1}{4} \frac{\hbar q_b}{m_0 c} \frac{\Pi_{b'}}{m_0 c} i \varepsilon_{bb'b''} \sigma_{b''} \\ + O(\alpha_{FS}^3) \end{pmatrix}
\end{aligned} \tag{258}$$

Such that for the matrix element  $\langle U_k^{(NW)} | \mathbb{T} e^{\pm i q_a x_a} \mathbb{T}^\dagger | U_{k'}^{(NW)} \rangle$  in the Newton–Wigner representation one finds [7]

$$\begin{aligned}
&\langle U_k^{(NW)} | \mathbb{T} e^{-i q_a x_a} \mathbb{T}^\dagger | U_{k'}^{(NW)} \rangle \\
&= \int \frac{d^3 q}{(2\pi)^3} \frac{e^{i \mathbf{q} \cdot \mathbf{R}}}{|\mathbf{q}|^2} \left( \int d^3 r \sum_{k, k'} U_\mu^{*(NW)}(\mathbf{r}, k) e^{\pm i \mathbf{q} \cdot \mathbf{r}} \begin{pmatrix} \left( 1 - \frac{1}{8} \frac{\hbar q_b}{m_0 c} \frac{\hbar q_b}{m_0 c} \right) \mathbf{1}_{4 \times 4} \\ \pm \frac{1}{4} \frac{\hbar q_b}{m_0 c} \frac{\Pi_{b'}}{m_0 c} i \varepsilon_{bb'b''} \sigma_{b''} \\ + O(\alpha_{FS}^3) \end{pmatrix}_{\mu, \mu'} U_{\mu'}^{(NW)}(\mathbf{r}, k') \right)
\end{aligned} \tag{259}$$

Here it has been used that the nondiagonal terms in (258) do not contribute, as has been explained in section 5, see (178).

Furthermore it has been switched to the position representation  $U_\mu^{*(NW)}(\mathbf{r}, k)$  according to (106) so that one can more easily identify the contributions (e.g. the first line in (259) will yield the Coulomb interaction, the second line will yield the spin-orbit coupling in the presence of the other electrons).

The operator  $\mathbb{T} \circ \alpha_b e^{\pm i q_{a'} x_{a'}} \circ \mathbb{T}^\dagger$  can be rearranged according to [7]

$$\begin{aligned} \mathbb{T} \circ \alpha_a e^{\pm i q_{a'} x_{a'}} \circ \mathbb{T}^\dagger &= \mathbb{T} \circ e^{\pm i q_{a'} x_{a'}} \alpha_a \circ \mathbb{T}^\dagger \\ &= (\mathbb{T} \circ e^{\pm i q_{a'} x_{a'}} \circ \mathbb{T}^\dagger) \circ (\mathbb{T} \circ \alpha_a \circ \mathbb{T}^\dagger) \end{aligned} \quad (260)$$

The evaluation of the part  $(\mathbb{T} \circ e^{\pm i q_{a'} x_{a'}} \circ \mathbb{T}^\dagger)$  is given in (258). The evaluation of the part  $(\mathbb{T} \circ \alpha_a \circ \mathbb{T}^\dagger)$  is given in the appendix section B, see (350). Therefore, one finds up to the order  $\alpha_{FS}^3$  [7]

$$\begin{aligned} &\mathbb{T} \circ \alpha_a e^{\pm i q_{a'} x_{a'}} \circ \mathbb{T}^\dagger \\ &= e^{\pm i q_a \hat{x}_a} \circ \left( \begin{aligned} &\left( 1 - \frac{1}{8} \frac{\hbar q_{a'}}{m_0 c} \frac{\hbar q_{a'}}{m_0 c} \right) \alpha_b - \frac{1}{4} \frac{\Pi_b}{m_0 c} \frac{\Pi_{b'}}{m_0 c} \left( \alpha_b \alpha_{b'} \alpha_a + \underbrace{\left( \alpha_b \alpha_a + \alpha_a \alpha_b \right)}_{2\delta_{a,b}} \right) \alpha_{b'} \right) \\ &\mp \frac{1}{2} \frac{\hbar q_{a'}}{m_0 c} \frac{\Pi_b}{m_0 c} \alpha_{a'} \pm \frac{1}{4} \frac{\hbar q_{a'}}{m_0 c} \frac{\Pi_a}{m_0 c} i \varepsilon_{a' a a''} \sigma_{a''} \alpha_b \\ &\pm \frac{\hbar q_{a'}}{m_0 c} \frac{\beta}{2} (\delta_{a',b} + i \varepsilon_{a',b,a''} \sigma_{a''}) \\ &+ \frac{\Pi_b}{m_0 c} \beta \\ &+ O(\alpha_{FS}^3) \end{aligned} \right) \end{aligned} \quad (261)$$

Inserting (261) into the matrix elements  $\langle U_k^{(NW)} | \mathbb{T} \circ \alpha_b e^{\pm i q_a x_a} \circ \mathbb{T}^\dagger | U_{k'}^{(NW)} \rangle$ , and using that nondiagonal parts do again not contribute in the Newton–Wigner representation then [7]

$$\begin{aligned} &\langle U_k^{(NW)} | \mathbb{T} \circ \alpha_b e^{\pm i q_{a'} x_{a'}} \circ \mathbb{T}^\dagger | U_{k'}^{(NW)} \rangle \\ &= \int d^3 r U_\mu^{*(NW)}(\mathbf{r}, k) e^{\pm i \mathbf{q} \cdot \mathbf{r}} \left( \begin{aligned} &\left( \pm \frac{1}{2} \frac{\hbar q_a}{m_0 c} + \frac{\Pi_a}{m_0 c} \right) \mathbf{1}_{4 \times 4} \\ &\pm \frac{1}{2} \frac{\hbar q_{a'}}{m_0 c} i \varepsilon_{a',a,a''} \sigma_{a''} \\ &+ O(\alpha_{FS}^3) \end{aligned} \right)_{\mu,\mu'} U_{\mu'}^{(NW)}(\mathbf{r}, k') \end{aligned} \quad (262)$$

### 6.4.1 The First Order Effective Interaction

Here, the coupling of the matter fields to the photons described by  $\hat{\mathcal{H}}_{\perp}^{(low,0)}$  in the Hamiltonian  $\hat{\mathcal{H}}_{LM}$  of (181) is expressed in the Newton–Wigner representation. This is quite analogue to the procedure above.

The coupling term is given by [7]

$$\hat{\mathcal{H}}_{\perp}^{(low,0)} = -\frac{1}{m_0 c^2} \int d^3 r \hat{j}_b^{(0)}(\mathbf{r}) \mathcal{A}_b^{(T,low)}(\mathbf{r}) \quad (263)$$

Or, explicitey, [7]

$$\hat{\mathcal{H}}_{\perp}^{(low,0)} = \left( -\frac{q_e}{m_0 c} \right) \sum_{k,k'} \frac{1}{\sqrt{V}} \sum_{q < q_B} \sum_b \mathcal{A}_b(q) \begin{pmatrix} \langle U_k | \alpha_b e^{iq_a x_a} | U_{k'} \rangle \hat{c}_k^{\dagger} \hat{c}_{k'} \hat{a}_q \\ + \langle U_k | \alpha_b e^{-iq_a x_a} | U_{k'} \rangle \hat{c}_k^{\dagger} \hat{c}_{k'}^{\dagger} \hat{a}_q^{\dagger} \\ - \langle V_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \hat{b}_{k'}^{\dagger} \hat{b}_{\tilde{k}} \hat{a}_q \\ - \langle V_k | \alpha_b e^{-iq_a x_a} | V_{k'} \rangle \hat{b}_{k'}^{\dagger} \hat{b}_{\tilde{k}} \hat{a}_q^{\dagger} \end{pmatrix} \quad (264)$$

It is again the matrix elements  $\langle U_k | \alpha_b e^{\pm iq_a x_a} | U_{k'} \rangle$  or  $\langle V_k | \alpha_b e^{\pm iq_a x_a} | V_{k'} \rangle$  which yield the corrections in the nonrelativistic limit. Using (262) one can interpret the nonrelativistic current density  $\hat{j}_b^{(0)}(\mathbf{r})$  [7]

$$\hat{\mathcal{H}}_{\perp}^{(low,0)} = \left( -\frac{q_e}{m_0 c} \right) \sum_{k,k'} \frac{1}{\sqrt{V}} \sum_{q < q_B} \sum_b \mathcal{A}_b(q) \begin{pmatrix} \int d^3 r U_{\mu}^{*(NW)}(\mathbf{r}, k) e^{+i\mathbf{q}\cdot\mathbf{r}} \begin{pmatrix} \left( +\frac{1}{2} \frac{\hbar q_b}{m_0 c} + \frac{\Pi_b}{m_0 c} \right) \mathbf{1}_{4 \times 4} \\ + \frac{1}{2} \frac{\hbar q_{a'}}{m_0 c} i \varepsilon_{a',b,a''} \sigma_{a''} \end{pmatrix}_{\mu,\mu'} U_{\mu'}^{(NW)}(\mathbf{r}, k') \hat{c}_k^{\dagger} \hat{c}_{k'} \hat{a}_q \\ + \int d^3 r U_{\mu}^{*(NW)}(\mathbf{r}, k) e^{-i\mathbf{q}\cdot\mathbf{r}} \begin{pmatrix} \left( -\frac{1}{2} \frac{\hbar q_b}{m_0 c} + \frac{\Pi_b}{m_0 c} \right) \mathbf{1}_{4 \times 4} \\ - \frac{1}{2} \frac{\hbar q_{a'}}{m_0 c} i \varepsilon_{a',b,a''} \sigma_{a''} \end{pmatrix}_{\mu,\mu'} U_{\mu'}^{(NW)}(\mathbf{r}, k') \hat{c}_k^{\dagger} \hat{c}_{k'}^{\dagger} \hat{a}_q^{\dagger} \\ + \int d^3 r V_{\mu}^{*(NW)}(\mathbf{r}, \tilde{k}) e^{+i\mathbf{q}\cdot\mathbf{r}} \begin{pmatrix} \left( \frac{1}{2} \frac{\hbar q_b}{m_0 c} + \frac{\Pi_b}{m_0 c} \right) \mathbf{1}_{4 \times 4} \\ + \frac{1}{2} \frac{\hbar q_{a'}}{m_0 c} i \varepsilon_{a',b,a''} \sigma_{a''} \end{pmatrix}_{\mu,\mu'} V_{\mu'}^{(NW)}(\mathbf{r}, \tilde{k}') \hat{b}_{k'}^{\dagger} \hat{b}_{\tilde{k}} \hat{a}_q \\ + \int d^3 r V_{\mu}^{*(NW)}(\mathbf{r}, \tilde{k}) e^{-i\mathbf{q}\cdot\mathbf{r}} \begin{pmatrix} \left( -\frac{1}{2} \frac{\hbar q_b}{m_0 c} + \frac{\Pi_b}{m_0 c} \right) \mathbf{1}_{4 \times 4} \\ - \frac{1}{2} \frac{\hbar q_{a'}}{m_0 c} i \varepsilon_{a',b,a''} \sigma_{a''} \end{pmatrix}_{\mu,\mu'} V_{\mu'}^{(NW)}(\mathbf{r}, \tilde{k}') \hat{b}_{k'}^{\dagger} \hat{b}_{\tilde{k}} \hat{a}_q^{\dagger} \end{pmatrix} \quad (265)$$

Neglecting the antimatter part and using the transversality condition  $\sum_b \mathcal{A}_b(q) q_b = 0$  there follows [7]

$$\begin{aligned}
\hat{\mathcal{H}}_{\perp}^{(low,0,el)} &= \left(-\frac{q_e}{m_0 c}\right) \sum_{k,k'} \frac{1}{\sqrt{V}} \sum_{q < q_B} \sum_b \mathcal{A}_b(q) \\
&\times \left( \int d^3 r U_{\mu}^{*(NW)}(\mathbf{r}, k) e^{+i\mathbf{q}\cdot\mathbf{r}} \left( \frac{\Pi_b}{m_0 c} \mathbf{1}_{4\times 4} + \frac{1}{2} \frac{\hbar q_{a'}}{m_0 c} i\varepsilon_{a',b,a''} \sigma_{a''} \right)_{\mu,\mu'} U_{\mu'}^{(NW)}(\mathbf{r}, k') \hat{c}_k^{\dagger} \hat{c}_{k'} \hat{a}_q \right) \\
&+ \int d^3 r U_{\mu}^{*(NW)}(\mathbf{r}, k) e^{-i\mathbf{q}\cdot\mathbf{r}} \left( \frac{\Pi_b}{m_0 c} \mathbf{1}_{4\times 4} - \frac{1}{2} \frac{\hbar q_{a'}}{m_0 c} i\varepsilon_{a',b,a''} \sigma_{a''} \right)_{\mu,\mu'} U_{\mu'}^{(NW)}(\mathbf{r}, k') \hat{c}_k^{\dagger} \hat{c}_{k'} \hat{a}_q^{\dagger} \Big) \\
&= \left(-\frac{q_e}{m_0 c}\right) \frac{1}{\sqrt{V}} \sum_{q < q_B} \sum_b \mathcal{A}_b(q) \\
&\times \sum_{s,s'} \left( \int d^3 r \hat{\psi}_s^{\dagger}(\mathbf{r}) e^{+i\mathbf{q}\cdot\mathbf{r}} \left( \frac{\Pi_b}{m_0 c} \mathbf{1}_{2\times 2} + \frac{1}{2} \frac{\hbar q_{a'}}{m_0 c} i\varepsilon_{a',b,a''} \sigma_{a''}^{(P)} \right)_{s,s'} \hat{\psi}_{s'}(\mathbf{r}) \hat{a}_q \right) \\
&+ \int d^3 r \hat{\psi}_s^{\dagger}(\mathbf{r}) e^{-i\mathbf{q}\cdot\mathbf{r}} \left( \frac{\Pi_b}{m_0 c} \mathbf{1}_{2\times 2} - \frac{1}{2} \frac{\hbar q_{a'}}{m_0 c} i\varepsilon_{a',b,a''} \sigma_{a''}^{(P)} \right)_{s,s'} \hat{\psi}_{s'}(\mathbf{r}) \hat{a}_q^{\dagger} \Big)
\end{aligned} \tag{266}$$

where the Schrödinger–Pauli field operators (228) have now been inserted.

Once the matrix elements have been evaluated one can separate the current density from the vector potential [7]:

$$\begin{aligned}
\hat{\mathcal{H}}_{\perp}^{(low,0,el)} &= \left(-\frac{q_e}{m_0 c}\right) \\
&\times \left( \int d^3 r \sum_b \left( \frac{1}{\sqrt{V}} \sum_{q < q_B} \mathcal{A}_b(q) (e^{+i\mathbf{q}\cdot\mathbf{r}} \hat{a}_q + e^{-i\mathbf{q}\cdot\mathbf{r}} \hat{a}_q^{\dagger}) \right) \left( \sum_s \hat{\psi}_s^{\dagger}(\mathbf{r}) \frac{\Pi_b}{m_0 c} \hat{\psi}_s(\mathbf{r}) \right) \right. \\
&+ \int d^3 r \sum_b \frac{1}{m_0 c} \varepsilon_{a',b,a''} \frac{\partial}{\partial r_{a'}} \left( \frac{1}{\sqrt{V}} \sum_{q < q_B} \mathcal{A}_b(q) (e^{+i\mathbf{q}\cdot\mathbf{r}} \hat{a}_q + e^{-i\mathbf{q}\cdot\mathbf{r}} \hat{a}_q^{\dagger}) \right) \left. \left( \sum_{s,s'} \hat{\psi}_s^{\dagger}(\mathbf{r}) \left( \frac{\hbar}{2} \sigma_{a''}^{(P)} \right)_{s,s'} \hat{\psi}_{s'}(\mathbf{r}) \right) \right)
\end{aligned} \tag{267}$$

The following definitions for the operator of the vector potential  $\hat{\mathfrak{A}}_b(\mathbf{x})$  of the low energy photons, and paramagnetic current density of the matter  $\hat{j}_a^{(e,para)}(\mathbf{r})$ , the diamagnetic current density  $\hat{j}_a^{(e,dia)}(\mathbf{r})$  and the magnetization current density  $j_b^{(e,spin)}(\mathbf{r})$  [7],

$$\begin{aligned}
\hat{\mathfrak{A}}_b(\mathbf{x}) &= \frac{1}{\sqrt{V}} \sum_{q < q_B} \mathcal{A}_b(q) \left( e^{iq_a x_a} \hat{a}_q + e^{-iq_a x_a} \hat{a}_q^\dagger \right) \\
\hat{j}_a^{(e,para)}(\mathbf{r}) &= \frac{q_e}{2m_0} \frac{\hbar}{i} \sum_s \left( \hat{\psi}_s^\dagger(\mathbf{r}) \frac{\partial}{\partial r_a} \hat{\psi}_s(\mathbf{r}) - \left( \frac{\partial}{\partial r_a} \hat{\psi}_s^\dagger(\mathbf{r}) \right) \hat{\psi}_s(\mathbf{r}) \right) \\
\hat{j}_a^{(e,dia)}(\mathbf{r}) &= -\frac{q_e^2}{m_0} \left( \sum_s \hat{\psi}_s^\dagger(\mathbf{r}) \hat{\psi}_s(\mathbf{r}) \right) A_a^{(ext)}(\mathbf{r}) \\
j_b^{(e,spin)}(\mathbf{r}) &= \frac{q_e}{m_0} \varepsilon_{b,a',a''} \frac{\partial}{\partial r_{a'}} \hat{S}_{a''}^{(e)}(\mathbf{r}) = \left( \frac{q_e}{m_0} \text{rot} \mathbf{S}^{(e)}(\mathbf{r}) \right)_b
\end{aligned} \tag{268}$$

where  $q$  is a multiindex meaning  $\sum_{q < q_B} = \sum_{\mathbf{q} < \mathbf{q}_B} \sum_{\lambda \in \{I, II\}}$ , and where  $\lambda$  counts the polarizations, finally lead to [7]

$$\begin{aligned}
\hat{\mathcal{H}}_\perp^{(low,0,el)} &= \frac{1}{m_0 c^2} \left( \begin{array}{l} - \int d^3 r \sum_b \left( \hat{j}_b^{(e,para)}(\mathbf{r}) + \hat{j}_b^{(e,dia)}(\mathbf{r}) \right) \hat{\mathfrak{A}}_b(\mathbf{r}) \\ - \frac{q_e}{m_0} \int d^3 r \sum_b \hat{\mathfrak{A}}_b(\mathbf{r}) \left( \varepsilon_{b,a',a''} \frac{\partial}{\partial r_{a'}} \hat{S}_{a''}^{(e)}(\mathbf{r}) \right) \end{array} \right) \\
&= -\frac{1}{m_0 c^2} \left( \int d^3 r \sum_b \left( \hat{j}_b^{(e,para)}(\mathbf{r}) + \hat{j}_b^{(e,dia)}(\mathbf{r}) + j_b^{(e,spin)}(\mathbf{r}) \right) \hat{\mathfrak{A}}_b(\mathbf{r}) \right)
\end{aligned} \tag{269}$$

The Hamiltonian (269) can now be retranslated to first quantization.

#### 6.4.2 The Second Order Effective Interactions

In the following the effective interaction terms  $\hat{\mathcal{U}}_C^{(0)}$  and  $\hat{\mathcal{V}}_{\perp,ee}$ , and the term  $\hat{\mathcal{V}}_{ext}^{(0)}$  are expressed in the Newton–Wigner representation. The beginning is made with  $\hat{\mathcal{U}}_C^{(0)}$  and then the term describing the coupling to external sources  $\hat{\mathcal{V}}_{ext}^{(0)}$  is expressed in the Newton–Wigner representation, because the procedure is similar to  $\hat{\mathcal{U}}_C^{(0)}$ . Finally, the term  $\hat{\mathcal{V}}_{\perp,ee}$  is evaluated. Having done that everything can be put together to go back to first quantization.

##### The Effective Longitudinal Interaction $\hat{\mathcal{U}}_C^{(0)}$

The effective QED Coulomb interaction term  $\hat{\mathcal{U}}_C^{(0)} = \mathcal{N} \left( \hat{\mathcal{V}}_C^{(0)} \right)$  is part of the solution of the homogeneous differential equation in the ansatz

for the second order solution of the flow equation. It is derived in section 4.1.3 and the result is given by (142).

Making use of the Eriksen transformation  $\mathbb{T}$  or by using (168) it decomposes into the following three contributions [7, 8]

$$\begin{aligned}
\mathcal{N}(\hat{\mathcal{V}}_C^{(0)}) &= \frac{q_e^2}{2\varepsilon_0} \int \frac{d^3q}{(2\pi)^3} \frac{1}{|\mathbf{q}|^2} \times \\
&\times \sum_{K,k} \sum_{K',k'} \left( \begin{aligned} &\langle U_K^{(NW)} | \mathbb{T} \circ e^{-iq_a x_a} \circ \mathbb{T}^\dagger | U_k^{(NW)} \rangle \langle U_{K'}^{(NW)} | \mathbb{T} \circ e^{iq_a x_a} \circ \mathbb{T}^\dagger | U_{k'}^{(NW)} \rangle \hat{c}_K^\dagger \hat{c}_{K'}^\dagger \hat{c}_{k'} \hat{c}_k \\ &+ \langle V_k^{(NW)} | \mathbb{T} \circ e^{-iq_a x_a} \circ \mathbb{T}^\dagger | V_K^{(NW)} \rangle \langle V_{k'}^{(NW)} | \mathbb{T} \circ e^{iq_a x_a} \circ \mathbb{T}^\dagger | V_{K'}^{(NW)} \rangle \hat{\delta}_{\bar{K}}^\dagger \hat{\delta}_{\bar{K}'}^\dagger \hat{b}_{\bar{k}'} \hat{b}_{\bar{k}} \\ &- 2 \langle U_K^{(NW)} | \mathbb{T} \circ e^{-iq_a x_a} \circ \mathbb{T}^\dagger | U_k^{(NW)} \rangle \langle V_{k'}^{(NW)} | \mathbb{T} \circ e^{iq_a x_a} \circ \mathbb{T}^\dagger | V_{K'}^{(NW)} \rangle \hat{c}_K^\dagger \hat{c}_k \hat{\delta}_{\bar{K}'}^\dagger \hat{b}_{\bar{k}'} \\ &+ 2 \langle U_K^{(NW)} | \mathbb{T} \circ e^{-iq_a x_a} \circ \mathbb{T}^\dagger | V_k^{(NW)} \rangle \langle V_{k'}^{(NW)} | \mathbb{T} \circ e^{iq_a x_a} \circ \mathbb{T}^\dagger | U_{K'}^{(NW)} \rangle \hat{c}_K^\dagger \hat{b}_{\bar{k}} \hat{\delta}_{\bar{K}'}^\dagger \hat{c}_{\bar{K}'} \end{aligned} \right) \\
&\equiv \hat{\mathcal{V}}_{C,ee} + \hat{\mathcal{V}}_{C,pp} + \hat{\mathcal{V}}_{C,ep}
\end{aligned} \tag{270}$$

$\hat{\mathcal{V}}_{C,ee}$  describes the effective Coulomb interaction between electrons,  $\hat{\mathcal{V}}_{C,pp}$  describes the effective Coulomb interaction between positrons, and  $\hat{\mathcal{V}}_{C,ep}$  describe an effective Coulomb interaction between pairs of electrons and positrons.

In the following the effective Coulomb interaction  $\hat{\mathcal{V}}_{C,ee}$  between the electrons is evaluated.

Using the identity (256) for the matrix elements  $\mathbb{T} \circ e^{-iq_a x_a} \circ \mathbb{T}^\dagger$  and neglecting contributions of the order  $\alpha_{FS}^3$  one finds [7, 8]

$$\begin{aligned}
\hat{\mathcal{V}}_{C,ee} &= \frac{q_e^2}{2\varepsilon_0} \int d^3r \int d^3r' \sum_{K,k} \sum_{K',k'} \hat{c}_K^\dagger \hat{c}_{K'}^\dagger \hat{c}_{k'} \hat{c}_k \times \int \frac{d^3q}{(2\pi)^3} \frac{e^{iq_a \cdot (r'_a - r_a)}}{|\mathbf{q}|^2} \\
&\left( \begin{aligned} &\left( 1 - \frac{\hbar q_b}{4 m_0 c} \frac{\hbar q_b}{m_0 c} \right) U_\mu^{*(NW)}(\mathbf{r}, K) U_\mu^{(NW)}(\mathbf{r}, k) U_\nu^{*(NW)}(\mathbf{r}', K') U_\nu^{(NW)}(\mathbf{r}', k') \\ &- \frac{i}{4} \varepsilon_{bb'b''} \frac{\hbar q_b}{m_0 c} U_\mu^{*(NW)}(\mathbf{r}, K) (\sigma_{b'\nu})_{\mu,\mu'} \left( \frac{\Pi_{b'}}{m_0 c} U_{\mu'}^{(NW)}(\mathbf{r}, k) \right) U_\nu^{*(NW)}(\mathbf{r}', K') U_\nu^{(NW)}(\mathbf{r}', k') \\ &+ U_\mu^{*(NW)}(\mathbf{r}, K) U_\mu^{(NW)}(\mathbf{r}, k) \frac{i}{4} \varepsilon_{aa'a''} \frac{\hbar q_a}{m_0 c} U_\nu^{*(NW)}(\mathbf{r}', K') (\sigma_{a'\nu'})_{\nu,\nu'} \left( \frac{\Pi_{a'}}{m_0 c} U_{\nu'}^{(NW)}(\mathbf{r}', k') \right) \\ &+ O(\alpha_{FS}^3) \end{aligned} \right)
\end{aligned} \tag{271}$$

With [8, 7]

$$\begin{aligned}
& \int \frac{d^3 q}{(2\pi)^3} \frac{e^{iqa \cdot (r'_a - r_a)}}{|\mathbf{q}|^2} = \frac{1}{4\pi|\mathbf{r}' - \mathbf{r}|} \\
& \int \frac{d^3 q}{(2\pi)^3} \frac{e^{iqa \cdot (r'_a - r_a)}}{|\mathbf{q}|^2} q_b = \frac{\nabla'_b}{i} \int \frac{d^3 q}{(2\pi)^3} \frac{e^{iqa \cdot (r'_a - r_a)}}{|\mathbf{q}|^2} = \frac{\nabla'_b}{i} \frac{1}{4\pi|\mathbf{r}' - \mathbf{r}|} = -\frac{1}{i} \frac{r'_b - r_b}{4\pi|\mathbf{r}' - \mathbf{r}|^3} \\
& \int \frac{d^3 q}{(2\pi)^3} \frac{e^{iqa \cdot (r'_a - r_a)}}{|\mathbf{q}|^2} q_b q_b = \delta^{(3)}(\mathbf{r} - \mathbf{r}')
\end{aligned} \tag{272}$$

there follows [8, 7]

$$\begin{aligned}
\hat{V}_{C,ee} = & \frac{q_e^2}{2\varepsilon_0} \int d^3 r \int d^3 r' \sum_{K,k} \sum_{K',k'} \hat{c}_K^\dagger \hat{c}_K \hat{c}_{k'}^\dagger \hat{c}_{k'} \times \\
& \left( \begin{aligned} & U_\mu^{*(NW)}(\mathbf{r}, K) U_\mu^{(NW)}(\mathbf{r}, k) \frac{1}{4\pi|\mathbf{r}' - \mathbf{r}|} U_\nu^{*(NW)}(\mathbf{r}', K') U_\nu^{(NW)}(\mathbf{r}', k') \\ & -\frac{1}{4} \left( \frac{\hbar}{m_0 c} \right)^2 U_\mu^{*(NW)}(\mathbf{r}, K) U_\mu^{(NW)}(\mathbf{r}, k) \delta^{(3)}(\mathbf{r} - \mathbf{r}') U_\nu^{*(NW)}(\mathbf{r}', K') U_\nu^{(NW)}(\mathbf{r}', k') \\ & -\frac{1}{2} \varepsilon_{bb'b''} \frac{\hbar}{m_0 c} \frac{r_b - r'_b}{4\pi|\mathbf{r}' - \mathbf{r}|^3} U_\mu^{*(NW)}(\mathbf{r}, K) (\sigma_{b''})_{\mu, \mu'} \left( \frac{\Pi_{b'}}{m_0 c} U_{\mu'}^{(NW)}(\mathbf{r}, k) \right) U_\nu^{*(NW)}(\mathbf{r}', K') U_\nu^{(NW)}(\mathbf{r}', k') \\ & + O(\alpha_{FS}^3) \end{aligned} \right)
\end{aligned} \tag{273}$$

Inserting the Schrödinger–Pauli amplitudes (172) finally gives [8, 7]

$$\begin{aligned}
\hat{V}_{C,ee} = & \frac{q_e^2}{2\varepsilon_0} \int d^3 r \int d^3 r' \left( \begin{aligned} & \hat{\psi}_s^\dagger(\mathbf{r}) \hat{\psi}_{s'}^\dagger(\mathbf{r}') \frac{1}{4\pi|\mathbf{r}' - \mathbf{r}|} \hat{\psi}_{s'}(\mathbf{r}') \hat{\psi}_s(\mathbf{r}) \\ & -\frac{1}{4} \left( \frac{\hbar}{m_0 c} \right)^2 \hat{\psi}_s^\dagger(\mathbf{r}) \hat{\psi}_{s'}^\dagger(\mathbf{r}') \delta^{(3)}(\mathbf{r} - \mathbf{r}') \hat{\psi}_{s'}(\mathbf{r}') \hat{\psi}_s(\mathbf{r}) \\ & -\hat{\psi}_s^\dagger(\mathbf{r}) \hat{\psi}_{s''}^\dagger(\mathbf{r}') \varepsilon_{bb'b''} \frac{\hbar}{m_0 c} \frac{r_b - r'_b}{8\pi|\mathbf{r}' - \mathbf{r}|^3} \hat{\psi}_{s''}(\mathbf{r}') \left( \sigma_{b''}^{(P)} \right)_{s, s'} \frac{\Pi_{b'}}{m_0 c} \hat{\psi}_{s'}(\mathbf{r}) \\ & + O(\alpha_{FS}^3) \end{aligned} \right)
\end{aligned} \tag{274}$$

$\hat{V}_{C,ee}$  is the nonrelativistic Coulomb interaction between electrons expressed in second quantization. It can now be reexpressed in first quantization, which is done in section 6.5.

### The Coupling to External Sources $\hat{V}_{ext}^{(0)}$

The contribution of the coupling of the matter fields to an external potential  $\tilde{\Phi}_{ext}(\mathbf{r})$  remaining in second order perturbation theory (see (127) in section 4.1.3) is given by



$$\hat{\mathcal{V}}_{ext}^{(0)} = \int \frac{d^3q}{(2\pi)^3} \tilde{\Phi}_{ext}(\mathbf{q}) \sum_{k,k'} \left( \langle U_k | e^{-iq_a x_a} | U_{k'} \rangle \hat{c}_k^\dagger c_{k'} - \langle V_k | e^{-iq_a x_a} | V_{k'} \rangle b_{\tilde{k}'}^\dagger \hat{b}_{\tilde{k}} \right) \quad (275)$$

The Fourier representation of an external Coulomb potential of an atomic nucleus is given by  $\tilde{\Phi}_{ext}(\mathbf{q}) = \frac{Z|q_e|}{4\pi\epsilon_0} e^{i\mathbf{q}\cdot\mathbf{R}} \frac{1}{|\mathbf{q}|^2}$ , see also (39).

By again using the relations (168) for switching to the Newton–Wigner representation of  $\hat{\mathcal{V}}_{ext}^{(0)}$  there follows [7]

$$\begin{aligned} \hat{\mathcal{V}}_{ext}^{(0)} &= \int \frac{d^3q}{(2\pi)^3} \tilde{\Phi}_{ext}(\mathbf{q}) \sum_{k,k'} \left( \langle U_k | e^{-iq_a x_a} | U_{k'} \rangle \hat{c}_k^\dagger c_{k'} - \langle V_k | e^{-iq_a x_a} | V_{k'} \rangle b_{\tilde{k}'}^\dagger \hat{b}_{\tilde{k}} \right) \\ &= \int \frac{d^3q}{(2\pi)^3} \tilde{\Phi}_{ext}(\mathbf{q}) \sum_{k,k'} \left( \langle U_k^{(NW)} | \mathbb{T} e^{-iq_a x_a} \mathbb{T}^\dagger | U_{k'}^{(NW)} \rangle \hat{c}_k^\dagger c_{k'} - \langle V_k^{(NW)} | \mathbb{T} e^{-iq_a x_a} \mathbb{T}^\dagger | V_{k'}^{(NW)} \rangle b_{\tilde{k}'}^\dagger \hat{b}_{\tilde{k}} \right) \\ &\equiv \hat{\mathcal{V}}_{ext}^{(el)} + \hat{\mathcal{V}}_{ext}^{(p)} \end{aligned} \quad (276)$$

Now for the electron part  $\hat{\mathcal{V}}_{ext}^{(el)}$  one finds with [7]

$$\begin{aligned} \tilde{\rho}_0^{(el)}(\mathbf{q}) &= \int d^3r e^{-i\mathbf{q}\cdot\mathbf{r}} \rho_0^{(el)}(\mathbf{r}) \\ \rho_0^{(el)}(\mathbf{r}) &= \sum_{k,k'} U_\nu^{*(NW)}(\mathbf{r}, k) | \mathbb{T} e^{-iq_a x_a} \mathbb{T}^\dagger | U_\nu^{(NW)}(\mathbf{r}, k') \hat{c}_k^\dagger c_{k'} \end{aligned} \quad (277)$$

and with the result (258) [7]

$$\begin{aligned} \hat{\mathcal{V}}_{ext}^{(el)} &= \int \frac{d^3q}{(2\pi)^3} \tilde{\Phi}_{ext}^{(el)}(\mathbf{q}) \tilde{\rho}_0^{(el)}(\mathbf{q}) \\ &= \int \frac{d^3q}{(2\pi)^3} \left( \frac{Z|q_e|}{4\pi\epsilon_0} e^{i\mathbf{q}\cdot\mathbf{R}} \frac{1}{|\mathbf{q}|^2} \right) \left( \sum_{k,k'} \langle U_k^{(NW)} | \mathbb{T} e^{-iq_a x_a} \mathbb{T}^\dagger | U_{k'}^{(NW)} \rangle \hat{c}_k^\dagger c_{k'} \right) \\ &= \frac{Z|q_e|}{4\pi\epsilon_0} \int \frac{d^3q}{(2\pi)^3} \frac{e^{i\mathbf{q}\cdot\mathbf{R}}}{|\mathbf{q}|^2} \left( \int d^3r \sum_{k,k'} U_\mu^{*(NW)}(\mathbf{r}, k) e^{-i\mathbf{q}\cdot\mathbf{r}} \begin{pmatrix} \left(1 - \frac{1}{8} \frac{\hbar q_b}{m_0 c} \frac{\hbar q_b}{m_0 c}\right) \mathbf{1}_{4 \times 4} \\ -\frac{1}{4} \frac{\hbar q_b}{m_0 c} \frac{\Pi_{b'}}{m_0 c} \quad i \varepsilon_{bb'b''} \sigma_{b''} \\ + O(\alpha_{FS}^3) \end{pmatrix}_{\mu,\mu'} U_{\mu'}^{(NW)}(\mathbf{r}, k') \right) \\ &= \frac{Z|q_e|}{4\pi\epsilon_0} \int d^3r \sum_{k,k'} U_\mu^{*(NW)}(\mathbf{r}, k) \left( \begin{array}{c} \int \frac{d^3q}{(2\pi)^3} \frac{e^{i\mathbf{q}\cdot(\mathbf{R}-\mathbf{r})}}{|\mathbf{q}|^2} \\ - \int \frac{d^3q}{(2\pi)^3} \frac{e^{i\mathbf{q}\cdot(\mathbf{R}-\mathbf{r})}}{|\mathbf{q}|^2} \frac{1}{8} \frac{\hbar q_b}{m_0 c} \frac{\hbar q_b}{m_0 c} \\ - \int \frac{d^3q}{(2\pi)^3} \frac{e^{i\mathbf{q}\cdot(\mathbf{R}-\mathbf{r})}}{|\mathbf{q}|^2} \left( \frac{1}{4} \frac{\hbar q_b}{m_0 c} \frac{\Pi_{b'}}{m_0 c} \quad i \varepsilon_{bb'b''} \sigma_{b''} \right)_{\mu,\mu'} \end{array} \right) U_\mu^{(NW)}(\mathbf{r}, k') \end{aligned} \quad (278)$$

Again inserting the integral relations (272) gives the result which can be reexpressed in first quantization [7]:

$$\hat{\mathcal{V}}_{ext}^{(el)} = \frac{Z|q_e|}{4\pi\epsilon_0} \int d^3r \hat{\psi}_s^\dagger(\mathbf{r}) \left( \begin{array}{c} -\frac{1}{8} \frac{\hbar}{m_0 c} \frac{\hbar}{m_0 c} \frac{1}{4\pi|\mathbf{R}-\mathbf{r}|} \delta^{(3)}(\mathbf{R}-\mathbf{r}) \\ +\frac{1}{4} \frac{\hbar}{m_0 c} \epsilon_{bb'b''} \left( \frac{R_b - r_b}{4\pi|\mathbf{R}-\mathbf{r}|^3} \right) \left( \frac{\Pi_{b'}}{m_0 c} \sigma_{b''}^{(P)} \right)_{\mu,\mu'} \end{array} \right) \hat{\psi}_{s'}(\mathbf{r}) \quad (279)$$

The first line is the Coulomb interaction with the atomic nucleus at the position  $\mathbf{R}$ . The second line is the Darwin-term, and the third line is the spin-orbit interaction of an electron in the Coulomb field of the nucleus.

### The Effective Transversal Interaction $\hat{\mathcal{V}}_{\perp,ee}$

The effective transversal interaction  $\hat{\mathcal{V}}_{\perp,ee}$  as a result of the solution of the inhomogeneous differential equation of second order perturbation expansion as deduced in section 4.1.3 follows as

$$\begin{aligned} \hat{\mathcal{V}}_{\perp,ee} &= m_0 c^2 \left( \frac{q_e}{m_0 c} \right)^2 \sum_{k,k'} \sum_{K,K'} \frac{1}{V} \sum_{\mathbf{q}} \kappa_q \frac{\hbar}{2\epsilon_0 \omega(\mathbf{q})} \sum_{b,b'} \left( \delta_{b,b'} - \frac{q_b q_{b'}}{|\mathbf{q}|^2} \right) \times \\ &\times \left\langle U_k^{(NW)} \left| \mathbb{T} \circ \alpha_b e^{iq_a x_a} \circ \mathbb{T}^\dagger \right| U_{k'}^{(NW)} \right\rangle \left\langle U_{K'}^{(NW)} \left| \mathbb{T} \circ \alpha_{b'} e^{-iq_a x_a} \circ \mathbb{T}^\dagger \right| U_K^{(NW)} \right\rangle \\ &\times \frac{(\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q) - (\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_q)}{(\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)^2 + (\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_q)^2} \hat{c}_k^\dagger \hat{c}_{K'}^\dagger \hat{c}_K \hat{c}_{k'} \end{aligned} \quad (280)$$

For the effective interaction  $\hat{\mathcal{V}}_{\perp,ee}$  one has to consider that in the nonrelativistic subspace of QED the difference in the fermionic energies is always very small compared to the rest energy [7]:

$$\begin{aligned} |E_k - E_{k'}| &\ll m_0 c^2 \\ |E_{K'} - E_K| &\ll m_0 c^2 \end{aligned} \quad (281)$$

Hence there holds [7]

$$\frac{(\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q) - (\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_q)}{(\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)^2 + (\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_q)^2} \simeq -\frac{1}{\tilde{\omega}_q} \quad (282)$$

The factor  $\kappa_q$  in (280) means that it is the high-energy photons, those with wave number  $|\mathbf{q}| > q_B$ , which cause the effective transversal interaction  $\hat{\mathcal{V}}_{\perp,ee}$ . Since these have been eliminated in favor for  $\hat{\mathcal{V}}_{\perp,ee}$  one can set  $\kappa_q \equiv 1$ .

Switching to the Newton–Wigner representation according to (168) this yields the following approximation [7]

$$\begin{aligned}
\hat{\mathcal{V}}_{\perp,ee} &= \simeq \frac{q_e^2}{2\varepsilon_0} \left( \frac{\hbar}{m_0c} \right)^2 \sum_{k,k'} \sum_{K,K'} \frac{1}{V} \sum_{\mathbf{q}} \frac{1}{\hbar\omega(\mathbf{q})} \sum_{b,b'} \left( \delta_{b,b'} - \frac{q_b q_{b'}}{|\mathbf{q}|^2} \right) \times \\
&\times \left\langle U_k^{(NW)} \left| \mathbb{T} \circ \alpha_b e^{iq_a x_a} \circ \mathbb{T}^\dagger \right| U_{k'}^{(NW)} \right\rangle \left\langle U_{K'}^{(NW)} \left| \mathbb{T} \circ \alpha_{b'} e^{-iq_a x_a} \circ \mathbb{T}^\dagger \right| U_K^{(NW)} \right\rangle \left( -\frac{1}{\bar{\omega}_q} \right) \hat{c}_k^\dagger \hat{c}_{K'}^\dagger \hat{c}_K \hat{c}_{k'} \\
&= \frac{q_e^2}{2\varepsilon_0} \left( \frac{\hbar}{m_0c} \right)^2 \sum_{k,k'} \sum_{K,K'} \hat{c}_k^\dagger \hat{c}_{K'}^\dagger \hat{c}_K \hat{c}_{k'} \frac{1}{V} \sum_{\mathbf{q}} \left( -\frac{1}{\bar{\omega}_q} \right) \sum_{b,b'} \left( \delta_{b,b'} - \frac{q_b q_{b'}}{|\mathbf{q}|^2} \right) \times \\
&\times \left\langle U_k^{(NW)} \left| \mathbb{T} \circ \alpha_b e^{iq_a x_a} \circ \mathbb{T}^\dagger \right| U_{k'}^{(NW)} \right\rangle \left\langle U_{K'}^{(NW)} \left| \mathbb{T} \circ \alpha_{b'} e^{-iq_a x_a} \circ \mathbb{T}^\dagger \right| U_K^{(NW)} \right\rangle
\end{aligned} \tag{283}$$

With the matrix elements (262) then [7]

$$\begin{aligned}
\hat{\mathcal{V}}_{\perp,ee} &= -\frac{q_e^2}{2\varepsilon_0} \sum_{k,k'} \sum_{K,K'} \hat{c}_k^\dagger \hat{c}_{K'}^\dagger \hat{c}_K \hat{c}_{k'} \frac{1}{V} \sum_{\mathbf{q}} \frac{1}{|\mathbf{q}|^2} \sum_{b,b'} \left( \delta_{a,b} - \frac{q_a q_b}{|\mathbf{q}|^2} \right) \times \\
&\times \int d^3r U_\mu^{*(NW)}(\mathbf{r}, k) e^{i\mathbf{q}\cdot\mathbf{r}} \left( \begin{array}{c} \left( \frac{1}{2} \frac{\hbar q_a}{m_0c} + \frac{\Pi_a}{m_0c} \right) \mathbf{1}_{4 \times 4} \\ + \frac{i}{2} \frac{\hbar q_{a'}}{m_0c} \varepsilon_{a',a,a''} \sigma_{a''} \\ + O(\alpha_{FS}^3) \end{array} \right)_{\mu,\mu'} U_{\mu'}^{(NW)}(\mathbf{r}, k') \\
&\times \int d^3r' U_\nu^{*(NW)}(\mathbf{r}', K') e^{-i\mathbf{q}\cdot\mathbf{r}'} \left( \begin{array}{c} \left( -\frac{1}{2} \frac{\hbar q_b}{m_0c} + \frac{\Pi'_b}{m_0c} \right) \mathbf{1}_{4 \times 4} \\ - \frac{i}{2} \frac{\hbar q_{b'}}{m_0c} \varepsilon_{b',b,b''} \sigma_{b''} \\ + O(\alpha_{FS}^3) \end{array} \right)_{\nu,\nu'} U_{\nu'}^{(NW)}(\mathbf{r}', K)
\end{aligned} \tag{284}$$

After several steps, and with the definition of the interaction potentials [7]

$$\begin{aligned}
V_{a,b}^{(o,o)}(\mathbf{r}-\mathbf{r}') &= \left(-\frac{q_e^2}{\varepsilon_0}\right) \frac{1}{V} \sum_{\mathbf{q}} \frac{1}{|\mathbf{q}|^2} e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} \left(\delta_{a,b} - \frac{q_a q_b}{|\mathbf{q}|^2}\right) \\
V_{a,b}^{(sp,sp)}(\mathbf{r}-\mathbf{r}') &= \left(-\frac{q_e^2}{\varepsilon_0}\right) \frac{1}{V} \sum_{\mathbf{q}} \frac{1}{|\mathbf{q}|^2} e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} \frac{1}{4} \left(\frac{\hbar|\mathbf{q}|}{m_0 c}\right)^2 \left(\delta_{a,b} - \frac{q_a q_b}{|\mathbf{q}|^2}\right) \\
V_{b'}^{(osp,o)}(\mathbf{r}-\mathbf{r}') &= \left(-\frac{q_e^2}{\varepsilon_0}\right) \frac{1}{V} \sum_{\mathbf{q}} \frac{1}{|\mathbf{q}|^2} e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} \left(\frac{i}{2} \frac{\hbar q_{b'}}{m_0 c}\right)
\end{aligned} \tag{285}$$

one finds, by inserting the Newton–Wigner amplitudes related to the Schrödinger–Pauli amplitudes (173) [7],

$$\hat{V}_{\perp,ee} = \frac{1}{2} \int d^3r \int d^3r' \left( \begin{aligned} &\hat{\psi}_s^\dagger(\mathbf{r}) \hat{\psi}_{s'}^\dagger(\mathbf{r}') V_{a,b}^{(o,o)}(\mathbf{r}-\mathbf{r}') \left(\frac{\Pi_b'}{m_0 c} \hat{\psi}_{s'}(\mathbf{r}')\right) \left(\frac{\Pi_a}{m_0 c} \hat{\psi}_s(\mathbf{r})\right) \\ &+ \hat{\psi}_s^\dagger(\mathbf{r}) \hat{\psi}_{s'}^\dagger(\mathbf{r}') V_{a,b}^{(sp,sp)}(\mathbf{r}-\mathbf{r}') \left(\sigma_b^{(P)}\right)_{s',\bar{s}'} \hat{\psi}_{\bar{s}'}(\mathbf{r}') \left(\sigma_a^{(P)}\right)_{s,\bar{s}} \hat{\psi}_{\bar{s}}(\mathbf{r}) \\ &+ \hat{\psi}_s^\dagger(\mathbf{r}) \hat{\psi}_{s'}^\dagger(\mathbf{r}') V_{b'}^{(osp,o)}(\mathbf{r}-\mathbf{r}') \varepsilon_{b',b,b''} \left(\frac{\Pi_b'}{m_0 c} \hat{\psi}_{s'}(\mathbf{r}')\right) \left(\sigma_{b''}^{(P)}\right)_{s,\bar{s}} \hat{\psi}_{\bar{s}}(\mathbf{r}) \\ &+ \hat{\psi}_s^\dagger(\mathbf{r}) \hat{\psi}_{s'}^\dagger(\mathbf{r}') \left(-V_{b'}^{(osp,o)}(\mathbf{r}-\mathbf{r}')\right) \varepsilon_{b',b,b''} \left(\sigma_{b''}^{(P)}\right)_{s',\bar{s}'} \hat{\psi}_{\bar{s}'}(\mathbf{r}') \left(\frac{\Pi_b}{m_0 c} \hat{\psi}_s(\mathbf{r})\right) \end{aligned} \right) \tag{286}$$

The meaning of the interaction potentials (285) is given as follows: the first line in (286) describes the orbit–orbit interaction between two electrons, the second line describes the magnetic dipole–dipole interaction, and the third and fourth lines describe the spin–other orbit interaction between the electrons.

The evaluation of the interaction potentials (285) can be found in the appendix section H. The result is given by [7]

$$\begin{aligned}
V_{a,b}^{(o,o)}(\mathbf{r}) &= \left(-\frac{q_e^2}{4\pi\varepsilon_0}\right) \frac{1}{2} \left(\frac{\delta_{a,b}}{r} + \frac{r_a r_b}{r^3}\right) \\
V_{a,b}^{(sp,sp)}(\mathbf{r}) &= \left(-\frac{q_e^2}{4\pi\varepsilon_0}\right) \frac{1}{4} \left(\frac{\hbar}{m_e c}\right)^2 \left(\frac{8}{3}\pi\delta^{(3)}(\mathbf{r}) \delta_{a,b} + \frac{3r_a r_b - 3|\mathbf{r}|^2 \delta_{a,b}}{|\mathbf{r}|^5}\right) \\
V_b^{(osp,o)}(\mathbf{r}) &= \frac{1}{2} \frac{\hbar}{m_e c} \frac{q_e^2}{4\pi\varepsilon_0} \frac{r_b}{r^3}
\end{aligned} \tag{287}$$

Inserting the transversal interaction potentials (287) yields the final result for the effective transversal interaction contribution [7, 8]

$$\hat{V}_{\perp,ee} = \frac{1}{2} \int d^3 r \int d^3 r' \left\{ \begin{array}{l} -\hat{\psi}_s^\dagger(\mathbf{r}) \hat{\psi}_{s'}^\dagger(\mathbf{r}') \left( \frac{q_e^2}{4\pi\epsilon_0} \right) \frac{1}{2} \left( \frac{\delta_{a,b}}{|\mathbf{r}-\mathbf{r}'|} + \frac{(r_a-r'_a)(r_b-r'_b)}{|\mathbf{r}-\mathbf{r}'|^3} \right) \left( \frac{\Pi'_b}{m_0 c} \hat{\psi}_{s'}(\mathbf{r}') \right) \left( \frac{\Pi_a}{m_0 c} \hat{\psi}_s(\mathbf{r}) \right) \\ -\hat{\psi}_s^\dagger(\mathbf{r}) \hat{\psi}_{s'}^\dagger(\mathbf{r}') \left( \frac{q_e^2}{4\pi\epsilon_0} \right) \frac{1}{4} \left( \frac{\hbar}{m_e c} \right)^2 \left( \frac{\frac{8}{3}\pi\delta^{(3)}(\mathbf{r}-\mathbf{r}')\delta_{a,b}}{3(r_a-r'_a)(r_b-r'_b)-3|\mathbf{r}-\mathbf{r}'|^2\delta_{a,b}} \right) (\sigma_b^{(P)})_{s',\bar{s}'} \hat{\psi}_{\bar{s}'}(\mathbf{r}') (\sigma_a^{(P)})_{s,\bar{s}} \hat{\psi}_{\bar{s}}(\mathbf{r}) \\ +\hat{\psi}_s^\dagger(\mathbf{r}) \hat{\psi}_{s'}^\dagger(\mathbf{r}') \frac{1}{2} \frac{\hbar}{m_e c} \frac{q_e^2}{4\pi\epsilon_0} \frac{(r_{b'}-r'_{b'})}{|\mathbf{r}-\mathbf{r}'|^3} \varepsilon_{b',b,b''} \left( \frac{\Pi'_b}{m_0 c} \hat{\psi}_{s'}(\mathbf{r}') \right) (\sigma_{b''}^{(P)})_{s,\bar{s}} \hat{\psi}_{\bar{s}}(\mathbf{r}) \\ -\hat{\psi}_s^\dagger(\mathbf{r}) \hat{\psi}_{s'}^\dagger(\mathbf{r}') \left( \frac{1}{2} \frac{\hbar}{m_e c} \frac{q_e^2}{4\pi\epsilon_0} \frac{(r_{b'}-r'_{b'})}{|\mathbf{r}-\mathbf{r}'|^3} \right) \varepsilon_{b',b,b''} (\sigma_{b''}^{(P)})_{s',\bar{s}'} \hat{\psi}_{\bar{s}'}(\mathbf{r}') \left( \frac{\Pi_b}{m_0 c} \hat{\psi}_s(\mathbf{r}) \right) \end{array} \right. \quad (288)$$

Now everything is put together for retranslating the Hamiltonian (181) to first quantization. This is done in the following subsection.

## 6.5 From Second Quantization to First Quantization: The Many–Electron Hamiltonian of Light–Matter Interactions

The nonrelativistic many–body Hamiltonian  $\hat{\mathcal{H}}_{LM}^{(el)}$  of a plurality of electrons has been introduced in section 6 according to [7, 8]

$$\begin{aligned} \hat{\mathcal{H}}_{LM}^{(el)} = & \hat{\mathcal{H}}_D^{(el)} + \hat{\mathcal{M}}_C^{(e)} + \hat{\mathcal{M}}_{\perp}^{(e)} + \hat{\mathcal{H}}_{rad} + \hat{\mathcal{H}}_{\perp}^{(low,el)} \\ & + \hat{\mathcal{V}}_{C,ee} + \hat{\mathcal{V}}_{ext}^{(el)} + \hat{\mathcal{V}}_{\perp,ee} \end{aligned} \quad (289)$$

In the last subsection these contributions have been evaluated as a gradient expansion by switching to the Newton–Wigner representation. This is the only representation in which a classical interpretation is possible, and at the same time it is the representation in which one can now quite simply reexpress the Hamiltonian (289) in first quantization, hence, as sum over *individual* particles. The switching to the Newton–Wigner representation is possible because the Eriksen transformation of a Dirac–particle in an external static magnetic induction field is known *exactly*, and because in the nonrelativistic subspace of QED it is reasonable to assume that the Newton–Wigner amplitudes vary slowly on the length scale of the Bohr radius  $a_B$  (atomic physics). These are given by the Schrödinger–Pauli amplitudes solving the Schrödinger–Pauli eigenvalue problem of a nonrelativistic spin  $\frac{1}{2}$  particle in an external magnetic induction field.

The results have been achieved as follows. The first three terms  $\hat{\mathcal{H}}_D^{(el)} + \hat{\mathcal{M}}_C^{(e)} + \hat{\mathcal{M}}_{\perp}^{(e)}$  in (289) yield the effective Schrödinger–Pauli Hamiltonian  $\hat{\mathcal{H}}_{SP}^{(el)}$  for an electron with mass  $m_e$ , charge  $q_e$  and spin  $\sigma_b = \hat{1}_{2 \times 2} \otimes \sigma_b^{(P)}$ . This has been evaluated in subsection 6.3 [7, 8]

$$\hat{\mathcal{H}}_{SP}^{(el)} = \int d^3r \hat{\psi}_s^{\dagger}(\mathbf{r}) \left( \begin{array}{c} m_e c^2 + \frac{\Pi_b \Pi_b}{2m_e} - \frac{1}{8} \frac{1}{m_e^3 c^2} \left( \hat{\Pi}_b \right)^4 \\ + \left( 2 + \frac{\alpha_{FS}}{\pi} \right) \left( \frac{q_e \hbar}{2m_e} B_b^{(ext)} \sigma_b \right)_{s,s'} \\ + O(\alpha_{FS}^3) \end{array} \right) \hat{\psi}_{s'}(\mathbf{r}) \quad (290)$$

The coupling of electrons to the low–energy photons  $\hat{\mathcal{H}}_{\perp}^{(low,0,el)}$  has been

deduced in subsection 6.4, see equation 269. The result is given by [7, 8]

$$\hat{\mathcal{H}}_{\perp}^{(low,0,el)} = -\frac{1}{m_e c^2} \int d^3 r \sum_b \left( \left( \hat{j}_b^{(e,para)}(\mathbf{r}) + \hat{j}_b^{(e,dia)}(\mathbf{r}) + j_b^{(e,spin)}(\mathbf{r}) \right) \hat{\mathcal{Q}}_b(\mathbf{r}) \right) \quad (291)$$

The effective Coulomb interaction  $\hat{\mathcal{V}}_{C,ee}$  has been deduced in subsection 6.4.2 [7, 8]:

$$\hat{\mathcal{V}}_{C,ee} = \frac{q_e^2}{2\varepsilon_0} \int d^3 r \int d^3 r' \left( \begin{array}{c} \hat{\psi}_s^\dagger(\mathbf{r}) \hat{\psi}_{s'}^\dagger(\mathbf{r}') \frac{1}{4\pi|\mathbf{r}'-\mathbf{r}|} \hat{\psi}_{s'}(\mathbf{r}') \hat{\psi}_s(\mathbf{r}) \\ -\frac{1}{4} \left( \frac{\hbar}{m_e c} \right)^2 \hat{\psi}_s^\dagger(\mathbf{r}) \hat{\psi}_{s'}^\dagger(\mathbf{r}') \delta^{(3)}(\mathbf{r}-\mathbf{r}') \hat{\psi}_{s'}(\mathbf{r}') \hat{\psi}_s(\mathbf{r}) \\ -\hat{\psi}_s^\dagger(\mathbf{r}) \hat{\psi}_{s''}^\dagger(\mathbf{r}') \varepsilon_{bb'b''} \frac{\hbar}{m_e c} \frac{r_b-r'_b}{8\pi|\mathbf{r}'-\mathbf{r}|^3} \hat{\psi}_{s''}(\mathbf{r}') \left( \sigma_{b''}^{(P)} \right)_{s,s'} \frac{\Pi_{b'}}{m_e c} \hat{\psi}_{s'}(\mathbf{r}) \\ +O(\alpha_{FS}^3) \end{array} \right) \quad (292)$$

The interaction  $\hat{\mathcal{V}}_{ext}^{(el)}$  of the electrons with an external source is found to be (see section 6.4.2) [7, 8]

$$\hat{\mathcal{V}}_{ext}^{(el)} = \frac{Z|q_e|}{4\pi\varepsilon_0} \int d^3 r \hat{\psi}_s^\dagger(\mathbf{r}) \left( \begin{array}{c} -\frac{1}{8} \frac{\hbar}{m_e c} \frac{\hbar}{m_e c} \delta^{(3)}(\mathbf{R}-\mathbf{r}) \\ +\frac{1}{4} \frac{\hbar}{m_e c} \varepsilon_{bb'b''} \left( \frac{R_b-r_b}{4\pi|\mathbf{R}-\mathbf{r}|^3} \right) \left( \sigma_{b''}^{(P)} \right)_{\mu,\mu'} \end{array} \right) \hat{\psi}_{s'}(\mathbf{r}) \quad (293)$$

And finally, the effective transversal interaction  $\hat{\mathcal{V}}_{\perp,ee}$  between the electrons is found to be [7, 8]

$$\hat{\mathcal{V}}_{\perp,ee} = \frac{1}{2} \int d^3 r \int d^3 r' \left\{ \begin{array}{l} -\hat{\psi}_s^\dagger(\mathbf{r}) \hat{\psi}_{s'}^\dagger(\mathbf{r}') \left( \frac{q_e^2}{4\pi\varepsilon_0} \right) \frac{1}{2} \left( \frac{\delta_{a,b}}{|\mathbf{r}-\mathbf{r}'|} + \frac{(r_a-r'_a)(r_b-r'_b)}{|\mathbf{r}-\mathbf{r}'|^3} \right) \left( \frac{\Pi'_b}{m_0 c} \hat{\psi}_{s'}(\mathbf{r}') \right) \left( \frac{\Pi_a}{m_e c} \hat{\psi}_s(\mathbf{r}) \right) \\ -\hat{\psi}_s^\dagger(\mathbf{r}) \hat{\psi}_{s'}^\dagger(\mathbf{r}') \left( \frac{q_e^2}{4\pi\varepsilon_0} \right) \frac{1}{4} \left( \frac{\hbar}{m_e c} \right)^2 \left( \begin{array}{c} \frac{8}{3} \pi \delta^{(3)}(\mathbf{r}-\mathbf{r}') \delta_{a,b} \\ + \frac{3(r_a-r'_a)(r_b-r'_b)-3|\mathbf{r}-\mathbf{r}'|^2 \delta_{a,b}}{|\mathbf{r}-\mathbf{r}'|^5} \end{array} \right) \left( \sigma_b^{(P)} \right)_{s',\bar{s}'} \hat{\psi}_{\bar{s}'}(\mathbf{r}') \left( \sigma_a^{(P)} \right)_{s,\bar{s}} \hat{\psi}_{\bar{s}}(\mathbf{r}) \\ +\hat{\psi}_s^\dagger(\mathbf{r}) \hat{\psi}_{s'}^\dagger(\mathbf{r}') \frac{1}{2} \frac{\hbar}{m_e c} \frac{q_e^2}{4\pi\varepsilon_0} \frac{(r_{b'}-r'_{b'})}{|\mathbf{r}-\mathbf{r}'|^3} \varepsilon_{b',b,b''} \left( \frac{\Pi'_b}{m_0 c} \hat{\psi}_{s'}(\mathbf{r}') \right) \left( \sigma_{b''}^{(P)} \right)_{s,\bar{s}} \hat{\psi}_{\bar{s}}(\mathbf{r}) \\ -\hat{\psi}_s^\dagger(\mathbf{r}) \hat{\psi}_{s'}^\dagger(\mathbf{r}') \left( \frac{1}{2} \frac{\hbar}{m_e c} \frac{q_e^2}{4\pi\varepsilon_0} \frac{(r_{b'}-r'_{b'})}{|\mathbf{r}-\mathbf{r}'|^3} \right) \varepsilon_{b',b,b''} \left( \sigma_{b''}^{(P)} \right)_{s',\bar{s}'} \hat{\psi}_{\bar{s}'}(\mathbf{r}') \left( \frac{\Pi_b}{m_e c} \hat{\psi}_s(\mathbf{r}) \right) \end{array} \right. \quad (294)$$

See (286).

Please note that the bare mass  $m_0$  has been replaced by the “true” electron mass  $m_e$  in the relativistic correction to the kinetic energy,

the relativistic corrections to the QED Coulomb interaction, and the relativistic corrections to the QED transversal interaction. It is in the nature of the perturbation theory that one gains in the order  $\alpha_{FS}^2$  contributions which are not renormalized in this order but in higher orders of the perturbation expansion. However, the error one makes in the replacement  $m_0 \rightarrow m_e$  is small of the order  $\alpha_{FS}$ , and it does not exceed the order of the particular term. Consider for example the coupling term  $\hat{\mathcal{H}}_{\perp}^{(low,el)}$ . By construction this term of the order  $\alpha_{FS}$ . In section 6.3 it has been shown that the first order renormalization of the bare mass itself is of order  $\alpha_{FS}$ , hence, the error by replacing  $m_0 \rightarrow m_e$  is not larger than  $\alpha_{FS}$ , e.g. the order of the term  $\hat{\mathcal{H}}_{\perp}^{(low,el)}$ . In this sense the renormalization is closed.

Having said that we now go to the first quantization. For a general one-particle operator  $\mathcal{O}^{(1)}$  in second quantization there holds

$$\mathcal{O}^{(1)} = \int d^3r \sum_{s,s'} \hat{\psi}_s^\dagger(\mathbf{r}) \hat{O}(\mathbf{r}) \hat{\psi}_{s'}(\mathbf{r}) \quad (295)$$

And for a general two-particle operator  $\mathcal{O}^{(2)}$  in second quantization

$$\mathcal{O}^{(2)} = \int d^3r \int d^3r' \sum_{s,s'} \hat{\psi}_s^\dagger(\mathbf{r}) \hat{\psi}_{s'}^\dagger(\mathbf{r}') \hat{O}(\mathbf{r}, \mathbf{r}') \hat{\psi}_s(\mathbf{r}') \hat{\psi}_{s'}(\mathbf{r}) \quad (296)$$

There readily follows for (295) in the first quantization

$$\hat{O}^{(1)} = \sum_{j=1}^N \hat{O}(\mathbf{r}^{(j)}) \quad (297)$$

and for (296) accordingly

$$\hat{O}^{(2)} = \frac{1}{2} \sum_{j \neq j'=1}^N \hat{O}(\mathbf{r}^{(j)}, \mathbf{r}^{(j')}) \quad (298)$$

With that we one can reexpress the terms (290), (291), (292), (293) and (294) in first quantization as [7, 8]



$$\hat{H}_{SP}^{(el)} = \sum_{j=1}^N \left( \begin{aligned} & m_e c^2 + \frac{(\Pi_b^{(j)})(\Pi_b^{(j)})}{2m_e} - \frac{1}{8} \frac{1}{m_e^3 c^2} \left( \Pi_b^{(j)} \right)^4 \\ & + \left( 2 + \frac{\alpha_{FS}}{\pi} \right) \left( \frac{q_e \hbar}{2m_e} B_b^{(ext)} \sigma_b^{(P,j)} \right)_{s,s'} \\ & + O(\alpha_{FS}^3) \end{aligned} \right) \quad (299)$$

$$\hat{H}_{\perp}^{(low,el)} = -\frac{1}{m_e c^2} \sum_{j=1}^N \left( \hat{j}_b^{(e,para)} \left( \mathbf{r}^{(j)} \right) + \hat{j}_b^{(e,dia)} \left( \mathbf{r}^{(j)} \right) + j_b^{(e,spin)} \left( \mathbf{r}^{(j)} \right) \right) \hat{\mathcal{U}}_b \left( \mathbf{r}^{(j)} \right) \quad (300)$$

where

$$\begin{aligned} \hat{j}_b^{(e,para)} \left( \mathbf{r}^{(j)} \right) &= \frac{q_e}{m_e} \hat{p}^{(j)} \\ \hat{j}_b^{(e,dia)} \left( \mathbf{r}^{(j)} \right) &= -\frac{q_e^2}{m_e} A_b^{(ext)} \left( \mathbf{r}^{(j)} \right) \\ j_b^{(e,spin)} \left( \mathbf{r}^{(j)} \right) &= \frac{q_e}{m_e} \varepsilon_{b,a',a''} \frac{\partial}{\partial r_{a'}^{(j)}} \hat{S}_{a''}^{(e)} \left( \mathbf{r} \right) = \left( \frac{q_e}{m_e} \text{rot} \mathbf{S}^{(e)} \left( \mathbf{r}^{(j)} \right) \right)_b \end{aligned} \quad (301)$$

$$\hat{V}_{C,ee} = \frac{1}{2} \sum_{j \neq j'}^N \left( \begin{aligned} & \frac{q_e^2}{4\pi\varepsilon_0 |\mathbf{r}^{(j')} - \mathbf{r}^{(j)}|} \\ & - \frac{q_e^2}{4\pi\varepsilon_0} \left( \frac{\hbar}{m_e c} \right)^2 \pi \delta^{(3)} \left( \mathbf{r}^{(j)} - \mathbf{r}^{(j')} \right) \\ & - \frac{q_e^2}{8\pi\varepsilon_0} \frac{\hbar}{m_e c} \sigma_{b''}^{(P,j)} \varepsilon_{bb'b''} \frac{r_b^{(j)} - r_b^{(j')}}{|\mathbf{r}^{(j)} - \mathbf{r}^{(j')}|^3} \frac{\Pi_{b'}^{(j)}}{m_e c} \end{aligned} \right) \quad (302)$$

$$\hat{V}_{ext}^{(el)} = \frac{Z |q_e|}{4\pi\varepsilon_0} \sum_{j=1}^N \left( \begin{aligned} & \frac{1}{4\pi |\mathbf{R} - \mathbf{r}^{(j)}|} \\ & - \frac{1}{8} \frac{\hbar}{m_e c} \frac{\hbar}{m_e c} \delta^{(3)} \left( \mathbf{R} - \mathbf{r}^{(j)} \right) \\ & + \frac{1}{4} \frac{\hbar}{m_e c} \varepsilon_{bb'b''} \left( \frac{R_b - r_b^{(j)}}{4\pi |\mathbf{R} - \mathbf{r}^{(j)}|^3} \right) \left( \frac{\Pi_{b'}}{m_e c} \sigma_{b''}^{(P,j)} \right)_{\mu,\mu'} \end{aligned} \right) \quad (303)$$

$$\hat{V}_{\perp,ee} = \frac{1}{2} \sum_{j \neq j'}^N \left( \begin{aligned} & \left( -\frac{q_e^2}{4\pi\epsilon_0} \right) \frac{1}{2} \left( \frac{\delta_{a,b}}{|\mathbf{r}^{(j)} - \mathbf{r}^{(j')}|} + \frac{(r_a^{(j)} - r_a^{(j')})(r_b^{(j)} - r_b^{(j')})}{|\mathbf{r}^{(j)} - \mathbf{r}^{(j')}|^3} \right) \frac{\Pi_b^{(j')} \Pi_a^{(j)}}{m_e c} \\ & + \left( -\frac{q_e^2}{4\pi\epsilon_0} \right) \frac{1}{4} \left( \frac{\hbar}{m_e c} \right)^2 \left( \begin{aligned} & \frac{\frac{8}{3} \pi \delta^{(3)}(\mathbf{r}^{(j)} - \mathbf{r}^{(j')}) \delta_{a,b}}{3(r_a^{(j)} - r_a^{(j')})(r_b^{(j)} - r_b^{(j')}) - 3|\mathbf{r}^{(j)} - \mathbf{r}^{(j')}|^2 \delta_{a,b}} \\ & + \frac{\delta_{a,b}}{|\mathbf{r}^{(j)} - \mathbf{r}^{(j')}|^5} \end{aligned} \right) \sigma_b^{(P,j')} \sigma_a^{(P,j)} \\ & + \frac{1}{2} \frac{\hbar}{m_e c} \frac{q_e^2}{4\pi\epsilon_0} \frac{r_b^{(j)} - r_b^{(j')}}{|\mathbf{r}^{(j)} - \mathbf{r}^{(j')}|^3} \varepsilon_{b',b,b''} \left( \Pi_b^{(j')} \sigma_{b''}^{(P,j)} - \Pi_b^{(P,j)} \sigma_{b''}^{(j')} \right) \end{aligned} \right) \quad (304)$$

Note that  $N$  is the **number of electrons!** Hence, one can now **count the particles!** Furthermore,  $\sigma_b^{(P)}$  was used instead of its relativistic sister  $\sigma_b = 1 \otimes \sigma_b^{(P)}$  because now the (empty) positron block can be ignored (although it is actually always there! Only hidden!)

Hence, the nonrelativistic Hamiltonian of many-electron light matter interactions expressed in first quantization, deduced from full QED, assumes the following guise [7, 8]:

$$\hat{H}_{LM}^{(el)} = \hat{H}_{SP}^{(el)} + \hat{H}_{\perp}^{(low,el)} + \hat{V}_{C,ee} + \hat{V}_{\perp,ee} + H_{rad} + \hat{V}_{ext}^{(el)} \quad (305)$$

The nonrelativistic Hamiltonian  $\hat{H}_{LM}^{(pos)}$  of many-positron light matter interactions in first quantization can be derived in a fully complete consideration from the second quantized Hamiltonian  $\hat{\mathcal{H}}_{LM}^{(pos)}$  as has been done for the electron Hamiltonian  $\hat{H}_{LM}^{(el)}$  from  $\hat{\mathcal{H}}_{LM}^{(el)}$ .

It should also be possible, as indicated in (238), to start from the second quantized Hamiltonian  $\hat{\mathcal{H}}_{LM}^{(el)}$  of the electrons and apply the charge conjugation operation  $\hat{\mathcal{C}}_F$  given in (408), and introduced in the appendix F.

The second quantized Hamiltonian  $\hat{\mathcal{H}}_{LM}^{(pos)}$  of the positrons can then be readily reexpressed in first quantization with the prescriptions (297) and (298). This makes it manifest that the renormalization of the positron attributes is equal to the renormalization of the electron, such that the positron is equal to the electron.

Now the Hamiltonian (305) of the electrons does not coincide with the solution of T. Itoh [13]. The main difference is that Itoh eliminates all photons from the QED Hamiltonian, such that it is not comprehensible how Itoh comes from the bare mass in the QED Hamiltonian to the

renormalized true electron mass, and therefore, how he achieves the anomalous  $g$ -factor of the electrons.

Furthermore, Itoh drops terms which violate the particle number conservation. Proceeding in this way one can first never be sure that one misses contributions that belong to the result in the respective order. And second, it is impossible to obtain a Hamiltonian describing the positrons and therefore one cannot treat electrons and positrons on equal footing.

The same is true for the derivation of Bialynicki–Birula [14], who also does not take into account terms which violate the particle number conservation by starting from Dirac field operators which describe particles and antiparticles separately. The mass renormalization of the electron is then explained by the normal ordering of the nonrelativistic Coulomb–interaction.

As has been shown here, the renormalization comprises two contributions: one part stems from the QED Coulomb interaction, the longitudinal interaction, and the other part stems from the QED transversal interaction, the one between the (anti-)matter fields and the high-energy photons. Eliminating this particle number violating contributions of the QED Hamiltonian by applying the flow equation yields mass renormalization and the renormalization of the  $g$ -factor (which coincides with the Schwinger result), and additionally the well-known effective longitudinal interactions (Coulomb interaction, Darwin term in the external field, spin–orbit interaction in the electric field of the other electrons) and the effective transversal interactions (dipole–dipole interaction, spin–other orbit interaction and orbit–orbit interaction) [37]. Here one has to emphasize that it is not the ultra-high energy photon modes which renormalize the bare mass  $m_0$  and the  $g$ -factor. From the graph 2 it can be seen which photons contribute to the renormalization: it is the photons between the energy scale  $\alpha_{FS}m_e c^2$  and the pair creation threshold  $\hbar c q_C$  !

With the derivation of the nonrelativistic limit of the QED Hamiltonian (8) presented here one can treat each constituent on equal footing, hence, the positrons are particles equal to the electrons.

The result (305) is crystal clear in its derivation, where each step can be understood. One does not have to omit terms which violate the particle number conservation, and all contributions important for

the respective order of the perturbation expansion in the finestructure constant  $\alpha_{FS}$  have been kept.

The result (305) also makes one thing clear: it would be *wrong* to start from the classical Hamilton function of light–matter interaction and quantize it by making use of the correspondence principle, because in progressing so, one would implement all photons into this Hamiltonian. It is, however, obvious, that the true Hamiltonian of light–matter interactions comprises only the low–energy photons, hence, all photons whose wave number  $q$  is smaller then the Bohr wave number  $q_B$  defined by  $\hbar cq_B \equiv \alpha_{FS} m_e c^2$ .

For  $N = 2$ ,  $A_a^{(ext)}(\mathbf{r}) = 0$ ,  $\hat{\mathfrak{A}}_b(\mathbf{r}^{(j)}) = \hat{0}$  and without the radiation contribution  $H_{rad}$  the Hamiltonian (305) coincides with the so–called Breit–Dirac–Pauli Hamiltonian<sup>3</sup>, see for example [37]. For the derivation of the Breit–Dirac–Pauli Hamiltonian, the photons have to be eliminated completely. However, since we are living in a world where there are always photons present, the Hamiltonian (305) is physically more sensible, since it describes the interaction of the electrons with the low–energy photons and includes the radiation field.

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<sup>3</sup> The Breit–Dirac–Pauli Hamiltonian can also be constructed by starting from relativistic classical mechanics. One constructs a Lagrange function (the so–called Darwin Lagrange function) of two interacting electrons. These interact via the electromagnetic fields they produce due to their motion, hence, due to the Lorentz force felt of by electron due to the electromagnetic field of the respective other electron and vice versa. From this Lagrange function then the Breit Hamiltonian is derived in analogy to the derivation of the Dirac Hamiltonian of one electron. The Breit Hamiltonian subsequently is a  $16 \times 16$  matrix operator and thus acts on 16–component spinors. This gives then a system of sixteen coupled equations which can be decoupled by replacing the “large” components by the “small” components, just as in case of the free Dirac Hamiltonian. Proceeding in this guise finally yields the Breit–Pauli–Dirac Hamiltonian [52, 53]. However, starting from classical mechanics for two interacting particles leads to serious problems, e.g. an unphysical  $|e|^4$  term in the Breit–Dirac–Pauli Hamiltonian. This is also discussed in section 7. The flow equation method does not provide such an unphysical contribution to the nonrelativistic limit of QED.

## 7 Summary and Discussion

This dissertation was dedicated to the goal of deducing the nonrelativistic limit from Quantum Electrodynamics as a high energy field theory.

The central problem breaks thereby down into two subproblems of which, thinking in classical physical terms, one would assume to be related to each other: the first, fundamental subproblem is that in QED, the particle number conservation is violated. Whatever one wants to understand by a particle in the context of QED – be it an occupied (anti-)matter mode or the (anti-)matter field itself – the particle number operator  $\hat{N}$  counting occupied (anti-)matter modes is well defined, and it does not commute with the Hamiltonian of QED. Hence, the particle number is not conserved, which is a profoundly unclassical property.

The second subproblem is the coherent superposition of matter and antimatter modes in the Dirac field operators describing the creation and annihilation of matter and antimatter in the QED Hamiltonian. Assuming that there are particles and antiparticles, one would also assume that there is a clear distinction between matter and antimatter. However, it is (unfortunately deeply) hidden in the formalism of QED that there is *no clear distinction*. This is due to the fact that the Dirac field operators comprise four components matter and antimatter are at first indissolubly interwoven with each other which on the other hand goes back to the structure and the properties of the Dirac Hamiltonian.

It was now possible to achieve the goal of deducing the nonrelativistic limit of QED by taking two separate steps: first the QED Hamiltonian has been unitarily transformed in such a way that an equivalent Hamiltonian that *conserves the particle number* emerged. This Hamiltonian is a many-body Hamiltonian describing the interaction with (possibly fast moving) matter and antimatter fields, and low energy photons (such with wave numbers  $q < q_B$ ). But in this Hamiltonian the matter and antimatter degrees of freedom are still coherently superposed.

Therefore, in a second step, the matter and antimatter degrees of freedom in the particle number conserving unitary equivalent QED Hamiltonian have been decoupled.

In this guise then the nonrelativistic Hamiltonian of light-matter inter-

actions emerged as a many–body field theory Hamiltonian for electrons and positrons separately. The resulting many–body field theory Hamiltonian for electrons has been retranslated to first quantization, hence, it has been expressed as a sum over *individual point-like particles carrying mass, charge and spin*.

It was possible to achieve a unitarily equivalent QED Hamiltonian which conserves the particle number by the help of the Wegner flow equation, which is a differential equation for unitarily transforming a matrix or an operator.

The generator of this flow equation made it possible to remove the pair terms of the QED Coulomb interaction and the high energy photons. With high energy photons hard X–ray photons and gamma ray photons are meant. However, this flow equation is initially a nonlinear ordinary differential equation, such that it could only be solved perturbatively. For this the QED Hamiltonian has been expanded into a series in the finestructure constant, and the initial data has been chosen accordingly. The latter means that it has been assumed that the radiation field energy is of the same strength as the contribution of the rest energy and the kinetic energy of the matter and antimatter fields (else one would ignore the high energy photons from the beginning, which would thus be inconsistent).

Now this expansion led to a system of recursively coupled differential equations still being nonlinear. Since the zeroth order differential equation could be solved exactly, all higher order differential equations occurred as *linear* ones. It was possible to solve these linear ordinary differential equations up to the second order in the finestructure constant by the help of an ansatz which reproduced the eigenvalue character of multiple interacted commutators.

Indeed, in this guise, all pair terms and high energy photons have been removed from the QED Hamiltonian and a unitarily equivalent Hamiltonian emerged which conserves the particle number.

This elimination of the pair terms of the QED Coulomb interaction and the high energy photons yielded effective interactions in a completely symmetric fashion for both matter and antimatter, as well as for the photons. Next to that a term has been gained which describes the interaction of electrons with positrons (positronium).

Moreover, terms have been gained which renormalize the bare

attributes mass  $m_0$  and with that the  $g$ -factor of the fermions. These so-called self-energy terms are present due to the requirement that one has to normally order the creation and annihilation operators for the fermions and the photons. This, on the other hand, is necessary because only in the normally ordered form it is possible to reexpress the field operators in first quantization.

One such renormalization contribution is due to the elimination of the interaction between the (anti-)matter fields and the high-energy photons, the transversal coupling. The second renormalization contribution is due to the elimination of the high-energy interaction between the matter and antimatter fields, the QED Coulomb interaction.

Altogether, the unitarily equivalent QED Hamiltonian which conserves the particle number then comprises the effective Pauli Hamiltonian, the effective Coulomb interaction, the effective transversal interaction, the coupling of the matter and antimatter fields to the low energy photons, and the radiation field.

Besides one gets an effective fermion-photon interaction describing stimulated emission, a constant spectral shift and an effective electron-positron interaction. The evaluation of these contributions has been postponed.

The focus has been set on evaluating the part of the Hamiltonian that describes matter only, the many-electron QED Hamiltonian. Analogous considerations regarding positrons have also been postponed.

The many-fermion QED Hamiltonian in second quantization can be found by expressing the contributions of the particle number conserving unitarily equivalent QED Hamiltonian in the Newton-Wigner representation. This is the representation in which matter and antimatter degrees of freedom fall apart.

The Newton-Wigner representation follows from the Eriksen transformation, which is a unitary transformation that blockdiagonalizes the single-particle Dirac Hamiltonian, leading to a decomposition of the field operators into upper and lower components for matter and antimatter respectively.

The renormalization terms together with the Dirac quantum field which, in the Newton-Wigner representation, is nothing but the

relativistic, second quantized Schrödinger–Pauli Hamiltonian, then renormalize the bare mass  $m_0$  and the  $g$ -factor of the fermions. For the latter the Schwinger result has been found.

The evaluation of the renormalization terms showed that the anomalous  $g$ -factor is due to the renormalization of the fermionic bare mass. The renormalization of the bare mass could be achieved in a physically consistent manner by introducing the physical cut-off. This cut-off truncates both the kinetic energy of the fermions and the photon energy and led to the important numerical factor  $\frac{1}{3}$  due to which the bare rest mass is renormalized equally as the bare kinetic mass.

Since the single-particle Dirac Hamiltonian in the Newton–Wigner representation is blockdiagonal, where the blocks are given by the relativistic Schrödinger–Pauli Hamiltonian, it is possible to set the Newton–Wigner amplitudes in relation to the Schrödinger–Pauli amplitudes describing the nonrelativistic electron in an external magnetic induction field. The related Schrödinger–Pauli wave functions vary slowly on the atomic length scale, compared to the Compton wavelength. It was therefore possible to evaluate the matrix elements which give the corrections to the Dirac representation as a gradient expansion.

Finally, the low-energy QED Hamiltonian in the Newton–Wigner representation describes a plurality of electrons interacting with each other and with low-energy photons. With that the many-electron Hamiltonian of nonrelativistic light–matter interactions in its second quantized guise has been derived, which could then be reexpressed in first quantization, hence, as a sum over individual point particles.

The result extends that of Cohen–Tannoudji et al. presented in their textbook on QED [6] by one order (though the technical procedure was different there, e.g. perturbation theory has been applied by starting from a particle picture from the beginning). This means that the first relativistic corrections to the Schrödinger–Pauli Hamiltonian have been derived. However, it has to be emphasized that with the method presented here, one has at no point assumed particle number conservation, it has been *demande*d by unitarily transforming the QED Hamiltonian. By solving the flow equation, using the generator which demands particle number conservation, one can proceed in a



technically clean manner and treat all constituents involved on equal footing. This sharply distinguishes the method presented here from all previous derivations of the nonrelativistic limit from the QED Hamiltonian like the work of I. Bialynicky–Birula [14], by T. Itoh [13], and by Cohen–Tannoudji et al. [6, 45].

The derivation of the nonrelativistic limit of full QED has the great advantage that one does not have to start from the single–particle theory of classical mechanics or relativistic quantum mechanics and try to extend it to multiple interacting particles, in order to derive from it its nonrelativistic limit. Such a Hamiltonian exists, it is the Breit–Dirac–Pauli Hamiltonian. It has been derived the early 1929 work of Gregory Breit [52]. Breit worked out this Hamiltonian by proceeding similarly as Dirac with this single–electron approach. Breit imagined that two electrons interact with each other due to the electromagnetic field generated by the respective other, moving electron (see also footnote 3). With that he suggested for the description of two interacting electrons an effective Hamiltonian operating on a sixteen-component two–particle wavefunction. From Breit’s wave equation for that wavefunction emerged in the nonrelativistic limit the well known Schrödinger–Pauli Hamiltonian for two interacting electrons carrying mass, charge and spin. However, the lowest order relativistic corrections to the particles Coulomb interaction yielded not only the physical interaction terms (e.g. the magnetic dipole–dipole interaction), but also an interaction term proportional to  $|e|^4$  that contradicts experiment [53].

The result derived here coincides with the Breit–Dirac–Pauli Hamiltonian (however, without the unphysical term) iff one sets  $N = 2$ , puts the radiation field to zero, as well as the external magnetic induction field and the photon vector field (the correct version of the Breit–Dirac–Pauli Hamiltonian is also known as the Bethe–Salpeter Hamiltonian, see below). Conversely, it would probably not be immediately obvious how to integrate the photons into the Breit–Dirac Pauli Hamiltonian or into the Bethe–Salpeter Hamiltonian in order to get a nonrelativistic light–matter interaction Hamiltonian; especially would it not be clear that these photons are then limited in their energy, e.g. that X-ray photons and gamma photons must be excluded from the Breit–Dirac–Pauli Hamiltonian or the Bethe–Salpeter Hamiltonian.

Hence, proceeding the opposite way, namely starting from the classical quantum mechanics and the special theory of relativity, or from the relativistic quantum mechanics of Paul Dirac, and trying to extend it to a plurality of interacting particles yields numerous and serious problems, see also [15] and the references therein.

It is also not necessary to start from a two-particle Bethe-Salpeter equation describing bound states of a two-particle field theoretical system in terms of propagators. This might be a useful equation, however, as has hopefully become clear, it is questionable how the field theory formalism and the particle picture come together here. The covariant derivation of the results of Breit was established by Bethe and Salpeter on the basis of QED, thus obtaining (in a frame of reference with the total center of mass momentum being zero) a correct version of the nonrelativistic Hamiltonian derived by G. Breit without the unphysical  $|e|^4$  term [54]. An extension of the fully relativistic Bethe-Salpeter equation to more than two interacting fermions seems to be a hard problem, one aspect being the normalization of the many-body wave function. Any Hamiltonian which involves a sum of Dirac Hamiltonians for three or more particles plus local interactions suffers from the so called continuum disease, that is normalizable eigenfunctions don't exist because of the coherent superposition of positive- and negative-energy states [55]. To get from there via the Bethe-Salpeter approach back to the Schrödinger-Pauli Hamiltonian for a plurality of electrons, together with the lowest order relativistic corrections, requires to intrude in an ad hoc manner positive-energy projection operators collecting the interaction terms of the electrons [54], for a recent summary see [56].

Altogether, applying the flow equation method to the nonrelativistic limit problem of QED is the most general method for attacking this problem. With it it is possible to always stay on the level of the Hamiltonian as the generator of the dynamics of the system. Here one does not have to evaluate matrix elements of operators with the help of the S-matrix as time ordered products in the interaction picture of the QED interactions. For the S-matrix method it is necessary to choose initial and final states, which is not necessary iff one remains on the level of the Hamiltonian. The flow equation method also differs from the “method 2” of Dirac who starts from the Heisenberg equation of motion of a field operator describing the emission of *one* electron with

respect to the QED Hamiltonian and solves it perturbatively [32].

In this dissertation it has been started from the full QED Hamiltonian as a second quantized field theory including all interactions, and it has been asked how one can retrieve the classical point particle carrying mass, charge and spin from it. By applying the flow equation to the problem it was possible, always treating the constituents of the QED soup on equal footing, to derive a many-fermion Hamiltonian of nonrelativistic light matter interactions, including the Schwinger result of the magnetic moment of the fermions.

# Appendix

# A Spectral Representation of the Dirac Hamiltonian

With the Dirac Amplitudes  $U_\mu(\mathbf{r}; k)$  and  $V_\mu(\mathbf{r}; k)$  in the compact Dirac bracket notation [7],

$$\begin{aligned}
 U_\mu(\mathbf{r}; k) &= \langle (\mathbf{r}, \mu) | U_k \rangle \\
 U_{\mu'}^*(\mathbf{r}'; k) &= \langle U_k | (\mathbf{r}', \mu') \rangle \\
 V_\mu(\mathbf{r}; k) &= \langle (\mathbf{r}, \mu) | V_k \rangle \\
 V_{\mu'}^*(\mathbf{r}'; k) &= \langle V_k | (\mathbf{r}', \mu') \rangle
 \end{aligned} \tag{306}$$

$$\int d^3 r' \sum_{\mu'} |(\mathbf{r}', \mu')\rangle \langle (\mathbf{r}', \mu')| = \mathbf{1}$$

and the completeness relations (18) it is possible to define projection operators [7]

$$\begin{aligned}
 \mathbf{P}^{(+)} &= \sum_{k'} |U_{k'}\rangle \langle U_{k'}| \\
 \mathbf{P}^{(-)} &= \sum_{k'} |V_{k'}\rangle \langle V_{k'}|
 \end{aligned} \tag{307}$$

that project onto the subspaces of positive energy or negative energy of  $\mathbf{H}^{(D)}$  according to (16). These projection operators have the following properties [7]

$$\begin{aligned}
 \left(\mathbf{P}^{(+)}\right)^\dagger &= \mathbf{P}^{(+)} \\
 \left(\mathbf{P}^{(-)}\right)^\dagger &= \mathbf{P}^{(-)} \\
 \mathbf{P}^{(+)} + \mathbf{P}^{(-)} &= \mathbf{1}_{4 \times 4} \\
 \mathbf{P}^{(+)} \circ \mathbf{P}^{(-)} &= \mathbf{0}_{4 \times 4} = \mathbf{P}^{(-)} \circ \mathbf{P}^{(+)}
 \end{aligned} \tag{308}$$

The projection operators (307) commute furthermore with the Dirac Hamiltonian,  $[\mathbf{H}^{(D)}, \mathbf{P}^{(\pm)}] = 0$

From these one finds the spectra representation of the Dirac Hamiltonian  $\mathbf{H}^{(D)}$  as follows [7]

$$\begin{aligned}
\mathbf{H}^{(D)} &= \mathbf{H}^{(D)} \circ (\mathbf{P}^{(+)} + \mathbf{P}^{(-)}) \\
&= \sum_{k'} |E_{k'}| (|U_{k'}\rangle \langle U_{k'}| - |V_{k'}\rangle \langle V_{k'}|)
\end{aligned} \tag{309}$$

And for the square of the Dirac Hamiltonian [7]

$$\begin{aligned}
\mathbf{H}^{(D)} \circ \mathbf{H}^{(D)} &= \sum_{k'} |E_{k'}| (|U_{k'}\rangle \langle U_{k'}| - |V_{k'}\rangle \langle V_{k'}|) \circ \sum_{k''} |E_{k''}| (|U_{k''}\rangle \langle U_{k''}| - |V_{k''}\rangle \langle V_{k''}|) \\
&= \sum_{k'} |E_{k'}|^2 (|U_{k'}\rangle \langle U_{k'}| + |V_{k'}\rangle \langle V_{k'}|)
\end{aligned} \tag{310}$$

Note that (310) is always positive. Thus, one can take the square root [7]:

$$\sqrt{\mathbf{H}^{(D)} \circ \mathbf{H}^{(D)}} = \sum_{k'} |E_{k'}| (|U_{k'}\rangle \langle U_{k'}| + |V_{k'}\rangle \langle V_{k'}|) \tag{311}$$

Since [7]

$$\begin{aligned}
&\sqrt{\mathbf{H}^{(D)} \circ \mathbf{H}^{(D)}} \circ \sqrt{\mathbf{H}^{(D)} \circ \mathbf{H}^{(D)}} \\
&= \sum_{k'} |E_{k'}|^2 (|U_{k'}\rangle \langle U_{k'}| + |V_{k'}\rangle \langle V_{k'}|) \\
&= \mathbf{H}^{(D)} \circ \mathbf{H}^{(D)}
\end{aligned} \tag{312}$$

$$\sqrt{\mathbf{H}^{(D)} \circ \mathbf{H}^{(D)}} |U_k\rangle = \sum_{k'} |E_{k'}| (|U_{k'}\rangle \langle U_{k'}| + |V_{k'}\rangle \langle V_{k'}|) |U_k\rangle = E_k |U_k\rangle$$

$$\sqrt{\mathbf{H}^{(D)} \circ \mathbf{H}^{(D)}} |V_k\rangle = \sum_{k'} |E_{k'}| (|U_{k'}\rangle \langle U_{k'}| + |V_{k'}\rangle \langle V_{k'}|) |V_k\rangle = E_k |V_k\rangle$$

$$\begin{aligned}
\mathbf{H}^{(D)} &= \sum_{k'} |E_{k'}| (|U_{k'}\rangle \langle U_{k'}| - |V_{k'}\rangle \langle V_{k'}|) \\
&= \sqrt{\mathbf{H}^{(D)} \circ \mathbf{H}^{(D)}} \circ \sum_{k'} (|U_{k'}\rangle \langle U_{k'}| - |V_{k'}\rangle \langle V_{k'}|) \\
&= \sqrt{\mathbf{H}^{(D)} \circ \mathbf{H}^{(D)}} \circ (\mathbf{P}^{(+)} - \mathbf{P}^{(-)})
\end{aligned} \tag{313}$$

This relation between the projection operators (307) and the Dirac Hamiltonian can be also found in [50].

The identity (313) is important, since there follows a formal representation of the nonlocal operator  $\frac{H^{(D)}}{\sqrt{H^{(D)} \circ H^{(D)}}}$  as [7]

$$P^{(+)} - P^{(-)} = \frac{H^{(D)}}{\sqrt{H^{(D)} \circ H^{(D)}}} \quad (314)$$

and for the projection operators [7]

$$P^{(\pm)} = \frac{1}{2} \left( \mathbf{1}_{4 \times 4} \pm \frac{H^{(D)}}{\sqrt{H^{(D)} \circ H^{(D)}}} \right) \quad (315)$$

Note that in the nonrelativistic limit  $m_0 c^2 \rightarrow \infty$  there follows  $\lim_{m_0 c^2 \rightarrow \infty} P^{(\pm)} = \frac{1}{2} (\mathbf{1}_{4 \times 4} \pm \beta)$ . Remark the  $\beta$  matrix as the operator indicating particles  $\mathbf{1}_{2 \times 2}$  in its first argument and antiparticles  $-\mathbf{1}_{2 \times 2}$  in its last argument.

## B The Derivation of the Eriksen Transformation

A unitary transformation is searched for which blockdiagonalizes the single-particle Dirac Hamiltonian, and which separates the matter degrees of freedom and the antimatter degrees of freedom in the Dirac modes.

Now since the operator  $\beta$  is blockdiagonal in the Dirac representation it is reasonable to assume that a unitarily equivalent Dirac Hamiltonian commutes with  $\beta$ , because in that case, this new Hamiltonian must also be blockdiagonal. However, there might be several unitary transformations which lead to a blockdiagonal Dirac Hamiltonian, but for which matter and antimatter degrees of freedom are still coupled [8]. Therefore, the unitary transformation must also yield new amplitudes which are energy-separated in the sense as indicated in (163). Both requirements, the blockdiagonalization of the Dirac Hamiltonian and the energy separation of the Dirac amplitudes define the Eriksen transformation [10, 7].

In the following it will be shown that the generator of a flow equation which yields the Eriksen transformation  $\mathbb{T}$  in the limit  $s \rightarrow \infty$  is given by [7]

$$\eta^{(T)}(s) = [\beta, \mathbf{H}(s)] \quad (316)$$

Since the generator  $\eta^{(T)}(s)$  depends only linearly on the Hamiltonian  $\mathbf{H}(s)$ , it induces a Brockett type of flow equation for the gauge invariant Dirac Hamiltonian [7]:

$$\begin{aligned} \frac{d}{ds} \mathbf{H}(s) &= [\eta^{(T)}(s), \mathbf{H}(s)] \\ \eta^{(T)}(s) &= [\beta, \mathbf{H}(s)] \\ \mathbf{H}(s=0) &= \mathbf{H}^{(D)} = m_0 c^2 \beta + c \alpha_b \Pi_b \end{aligned} \quad (317)$$

And, as a reminder,



$$\begin{aligned}
\hat{\Pi}_b &= p_b - q_e A_b(\hat{\mathbf{x}}) \\
[\hat{p}_b, \hat{x}_a] &= \frac{\hbar}{i} \delta_{b,a} \hat{1} \\
\text{rot} \mathbf{A}(\mathbf{r}) &= \mathbf{B}^{(ext)}(\mathbf{r}) \\
\beta \alpha_b + \alpha_b \beta &= \mathbf{0}_{4 \times 4}
\end{aligned}$$

It will now now be proven that the ansatz [7]

$$\begin{aligned}
\mathbf{H}(s) &= \beta \mathbf{E}(s) + D_A \mathbf{F}(s) \\
D_A &= \frac{\alpha_b \Pi_b}{\sqrt{(\alpha_a \Pi_a)^2}} \tag{318}
\end{aligned}$$

solves the differential equation (317) exactly. Here,  $\mathbf{E}(s)$  and  $\mathbf{F}(s)$  are four-dimensional blockdiagonal (!) operators that have to be specified. The operator  $D_A$  might be non-local.

The properties of the involved operators  $\beta$  and  $\alpha_b \Pi_b$  are the following [7]

$$\begin{aligned}
D_A D_A &= \mathbf{1}_{4 \times 4} \\
\beta \beta &= \mathbf{1}_{4 \times 4} \\
\beta D_A + D_A \beta &= \mathbf{0}_{4 \times 4} \\
\left[ \beta, (\alpha_b \Pi_b)^2 \right] &= \mathbf{0}_{4 \times 4} \tag{319}
\end{aligned}$$

Now one assumes that the operators  $\mathbf{E}(s)$  and  $\mathbf{F}(s)$  are only dependent on the square  $(\alpha_a \Pi_a)^2$  which will be verified once their explicit shape has been constructed.

Iff the assumption holds true then [7]

$$\begin{aligned}
[\beta, \mathbf{E}(s)] &= \mathbf{0}_{4 \times 4} = [\beta, \mathbf{F}(s)] \\
[D_A, \mathbf{E}(s)] &= \mathbf{0}_{4 \times 4} = [D_A, \mathbf{F}(s)] \\
[\mathbf{E}(s), \mathbf{F}(s)] &= \mathbf{0}_{4 \times 4} \tag{320}
\end{aligned}$$

And the generator (316) assumes the following guise [7]

$$\eta^{(T)}(s) = 2\beta D_A \mathbf{F}(s) \tag{321}$$

One can now explicitly write for the flow equation (317)

$$\begin{aligned}
\frac{d}{ds}\mathbf{H}(s) &= \beta\frac{d}{ds}\mathbf{E}(s) + D_A\frac{d}{ds}\mathbf{F}(s) \\
&\stackrel{!}{=} \left[\eta^{(T)}(s), \mathbf{H}(s)\right] \\
&= [2\beta D_A\mathbf{F}(s), \beta\mathbf{E}(s) + D_A\mathbf{F}(s)] \\
&= -4D_A\mathbf{F}(s)\mathbf{E}(s) + 4\beta\mathbf{F}(s)\mathbf{F}(s)
\end{aligned} \tag{322}$$

where the relations (320) have been used.

Rewriting this one finds [7]

$$\beta\left(\frac{d}{ds}\mathbf{E}(s) - 4\mathbf{F}(s)\mathbf{F}(s)\right) + D_A\left(\frac{d}{ds}\mathbf{F}(s) + 4\mathbf{F}(s)\mathbf{E}(s)\right) = \mathbf{0}_{4\times 4} \tag{323}$$

This equation (323) decomposes into two coupled nonlinear differential equations for determining the operators  $\mathbf{E}(s)$  and  $\mathbf{F}(s)$  [7]

$$\begin{aligned}
\frac{d}{ds}\mathbf{E}(s) &= 4\mathbf{F}(s)\mathbf{F}(s) \\
\frac{d}{ds}\mathbf{F}(s) &= -4\mathbf{E}(s)\mathbf{F}(s)
\end{aligned} \tag{324}$$

One can show this by applying the lemma  $\mathbf{X}\beta + \mathbf{Y}D_A = \mathbf{0}_{4\times 4} \Rightarrow (\mathbf{X} = \mathbf{0}_{4\times 4}) \wedge (\mathbf{Y} = \mathbf{0}_{4\times 4})$  for two  $4 \times 4$  matrix operators  $\mathbf{X}$  and  $\mathbf{Y}$  with the property  $[\mathbf{X}, \beta] = \mathbf{0}_{4\times 4} = [\mathbf{Y}, \beta]$  [7].

From the chosen initial values for  $s = 0$  one finds [7]

$$\begin{aligned}
\mathbf{H}(0) &= \beta\mathbf{E}(0) + D_A\mathbf{F}(0) \\
&\stackrel{!}{=} \mathbf{H}^{(D)} \\
&= m_0c^2\beta + c\alpha_b\Pi_b
\end{aligned} \tag{325}$$

which implies for the initial values for  $\mathbf{E}(s)$  and  $\mathbf{F}(s)$  [7]

$$\begin{aligned}
\mathbf{F}(0) &= c\sqrt{(\alpha_a\Pi_a)^2} \\
\mathbf{E}(0) &= m_0c^2\mathbf{1}_{4\times 4}
\end{aligned} \tag{326}$$

The coupled equations (324) can now be solved by observing that the square  $\mathbf{H}(s)\mathbf{H}(s) = \mathbf{E}(s)\mathbf{E}(s) + \mathbf{F}(s)\mathbf{F}(s) \equiv \mathcal{Q}(s)$  is a constant of motion [7]:

$$\begin{aligned}
\frac{d}{ds}\mathcal{Q}(s) &= \mathbf{E}(s)\left(\frac{d}{ds}\mathbf{E}(s)\right) + \left(\frac{d}{ds}\mathbf{E}(s)\right)\mathbf{E}(s) + \mathbf{F}(s)\left(\frac{d}{ds}\mathbf{F}(s)\right) + \left(\frac{d}{ds}\mathbf{F}(s)\right)\mathbf{F}(s) \\
&= \mathbf{E}(s)\mathbf{F}(s)\mathbf{F}(s) + 4\mathbf{F}(s)\mathbf{F}(s)\mathbf{E}(s) - 4\mathbf{F}(s)\mathbf{E}(s)\mathbf{F}(s) - 4\mathbf{E}(s)\mathbf{F}(s)\mathbf{F}(s) \\
&= 4\mathbf{F}(s)(\mathbf{F}(s)\mathbf{E}(s) - \mathbf{E}(s)\mathbf{F}(s)) \\
&= \mathbf{0}_{4\times 4}
\end{aligned} \tag{327}$$

Hence [7],

$$\begin{aligned}
\mathcal{Q}(s) &= \mathcal{Q}(0) \\
&= \mathbf{E}(0)\mathbf{E}(0) + \mathbf{F}(0)\mathbf{F}(0) \\
&= (m_0c^2)^2 \mathbf{1}_{4\times 4} + c^2(\alpha_a\Pi_a)^2 \\
&= \mathbf{H}^{(D)}(0)\mathbf{H}^{(D)}(0)
\end{aligned} \tag{328}$$

The formal solution for  $\mathbf{F}(s)$  for the differential equation (324) [7]

$$\mathbf{F}(s) = \exp\left[-4\int_0^s ds'\mathbf{E}(s')\right]\mathbf{F}(0) \tag{329}$$

which is true iff  $[\mathbf{E}(s_1), \mathbf{E}(s_2)] = \mathbf{0}_{4\times 4}$  for  $s_1, s_2 \in \epsilon[0, \infty]$ . This condition holds true once one has found the explicit solution of  $\mathbf{E}(s)$ .

Since  $\mathbf{E}(s)$  is positive and increases as a function of  $s$ ,  $\mathbf{F}(s)$  necessarily vanishes for  $s \rightarrow \infty$  [7]:

$$\lim_{s \rightarrow \infty} \mathbf{F}(s) = \mathbf{0}_{4\times 4} = \mathbf{F}(\infty) \tag{330}$$

For  $\mathcal{Q}(s)$  then [7]

$$\begin{aligned}
\mathbf{E}(s)\mathbf{E}(s) + \mathbf{F}(s)\mathbf{F}(s) &= \lim_{s \rightarrow \infty} (\mathbf{E}(s)\mathbf{E}(s) + \mathbf{F}(s)\mathbf{F}(s)) \\
&= \mathbf{E}(\infty)\mathbf{E}(\infty) \\
&= \lim_{s \rightarrow 0} (\mathbf{E}(s)\mathbf{E}(s) + \mathbf{F}(s)\mathbf{F}(s)) \\
&= \mathbf{H}^{(D)}(0)\mathbf{H}^{(D)}(0)
\end{aligned} \tag{331}$$

So, altogheter for  $\mathbf{E}(\infty)$  [7]

$$\begin{aligned}
\mathbf{E}(\infty) &= \sqrt{\mathbf{H}^{(D)} \circ \mathbf{H}^{(D)}} \\
&= \sqrt{(m_0 c^2)^2 \mathbf{1}_{4 \times 4} + c^2 (\alpha_a \Pi_a)^2} \\
&\equiv \mathbf{E}(\Pi)
\end{aligned} \tag{332}$$

$\mathbf{E}(\infty)$  only depends on  $(\alpha_a \Pi_a)^2$  as has been assumed above.

Inserting the result (332) into the differential equation (324) for  $\mathbf{E}(s)$  then gives [7]

$$\begin{aligned}
\frac{d}{ds} \mathbf{E}(s) &= 4 \mathbf{F}(s) \mathbf{F}(s) \\
&= 4 [\mathbf{E}(\infty)]^2 - 4 [\mathbf{E}(s)]^2
\end{aligned} \tag{333}$$

This holds because  $\mathbf{F}(s) \mathbf{F}(s) = \mathbf{E}(\infty) \mathbf{E}(\infty) - \mathbf{E}(s) \mathbf{E}(s)$ , which follows from (331).

The differential equation (333) can be solved exactly by the function [7]

$$\mathbf{E}(s) = \mathbf{E}(\infty) \tanh \left( 4 \mathbf{E}(\infty) s + \operatorname{artanh} \left( \frac{m_e c^2}{\mathbf{E}(\infty)} \right) \right) \tag{334}$$

This can be seen by calculating [7]

$$\begin{aligned}
\frac{d}{ds} \mathbf{E}(s) &= \frac{4 [\mathbf{E}(\infty)]^2}{\cosh^2 \left( 4 \mathbf{E}(\infty) s + \operatorname{artanh} \left( \frac{m_e c^2}{\mathbf{E}(\infty)} \right) \right)} \\
&= 4 [\mathbf{E}(\infty)]^2 \frac{\cosh^2 \left( 4 \mathbf{E}(\infty) s + \operatorname{artanh} \left( \frac{m_e c^2}{\mathbf{E}(\infty)} \right) \right) - \sinh^2 \left( 4 \mathbf{E}(\infty) s + \operatorname{artanh} \left( \frac{m_e c^2}{\mathbf{E}(\infty)} \right) \right)}{\cosh^2 \left( 4 \mathbf{E}(\infty) s + \operatorname{artanh} \left( \frac{m_e c^2}{\mathbf{E}(\infty)} \right) \right)} \\
&= 4 [\mathbf{E}(\infty)]^2 \left( 1 - \tanh^2 \left( 4 \mathbf{E}(\infty) s + \operatorname{artanh} \left( \frac{m_e c^2}{\mathbf{E}(\infty)} \right) \right) \right) \\
&= 4 [\mathbf{E}(\infty)]^2 - 4 [\mathbf{E}(s)]^2
\end{aligned}$$

Since  $s$  is only a number one can see immediately that the condition  $[\mathbf{E}(s_1), \mathbf{E}(s_2)] = \mathbf{0}_{4 \times 4}$  indeed holds true! Furthermore, the solution (334) for  $\mathbf{E}(s)$  is, too, a function depending on the square  $(\alpha_a \Pi_a)^2$ , as has been assumed above.

Now an explicit solution for the function  $\mathbf{F}(s)$  can be given, too [7]:

$$\begin{aligned}
F(s) &= \frac{1}{2} \sqrt{\frac{d}{ds} E(s)} \\
&= \frac{E(\infty)}{\cosh\left(4E(\infty)s + \operatorname{artanh}\left(\frac{m_e c^2}{E(\infty)}\right)\right)} \\
&= \sqrt{[E(\infty)]^2 - [E(s)]^2}
\end{aligned} \tag{335}$$

The explicit and exact solution to the differential equations (324) is very lucky, because now one can explicitly find the unitary transformation  $\mathbf{U}(s)$  yielding the blockdiagonalized Dirac Hamiltonian. Why is that? For that one has to understand the notion "generator" in a more formal way.

For each step  $s$  the unitarily transformed Hamiltonian  $\mathbf{H}(s)$  is given by [7]

$$\mathbf{H}(s) = \mathbf{U}(s) \circ \mathbf{H}^{(D)} \circ \mathbf{U}^\dagger(s) \tag{336}$$

(336) is a *formal* solution to the flow equation (317) for (318) with the generator  $\eta^{(E)}(s) \equiv 2\beta D_A F(s)$ . You can see this by regarding the equation of motion for the unitary transformation  $\mathbf{U}(s)$ :

$$\frac{d}{ds} \mathbf{U}(s) = \hat{\eta}^{(E)}(s) \mathbf{U}(s) \tag{337}$$

with the initial value  $\mathbf{U}(0) = \mathbf{1}_{4 \times 4}$  guaranteeing  $\mathbf{H}(s=0) = \mathbf{H}(0)$ .

With that then [7]

$$\begin{aligned}
\frac{d}{ds} \mathbf{H}(s) &= \frac{d}{ds} \mathbf{U}(s) \circ \mathbf{H}^{(D)} \circ \mathbf{U}^\dagger(s) + \mathbf{U}(s) \circ \mathbf{H}^{(D)} \circ \frac{d}{ds} \mathbf{U}^\dagger(s) \\
&= \hat{\eta}^{(E)}(s) \circ \mathbf{U}(s) \circ \mathbf{H}^{(D)} \circ \mathbf{U}^\dagger(s) + \mathbf{U}(s) \circ \mathbf{H}^{(D)} \circ \mathbf{U}^\dagger(s) \circ \left(-\hat{\eta}^{(E)}(s)\right) \\
&= \left[ \hat{\eta}^{(E)}(s), \mathbf{U}(s) \circ \mathbf{H}^{(D)} \circ \mathbf{U}^\dagger(s) \right] \\
&= \left[ \hat{\eta}^{(E)}(s), \mathbf{H}(s) \right]
\end{aligned} \tag{338}$$

The equation of motion (337) can be solved formally by [7]

$$\begin{aligned}
\mathbf{U}(s) &\equiv \exp \left[ \int_0^s ds' \hat{\eta}(s') \right] \\
&= \exp [\beta D_A \phi_{4 \times 4}(s)] \\
\phi_{4 \times 4}(s) &\equiv 2 \int_0^s ds' \mathbf{F}(s')
\end{aligned} \tag{339}$$

because in here  $[\hat{\eta}(s_1), \hat{\eta}(s_2)] = \hat{0}$  for  $s_1 \neq s_2$ .

In the limit  $s \rightarrow \infty$  of  $\mathbf{U}(s)$  this will give the Newton–Wigner representation  $\mathbf{H}^{(NW)}$  of the Dirac Hamiltonian (10) according to  $\mathbf{H}^{(NW)} = \mathbf{T} \circ \mathbf{H}^{(D)} \circ \mathbf{T}^\dagger$ , where the  $\mathbf{T} = \lim_{s \rightarrow \infty} \mathbf{U}(s)$ . This is done in the following.

Hence, one has to calculate the matrix valued phase  $\phi_{4 \times 4}(s)$ . Since it is a function  $\beta D_A$  of there holds  $[\phi_{4 \times 4}(s), \beta D_A] = \mathbf{0}_{4 \times 4}$ . From that follows for  $\mathbf{U}(s)$  [7]

$$\begin{aligned}
\mathbf{U}(s) &= \sum_{j=0}^{\infty} \frac{(\phi_{4 \times 4}(s))^j}{j!} (\beta D_A)^j \\
&= \sum_{n=0}^{\infty} \frac{(\phi_{4 \times 4}(s))^{2n}}{(2n)!} (\beta D_A)^{2n} + \sum_{n=0}^{\infty} \frac{(\phi_{4 \times 4}(s))^{2n+1}}{(2n+1)!} (\beta D_A)^{2n+1} \\
&= \sum_{n=0}^{\infty} \frac{(\phi_{4 \times 4}(s))^{2n}}{(2n)!} (-1)^n \mathbf{1}_{4 \times 4} + \beta D_A \sum_{n=0}^{\infty} \frac{(\phi_{4 \times 4}(s))^{2n+1}}{(2n+1)!} (-1)^n \mathbf{1}_{4 \times 4} \\
&= \cos [\phi_{4 \times 4}(s)] \mathbf{1}_{4 \times 4} + \beta D_A \sin [\phi_{4 \times 4}(s)]
\end{aligned} \tag{340}$$

where  $(\beta D_A)^{2n} = (-1)^n \mathbf{1}_{4 \times 4}$  and  $(\beta D_A)^{2n+1} = \beta D_A (-1)^n \mathbf{1}_{4 \times 4}$  has been used.

The matrix valued phase  $\phi_{4 \times 4}(s)$  is the solution of the integral equation (339). Hence, its derivative with respect to  $s$  is given by [7]

$$\begin{aligned}
\frac{d}{ds} \phi_{4 \times 4}(s) &= 2\mathbf{F}(s) \\
\phi_{4 \times 4}(0) &= \mathbf{0}_{4 \times 4}
\end{aligned} \tag{341}$$

Now using the solution (335) for  $F(s)$  there holds [7]

$$\begin{aligned}
2F(s) &= \frac{2E(\infty)}{\cosh\left(4E(\infty)s + \operatorname{artanh}\left(\frac{m_e c^2}{E(\infty)}\right)\right)} \\
&= 4E(\infty) \frac{\exp\left(-4E(\infty)s - \operatorname{artanh}\left(\frac{m_e c^2}{E(\infty)}\right)\right)}{1 + \left(\exp\left(-4E(\infty)s - \operatorname{artanh}\left(\frac{m_e c^2}{E(\infty)}\right)\right)\right)^2} \\
&= -\frac{d}{ds} \operatorname{arctan}\left(\exp\left(-4E(\infty)s - \operatorname{artanh}\left(\frac{m_e c^2}{E(\infty)}\right)\right)\right)
\end{aligned} \tag{342}$$

Comparing the last line in (342) with (341) we find the solution for the matrix valued phase [7]

$$\phi_{4 \times 4}(s) = \operatorname{arctan}\left(\exp\left(-\operatorname{artanh}\left(\frac{m_e c^2}{E(\infty)}\right)\right)\right) - \operatorname{arctan}\left(\exp\left(-4E(\infty)s - \operatorname{artanh}\left(\frac{m_e c^2}{E(\infty)}\right)\right)\right) \tag{343}$$

with  $\phi_{4 \times 4}(0) = \mathbf{0}_{4 \times 4}$  as it should be!

The solution (343) can be reexpressed by the help of the identity  $\operatorname{artanh}z = \ln \sqrt{\frac{1+z}{1-z}}$ , such that we can write  $\exp(-\operatorname{artanh}(z)) = \sqrt{\frac{1-z}{1+z}}$ . Hence [7],

$$\phi_{4 \times 4}(s) = \operatorname{arctan}\left(\sqrt{\frac{\mathbf{1}_{4 \times 4} - \frac{m_e c^2}{E(\infty)}}{\mathbf{1}_{4 \times 4} + \frac{m_e c^2}{E(\infty)}}}\right) - \operatorname{arctan}\left(\sqrt{\frac{\mathbf{1}_{4 \times 4} - \frac{m_e c^2}{E(\infty)}}{\mathbf{1}_{4 \times 4} + \frac{m_e c^2}{E(\infty)}}} e^{-4E(\infty)s}\right) \tag{344}$$

Note that  $\phi_{4 \times 4}(\infty) = \operatorname{arctan}\left(\sqrt{\frac{\mathbf{1}_{4 \times 4} - \frac{m_e c^2}{E(\infty)}}{\mathbf{1}_{4 \times 4} + \frac{m_e c^2}{E(\infty)}}}\right)$ . From this follows readily [7]

$$\tan[\phi_{4 \times 4}(\infty)] = \sqrt{\frac{\mathbf{1}_{4 \times 4} - \frac{m_e c^2}{E(\infty)}}{\mathbf{1}_{4 \times 4} + \frac{m_e c^2}{E(\infty)}}} = \frac{\sin[\phi_{4 \times 4}(\infty)]}{\cos[\phi_{4 \times 4}(\infty)]} \tag{345}$$

One can thus conclude [7]

$$\begin{aligned}
\sin [\phi_{4 \times 4}(\infty)] &= \sqrt{\frac{1}{2} \left( \mathbf{1}_{4 \times 4} - \frac{m_e c^2}{\mathbf{E}(\infty)} \right)} \\
\cos [\phi_{4 \times 4}(\infty)] &= \sqrt{\frac{1}{2} \left( \mathbf{1}_{4 \times 4} + \frac{m_e c^2}{\mathbf{E}(\infty)} \right)}
\end{aligned} \tag{346}$$

The factor  $\sqrt{\frac{1}{2}}$  assures that the Pythagorean theorem  $\sin^2 [\phi_{4 \times 4}(\infty)] + \cos^2 [\phi_{4 \times 4}(\infty)] = \mathbf{1}_{4 \times 4}$  holds true.

Finally, for  $s \rightarrow \infty$  of the unitary transformation  $\mathbf{U}(s)$  one harvests the unitary transformation yielding the blockdiagonalized Dirac Hamiltonian, the so-called Newton–Wigner Hamiltonian, according to [7]

$$\begin{aligned}
\mathbf{T} &= \lim_{s \rightarrow \infty} \mathbf{U}(s) = \exp [\beta D_A \phi_{4 \times 4}(\infty)] \\
&= \cos [\phi_{4 \times 4}(\infty)] \mathbf{1}_{4 \times 4} + \beta D_A \sin [\phi_{4 \times 4}(\infty)] \\
&= \sqrt{\frac{1}{2} \left( \mathbf{1}_{4 \times 4} + \frac{m_e c^2}{\mathbf{E}(\infty)} \right)} + \beta D_A \sqrt{\frac{1}{2} \left( \mathbf{1}_{4 \times 4} - \frac{m_e c^2}{\mathbf{E}(\infty)} \right)}
\end{aligned} \tag{347}$$

and [7]

$$\begin{aligned}
\mathbf{T}^\dagger &= \cos [\phi_{4 \times 4}(\infty)] \mathbf{1}_{4 \times 4} - \beta D_A \sin [\phi_{4 \times 4}(\infty)] \\
&= \sqrt{\frac{1}{2} \left( \mathbf{1}_{4 \times 4} + \frac{m_e c^2}{\mathbf{E}(\infty)} \right)} - \beta D_A \sqrt{\frac{1}{2} \left( \mathbf{1}_{4 \times 4} - \frac{m_e c^2}{\mathbf{E}(\infty)} \right)}
\end{aligned} \tag{348}$$

with  $\mathbf{E}(\infty) = \sqrt{\mathbf{H}^{(D)} \circ \mathbf{H}^{(D)}} = m_0 c^2 \sqrt{\mathbf{1}_{4 \times 4} + \frac{2}{m_0 c^2} \mathbf{H}_{4 \times 4}^{(P,0)}}$  and  $\mathbf{H}_{4 \times 4}^{(P,0)} = \frac{\Pi_b \Pi_b}{2m_0} \mathbf{1}_{4 \times 4} - \frac{q_e \hbar}{2m_0} B_b^{(ext)} \sigma_b$ .

From these results the Newton–Wigner Hamiltonian  $\mathbf{H}^{(NW)}$  arises as [7]



$$\begin{aligned}
\mathbf{H}^{(NW)} &= \lim_{s \rightarrow \infty} \mathbf{H}(s) \\
&= \lim_{s \rightarrow \infty} \left( \mathbf{U}(s) \circ \mathbf{H}^{(D)} \circ \mathbf{U}^\dagger(s) \right) \\
&= \mathbf{T} \circ \mathbf{H}^{(D)} \circ \mathbf{T}^\dagger \\
&= \beta \circ \sqrt{\mathbf{H}^{(D)} \circ \mathbf{H}^{(D)}} \\
&= \beta \circ \mathbf{E}(\infty) \\
&= m_0 c^2 \beta \circ \sqrt{\mathbf{1}_{4 \times 4} + \frac{2}{m_0 c^2} \mathbf{H}_{4 \times 4}^{(P,0)}}
\end{aligned} \tag{349}$$

In the following the Newton–Wigner representation of the Dirac operators  $\alpha_a$ ,  $\alpha_b \frac{\Pi_b}{m_0 c}$ ,  $\beta$  and  $\frac{2}{m_0 c^2} \mathbf{H}_{4 \times 4}^{(P,0)}$  will be deduced, as this is useful.

Now for the Dirac  $\alpha_a$  operator we can evaluate [7]

$$\begin{aligned}
\mathbf{T} \alpha_a \mathbf{T}^\dagger &= \mathbf{T} (\mathbf{\Pi}) \alpha_a \mathbf{T}^\dagger (\mathbf{\Pi}) \\
&= \alpha_a + \frac{\Pi_a}{m_0 c} \beta - \frac{1}{4} \frac{\Pi_b}{m_0 c} \frac{\Pi_{b'}}{m_0 c} \left( \alpha_b \alpha_{b'} \alpha_a + \underbrace{\left( \alpha_b \alpha_a + \alpha_a \alpha_b \right)}_{2\delta_{a,b}} \alpha_{b'} \right)
\end{aligned} \tag{350}$$

For transforming the other Dirac operators into the Newton–Wigner representation the following abbreviations are useful [7]

$$\begin{aligned}
\mathbf{C} &= \cos [\phi_{4 \times 4}(\infty)] = \sqrt{\frac{1}{2} \left( \mathbf{1}_{4 \times 4} + \frac{m_0 c^2}{\mathbf{E}(\infty)} \right)} \\
\mathbf{S} &= \sin [\phi_{4 \times 4}(\infty)] = \sqrt{\frac{1}{2} \left( \mathbf{1}_{4 \times 4} - \frac{m_0 c^2}{\mathbf{E}(\infty)} \right)} \\
\mathbf{E}(\infty) &= \sqrt{\mathbf{H}^{(D)} \circ \mathbf{H}^{(D)}} = m_0 c^2 \sqrt{\mathbf{1}_{4 \times 4} + \frac{2}{m_0 c^2} \mathbf{H}_{4 \times 4}^{(P,0)}}
\end{aligned} \tag{351}$$

because for (347) and (348) then [7]

$$\begin{aligned}
\mathbf{T} &= \mathbf{C} + \beta \mathbf{D}_A \mathbf{S} \\
\mathbf{T}^\dagger &= \mathbf{C} - \beta \mathbf{D}_A \mathbf{S}
\end{aligned} \tag{352}$$

Now the properties [7]

$$\begin{aligned}
\{\beta, D_A\} &= \mathbf{0}_{4 \times 4} \\
D_A D_A &= \mathbf{1}_{4 \times 4} = \beta \beta \\
[D_A, \phi_{4 \times 4}(\infty)] &= \mathbf{0}_{4 \times 4} = [\beta, \phi_{4 \times 4}(\infty)]
\end{aligned} \tag{353}$$

readily give [7]

$$\begin{aligned}
\mathbb{T} D_A \mathbb{T}^\dagger &= (\mathbb{C} + \beta D_A \mathbb{S}) D_A (\mathbb{C} - \beta D_A \mathbb{S}) \\
&= D_A (\mathbb{C}^2 - \mathbb{S}^2) + \beta (2\mathbb{C}\mathbb{S}) \\
&= D_A \frac{1}{\sqrt{\mathbf{1}_{4 \times 4} + \frac{2}{m_0 c^2} \mathbb{H}_{4 \times 4}^{(P,0)}}} + \beta \sqrt{\frac{\frac{2}{m_0 c^2} \mathbb{H}_{4 \times 4}^{(P,0)}}{\mathbf{1}_{4 \times 4} + \frac{2}{m_0 c^2} \mathbb{H}_{4 \times 4}^{(P,0)}}}
\end{aligned} \tag{354}$$

Since  $D_A = \frac{\alpha_b \frac{\Pi_b}{m_0 c}}{\sqrt{\left(\alpha_b \frac{\Pi_b}{m_0 c}\right)^2}}$  and  $\left(\alpha_b \frac{\Pi_b}{m_0 c}\right)^2 = \frac{2}{m_0 c^2} \mathbb{H}_{4 \times 4}^{(P,0)}$  there follows for the unitary transformation of the operator  $\alpha_b \frac{\Pi_b}{m_0 c}$  [7]

$$\begin{aligned}
\mathbb{T} \left( \alpha_b \frac{\Pi_b}{m_0 c} \right) \mathbb{T}^\dagger &= \mathbb{T} \left( \sqrt{\left(\alpha_b \frac{\Pi_b}{m_0 c}\right)^2} D_A \right) \mathbb{T}^\dagger \\
&= \sqrt{\left(\alpha_b \frac{\Pi_b}{m_0 c}\right)^2} \mathbb{T} D_A \mathbb{T}^\dagger \\
&= \frac{1}{\sqrt{\mathbf{1}_{4 \times 4} + \frac{2}{m_0 c^2} \mathbb{H}_{4 \times 4}^{(P,0)}}} \left( \frac{\Pi_b}{m_0 c} \alpha_b + \frac{2}{m_0 c^2} \mathbb{H}_{4 \times 4}^{(P,0)} \beta \right)
\end{aligned} \tag{355}$$

For the unitary transformation of the Dirac  $\beta$  matrix then [7]

$$\begin{aligned}
\mathbb{T} \beta \mathbb{T}^\dagger &= \beta (\mathbb{C}^2 - \mathbb{S}^2) - D_A (2\mathbb{C}\mathbb{S}) \\
&= \beta \frac{m_0 c^2}{\mathbb{E}(\infty)} - D_A \sqrt{\left(\mathbf{1}_{4 \times 4} - \frac{m_0 c^2}{\mathbb{E}(\infty)}\right) \left(\mathbf{1}_{4 \times 4} + \frac{m_0 c^2}{\mathbb{E}(\infty)}\right)} \\
&= \beta \frac{1}{\sqrt{\mathbf{1}_{4 \times 4} + \frac{2}{m_0 c^2} \mathbb{H}_{4 \times 4}^{(P,0)}}} - \alpha_b \frac{\Pi_b}{m_0 c} \frac{1}{\sqrt{\mathbf{1}_{4 \times 4} + \frac{2}{m_0 c^2} \mathbb{H}_{4 \times 4}^{(P,0)}}}
\end{aligned} \tag{356}$$

And finally, the unitary transformation of the operator  $\frac{2}{m_0 c^2} \mathbb{H}_{4 \times 4}^{(P,0)}$  [7]

$$\begin{aligned}
\mathbb{T} \left( \frac{2}{m_0 c^2} \mathbb{H}_{4 \times 4}^{(P,0)} \right) \mathbb{T}^\dagger &= \mathbb{T} \left( \alpha_b \frac{\Pi_b}{m_0 c} \right)^2 \mathbb{T}^\dagger \\
&= \mathbb{T} \left( \alpha_b \frac{\Pi_b}{m_0 c} \right) \mathbb{T}^\dagger \mathbb{T} \left( \alpha_b \frac{\Pi_b}{m_0 c} \right) \mathbb{T}^\dagger \\
&= \frac{2}{m_0 c^2} \mathbb{H}_{4 \times 4}^{(P,0)}
\end{aligned} \tag{357}$$

As expected, since the relativistic Pauli Hamiltonian is blockdiagonal.

## C Properties of the Dirac Operators in the Newton–Wigner Representation

As has been shown in section 5, the Newton–Wigner representation of the Dirac–Hamiltonian has very nice properties regarding the possibility to interpret the Dirac–particle. It can be achieved by the help of the Eriksen transformation  $\mathbb{T}$ .

Here some useful identities between the Dirac–operators and their analogues in the Newton–Wigner representation are given.

Now the relation between the Dirac Hamiltonian and the Newton–Wigner Hamiltonian is given by [10, 7]

$$\mathbf{H}^{(NW)} = \beta \circ \sqrt{\mathbf{H}^{(D)} \circ \mathbf{H}^{(D)}} \quad (358)$$

The reverse is then true [7]

$$\mathbf{H}^{(D)} = \mathbb{T}^\dagger \circ \left( \beta \circ \sqrt{\mathbf{H}^{(D)} \circ \mathbf{H}^{(D)}} \right) \circ \mathbb{T} \quad (359)$$

Now since  $[\mathbb{T}, \sqrt{\mathbf{H}^{(D)} \circ \mathbf{H}^{(D)}}] = \mathbf{0}_{4 \times 4}$  one can write for (359) [7]

$$\mathbf{H}^{(D)} = \sqrt{\mathbf{H}^{(D)} \circ \mathbf{H}^{(D)}} \circ \mathbb{T}^\dagger \circ \beta \circ \mathbb{T} \quad (360)$$

From the spectral representation of the Dirac Hamiltonian follows on the other hand [7]

$$\mathbf{H}^{(D)} = \sqrt{\mathbf{H}^{(D)} \circ \mathbf{H}^{(D)}} \circ \left( \mathbf{P}^{(+)} - \mathbf{P}^{(-)} \right) \quad (361)$$

which has been shown in section A of the appendix, see (313)!

Hence [7],

$$\begin{aligned} \mathbb{T}^\dagger \circ \beta \circ \mathbb{T} &= \mathbf{P}^{(+)} - \mathbf{P}^{(-)} \\ &= \frac{\mathbf{H}^{(D)}}{\sqrt{\mathbf{H}^{(D)} \circ \mathbf{H}^{(D)}}} \end{aligned} \quad (362)$$

The validity of the last line has been also shown in section A of the appendix, see (314).

**Justification of the Identity (255)**

The following considerations were inspired by [51]. There holds [7]

$$\langle \mathbf{r}', \mu' | \mathbf{r}, \mu \rangle = \delta_{\mu', \mu} \delta^3(\mathbf{r}' - \mathbf{r}) \quad (363)$$

From the eigenvalue relation  $\langle \mathbf{r}', \mu' | \mathbf{x}_a = \langle \mathbf{r}', \mu' | r'_a$  there follows for the matrix element of the position operator  $\mathbf{x}_a$  with respect to a fixed position state  $|\mathbf{r}, \mu\rangle$  then [7]

$$\begin{aligned} \langle \mathbf{r}', \mu' | \mathbf{x}_a | \mathbf{r}, \mu \rangle &= \langle \mathbf{r}', \mu' | r'_a | \mathbf{r}, \mu \rangle \\ &= r'_a \langle \mathbf{r}', \mu' | \mathbf{r}, \mu \rangle \\ &= r'_a \delta_{\mu', \mu} \delta^3(\mathbf{r}' - \mathbf{r}) \end{aligned} \quad (364)$$

And accordingly [7]

$$\begin{aligned} \langle \mathbf{r}', \mu' | \mathbf{x}_b \mathbf{x}_a | \mathbf{r}, \mu \rangle &= \langle \mathbf{r}', \mu' | r'_b \mathbf{x}_a | \mathbf{r}, \mu \rangle \\ &= r'_b \langle \mathbf{r}', \mu' | \mathbf{x}_b | \mathbf{r}, \mu \rangle \\ &= r'_b r'_a \delta_{\mu', \mu} \delta^3(\mathbf{r}' - \mathbf{r}) \end{aligned} \quad (365)$$

Hence, for a general function  $V(\mathbf{x})$  there holds [7]

$$\begin{aligned} \langle \mathbf{r}', \mu' | V(\mathbf{x}) | \mathbf{r}, \mu \rangle &= V(\mathbf{r}') \langle \mathbf{r}', \mu' | \mathbf{r}, \mu \rangle \\ &= V(\mathbf{r}') \delta_{\mu', \mu} \delta^3(\mathbf{r}' - \mathbf{r}) \end{aligned} \quad (366)$$

Using the completeness relation [7]

$$\sum_{\mu'} \int d^3 r' |\mathbf{r}', \mu'\rangle \langle \mathbf{r}', \mu'| = \hat{\mathbf{1}}_{4 \times 4} \quad (367)$$

The matrix element of the function  $V(\mathbf{x})$  with respect to the Newton–Wigner eigenfunctions  $|U_k^{(NW)}\rangle$  is therefore given by [7]

$$\begin{aligned}
& \langle U_K^{(NW)} | V(\mathbf{x}) | U_k^{(NW)} \rangle \\
&= \langle U_K^{(NW)} | \left( \sum_{\mu'} \int d^3 r' | \mathbf{r}', \mu' \rangle \langle \mathbf{r}', \mu' | \right) V(\mathbf{x}) \left( \sum_{\mu} \int d^3 r | \mathbf{r}, \mu \rangle \langle \mathbf{r}, \mu | \right) | U_k^{(NW)} \rangle \\
&= \sum_{\mu', \mu} \int d^3 r' \int d^3 r \langle U_K^{(NW)} | \mathbf{r}', \mu' \rangle \langle \mathbf{r}', \mu' | V(\mathbf{x}) | \mathbf{r}, \mu \rangle \langle \mathbf{r}, \mu | U_k^{(NW)} \rangle \\
&= \sum_{\mu', \mu} \int d^3 r' \int d^3 r \left( U_{\mu'}^{(NW)}(\mathbf{r}', K) \right)^* \langle \mathbf{r}', \mu' | V(\mathbf{x}) | \mathbf{r}, \mu \rangle U_{\mu}^{(NW)}(\mathbf{r}, k) \\
&= \sum_{\mu', \mu} \int d^3 r' \int d^3 r \left( U_{\mu'}^{(NW)}(\mathbf{r}', K) \right)^* V(\mathbf{r}') \delta_{\mu', \mu} \delta^3(\mathbf{r}' - \mathbf{r}) U_{\mu}^{(NW)}(\mathbf{r}, k) \\
&= \sum_{\mu'} \int d^3 r' \left( U_{\mu'}^{(NW)}(\mathbf{r}', K) \right)^* V(\mathbf{r}') U_{\mu'}^{(NW)}(\mathbf{r}', k)
\end{aligned} \tag{368}$$

For the analogue relations of the momentum operator  $\mathbf{p}_b$  one starts with the fundamental commutation relation

$$[\mathbf{p}_b, \mathbf{x}_a] = \frac{\hbar}{i} \delta_{b,a} \mathbf{1} \tag{369}$$

where  $\mathbf{x}_a$  is the position operator.

The matrix element of the momentum operator in the position representation, with respect to the fixed position eigenstate  $|\mathbf{r}, \mu\rangle$ , assumes the following guise [7]

$$\begin{aligned}
\langle \mathbf{r}', \mu' | \mathbf{p}_b | \mathbf{r}, \mu \rangle &= \left\langle \mathbf{r}', \mu' \left| \frac{\hbar}{i} \frac{\partial}{\partial r'_b} \right| \mathbf{r}, \mu \right\rangle \\
&= \lim_{\tau \rightarrow 0} \frac{\hbar}{i} \frac{1}{2\tau} \left( \langle \mathbf{r}' + \tau \mathbf{e}^{(b)}, \mu' | - \langle \mathbf{r}' - \tau \mathbf{e}^{(b)}, \mu' | \right) | \mathbf{r}, \mu \rangle \\
&= \delta_{\mu', \mu} \lim_{\tau \rightarrow 0} \frac{\hbar}{i} \frac{1}{2\tau} \left( \delta^3(\mathbf{r}' + \tau \mathbf{e}^{(b)} - \mathbf{r}) - \delta^3(\mathbf{r}' - \tau \mathbf{e}^{(b)} - \mathbf{r}) \right)
\end{aligned} \tag{370}$$

Therefore [7]

$$\begin{aligned}
& \langle \mathbf{r}', \mu' | \mathbf{p}_b \mathbf{p}_a | \mathbf{r}, \mu \rangle \\
&= \left( \langle \mathbf{r}', \mu' | \frac{\hbar}{i} \frac{\partial}{\partial r'_b} \right) \mathbf{p}_a | \mathbf{r}, \mu \rangle \\
&= \lim_{\tau \rightarrow 0} \frac{\hbar}{i} \frac{1}{2\tau} \left( \langle \mathbf{r}' + \tau \mathbf{e}^{(b)}, \mu' | - \langle \mathbf{r}' - \tau \mathbf{e}^{(b)}, \mu' | \right) \mathbf{p}_a | \mathbf{r}, \mu \rangle \\
&= \lim_{\tau \rightarrow 0} \frac{\hbar}{i} \frac{1}{2\tau} \left( \langle \mathbf{r}' + \tau \mathbf{e}^{(b)}, \mu' | \mathbf{p}_a - \langle \mathbf{r}' - \tau \mathbf{e}^{(b)}, \mu' | \mathbf{p}_a \right) | \mathbf{r}, \mu \rangle \\
&= \lim_{\tau \rightarrow 0} \frac{\hbar}{i} \frac{1}{2\tau} \left( \langle \mathbf{r}' + \tau \mathbf{e}^{(b)}, \mu' | \mathbf{p}_a | \mathbf{r}, \mu \rangle - \langle \mathbf{r}' - \tau \mathbf{e}^{(b)}, \mu' | \mathbf{p}_a | \mathbf{r}, \mu \rangle \right) \\
&= \delta_{\mu', \mu} \lim_{\tau \rightarrow 0} \lim_{\tau' \rightarrow 0} \left( \frac{\hbar}{i} \right)^2 \frac{1}{2\tau} \frac{1}{2\tau'} \left( \begin{aligned} & \delta^3(\mathbf{r}' + \tau \mathbf{e}^{(b)} + \tau' \mathbf{e}^{(a)} - \mathbf{r}) - \delta^3(\mathbf{r}' + \tau \mathbf{e}^{(b)} - \tau' \mathbf{e}^{(a)} - \mathbf{r}) \\ & - \delta^3(\mathbf{r}' - \tau \mathbf{e}^{(b)} + \tau' \mathbf{e}^{(a)} - \mathbf{r}) + \delta^3(\mathbf{r}' - \tau \mathbf{e}^{(b)} - \tau' \mathbf{e}^{(a)} - \mathbf{r}) \end{aligned} \right) \quad (371)
\end{aligned}$$

Now, in the Newton Wigner representation then [7]

$$\begin{aligned}
& \left\langle U_K^{(NW)} \middle| \mathbf{p}_b \mathbf{p}_a \middle| U_k^{(NW)} \right\rangle \\
&= \left\langle U_K^{(NW)} \middle| \left( \sum_{\mu'} \int d^3 r' | \mathbf{r}', \mu' \rangle \langle \mathbf{r}', \mu' | \right) \mathbf{p}_b \mathbf{p}_a \left( \sum_{\mu} \int d^3 r | \mathbf{r}, \mu \rangle \langle \mathbf{r}, \mu | \right) \middle| U_k^{(NW)} \right\rangle \\
&= \sum_{\mu', \mu} \int d^3 r' \int d^3 r \left\langle U_K^{(NW)} \middle| \mathbf{r}', \mu' \right\rangle \langle \mathbf{r}', \mu' | \mathbf{p}_b \mathbf{p}_a | \mathbf{r}, \mu \rangle \langle \mathbf{r}, \mu | U_k^{(NW)} \rangle \\
&= \sum_{\mu', \mu} \int d^3 r' \int d^3 r \left( U_{\mu'}^{(NW)}(\mathbf{r}', K) \right)^* \langle \mathbf{r}', \mu' | \mathbf{p}_b \mathbf{p}_a | \mathbf{r}, \mu \rangle U_{\mu}^{(NW)}(\mathbf{r}, k) \\
&= \sum_{\mu', \mu} \int d^3 r' \int d^3 r \left( U_{\mu'}^{(NW)}(\mathbf{r}', K) \right)^* \delta_{\mu', \mu} \lim_{\tau \rightarrow 0} \lim_{\tau' \rightarrow 0} \left( \frac{\hbar}{i} \right)^2 \frac{1}{2\tau} \frac{1}{2\tau'} \times \\
&\quad \times \left( \begin{aligned} & \delta^3(\mathbf{r}' + \tau \mathbf{e}^{(b)} + \tau' \mathbf{e}^{(a)} - \mathbf{r}) - \delta^3(\mathbf{r}' + \tau \mathbf{e}^{(b)} - \tau' \mathbf{e}^{(a)} - \mathbf{r}) \\ & - \delta^3(\mathbf{r}' - \tau \mathbf{e}^{(b)} + \tau' \mathbf{e}^{(a)} - \mathbf{r}) + \delta^3(\mathbf{r}' - \tau \mathbf{e}^{(b)} - \tau' \mathbf{e}^{(a)} - \mathbf{r}) \end{aligned} \right) U_{\mu}^{(NW)}(\mathbf{r}, k) \\
&= \sum_{\mu'} \int d^3 r' \left( U_{\mu'}^{(NW)}(\mathbf{r}', K) \right)^* \lim_{\tau \rightarrow 0} \lim_{\tau' \rightarrow 0} \left( \frac{\hbar}{i} \right)^2 \frac{1}{2\tau} \frac{1}{2\tau'} \\
&\quad \times \left( \begin{aligned} & U_{\mu}^{(NW)}(\mathbf{r}' + \tau \mathbf{e}^{(b)} + \tau' \mathbf{e}^{(a)}, k) - U_{\mu'}^{(NW)}(\mathbf{r}' + \tau \mathbf{e}^{(b)} - \tau' \mathbf{e}^{(a)}, k) \\ & - U_{\mu}^{(NW)}(\mathbf{r}' - \tau \mathbf{e}^{(b)} + \tau' \mathbf{e}^{(a)}, k) + U_{\mu}^{(NW)}(\mathbf{r}' - \tau \mathbf{e}^{(b)} - \tau' \mathbf{e}^{(a)}, k) \end{aligned} \right) \\
&= \sum_{\mu'} \int d^3 r' \left( U_{\mu'}^{(NW)}(\mathbf{r}', K) \right)^* \left( \frac{\hbar}{i} \frac{\partial}{\partial r'_a} \frac{\hbar}{i} \frac{\partial}{\partial r'_b} U_{\mu'}^{(NW)}(\mathbf{r}', k) \right) \quad (372)
\end{aligned}$$

Hence, for a general polynomia  $Y(\mathbf{p})$ , applying the superpositon principle [7],

$$\begin{aligned}
& \langle U_K^{(NW)} | Y(\mathbf{p}) | U_k^{(NW)} \rangle \\
&= \langle U_K^{(NW)} | \left( \sum_{\mu'} \int d^3 r' | \mathbf{r}', \mu' \rangle \langle \mathbf{r}', \mu' | \right) Y(\mathbf{p}) \left( \sum_{\mu} \int d^3 r | \mathbf{r}, \mu \rangle \langle \mathbf{r}, \mu | \right) | U_k^{(NW)} \rangle \\
&= \sum_{\mu', \mu} \int d^3 r' \int d^3 r \langle U_K^{(NW)} | \mathbf{r}', \mu' \rangle \langle \mathbf{r}', \mu' | Y(\mathbf{p}) | \mathbf{r}, \mu \rangle \langle \mathbf{r}, \mu | U_k^{(NW)} \rangle \\
&= \sum_{\mu'} \int d^3 r' \left( U_{\mu'}^{(NW)}(\mathbf{r}', K) \right)^* \langle \mathbf{r}', \mu' | Y(\mathbf{p}) | \mathbf{r}, \mu \rangle U_{\mu'}^{(NW)}(\mathbf{r}', k) \\
&= \sum_{\mu'} \int d^3 r' \left( U_{\mu'}^{(NW)}(\mathbf{r}', K) \right)^* \left( Y \left( \frac{\hbar}{i} \nabla' \right) U_{\mu'}^{(NW)}(\mathbf{r}', k) \right)
\end{aligned} \tag{373}$$

So that finally for a function  $F_{\mu', \mu}(\mathbf{x}, \mathbf{p})$  the matrix element with respect to a Newton–Wigner eigenstate [7]

$$\begin{aligned}
& \langle U_K^{(NW)} | F_{4 \times 4}(\mathbf{x}, \mathbf{p}) | U_k^{(NW)} \rangle \\
&= \langle U_K^{(NW)} | \left( \sum_{\mu'} \int d^3 r' | \mathbf{r}', \mu' \rangle \langle \mathbf{r}', \mu' | \right) F_{4 \times 4}(\mathbf{x}, \mathbf{p}) \left( \sum_{\mu} \int d^3 r | \mathbf{r}, \mu \rangle \langle \mathbf{r}, \mu | \right) | U_k^{(NW)} \rangle \\
&= \sum_{\mu', \mu} \int d^3 r' \int d^3 r \langle U_K^{(NW)} | \mathbf{r}', \mu' \rangle \langle \mathbf{r}', \mu' | F_{4 \times 4}(\mathbf{x}, \mathbf{p}) | \mathbf{r}, \mu \rangle \langle \mathbf{r}, \mu | U_k^{(NW)} \rangle \\
&= \sum_{\mu'} \int d^3 r' \left( U_{\mu'}^{(NW)}(\mathbf{r}', K) \right)^* \left( F_{\mu', \mu} \left( \mathbf{r}', \frac{\hbar}{i} \nabla' \right) U_{\mu}^{(NW)}(\mathbf{r}', k) \right)
\end{aligned} \tag{374}$$

## D Relation between the Dirac Hamiltonian and the Schrödinger Pauli Hamiltonian in a static external magnetic field

For the square of the Dirac Hamiltonian we find explicetly [7]

$$\begin{aligned} \mathbf{H}^{(D)} \circ \mathbf{H}^{(D)} &= (m_0 c^2 \beta + c \alpha_b \Pi_b) \circ (m_0 c^2 \beta + c \alpha_{b'} \Pi_{b'}) \\ &= \left( (m_0 c^2)^2 + c^2 \Pi_b \Pi_b \right) \mathbf{1}_{4 \times 4} - q_e \hbar c^2 B_{b''}^{(ext)} \sigma_{b''} \end{aligned} \quad (375)$$

where we have used the anticommutation relation  $\{\alpha_b, \beta\} = 0_{4 \times 4}$ ,  $b \in \{x, y, z\}$ .  $\sigma_b$  is the relativistic spin operator given in (158).

The square of the Dirac Hamiltonian, represented by a matrix, assumes the following guise [7]

$$\begin{aligned} & \left( (m_0 c^2)^2 + c^2 \Pi_b \Pi_b \right) \mathbf{1}_{4 \times 4} - q_e \hbar c^2 B_{b''}^{(ext)} \sigma_{b''} \\ &= \left( \begin{array}{cc} \left( (m_0 c^2)^2 + c^2 \Pi_b \Pi_b \right) \mathbf{1}_{2 \times 2} - q_e \hbar c^2 B_b^{(ext)} \sigma_b^{(P)} & 0_{2 \times 2} \\ 0_{2 \times 2} & \left( (m_0 c^2)^2 + c^2 \Pi_b \Pi_b \right) \mathbf{1}_{2 \times 2} - q_e \hbar c^2 B_b^{(ext)} \sigma_b^{(P)} \end{array} \right) \\ &= (m_0 c^2)^2 \left( \mathbf{1}_{4 \times 4} + \frac{2}{m_0 c^2} \mathbf{H}_{4 \times 4}^{(P,0)} \right) \end{aligned} \quad (376)$$

Where the  $4 \times 4$  Pauli Hamiltonian is given by

$$\mathbf{H}_{4 \times 4}^{(P,0)} = \mathbf{1}_{2 \times 2} \otimes \mathbf{H}_{2 \times 2}^{(SP,0)} \quad (377)$$

and the  $2 \times 2$  Schrödinger Pauli Hamiltonian describing the nonrelativistic electron in an external magnet induction field is given by

$$\mathbf{H}_{2 \times 2}^{(SP,0)} = \frac{\Pi_b \Pi_b}{2m_0} \mathbf{1}_{2 \times 2} - \frac{q_e \hbar}{2m_0} B_b^{(ext)} \sigma_b^{(P)} \quad (378)$$

Hence, the square root of the Dirac Hamiltonian is related to the Schrödinger Pauli Hamiltonian according to

$$\sqrt{\mathbf{H}^{(D)} \circ \mathbf{H}^{(D)}} = m_0 c^2 \times \mathbf{1}_{2 \times 2} \otimes \sqrt{\mathbf{1}_{2 \times 2} + \frac{2}{m_0 c^2} \mathbf{H}_{2 \times 2}^{(SP,0)}} \quad (379)$$



It is now possible to expand the square root  $\sqrt{\mathbf{1}_{2 \times 2} + \frac{2}{m_0 c^2} \mathbf{H}_{2 \times 2}^{(SP,0)}}$  as a Taylor series:

$$\sqrt{\mathbf{1}_{2 \times 2} + \frac{2}{m_0 c^2} \mathbf{H}_{2 \times 2}^{(SP,0)}} = \mathbf{1}_{2 \times 2} + \frac{1}{m_0 c^2} \mathbf{H}_{2 \times 2}^{(SP,0)} - \frac{1}{2} \left( \frac{1}{m_0 c^2} \mathbf{H}_{2 \times 2}^{(SP,0)} \right)^2 + \dots \quad (380)$$

With the expansion (380) one finds a nonlocal, gauge invariant representation of  $\sqrt{\mathbf{H}^{(D)} \circ \mathbf{H}^{(D)}}$  according to

$$\sqrt{\mathbf{H}^{(D)} \circ \mathbf{H}^{(D)}} = \sqrt{\left( (m_0 c^2)^2 + c^2 \Pi_b \Pi_b \right) \mathbf{1}_{4 \times 4} - q_e \hbar c^2 B_b^{(ext)} \sigma_b} \quad (381)$$

With the ansatz  $\sqrt{\mathbf{H}^{(D)} \circ \mathbf{H}^{(D)}} = W_0 \mathbf{1}_{4 \times 4} + W_b \sigma_b$  [7] it is possible to find the coefficients  $W_0$  and  $W_b$  for a linear representation of (381).

Squaring the ansatz then [7]

$$\begin{aligned} \left( (m_0 c^2)^2 + c^2 \Pi_b \Pi_b \right) \mathbf{1}_{4 \times 4} - q_e \hbar c^2 B_b^{(ext)} \sigma_b &= (W_0 \mathbf{1}_{4 \times 4} + W_b \sigma_b)^2 \\ &= (W_0^2 + W_b W_b) \mathbf{1}_{4 \times 4} + (W_0 W_b + W_b W_0) \sigma_b \end{aligned} \quad (382)$$

Hence, by comparing the linearly independent matrices  $\mathbf{1}_{4 \times 4}$  and of  $\sigma_b$  [7],

$$\begin{aligned} W_0^2 + W_b W_b &= (m_0 c^2)^2 + c^2 \Pi_b \Pi_b \\ W_0 W_b + W_b W_0 &= -q_e \hbar c^2 B_b^{(ext)} \end{aligned} \quad (383)$$

If the external magnetic induction field  $B_b^{(ext)}$  is constant then  $\Pi_b \Pi_b$  commutes with  $B_b^{(ext)}$  and there holds  $W_0 W_b + W_b W_0 = 2W_0 W_b$ .

In that case then [7]

$$W_b = -\frac{q_e \hbar c^2 B_b^{(ext)}}{2W_0} \quad (384)$$

and [7]

$$W_0^2 + W_b W_b = W_0^2 + \frac{1}{W_0^2} \left( -\frac{q_e \hbar c^2}{2} |\mathbf{B}^{(ext)}| \right)^2 \quad (385)$$

$$\stackrel{!}{=} (m_0 c^2)^2 + c^2 \Pi_b \Pi_b$$

This leads then to [7]

$$W_0^4 - W_0^2 \left( (m_0 c^2)^2 + c^2 \Pi_b \Pi_b \right) + \left( -\frac{q_e \hbar c^2}{2} |\mathbf{B}^{(ext)}| \right)^2 = 0 \quad (386)$$

$$\left( W_0^2 - \frac{1}{2} \left( (m_0 c^2)^2 + c^2 \Pi_b \Pi_b \right) \right)^2 = \frac{1}{4} \left( (m_0 c^2)^2 + c^2 \Pi_b \Pi_b \right)^2 - \frac{(q_e \hbar c^2 |\mathbf{B}^{(ext)}|)^2}{4}$$

Since  $W_0$  is real one can ignore the solution with the minus sign and find [7]

$$W_0^2 = \frac{1}{2} \left( (m_0 c^2)^2 + c^2 \Pi_b \Pi_b + \sqrt{\left( (m_0 c^2)^2 + c^2 \Pi_b \Pi_b \right)^2 - \frac{(q_e \hbar c^2 |\mathbf{B}^{(ext)}|)^2}{4}} \right) \quad (387)$$

which can be represented as a square according to [7]

$$W_0^2 = \left( \frac{1}{2} \sqrt{\left( (m_0 c^2)^2 + c^2 \Pi_b \Pi_b \right) + \frac{q_e \hbar c^2 |\mathbf{B}^{(ext)}|}{2}} + \frac{1}{2} \sqrt{\left( (m_0 c^2)^2 + c^2 \Pi_b \Pi_b \right) - \frac{q_e \hbar c^2 |\mathbf{B}^{(ext)}|}{2}} \right)^2 \quad (388)$$

Altogether then [7]

$$W_0 = \frac{w_+ + w_-}{2}$$

$$w_{\pm} = \sqrt{\left( (m_0 c^2)^2 + c^2 \Pi_b \Pi_b \right) \pm \frac{q_e \hbar c^2 |\mathbf{B}^{(ext)}|}{2}} \quad (389)$$

$$W_b = -\frac{q_e \hbar c^2 B_b^{(ext)}}{2W_0} = -\frac{q_e \hbar c^2 B_b^{(ext)}}{w_+ + w_-}$$

This means that for a homogenous static magnetic induction field  $B_b^{(ext)}$  we find exactly [7]

$$\sqrt{\mathbf{H}^{(D)} \circ \mathbf{H}^{(D)}} = \frac{w_+ + w_-}{2} \mathbf{1}_{4 \times 4} - \frac{q_e \hbar c^2 B_b^{(ext)}}{w_+ + w_-} \sigma_b \quad (390)$$

which is *not* the Dirac Hamiltonian  $\mathbf{H}^{(D)}$ .

Since  $\left[ \sqrt{\mathbf{H}^{(D)} \circ \mathbf{H}^{(D)}}, B_b^{(ext)} \sigma_b \right] = \hat{0}$  there exists a common basis of eigenfunctions of  $B_b^{(ext)} \sigma_b$  and  $\Pi_b \Pi_b$ .

For a weak magnetic induction field there still holds [7]

$$\begin{aligned} \sqrt{\mathbf{H}^{(D)} \circ \mathbf{H}^{(D)}} &= \sqrt{(m_0 c^2)^2 + c^2 \Pi_b \Pi_b} \times \mathbf{1}_{4 \times 4} - \frac{q_e \hbar c^2}{2 \sqrt{(m_0 c^2)^2 + c^2 \Pi_b \Pi_b}} B_b^{(ext)} \sigma_b \\ &+ O\left(\left| \mathbf{B}^{(ext)} \right|^2\right) \end{aligned} \quad (391)$$

Weak means here that the magnetic length  $L_B = \sqrt{\frac{2\hbar}{|q_e| B^{(ext)}}}$  is much larger than the Bohr radius  $a_B$ , hence  $L_B \gg a_B$ .

## E Orders of Magnitude in the QED Hamiltonian

Here it is explained why the transversal coupling contribution  $\hat{\mathcal{H}}_{\perp}$  to the QED Hamiltonian is of first order in the finestructure constant whereas the Coulomb–interaction contribution  $\hat{\mathcal{V}}_C$  is of second order. The notation is taken from [7].

Now with the electron mass  $m_e$ , the vacuum speed of light  $c$  and Plancks constant  $\hbar$  the Compton wavelength of the electron is given by

$$\begin{aligned} k_C &= \frac{m_e c}{\hbar} = \frac{2\pi}{\lambda_C} \\ \lambda_C &= \frac{h}{m_e c} \simeq 2.4 \times 10^{-12} [m] \end{aligned} \quad (392)$$

Multiplying this with the Bohr radius  $a_B$  of the hydrogen atom

$$a_B = \frac{4\pi\epsilon_0 \hbar^2}{|e|^2 m_e} \quad (393)$$

the product  $k_C a_B$  is a dimensionless number

$$\begin{aligned} k_C a_B &= \frac{m_e c}{\hbar} \frac{4\pi\epsilon_0 \hbar^2}{|e|^2 m_e} = \frac{4\pi\epsilon_0 \hbar c}{|e|^2} = \frac{1}{\alpha_{FS}} = 137.036 \\ \alpha_{FS} &= \frac{|e|^2}{4\pi\epsilon_0 \hbar c} = \frac{1}{k_C a_B} \end{aligned} \quad (394)$$

hence, nothing but the finestructure constant  $\alpha_{FS}$ .

The Hamiltonian of the Schrödinger eigenvalue problem of one electron in the Coulomb field of the (infinitely heavy, resting) proton is given by

$$H = -\frac{\hbar^2}{2m_e} \nabla_r^2 - \frac{|e|^2}{4\pi\epsilon_0 r} \quad (395)$$

One can now rewrite the components  $r_a$  of the positon operator, where  $a \in \{x, y, z\}$ , as a multiple of the Bohr radius according to  $r_a = a_B \bar{r}_a$ . For the Hamiltonian (395) follows

$$H = \frac{|e|^2}{4\pi\epsilon_0} \frac{1}{a_B} \left[ -\frac{4\pi\epsilon_0}{|e|^2} a_B \frac{\hbar^2}{2m_e} \frac{1}{a_B^2} \nabla_{\vec{r}}^2 - \frac{1}{\vec{r}} \right] \quad (396)$$

Note that  $\frac{4\pi\epsilon_0}{|e|^2} a_B \frac{\hbar^2}{2m_e} \frac{1}{a_B^2} = \frac{4\pi\epsilon_0}{|e|^2} \frac{\hbar^2}{m_e} \frac{1}{2a_B} = \frac{1}{2}$ . Hence, the Hamiltonian can be rewritten according to  $H = E_C \bar{H}$  with  $E_C = \frac{|e|^2}{4\pi\epsilon_0} \frac{1}{a_B}$ . In atomic units one readily finds

$$\bar{H} = -\frac{1}{2} \nabla_{\vec{r}}^2 - \frac{1}{\vec{r}} \quad (397)$$

The Hamiltonian (397) is the dimensionless Hamiltonian of the hydrogen atom. The constant  $E_C$ , the Hartree, is the double of the expectation value of the electron in the ground state  $1s$  :

$$\begin{aligned} E_C = -2E_{1s} &= \frac{|e|^2}{4\pi\epsilon_0} \left\langle \frac{1}{r} \right\rangle_{1s} = \frac{|e|^2}{4\pi\epsilon_0} \frac{1}{a_B} = \frac{|e|^2}{4\pi\epsilon_0} \frac{4\pi\epsilon_0}{|e|^2} \frac{\hbar^2}{m_e} = \left( \frac{|e|^2}{4\pi\epsilon_0} \frac{1}{\hbar c} \right)^2 m_e c^2 \\ &= \alpha_{FS}^2 m_e c^2 = 2 \times 13.606 [eV] \end{aligned} \quad (398)$$

In atomic units the action is measured as a multiple of the Planck constant  $\hbar$ , charge as a multiple of the elementary charge  $|e|$ , mass as a multiple of the electron mass  $m_e$ , length as a multiple of the Bohr radius  $a_B$ , energy as a multiple of the Hartree  $E_C$ , velocity as a multiple of the velocity  $v_{1s}$  of the hydrogen–electron in its ground state  $1s$ . It thus seems like  $\hbar = 1$ ,  $|e| = 1$ ,  $m_e = 1$ ,  $a_B = 1$ ,  $E_C = 1$ . The Bohr magneton  $\mu_B \equiv \frac{|e|\hbar}{2m_e}$  in atomic units is given by  $\mu_B = \frac{1}{2}$ .

The electric field strength in atomic units is therefore given by

$$\mathcal{E}_0 = \frac{E_C}{|e| a_B} = \frac{|e|}{4\pi\epsilon_0} \frac{1}{a_B^2} \quad (399)$$

From the Lorentz equation of motion follows for the magnetic induction field strength

$$\mathcal{B}_0 = \frac{\mathcal{E}_0}{c} \quad (400)$$

The virial theorem yields for the kinetic energy of the electron in the groundstate  $1s$

$$\frac{m_e}{2} v_{1s}^2 = -E_{1s} = \frac{E_C}{2} \quad (401)$$

giving

$$v_{1s} = \sqrt{\frac{E_C}{m_e}} = \sqrt{\frac{\alpha_{FS}^2 m_e c^2}{m_e}} = \alpha_{FS} c \simeq \frac{c}{137} \quad (402)$$

The speed of light  $c$  in atomic units is thus given by  $\bar{c} = \frac{c}{v_{1s}} = \frac{1}{\alpha_{FS}} \simeq 137!$

Therefore one finds for magnetic induction field strength (400)

$$\begin{aligned} \mathcal{B}_0 &= \frac{\mathcal{E}_0}{v_{1s}} = \frac{E_C}{|e| a_B v_{1s}} = \frac{\alpha_{FS}^2 m_e c^2}{|e| a_B} \frac{1}{v_{1s}} \\ &= \frac{\hbar}{2|e|} = \frac{\Phi_0}{\pi a_B^2} \end{aligned} \quad (403)$$

This is magnetic induction field with one magnetic flux quantum  $\Phi_0 = \frac{\hbar}{2|e|}$  per area of radius  $a_B$ . In SI units this is a very high field strength  $\mathcal{B}_0 \simeq 2.3 \times 10^5 [T]!$  The values we can have in the laboratory are at least four orders of magnitude smaller!

Finally one finds for gauge invariant velocity operator  $\hat{\Pi}_a$  in atomic units:

$$\begin{aligned} \frac{\hat{\Pi}_a}{m_0 c} &= \left( \frac{\hbar}{m_0 c a_B} \right) \frac{1}{i} \frac{\partial}{\partial \left( \frac{r_a}{a_B} \right)} - \frac{|e|}{m_0 c} a_B \mathcal{B}_0 \left( \frac{q}{|e|} \frac{\hat{A}_a^{(T)}(\mathbf{r}) + A_a^{(ext)}(\mathbf{r}, t)}{\mathcal{B}_0 a_B} \right) \\ &= \alpha_{FS} \bar{\Pi}_a \end{aligned} \quad (404)$$

Here the identity  $\frac{|e| a_B}{m_0 c} \mathcal{B}_0 = \frac{|e| a_B}{m_0 c} \left( \frac{\hbar}{|e| a_B^2} \right) = \frac{1}{k_C a_B} = \alpha_{FS}$  has been used.

Furthermore,  $\bar{q} = \frac{q}{|e|} = \frac{q}{|e|}$  is the coupling constant of the electromagnetic fields in atomic units, and

$$\begin{aligned}
\bar{t} &= \frac{t}{t_B} \\
t_B &= \frac{a_B}{c} \\
\bar{A}_a(\bar{\mathbf{r}}, \bar{t}) &= \frac{\hat{A}_a^{(T)}(a_B \bar{\mathbf{r}}) + A_a^{(ext)}(a_B \bar{\mathbf{r}}, t_B \bar{t})}{\mathcal{B}_0 a_B} \\
\bar{\Pi}_a &= \frac{1}{i} \frac{\partial}{\partial \bar{r}_a} - \bar{q} \bar{A}_a(\bar{\mathbf{r}}, \bar{t})
\end{aligned} \tag{405}$$

Therefore, the contribution  $\hat{\mathcal{H}}_\perp$  is smaller by a factor  $\alpha_{FS}$  than  $\hat{\mathcal{H}}_D$ ! Using (405) there holds

$$\begin{aligned}
\frac{1}{m_0 c^2} \hat{\mathcal{H}}_\perp &= -\frac{1}{m_0 c^2} \int d^3 r \hat{j}_b(\mathbf{r}) \hat{A}_b^{(T)}(\mathbf{r}) \\
&= -\alpha_{FS} \int d^3 r \sum_{\mu, \mu' \in \{1, 2, 3, 4\}} \hat{\Psi}_\mu^\dagger(\mathbf{r}) (\alpha_b)_{\mu' \mu''} \hat{\Psi}_{\mu''}(\mathbf{r}) \bar{q} \bar{A}_a^{(T)}(\mathbf{r})
\end{aligned} \tag{406}$$

The Coulomb interaction  $\hat{\mathcal{V}}_C$  is smaller by a factor  $\alpha_{FS}^2$  than  $\hat{\mathcal{H}}_D$  or the rest energy  $m_e c^2$ :

$$\frac{1}{m_e c^2} \frac{|e|^2}{4\pi \epsilon_0 a_B} = \frac{E_C}{m_0 c^2} = \alpha_{FS}^2 \tag{407}$$

The term  $\hat{\mathcal{H}}_{rad}$  has to be a zeroth order term in the perturbation expansion, because if one would assume it to be of order  $\alpha_{FS}^2$  as is the Coulomb–interaction one would assume that there are no high energy photons in the QED soup! This would not be consistent. The energy of one photon might be small, however, the occupation number of the electromagnetic modes can take *any* value.

## F Charge Conjugation Symmetrie of QED, Normal Ordering and QED Ground State

It is searched for the operator  $\hat{\mathcal{C}}_F$  that causes the exchange of the matter annihilation operator  $\hat{c}_k$  with  $\hat{b}_k$ , and of the antimatter creation operator  $\hat{b}_k^\dagger$  with  $\hat{c}_k^\dagger$ .

In textbooks, the so-called charge conjugation operator is introduced according to

$$\hat{\mathcal{C}}_F = -i\beta\alpha_y \quad (408)$$

see for example [5]. The operator (408) acts on the amplitudes  $U_\mu(\mathbf{r}; k)$  and  $V_\mu(\mathbf{r}; k)$  and gives the charge conjugated amplitudes  $U_\mu^{(C)}(\mathbf{r}; k)$  and  $V_\mu^{(C)}(\mathbf{r}; k)$ .

For understanding the relation between the normal ordering operation  $\mathcal{N}$  and the operation  $\frac{1-\mathcal{C}_F}{2}$  for correctly defining the QED Hamiltonian (8), the charge conjugation operation  $\mathcal{C}_F$  acting on the creation and annihilation operators is introduced as [7]

$$\begin{aligned} \hat{\mathcal{C}}_F &= \exp \left[ i\frac{\pi}{2} \sum_{k'} \hat{X}_{k'} \right] \\ \hat{X}_k &= \left( \hat{c}_k^\dagger - \hat{b}_k^\dagger \right) \left( \hat{c}_k - \hat{b}_k \right) \\ \hat{\mathcal{C}}_F^\dagger &= \exp \left[ -i\frac{\pi}{2} \sum_{k'} \hat{X}_{k'} \right] \\ \hat{\mathcal{C}}_F^\dagger \hat{\mathcal{C}}_F &= \hat{1} = \hat{\mathcal{C}}_F \hat{\mathcal{C}}_F^\dagger \end{aligned} \quad (409)$$

Applied to the fermion creation and annihilation operators it results in their exchange according to [7]

$$\begin{aligned} \hat{\mathcal{C}}_F \hat{c}_k \hat{\mathcal{C}}_F^\dagger &= \hat{b}_k \\ \hat{\mathcal{C}}_F \hat{b}_k^\dagger \hat{\mathcal{C}}_F^\dagger &= \hat{c}_k^\dagger \end{aligned} \quad (410)$$

This can be proven by the help of the BCH expansion (see (629)). With [7]



$$\hat{\mathcal{C}}_F \hat{c}_k \hat{\mathcal{C}}_F^\dagger = \hat{c}_k + \sum_{n=1}^{\infty} \frac{\left(i\frac{\pi}{2}\right)^n}{n!} \left[\hat{X}_k, \hat{c}_k\right]^{(n)} \quad (411)$$

Now the  $n$ -th term is given recursively [7],

$$\left[\hat{X}_k, \hat{c}_k\right]^{(n)} = \left[\hat{X}_k, \left[\hat{X}_k, \hat{c}_k\right]^{(n-1)}\right]$$

and from  $\left[\hat{X}_k, \hat{c}_k\right]^{(1)} = \left[\hat{X}_k, \hat{c}_k\right] = -\left(\hat{c}_k - \hat{b}_k\right)$

one finds [7]

$$\left[\hat{X}_k, \hat{c}_k\right]^{(n)} = \frac{1}{2} (-2)^n \left(\hat{c}_k - \hat{b}_k\right)$$

Such that [7]

$$\begin{aligned} \hat{\mathcal{C}}_F \hat{c}_k \hat{\mathcal{C}}_F^\dagger &= \hat{c}_k + \sum_{n=1}^{\infty} \frac{\left(i\frac{\pi}{2}\right)^n}{n!} \frac{1}{2} (-2)^n \left(\hat{c}_k - \hat{b}_k\right) \\ &= \hat{c}_k + \frac{1}{2} \sum_{n=1}^{\infty} \frac{(-i\pi)^n}{n!} \left(\hat{c}_k - \hat{b}_k\right) \\ &= \hat{c}_k + \frac{1}{2} \left(e^{-i\pi} - 1\right) \left(\hat{c}_k - \hat{b}_k\right) \\ &= \hat{b}_k \end{aligned} \quad (412)$$

Now the question is what the charge conjugated Dirac field operator  $\hat{\Psi}_\mu^{(C)}(\mathbf{r})$ . In order to find it one has to apply the charge conjugation operation (409). Denoting the conjugated amplitudes with the superscript  $(C)$  then [7]

$$\begin{aligned} \hat{\Psi}_\mu^{(C)}(\mathbf{r}) &= \hat{\mathcal{C}}_F \hat{\Psi}_\mu(\mathbf{r}) \hat{\mathcal{C}}_F^\dagger \\ &= \hat{\mathcal{C}}_F \sum_k \left( U_\mu(\mathbf{r}; k) \hat{c}_k + V_\mu(\mathbf{r}; k) \hat{b}_k^\dagger \right) \hat{\mathcal{C}}_F^\dagger \\ &= \sum_k \left( U_\mu^{(C)}(\mathbf{r}; k) \hat{\mathcal{C}}_F \hat{c}_k \hat{\mathcal{C}}_F^\dagger + V_\mu^{(C)}(\mathbf{r}; k) \hat{\mathcal{C}}_F \hat{b}_k^\dagger \hat{\mathcal{C}}_F^\dagger \right) \\ &= \sum_k \left( U_\mu^{(C)}(\mathbf{r}; k) \hat{b}_k + V_\mu^{(C)}(\mathbf{r}; k) \hat{c}_k^\dagger \right) \end{aligned} \quad (413)$$

For finding charge conjugated amplitudes  $U_\mu^{(C)}(\mathbf{r}; k)$  and  $V_\mu^{(C)}(\mathbf{r}; k)$  one can has to compare the expressing (413) with [7]

$$\begin{aligned}
\hat{\Psi}_\mu^{(C)}(\mathbf{r}) &= (-i\beta\alpha_y)_{\mu,\mu'} \hat{\Psi}_{\mu'}^\dagger(\mathbf{r}) \\
&= (-i\beta\alpha_y)_{\mu,\mu'} \sum_k \left( U_{\mu'}^*(\mathbf{r}; k) \hat{c}_k^\dagger + V_{\mu'}^*(\mathbf{r}; k) \hat{b}_{\tilde{k}} \right) \\
&= \sum_k \left( (-i\beta\alpha_y)_{\mu,\mu'} V_{\mu'}^*(\mathbf{r}; k) \hat{b}_{\tilde{k}} + (-i\beta\alpha_y)_{\mu,\mu'} U_{\mu'}^*(\mathbf{r}; k) \hat{c}_k^\dagger \right) \\
&= \sum_k \left( (-i\beta\alpha_y)_{\mu,\mu'} V_{\mu'}^*(\mathbf{r}; \tilde{k}) \hat{b}_k + (-i\beta\alpha_y)_{\mu,\mu'} U_{\mu'}^*(\mathbf{r}; \tilde{k}) \hat{c}_{\tilde{k}}^\dagger \right) \\
&\stackrel{!}{=} \sum_k \left( U_\mu^{(C)}(\mathbf{r}; k) \hat{b}_k + V_\mu^{(C)}(\mathbf{r}; k) \hat{c}_{\tilde{k}}^\dagger \right)
\end{aligned} \tag{414}$$

In the third line it has been exchanged  $(k, \tilde{k}) \rightarrow (\tilde{k}, k)$ .

Hence, by comparing the respective last lines in (413) and (414) there has to hold [7]

$$\begin{aligned}
U_\mu^{(C)}(\mathbf{r}; k) &= (-i\beta\alpha_y)_{\mu,\mu'} V_{\mu'}^*(\mathbf{r}; \tilde{k}) \\
V_\mu^{(C)}(\mathbf{r}; k) &= (-i\beta\alpha_y)_{\mu,\mu'} U_{\mu'}^*(\mathbf{r}; \tilde{k})
\end{aligned} \tag{415}$$

Equipped with these relations one can show that the normal ordering rule  $\mathcal{N}$ , whose rule of application is explained in(44), is equal to the operation  $\frac{1-\mathcal{C}_F}{2}$  for defining the QED current density and the QED charge density operator.

The following identities being a direct consequence of (415) are useful [7]:

$$\begin{aligned}
\sum_{\mu,\nu} V_{\mu}^{\star}(\mathbf{r}; k') (\alpha_b)_{\mu\nu} U_{\nu}(\mathbf{r}; k) &= \sum_{\mu',\nu'} V_{\nu'}^{\star}(\mathbf{r}; \tilde{k}') (\alpha_b)_{\nu',\mu'} U_{\mu'}(\mathbf{r}; \tilde{k}') \\
\sum_{\mu,\nu} V_{\mu}^{\star}(\mathbf{r}; k') (\alpha_b)_{\mu\nu} V_{\nu}(\mathbf{r}; k) &= \sum_{\mu',\nu'} U_{\nu'}^{\star}(\mathbf{r}; \tilde{k}') (\alpha_b)_{\nu',\mu'} U_{\mu'}(\mathbf{r}; \tilde{k}') \\
\sum_{\mu,\nu} U_{\mu}^{\star}(\mathbf{r}; k') (\alpha_b)_{\mu\nu} U_{\nu}(\mathbf{r}; k) &= \sum_{\mu',\nu'} V_{\nu'}^{\star}(\mathbf{r}; \tilde{k}') (\alpha_b)_{\nu',\mu'} V_{\mu'}(\mathbf{r}; \tilde{k}') \\
\sum_{\mu,\nu} U_{\mu}^{\star}(\mathbf{r}; k') (\alpha_b)_{\mu,\nu} V_{\nu}(\mathbf{r}; k) &= \sum_{\mu',\nu'} U_{\nu'}^{\star}(\mathbf{r}; \tilde{k}') (\alpha_b)_{\nu',\mu'} V_{\mu'}(\mathbf{r}; \tilde{k}')
\end{aligned} \tag{416}$$

Any QED vector is thus charge conjugated as [7]

$$\begin{aligned}
\mathcal{C}_F \left( \Psi_{\mu}^{\dagger}(\mathbf{r}) (\alpha_b)_{\mu\nu} \Psi_{\nu}(\mathbf{r}) \right) &= \left( \hat{\mathcal{C}}_F \Psi_{\mu}^{\dagger}(\mathbf{r}) \hat{\mathcal{C}}_F^{\dagger} \right) (\alpha_b)_{\mu\nu} \left( \hat{\mathcal{C}}_F \Psi_{\nu}(\mathbf{r}) \hat{\mathcal{C}}_F^{\dagger} \right) \\
&= \sum_{k'} \left( U_{\mu}^{\star}(\mathbf{r}; k') \hat{b}_{k'}^{\dagger} + V_{\mu}^{\star}(\mathbf{r}; k') \hat{c}_{\tilde{k}'}^{\dagger} \right) (\alpha_b)_{\mu\nu} \sum_k \left( U_{\nu}(\mathbf{r}; k) \hat{b}_k + V_{\nu}(\mathbf{r}; k) \hat{c}_{\tilde{k}}^{\dagger} \right) \\
&= \sum_{k,k'} \begin{cases} U_{\mu}^{\star}(\mathbf{r}; k') (\alpha_b)_{\mu\nu} U_{\nu}(\mathbf{r}; k) \hat{b}_{k'}^{\dagger} \hat{b}_k \\ + U_{\mu}^{\star}(\mathbf{r}; k') (\alpha_b)_{\mu\nu} V_{\nu}(\mathbf{r}; k) \hat{b}_{k'}^{\dagger} \hat{c}_{\tilde{k}}^{\dagger} \\ + V_{\mu}^{\star}(\mathbf{r}; k') (\alpha_b)_{\mu\nu} U_{\nu}(\mathbf{r}; k) \hat{c}_{\tilde{k}'}^{\dagger} \hat{b}_k \\ + V_{\mu}^{\star}(\mathbf{r}; k') (\alpha_b)_{\mu\nu} V_{\nu}(\mathbf{r}; k) \hat{c}_{\tilde{k}'}^{\dagger} \hat{c}_{\tilde{k}}^{\dagger} \end{cases}
\end{aligned} \tag{417}$$

This has to be compared with [7]

$$\begin{aligned}
\hat{\Psi}_{\mu}^{\dagger}(\mathbf{r}) (\alpha_b)_{\mu\nu} \hat{\Psi}_{\nu}(\mathbf{r}) &= \sum_{k'} \left( U_{\mu}^{\star}(\mathbf{r}; k') \hat{c}_{k'}^{\dagger} + V_{\mu}^{\star}(\mathbf{r}; k') \hat{b}_{\tilde{k}'} \right) (\alpha_b)_{\mu\nu} \sum_k \left( U_{\nu}(\mathbf{r}; k) \hat{c}_k + V_{\nu}(\mathbf{r}; k) \hat{b}_{\tilde{k}}^{\dagger} \right) \\
&= \sum_{k,k'} \begin{cases} U_{\mu}^{\star}(\mathbf{r}; k') (\alpha_b)_{\mu\nu} U_{\nu}(\mathbf{r}; k) \hat{c}_{k'}^{\dagger} \hat{c}_k \\ + U_{\mu}^{\star}(\mathbf{r}; k') (\alpha_b)_{\mu\nu} V_{\nu}(\mathbf{r}; k) \hat{c}_{k'}^{\dagger} \hat{b}_{\tilde{k}}^{\dagger} \\ + V_{\mu}^{\star}(\mathbf{r}; k') (\alpha_b)_{\mu\nu} U_{\nu}(\mathbf{r}; k) \hat{b}_{\tilde{k}'} \hat{c}_k \\ + V_{\mu}^{\star}(\mathbf{r}; k') (\alpha_b)_{\mu\nu} V_{\nu}(\mathbf{r}; k) \hat{b}_{\tilde{k}'} \hat{b}_{\tilde{k}}^{\dagger} \end{cases}
\end{aligned} \tag{418}$$

And according to Pauli [33] then for the QED current density

$$\begin{aligned}
\hat{j}_b(\mathbf{r}) &= q_e \frac{1 - \mathcal{C}_F}{2} \hat{\Psi}_\mu^\dagger(\mathbf{r}) (c\alpha_b)_{\mu\nu} \hat{\Psi}_\nu(\mathbf{r}) \\
&= \frac{q_e c}{2} \sum_{k,k'} \sum_{\mu,\nu} (\alpha_b)_{\mu,\nu} \begin{cases} U_\mu^*(\mathbf{r}; k') U_\nu(\mathbf{r}; k) \left( \hat{c}_{k'}^\dagger \hat{c}_k - \hat{b}_{k'}^\dagger \hat{b}_k \right) \\ + U_\mu^*(\mathbf{r}; k') V_\nu(\mathbf{r}; k) \left( \hat{c}_{k'}^\dagger \hat{b}_k^\dagger + \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \right) \\ + V_\mu^*(\mathbf{r}; k') U_\nu(\mathbf{r}; k) \left( \hat{b}_{k'} \hat{c}_k + \hat{b}_k \hat{c}_{k'} \right) \\ + V_\mu^*(\mathbf{r}; k') V_\nu(\mathbf{r}; k) \left( \hat{c}_k^\dagger \hat{c}_{k'} - \hat{b}_k^\dagger \hat{b}_{k'} \right) \end{cases} \quad (419)
\end{aligned}$$

Applying the identities (416) one can rewrite (419) according to [7]

$$\hat{j}_b(\mathbf{r}) = q_e c \sum_{k,k'} \sum_{\mu,\nu} (\alpha_b)_{\mu,\nu} \begin{cases} U_\mu^*(\mathbf{r}; k') U_\nu(\mathbf{r}; k) \hat{c}_{k'}^\dagger \hat{c}_k - V_\mu^*(\mathbf{r}; k') V_\nu(\mathbf{r}; k) \hat{b}_{k'}^\dagger \hat{b}_k \\ + U_\mu^*(\mathbf{r}; k') V_\nu(\mathbf{r}; k) \hat{c}_{k'}^\dagger \hat{b}_k^\dagger + V_\mu^*(\mathbf{r}; k) U_\nu(\mathbf{r}; k') \hat{b}_k \hat{c}_{k'} \end{cases} \quad (420)$$

And applying the normal ordering rule  $\mathcal{N}(\hat{b}_{k'} \hat{b}_k^\dagger) = -\hat{b}_k^\dagger \hat{b}_{k'}$  for fermionic creation and annihilation operators one sees that [7]

$$\begin{aligned}
\hat{j}_b(\mathbf{r}) &= q_e \frac{1 - \mathcal{C}_F}{2} \hat{\Psi}_\mu^\dagger(\mathbf{r}) (c\alpha_b)_{\mu\nu} \hat{\Psi}_\nu(\mathbf{r}) \\
&= q_e c \sum_{\mu,\nu} \mathcal{N} \left( \sum_{k'} \left( U_\mu^*(\mathbf{r}; k') \hat{c}_{k'}^\dagger + V_\mu^*(\mathbf{r}; k') \hat{b}_{k'} \right) (\alpha_b)_{\mu,\nu} \sum_k \left( U_\nu(\mathbf{r}; k) \hat{c}_k + V_\nu(\mathbf{r}; k) \hat{b}_k^\dagger \right) \right) \\
&= q_e c \sum_{\mu,\nu} \mathcal{N} \left( \hat{\Psi}_\mu^\dagger(\mathbf{r}) (\alpha_b)_{\mu,\nu} \hat{\Psi}_\nu(\mathbf{r}) \right) \quad (421)
\end{aligned}$$

The representation of the current density operator  $\hat{j}_b(\mathbf{r})$  with the charge conjugation related operation  $\frac{1 - \mathcal{C}_F}{2}$  is completely equivalent to the representation with the normal ordering operation  $\mathcal{N}$ !

The same is true for the QED current density operator  $\hat{\varrho}(\mathbf{r})$ . According to W. Pauli [33] there holds

$$\begin{aligned}
\hat{\varrho}(\mathbf{r}) &= q_e \frac{1 - \mathcal{C}_F}{2} \sum_\mu \Psi_\mu^\dagger(\mathbf{r}) \Psi_\mu(\mathbf{r}) \\
&= q_e \sum_{k,k'} \sum_\mu \begin{cases} U_\mu^*(\mathbf{r}; k') U_\mu(\mathbf{r}; k) \hat{c}_{k'}^\dagger \hat{c}_k - V_\mu^*(\mathbf{r}; k) V_\mu(\mathbf{r}; k') \hat{b}_{k'}^\dagger \hat{b}_k \\ + U_\mu^*(\mathbf{r}; k') V_\mu(\mathbf{r}; k) \hat{c}_{k'}^\dagger \hat{b}_k^\dagger + V_\mu^*(\mathbf{r}; k) U_\mu(\mathbf{r}; k') \hat{b}_k \hat{c}_{k'} \end{cases} \quad (422)
\end{aligned}$$

whereas for the charge density operator as defined in (43) [7]

$$\begin{aligned}
\hat{\rho}(\mathbf{r}) &= q_e \frac{1 - \mathcal{C}_F}{2} \sum_{\mu} \Psi_{\mu}^{\dagger}(\mathbf{r}) \Psi_{\mu}(\mathbf{r}) \\
&= q_e \sum_{\mu} \mathcal{N} \left( \sum_{k'} \left( U_{\mu}^*(\mathbf{r}; k') \hat{c}_{k'}^{\dagger} + V_{\mu}^*(\mathbf{r}; k') \hat{b}_{k'} \right) \sum_k \left( U_{\nu}(\mathbf{r}; k) \hat{c}_k + V_{\nu}(\mathbf{r}; k) \hat{b}_k^{\dagger} \right) \right) \\
&= \mathcal{N} \left( q_e \sum_{\mu} \hat{\Psi}_{\mu}^{\dagger}(\mathbf{r}) \hat{\Psi}_{\mu}(\mathbf{r}) \right)
\end{aligned} \tag{423}$$

### Consequences of the Charge Conjugation Operation for the Ground State of QED

The charge conjugation operation  $\mathcal{C}_F$  applied to the QED current density operator  $\hat{j}_b(\mathbf{r})$  gives [7]

$$\begin{aligned}
\mathcal{C}_F \hat{j}_b(\mathbf{r}) &= \frac{q_e}{2} \mathcal{C}_F (1 - \mathcal{C}_F) \Psi_{\mu}^{\dagger}(\mathbf{r}) (c\alpha_b)_{\mu\nu} \Psi_{\nu}(\mathbf{r}) \\
&= \frac{q_e}{2} (\mathcal{C}_F - \mathcal{C}_F \mathcal{C}_F) \Psi_{\mu}^{\dagger}(\mathbf{r}) (c\alpha_b)_{\mu\nu} \Psi_{\nu}(\mathbf{r}) \\
&= \frac{q_e}{2} (\mathcal{C}_F - 1) \Psi_{\mu}^{\dagger}(\mathbf{r}) (c\alpha_b)_{\mu\nu} \Psi_{\nu}(\mathbf{r}) \\
&= -\frac{q_e}{2} (1 - \mathcal{C}_F) \Psi_{\mu}^{\dagger}(\mathbf{r}) (c\alpha_b)_{\mu\nu} \Psi_{\nu}(\mathbf{r}) \\
&= -\hat{j}_b(\mathbf{r})
\end{aligned} \tag{424}$$

and applied to the QED charge density operator  $\hat{\rho}(\mathbf{r})$  accordingly [7]

$$\begin{aligned}
\mathcal{C}_F \hat{\rho}(\mathbf{r}) &= \frac{q_e}{2} \mathcal{C}_F (1 - \mathcal{C}_F) \Psi_{\mu}^{\dagger}(\mathbf{r}) \Psi_{\mu}(\mathbf{r}) \\
&= -\frac{q_e}{2} (1 - \mathcal{C}_F) \Psi_{\mu}^{\dagger}(\mathbf{r}) \Psi_{\mu}(\mathbf{r}) \\
&= -\hat{\rho}(\mathbf{r})
\end{aligned} \tag{425}$$

Now the ground state  $|G\rangle$  of QED is defined to be the eigenstate of  $\mathcal{H}_{QED}$  to the lowest possible (positive) energy eigenvalue  $E_G$ . Demanding that  $|G\rangle$  is invariant under charge conjugation [7],

$$\hat{\mathcal{C}}_F^{\dagger} |G\rangle = |G\rangle \tag{426}$$

there follows necessarily [7]

$$\begin{aligned}
\langle G | \hat{\rho}(\mathbf{r}) | G \rangle &= \langle G | \hat{\mathcal{C}}_F \circ \hat{\rho}(\mathbf{r}) \circ \hat{\mathcal{C}}_F^\dagger | G \rangle = \langle G | \mathcal{C}_F \hat{\rho}(\mathbf{r}) | G \rangle = - \langle G | \hat{\rho}(\mathbf{r}) | G \rangle \\
\langle G | \hat{j}_b(\mathbf{r}) | G \rangle &= \langle G | \hat{\mathcal{C}}_F \circ \hat{j}_b(\mathbf{r}) \circ \hat{\mathcal{C}}_F^\dagger | G \rangle = \langle G | \mathcal{C}_F \hat{j}_b(\mathbf{r}) | G \rangle = - \langle G | \hat{j}_b(\mathbf{r}) | G \rangle
\end{aligned}
\tag{427}$$

Hence, the expectation values for the charge density and the current density with respect to the ground state  $|G\rangle$  *vanish* [7].

$$\begin{aligned}
\langle G | \hat{\rho}(\mathbf{r}) | G \rangle &= 0 \\
\langle G | \hat{j}_b(\mathbf{r}) | G \rangle &= 0
\end{aligned}
\tag{428}$$

These are physical properties, because if there would drop a current across QED we could make use of its energy, which is, of course, not the case! Or?

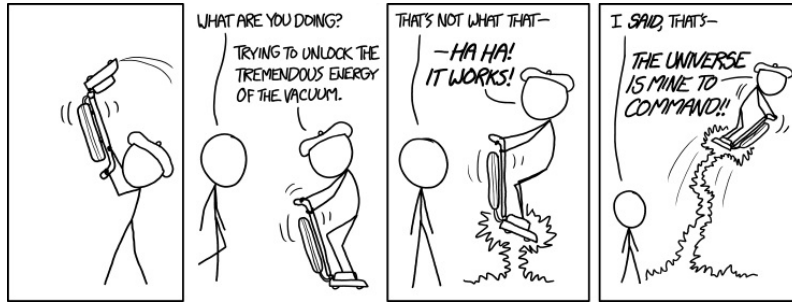


Figure 3: Taken from <https://www.explainxkcd.com/wiki/index.php/File:vacuum.png>, 24.04.2022

Please be aware that the ground state of QED is not the vacuum [46, 38].

These physical properties (428) are the true reason for the necessity to symmetrize the QED Hamiltonian with respect to the charge, as it has been introduced by W. Pauli. It now has become obvious that this is fully equivalent to the normal ordering operation. With that the normal ordering operation indeed has a physical meaning.

## G Complement to the Homogeneous Solution

$$\hat{H}^{(2,h)}(s)$$

In this part of the appendix the Coulomb–interaction is decomposed into a part which is normally ordered, and into a self energy part. This is very convenient for solving the homogeneous part of the second order differential equation.

The Fourier transform of the Coulomb interaction  $\mathcal{V}_C$ , by using  $\frac{1}{4\pi|\mathbf{r}|} = \int \frac{d^3q}{(2\pi)^3} \frac{e^{i\mathbf{q}\cdot\mathbf{r}}}{|\mathbf{q}|^2}$  is given by

$$\begin{aligned} \mathcal{V}_C &= \frac{1}{2\varepsilon_0} \int d^3r \int d^3r' \hat{\rho}(\mathbf{r}) \frac{1}{4\pi|\mathbf{r}-\mathbf{r}'|} \hat{\rho}(\mathbf{r}') \\ &= \frac{1}{2\varepsilon_0} \int \frac{d^3q}{(2\pi)^3} \tilde{\rho}(\mathbf{q}) \tilde{\rho}(-\mathbf{q}) \end{aligned} \quad (429)$$

with

$$\tilde{\rho}(\mathbf{q}) = \int d^3r e^{-i\mathbf{q}\cdot\mathbf{r}} \mathcal{N} \left( q_e \hat{\Psi}_\mu^\dagger(\mathbf{r}) \hat{\Psi}_\mu(\mathbf{r}) \right) \quad (430)$$

Now using

$$\begin{aligned} \hat{x}_a \hat{\Phi}_{\mu'}(\mathbf{r}) &= r_a \hat{\Phi}_{\mu'}(\mathbf{r}) \\ [\hat{\mathbf{p}}_b, \hat{x}_a] &= \frac{\hbar}{i} \delta_{a,b} \hat{\mathbf{1}} \\ \Pi_b &= \hat{\mathbf{p}}_b - q_e A_b(\hat{\mathbf{x}}) \end{aligned} \quad (431)$$

there follows for (430)

$$\tilde{\rho}(\mathbf{q}) = q_e \mathcal{N} \int d^3r \hat{\Psi}_\mu^\dagger(\mathbf{r}) e^{-iq_a \hat{x}_a} \hat{\Psi}_\mu(\mathbf{r}) \quad (432)$$

The following decomposition of the field operators  $\hat{\Psi}_\mu(\mathbf{r})$  and  $\hat{\Psi}_\mu^\dagger(\mathbf{r})$  is convenient [7]

$$\begin{aligned}
\hat{\Psi}_\mu(\mathbf{r}) &= \hat{\Gamma}_{e,\mu}(\mathbf{r}) + \hat{\Gamma}_{p,\mu}^\dagger(\mathbf{r}) \\
\hat{\Psi}_\mu^\dagger(\mathbf{r}) &= \hat{\Gamma}_{e,\mu}^\dagger(\mathbf{r}) + \hat{\Gamma}_{p,\mu}(\mathbf{r}) \\
\hat{\Gamma}_{e,\mu}(\mathbf{r}) &= \sum_k U_\mu(\mathbf{r}; k) \hat{c}_k \\
\hat{\Gamma}_{p,\mu}^\dagger(\mathbf{r}) &= \sum_k V_\mu(\mathbf{r}; k) \hat{b}_k^\dagger
\end{aligned} \tag{433}$$

The operators (433) obey to the anti commutation relations of fermionic field operators [7]:

$$\begin{aligned}
\left\{ \hat{\Gamma}_{e,\mu}(\mathbf{r}), \hat{\Gamma}_{e,\mu'}(\mathbf{r}') \right\} &= \hat{0} = \left\{ \hat{\Gamma}_{e,\mu}^\dagger(\mathbf{r}), \hat{\Gamma}_{e,\mu'}^\dagger(\mathbf{r}') \right\} \\
\left\{ \hat{\Gamma}_{e,\mu}(\mathbf{r}), \hat{\Gamma}_{e,\mu'}^\dagger(\mathbf{r}') \right\} &= \sum_k U_\mu(\mathbf{r}, k) U_{\mu'}^*(\mathbf{r}', k) \hat{1} \equiv P_{\mu,\mu'}^{(+)}(\mathbf{r}, \mathbf{r}') \\
\left\{ \hat{\Gamma}_{e,\mu}(\mathbf{r}), \hat{\Gamma}_{p,\mu'}^\dagger(\mathbf{r}') \right\} &= \hat{0} = \left\{ \hat{\Gamma}_{e,\mu}(\mathbf{r}), \hat{\Gamma}_{p,\mu'}(\mathbf{r}') \right\} \\
\left\{ \hat{\Gamma}_{e,\mu}^\dagger(\mathbf{r}), \hat{\Gamma}_{p,\mu'}^\dagger(\mathbf{r}') \right\} &= \hat{0} = \left\{ \hat{\Gamma}_{e,\mu}^\dagger(\mathbf{r}), \hat{\Gamma}_{p,\mu'}(\mathbf{r}') \right\}
\end{aligned} \tag{434}$$

$$\begin{aligned}
\left\{ \hat{\Gamma}_{p,\mu}(\mathbf{r}), \hat{\Gamma}_{p,\mu'}(\mathbf{r}') \right\} &= \hat{0} = \left\{ \hat{\Gamma}_{p,\mu}^\dagger(\mathbf{r}), \hat{\Gamma}_{p,\mu'}^\dagger(\mathbf{r}') \right\} \\
\left\{ \hat{\Gamma}_{p,\mu}(\mathbf{r}), \hat{\Gamma}_{p,\mu'}^\dagger(\mathbf{r}') \right\} &= \sum_k V_\mu^*(\mathbf{r}, k) V_{\mu'}(\mathbf{r}', k) \hat{1} \equiv P_{\mu',\mu}^{(-)}(\mathbf{r}', \mathbf{r})
\end{aligned}$$

Where  $P_{\mu,\mu'}^{(\pm)}(\mathbf{r}, \mathbf{r}')$  are the projection operators  $\mathbf{P}^{(\pm)}$  in position space

$$\begin{aligned}
P_{\mu,\mu'}^{(\pm)}(\mathbf{r}, \mathbf{r}') &= \langle \mathbf{r}, \mu | \mathbf{P}^{(\pm)} | \mathbf{r}', \mu' \rangle \\
\mathbf{P}^{(+)} &= \sum_k |U_k\rangle \langle U_k| \\
\mathbf{P}^{(-)} &= \sum_k |V_k\rangle \langle V_k|
\end{aligned} \tag{435}$$

However, the operators (433) are no field operators, because they do not build a complete system. This can be seen from the anticommutation relations yielding the projection operators in (434).

The completeness relation is only given by both  $P_{\mu,\mu'}^{(+)}(\mathbf{r}, \mathbf{r}')$  and  $P_{\mu,\mu'}^{(-)}(\mathbf{r}, \mathbf{r}')$ :



$$\begin{aligned}
P_{\mu,\mu'}^{(+)}(\mathbf{r}, \mathbf{r}') + P_{\mu,\mu'}^{(-)}(\mathbf{r}, \mathbf{r}') &= \langle \mathbf{r}, \mu | \mathbf{P}^{(+)} + \mathbf{P}^{(-)} | \mathbf{r}', \mu' \rangle \\
&= \langle \mathbf{r}, \mu | \mathbf{1}_{4 \times 4} | \mathbf{r}', \mu' \rangle \\
&= \delta_{\mu,\mu'} \delta^{(3)}(\mathbf{r} - \mathbf{r}')
\end{aligned} \tag{436}$$

Inserting the gamma operators (433) into the Fourier transform of the QED charge density operator (430) gives three contributions [7]:

$$\tilde{\rho}(\mathbf{q}) = q_e \int d^3r e^{-i\mathbf{q}\cdot\mathbf{r}} \sum_{\mu} \left( \hat{\Gamma}_{e,\mu}^{\dagger}(\mathbf{r}) \hat{\Gamma}_{e,\mu}(\mathbf{r}) - \hat{\Gamma}_{p,\mu}^{\dagger}(\mathbf{r}) \hat{\Gamma}_{p,\mu}(\mathbf{r}) + \hat{\Gamma}_{e,\mu}^{\dagger}(\mathbf{r}) \hat{\Gamma}_{p,\mu}^{\dagger}(\mathbf{r}) + \hat{\Gamma}_{p,\mu}(\mathbf{r}) \hat{\Gamma}_{e,\mu}(\mathbf{r}) \right) \tag{437}$$

These are abbreviated further as [7]

$$\begin{aligned}
\tilde{\rho}(\mathbf{q}) &= \tilde{\rho}_0(\mathbf{q}) + \tilde{\rho}_+(\mathbf{q}) + \tilde{\rho}_-(\mathbf{q}) \\
\tilde{\rho}_0(\mathbf{q}) &= q_e \int d^3r e^{-i\mathbf{q}\cdot\mathbf{r}} \left( \hat{\Gamma}_{e,\mu}^{\dagger}(\mathbf{r}) \hat{\Gamma}_{e,\mu}(\mathbf{r}) - \hat{\Gamma}_{p,\mu}^{\dagger}(\mathbf{r}) \hat{\Gamma}_{p,\mu}(\mathbf{r}) \right) \\
\tilde{\rho}_+(\mathbf{q}) &= q_e \int d^3r e^{-i\mathbf{q}\cdot\mathbf{r}} \hat{\Gamma}_{e,\mu}^{\dagger}(\mathbf{r}) \hat{\Gamma}_{p,\mu}^{\dagger}(\mathbf{r}) \\
\tilde{\rho}_-(\mathbf{q}) &= q_e \int d^3r e^{-i\mathbf{q}\cdot\mathbf{r}} \hat{\Gamma}_{p,\mu}(\mathbf{r}) \hat{\Gamma}_{e,\mu}(\mathbf{r})
\end{aligned} \tag{438}$$

and they share the following commutation relations with the particle number operator  $\hat{N} = \sum_k \left( \hat{c}_k^{\dagger} \hat{c}_k + \hat{b}_k^{\dagger} \hat{b}_k \right)$  [7]:

$$\begin{aligned}
\left[ \hat{N}_I, \tilde{\rho}_0(\mathbf{q}) \right] &= \hat{0} \\
\left[ \hat{N}_I, \tilde{\rho}_{\pm}(\mathbf{q}) \right] &= \pm 2 \tilde{\rho}_{\pm}(\mathbf{q})
\end{aligned} \tag{439}$$

With these relations one can now decompose the Coulomb–interaction  $\mathcal{V}_C$  and the coupling to an external source  $\hat{\mathcal{V}}_{ext}$  into particle number conserving and nonconserving parts.

The coupling to an external source, taking as such the Coulomb field of an atomic nucleus sitting at the point  $\mathbf{R}$  in space as given in (38), in its Fourier representation, is assumed the guise

$$\Phi^{(ext)}(\mathbf{r}) = \frac{Z |q_e|}{4\pi\epsilon_0} \int \frac{d^3q}{(2\pi)^3} e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{R})} \frac{1}{|\mathbf{q}|^2} \tag{440}$$

such that

$$\hat{\mathcal{V}}_{ext} = \frac{Z |q_e|}{4\pi\epsilon_0} \int \frac{d^3q}{(2\pi)^3} \frac{e^{i\mathbf{q}\cdot\mathbf{R}}}{|\mathbf{q}|^2} \tilde{\rho}(\mathbf{q}) \quad (441)$$

Inserting the identities (438) yields readily [7]

$$\begin{aligned} \hat{\mathcal{V}}_{ext} &= \hat{\mathcal{V}}_{ext}^{(0)} + \hat{\mathcal{V}}_{ext}^{(+)} + \hat{\mathcal{V}}_{ext}^{(-)} \\ \hat{\mathcal{V}}_{ext}^{(0)} &= \frac{Z |q_e|}{4\pi\epsilon_0} \int \frac{d^3q}{(2\pi)^3} \frac{e^{i\mathbf{q}\cdot\mathbf{R}}}{|\mathbf{q}|^2} \tilde{\rho}_0(\mathbf{q}) \\ \hat{\mathcal{V}}_{ext}^{(\pm)} &= \frac{Z |q_e|}{4\pi\epsilon_0} \int \frac{d^3q}{(2\pi)^3} \frac{e^{i\mathbf{q}\cdot\mathbf{R}}}{|\mathbf{q}|^2} \tilde{\rho}_{\pm}(\mathbf{q}) \end{aligned} \quad (442)$$

The commutation relations (439) now imply [7]

$$\begin{aligned} [\hat{N}_I, \hat{\mathcal{V}}_{ext}^{(0)}] &= \hat{0} \\ [\hat{N}_I, \hat{\mathcal{V}}_{ext}^{(\pm)}] &= \pm 2\hat{\mathcal{V}}_{ext}^{(\pm)} \end{aligned} \quad (443)$$

The decomposition of the QED Coulomb interaction is analogous. Here, one finds nine terms altogether [7]:

$$\begin{aligned} \tilde{\rho}(\mathbf{q}) \tilde{\rho}(-\mathbf{q}) &= (\tilde{\rho}_0(\mathbf{q}) + \tilde{\rho}_+(\mathbf{q}) + \tilde{\rho}_-(\mathbf{q})) (\tilde{\rho}_0(-\mathbf{q}) + \tilde{\rho}_+(-\mathbf{q}) + \tilde{\rho}_-(-\mathbf{q})) \\ &= \begin{cases} \tilde{\rho}_0(\mathbf{q}) \tilde{\rho}_0(-\mathbf{q}) + \tilde{\rho}_+(\mathbf{q}) \tilde{\rho}_-(-\mathbf{q}) + \tilde{\rho}_-(\mathbf{q}) \tilde{\rho}_+(-\mathbf{q}) \\ + \tilde{\rho}_0(\mathbf{q}) \tilde{\rho}_+(-\mathbf{q}) + \tilde{\rho}_+(\mathbf{q}) \tilde{\rho}_0(-\mathbf{q}) + \tilde{\rho}_0(\mathbf{q}) \tilde{\rho}_-(-\mathbf{q}) + \tilde{\rho}_-(\mathbf{q}) \tilde{\rho}_0(-\mathbf{q}) \\ + \tilde{\rho}_+(\mathbf{q}) \tilde{\rho}_+(-\mathbf{q}) + \tilde{\rho}_-(\mathbf{q}) \tilde{\rho}_-(-\mathbf{q}) \end{cases} \end{aligned} \quad (444)$$

Implying for the Coulomb interaction [7]

$$\mathcal{V}_C = \frac{1}{2\epsilon_0} \int \frac{d^3q}{(2\pi)^3} \frac{\tilde{\rho}(\mathbf{q}) \tilde{\rho}(-\mathbf{q})}{|\mathbf{q}|^2} = \mathcal{U}_C^{(0)} + \mathcal{U}_C^{(+)} + \mathcal{U}_C^{(-)} + \mathcal{U}_C^{(+,+)} + \mathcal{U}_C^{(-,-)} \quad (445)$$

Here [7]

$$\begin{aligned}
\mathcal{U}_C^{(0)} &= \frac{1}{2\varepsilon_0} \int \frac{d^3q}{(2\pi)^3} \frac{\tilde{\rho}_0(\mathbf{q})\tilde{\rho}_0(-\mathbf{q}) + \tilde{\rho}_+(\mathbf{q})\tilde{\rho}_-(-\mathbf{q}) + \tilde{\rho}_-(\mathbf{q})\tilde{\rho}_+(-\mathbf{q})}{|\mathbf{q}|^2} \\
\mathcal{U}_C^{(+)} &= \frac{1}{2\varepsilon_0} \int \frac{d^3q}{(2\pi)^3} \frac{\tilde{\rho}_0(\mathbf{q})\tilde{\rho}_+(-\mathbf{q}) + \tilde{\rho}_+(\mathbf{q})\tilde{\rho}_0(-\mathbf{q})}{|\mathbf{q}|^2} \\
\mathcal{U}_C^{(-)} &= \frac{1}{2\varepsilon_0} \int \frac{d^3q}{(2\pi)^3} \frac{\tilde{\rho}_0(\mathbf{q})\tilde{\rho}_-(-\mathbf{q}) + \tilde{\rho}_-(\mathbf{q})\tilde{\rho}_0(-\mathbf{q})}{|\mathbf{q}|^2} \\
\mathcal{U}_C^{(+,+)} &= \frac{1}{2\varepsilon_0} \int \frac{d^3q}{(2\pi)^3} \frac{\tilde{\rho}_+(\mathbf{q})\tilde{\rho}_+(-\mathbf{q})}{|\mathbf{q}|^2} \\
\mathcal{U}_C^{(-,-)} &= \frac{1}{2\varepsilon_0} \int \frac{d^3q}{(2\pi)^3} \frac{\tilde{\rho}_-(\mathbf{q})\tilde{\rho}_-(-\mathbf{q})}{|\mathbf{q}|^2}
\end{aligned} \tag{446}$$

with the commutation relations [7]

$$\begin{aligned}
\left[ \hat{N}_I, \mathcal{U}_C^{(0)} \right] &= \hat{0} \\
\left[ \hat{N}_I, \mathcal{U}_C^{(\pm)} \right] &= \pm 2\mathcal{U}_C^{(\pm)} \\
\left[ \hat{N}_I, \mathcal{U}_C^{(+,+)} \right] &= 4\mathcal{U}_C^{(+,+)} \\
\left[ \hat{N}_I, \mathcal{U}_C^{(-,-)} \right] &= 4\mathcal{U}_C^{(-,-)}
\end{aligned} \tag{447}$$

Such a decomposition into particle number conserving and nonconserving parts makes it possible express the Coulomb interaction as the sum of a normally ordered part and a self-energy contribution.

Inserting the gamma operators (433) into  $\tilde{\rho}_0(\mathbf{q})\tilde{\rho}_0(-\mathbf{q})$  and  $\tilde{\rho}_+(\mathbf{q})\tilde{\rho}_-(-\mathbf{q}) + \tilde{\rho}_-(\mathbf{q})\tilde{\rho}_+(-\mathbf{q})$  there follows, together with the anticommutation relations (434) of the gamma operators [7]

$$\begin{aligned}
\tilde{\rho}_0(\mathbf{q})\tilde{\rho}_0(-\mathbf{q}) &= q_e^2 \int d^3r \int d^3r' e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} \begin{pmatrix} \hat{\Gamma}_{e,\mu}^\dagger(\mathbf{r})\hat{\Gamma}_{e,\mu}(\mathbf{r})\hat{\Gamma}_{e,\mu'}^\dagger(\mathbf{r}')\hat{\Gamma}_{e,\mu'}(\mathbf{r}') \\ +\hat{\Gamma}_{p,\mu}^\dagger(\mathbf{r})\hat{\Gamma}_{p,\mu}(\mathbf{r})\hat{\Gamma}_{p,\mu'}^\dagger(\mathbf{r}')\hat{\Gamma}_{p,\mu'}(\mathbf{r}') \\ -\hat{\Gamma}_{p,\mu}^\dagger(\mathbf{r})\hat{\Gamma}_{p,\mu}(\mathbf{r})\hat{\Gamma}_{e,\mu'}^\dagger(\mathbf{r}')\hat{\Gamma}_{e,\mu'}(\mathbf{r}') \\ -\hat{\Gamma}_{e,\mu}^\dagger(\mathbf{r})\hat{\Gamma}_{e,\mu}(\mathbf{r})\hat{\Gamma}_{p,\mu'}^\dagger(\mathbf{r}')\hat{\Gamma}_{p,\mu'}(\mathbf{r}') \end{pmatrix} \\
&= q_e^2 \int d^3r \int d^3r' e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} \begin{pmatrix} P_{\mu,\mu'}^{(+)}(\mathbf{r},\mathbf{r}')\hat{\Gamma}_{e,\mu}^\dagger(\mathbf{r})\hat{\Gamma}_{e,\mu'}(\mathbf{r}') \\ +P_{\mu',\mu}^{(-)}(\mathbf{r},\mathbf{r}')\hat{\Gamma}_{p,\mu}^\dagger(\mathbf{r})\hat{\Gamma}_{p,\mu'}(\mathbf{r}') \\ +\mathcal{N}\left(\left(\hat{\Gamma}_{e,\mu}^\dagger(\mathbf{r})\hat{\Gamma}_{e,\mu}(\mathbf{r}) - \hat{\Gamma}_{p,\mu}^\dagger(\mathbf{r})\hat{\Gamma}_{p,\mu}(\mathbf{r})\right)\left(\hat{\Gamma}_{e,\mu'}^\dagger(\mathbf{r}')\hat{\Gamma}_{e,\mu'}(\mathbf{r}') - \hat{\Gamma}_{p,\mu'}^\dagger(\mathbf{r}')\hat{\Gamma}_{p,\mu'}(\mathbf{r}')\right)\right) \end{pmatrix}
\end{aligned} \tag{448}$$

and [7]

$$\begin{aligned}
& \tilde{\rho}_+(\mathbf{q})\tilde{\rho}_-(-\mathbf{q}) + \tilde{\rho}_-(\mathbf{q})\tilde{\rho}_+(-\mathbf{q}) \\
&= q_e^2 \int d^3r \int d^3r' e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} \left( + \left( P_{\mu,\mu'}^{(+)}(\mathbf{r},\mathbf{r}') - \hat{\Gamma}_{e,\mu'}^\dagger(\mathbf{r}')\hat{\Gamma}_{e,\mu}(\mathbf{r}) \right) \left( P_{\mu',\mu}^{(-)}(\mathbf{r}',\mathbf{r}) - \hat{\Gamma}_{p,\mu'}^\dagger(\mathbf{r}')\hat{\Gamma}_{p,\mu}(\mathbf{r}) \right) \right) \\
&= q_e^2 \int d^3r \int d^3r' e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} \left( \begin{array}{c} \hat{\Gamma}_{e,\mu}^\dagger(\mathbf{r})\hat{\Gamma}_{p,\mu}^\dagger(\mathbf{r}')\hat{\Gamma}_{p,\mu'}(\mathbf{r}')\hat{\Gamma}_{e,\mu'}(\mathbf{r}') \\ \hat{\Gamma}_{e,\mu}^\dagger(\mathbf{r})\hat{\Gamma}_{p,\mu}^\dagger(\mathbf{r}')\hat{\Gamma}_{p,\mu'}(\mathbf{r}')\hat{\Gamma}_{e,\mu'}(\mathbf{r}') \\ +\hat{\Gamma}_{e,\mu'}^\dagger(\mathbf{r}')\hat{\Gamma}_{p,\mu'}^\dagger(\mathbf{r}')\hat{\Gamma}_{p,\mu}(\mathbf{r})\hat{\Gamma}_{e,\mu}(\mathbf{r}) \\ -P_{\mu',\mu}^{(-)}(\mathbf{r}',\mathbf{r})\hat{\Gamma}_{e,\mu'}^\dagger(\mathbf{r}')\hat{\Gamma}_{e,\mu}(\mathbf{r}) - P_{\mu,\mu'}^{(+)}(\mathbf{r},\mathbf{r}')\hat{\Gamma}_{p,\mu'}^\dagger(\mathbf{r}')\hat{\Gamma}_{p,\mu}(\mathbf{r}) \\ +P_{\mu,\mu'}^{(+)}(\mathbf{r},\mathbf{r}')P_{\mu',\mu}^{(-)}(\mathbf{r}',\mathbf{r})\hat{\mathbb{1}} \end{array} \right) \tag{449}
\end{aligned}$$

Altogether one gets [7]

$$\begin{aligned}
\mathcal{U}_C^{(0)} &= \frac{1}{2\varepsilon_0} \int \frac{d^3q}{(2\pi)^3} \frac{\tilde{\rho}_0(\mathbf{q})\tilde{\rho}_0(-\mathbf{q}) + \tilde{\rho}_+(\mathbf{q})\tilde{\rho}_-(-\mathbf{q}) + \tilde{\rho}_-(\mathbf{q})\tilde{\rho}_+(-\mathbf{q})}{|\mathbf{q}|^2} \\
&= \frac{q_e^2}{2\varepsilon_0} \int \frac{d^3q}{(2\pi)^3} \frac{1}{|\mathbf{q}|^2} \int d^3r \int d^3r' e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} \times \\
&\quad \times \left( \begin{array}{c} P_{\mu,\mu'}^{(+)}(\mathbf{r},\mathbf{r}')\hat{\Gamma}_{e,\mu}^\dagger(\mathbf{r})\hat{\Gamma}_{e,\mu'}(\mathbf{r}') \\ +P_{\mu',\mu}^{(-)}(\mathbf{r}',\mathbf{r})\hat{\Gamma}_{p,\mu}^\dagger(\mathbf{r})\hat{\Gamma}_{p,\mu'}(\mathbf{r}') \\ +\mathcal{N} \left( \left( \hat{\Gamma}_{e,\mu}^\dagger(\mathbf{r})\hat{\Gamma}_{e,\mu}(\mathbf{r}) - \hat{\Gamma}_{p,\mu}^\dagger(\mathbf{r})\hat{\Gamma}_{p,\mu}(\mathbf{r}) \right) \left( \hat{\Gamma}_{e,\mu'}^\dagger(\mathbf{r}')\hat{\Gamma}_{e,\mu'}(\mathbf{r}') - \hat{\Gamma}_{p,\mu'}^\dagger(\mathbf{r}')\hat{\Gamma}_{p,\mu'}(\mathbf{r}') \right) \right) \\ +\hat{\Gamma}_{e,\mu}^\dagger(\mathbf{r})\hat{\Gamma}_{p,\mu}^\dagger(\mathbf{r}')\hat{\Gamma}_{p,\mu'}(\mathbf{r}')\hat{\Gamma}_{e,\mu'}(\mathbf{r}') \\ +\hat{\Gamma}_{e,\mu'}^\dagger(\mathbf{r}')\hat{\Gamma}_{p,\mu'}^\dagger(\mathbf{r}')\hat{\Gamma}_{p,\mu}(\mathbf{r})\hat{\Gamma}_{e,\mu}(\mathbf{r}) \\ -P_{\mu',\mu}^{(-)}(\mathbf{r}',\mathbf{r})\hat{\Gamma}_{e,\mu'}^\dagger(\mathbf{r}')\hat{\Gamma}_{e,\mu}(\mathbf{r}) - P_{\mu,\mu'}^{(+)}(\mathbf{r},\mathbf{r}')\hat{\Gamma}_{p,\mu'}^\dagger(\mathbf{r}')\hat{\Gamma}_{p,\mu}(\mathbf{r}) \\ +P_{\mu,\mu'}^{(+)}(\mathbf{r},\mathbf{r}')P_{\mu',\mu}^{(-)}(\mathbf{r}',\mathbf{r})\hat{\mathbb{1}} \end{array} \right) \tag{450}
\end{aligned}$$

In the second and sixth line we can substitute  $\{q_a, r_a, r'_a, \mu, \mu'\} \rightarrow \{-q_a, r'_a, r_a, \mu', \mu\}$  without changing the integrals. Further rearrangements finally give [7]

$$\mathcal{U}_C^{(0)} = \mathcal{N}(\mathcal{V}_C^{(0)}) + \frac{q_e^2}{2\varepsilon_0} \int \frac{d^3q}{(2\pi)^3} \frac{1}{|\mathbf{q}|^2} \left\{ \begin{array}{l} \int d^3r \int d^3r' e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} \left( P_{\mu,\mu'}^{(+)}(\mathbf{r},\mathbf{r}') - P_{\mu,\mu'}^{(-)}(\mathbf{r},\mathbf{r}') \right) \left( \hat{\Gamma}_{e,\mu}^\dagger(\mathbf{r})\hat{\Gamma}_{e,\mu'}(\mathbf{r}') - \hat{\Gamma}_{p,\mu'}^\dagger(\mathbf{r}')\hat{\Gamma}_{p,\mu}(\mathbf{r}) \right) \\ + \int d^3r \int d^3r' e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} P_{\mu,\mu'}^{(+)}(\mathbf{r},\mathbf{r}') P_{\mu',\mu}^{(-)}(\mathbf{r}',\mathbf{r}) \hat{\mathbb{1}} \end{array} \right. \tag{451}$$

The evaluation of the contributions  $\mathcal{U}_C^{(+)} + \mathcal{U}_C^{(-)} + \mathcal{U}_C^{(+,+)} + \mathcal{U}_C^{(-,-)}$  in  $\mathcal{U}_C^{(+)} + \mathcal{U}_C^{(-)}$  is similar.

Here, one needs to normally order the contributions  $\tilde{\rho}_0(\mathbf{q})\tilde{\rho}_+(-\mathbf{q}) + \tilde{\rho}_-(\mathbf{q})\tilde{\rho}_0(-\mathbf{q})$ , because the other ones are already normally ordered. Now [7]

$$\begin{aligned}
& \tilde{\rho}_0(\mathbf{q})\tilde{\rho}_+(-\mathbf{q}) + \tilde{\rho}_-(\mathbf{q})\tilde{\rho}_0(-\mathbf{q}) \\
&= q_e^2 \int d^3r \int d^3r' e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} \left( \begin{aligned} & \left( \hat{\Gamma}_{e,\mu}^\dagger(\mathbf{r})\hat{\Gamma}_{e,\mu}(\mathbf{r}) - \hat{\Gamma}_{p,\mu}^\dagger(\mathbf{r})\hat{\Gamma}_{p,\mu}(\mathbf{r}) \right) \hat{\Gamma}_{e,\mu'}^\dagger(\mathbf{r}')\hat{\Gamma}_{p,\mu'}^\dagger(\mathbf{r}') \\ & + \hat{\Gamma}_{p,\mu}^\dagger(\mathbf{r})\hat{\Gamma}_{e,\mu}(\mathbf{r}) \left( \hat{\Gamma}_{e,\mu'}^\dagger(\mathbf{r}')\hat{\Gamma}_{e,\mu'}(\mathbf{r}') - \hat{\Gamma}_{p,\mu'}^\dagger(\mathbf{r}')\hat{\Gamma}_{p,\mu'}(\mathbf{r}') \right) \end{aligned} \right) \\
&= \begin{cases} \mathcal{N}(\tilde{\rho}_0(\mathbf{q})\tilde{\rho}_+(-\mathbf{q}) + \tilde{\rho}_-(\mathbf{q})\tilde{\rho}_0(-\mathbf{q})) \\ + q_e^2 \int d^3r \int d^3r' e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} \left( \begin{aligned} & \hat{\Gamma}_{e,\mu}^\dagger(\mathbf{r})\hat{\Gamma}_{p,\mu'}^\dagger(\mathbf{r}')P_{\mu,\mu'}^{(+)}(\mathbf{r},\mathbf{r}') \\ & + \hat{\Gamma}_{p,\mu}^\dagger(\mathbf{r})\hat{\Gamma}_{e,\mu'}^\dagger(\mathbf{r}')P_{\mu',\mu}^{(-)}(\mathbf{r}',\mathbf{r}) \\ & - P_{\mu,\mu'}^{(+)}(\mathbf{r},\mathbf{r}')\hat{\Gamma}_{e,\mu'}(\mathbf{r}')\hat{\Gamma}_{p,\mu}(\mathbf{r}) \\ & - P_{\mu',\mu}^{(-)}(\mathbf{r}',\mathbf{r})\hat{\Gamma}_{p,\mu'}(\mathbf{r}')\hat{\Gamma}_{e,\mu}(\mathbf{r}) \end{aligned} \right) \end{cases} \quad (452)
\end{aligned}$$

Therefore one finds [7]

$$\begin{aligned}
& \mathcal{U}_C^{(+)} + \mathcal{U}_C^{(-)} \\
&= \begin{cases} \mathcal{N}(\mathcal{U}_C^{(+)} + \mathcal{U}_C^{(-)}) \\ + \frac{q_e^2}{2\varepsilon_0} \int \frac{d^3q}{(2\pi)^3} \frac{1}{|\mathbf{q}|^2} \int d^3r \int d^3r' e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} \left( P_{\mu,\mu'}^{(+)}(\mathbf{r},\mathbf{r}') - P_{\mu,\mu'}^{(-)}(\mathbf{r},\mathbf{r}') \right) \left( \hat{\Gamma}_{e,\mu}^\dagger(\mathbf{r})\hat{\Gamma}_{p,\mu'}^\dagger(\mathbf{r}') + \hat{\Gamma}_{p,\mu}(\mathbf{r})\hat{\Gamma}_{e,\mu'}(\mathbf{r}') \right) \end{cases} \quad (453)
\end{aligned}$$

The contributions  $\mathcal{U}_C^{(+,+)}$  and  $\mathcal{U}_C^{(-,-)}$  are already normally ordered.

Summarizing these results yields [7]

$$\begin{aligned}
\mathcal{V}_C &= \mathcal{U}_C^{(0)} + \mathcal{U}_C^{(+)} + \mathcal{U}_C^{(-)} + \mathcal{U}_C^{(+,+)} + \mathcal{U}_C^{(-,-)} \\
&= \begin{cases} \mathcal{N}(\mathcal{U}_C^{(0)} + \mathcal{U}_C^{(+)} + \mathcal{U}_C^{(-)} + \mathcal{U}_C^{(+,+)} + \mathcal{U}_C^{(-,-)}) \\ + \frac{q_e^2}{2\varepsilon_0} \int \frac{d^3q}{(2\pi)^3} \frac{1}{|\mathbf{q}|^2} \int d^3r \int d^3r' e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} \left( P_{\mu,\mu'}^{(+)}(\mathbf{r},\mathbf{r}') - P_{\mu,\mu'}^{(-)}(\mathbf{r},\mathbf{r}') \right) \times \\ \times \left( \hat{\Gamma}_{e,\mu}^\dagger(\mathbf{r})\hat{\Gamma}_{e,\mu'}(\mathbf{r}') - \hat{\Gamma}_{p,\mu'}^\dagger(\mathbf{r}')\hat{\Gamma}_{p,\mu}(\mathbf{r}) + \hat{\Gamma}_{e,\mu}(\mathbf{r})\hat{\Gamma}_{p,\mu'}^\dagger(\mathbf{r}') + \hat{\Gamma}_{p,\mu}(\mathbf{r})\hat{\Gamma}_{e,\mu'}(\mathbf{r}') \right) \\ + \underbrace{\frac{q_e^2}{2\varepsilon_0} \int \frac{d^3q}{(2\pi)^3} \frac{1}{|\mathbf{q}|^2} \int d^3r \int d^3r' e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} P_{\mu,\mu'}^{(+)}(\mathbf{r},\mathbf{r}') P_{\mu',\mu}^{(-)}(\mathbf{r}',\mathbf{r}) \hat{1}}_{=const.} \end{cases} \quad (454)
\end{aligned}$$

Since  $\mathcal{N} \left( \hat{\Psi}_\mu^\dagger(\mathbf{r}) \hat{\Psi}_{\mu'}(\mathbf{r}') \right) = \hat{\Gamma}_{e,\mu}^\dagger(\mathbf{r}) \hat{\Gamma}_{e,\mu'}(\mathbf{r}') - \hat{\Gamma}_{p,\mu'}^\dagger(\mathbf{r}') \hat{\Gamma}_{p,\mu}(\mathbf{r}) + \hat{\Gamma}_{e,\mu}^\dagger(\mathbf{r}) \hat{\Gamma}_{p,\mu'}^\dagger(\mathbf{r}') + \hat{\Gamma}_{p,\mu}(\mathbf{r}) \hat{\Gamma}_{e,\mu'}(\mathbf{r}')$  one can write for (454) [7]

$$\begin{aligned} \hat{\mathcal{V}}_C &= \text{const} \times \hat{1} + \mathcal{N} \left( \hat{\mathcal{V}}_C \right) \\ &+ \frac{q_e^2}{2\varepsilon_0} \int \frac{d^3q}{(2\pi)^3} \frac{1}{|\mathbf{q}|^2} \times \mathcal{N} \left( \sum_{\mu,\mu'} \int d^3r \int d^3r' \hat{\Psi}_\mu^\dagger(\mathbf{r}) e^{-i\mathbf{q}\cdot\mathbf{r}} \left( P_{\mu,\mu'}^{(+)}(\mathbf{r},\mathbf{r}') - P_{\mu,\mu'}^{(-)}(\mathbf{r},\mathbf{r}') \right) e^{i\mathbf{q}\cdot\mathbf{r}'} \hat{\Psi}_{\mu'}(\mathbf{r}') \right) \end{aligned} \quad (455)$$

Defining, with position operator  $\hat{x}_a$  and the projection operators  $\mathbf{P}^{(\pm)}$  [7]

$$\begin{aligned} &\sum_{\mu,\mu'} \int d^3r \int d^3r' \hat{\Psi}_\mu^\dagger(\mathbf{r}) e^{-i\mathbf{q}\cdot\mathbf{r}} \left( P_{\mu,\mu'}^{(+)}(\mathbf{r},\mathbf{r}') - P_{\mu,\mu'}^{(-)}(\mathbf{r},\mathbf{r}') \right) e^{i\mathbf{q}\cdot\mathbf{r}'} \hat{\Psi}_{\mu'}(\mathbf{r}') \\ &= \sum_{\mu,\mu'} \int d^3r \int d^3r' \hat{\Psi}_\mu^\dagger(\mathbf{r}) \langle \mathbf{r}, \mu | e^{-iq_a \hat{x}_a} \left( \mathbf{P}^{(+)} - \mathbf{P}^{(-)} \right) \circ e^{iq_a \hat{x}_a} | \mathbf{r}', \mu' \rangle \hat{\Psi}_{\mu'}(\mathbf{r}') \end{aligned} \quad (456)$$

(455) decomposes into [7]

$$\hat{\mathcal{V}}_C = \mathcal{N} \left( \hat{\mathcal{V}}_C \right) + \hat{\mathcal{M}}_C \quad (457)$$

where the self energy contribution  $\hat{\mathcal{M}}_C$  is given by [7]

$$\begin{aligned} \hat{\mathcal{M}}_C &= \mathcal{N} \left( \sum_{\mu,\mu'} \int d^3r \int d^3r' \hat{\Psi}_\mu^\dagger(\mathbf{r}) \mathbf{M}_{\mu,\mu'}^{(C)}(\mathbf{r},\mathbf{r}') \hat{\Psi}_{\mu'}(\mathbf{r}') \right) \\ \mathbf{M}_{\mu,\mu'}^{(C)}(\mathbf{r},\mathbf{r}') &= \frac{q_e^2}{2\varepsilon_0} \langle \mathbf{r}, \mu | \left( \int \frac{d^3q}{(2\pi)^3} \frac{1}{|\mathbf{q}|^2} e^{-iq_a \hat{x}_a} \left( \mathbf{P}^{(+)} - \mathbf{P}^{(-)} \right) \circ e^{iq_a \hat{x}_a} \right) | \mathbf{r}', \mu' \rangle \end{aligned} \quad (458)$$

One can now decompose the self energy (458) further into particle number conserving and violating terms. For this one has to insert the gamma operators (433) into (458) [7]:

$$\begin{aligned}
\hat{\mathcal{M}}_C &= \hat{\mathcal{M}}_C^{(0)} + \hat{\mathcal{M}}_C^{(+)} + \hat{\mathcal{M}}_C^{(-)} \\
\hat{\mathcal{M}}_C^{(0)} &= \sum_{\mu, \mu'} \int d^3r \int d^3r' \mathbf{M}_{\mu, \mu'}^{(C)}(\mathbf{r}, \mathbf{r}') \left( \hat{\Gamma}_{e, \mu}^\dagger(\mathbf{r}) \hat{\Gamma}_{e, \mu'}(\mathbf{r}') - \hat{\Gamma}_{p, \mu'}^\dagger(\mathbf{r}') \hat{\Gamma}_{p, \mu}(\mathbf{r}) \right) \\
\hat{\mathcal{M}}_C^{(+)} &= \sum_{\mu, \mu'} \int d^3r \int d^3r' \mathbf{M}_{\mu, \mu'}^{(C)}(\mathbf{r}, \mathbf{r}') \hat{\Gamma}_{e, \mu}^\dagger(\mathbf{r}) \hat{\Gamma}_{p, \mu'}^\dagger(\mathbf{r}') \\
\hat{\mathcal{M}}_C^{(-)} &= \sum_{\mu, \mu'} \int d^3r \int d^3r' \mathbf{M}_{\mu, \mu'}^{(C)}(\mathbf{r}, \mathbf{r}') \hat{\Gamma}_{p, \mu}(\mathbf{r}) \hat{\Gamma}_{e, \mu'}(\mathbf{r}')
\end{aligned} \tag{459}$$

The eigenvalue or commutation relations are readily provided by [7]

$$\begin{aligned}
\left[ \hat{N}, \hat{\mathcal{M}}_C^{(0)} \right] &= \hat{0} \\
\left[ \hat{N}, \hat{\mathcal{M}}_C^{(\pm)} \right] &= \pm 2 \hat{\mathcal{M}}_C^{(\pm)}
\end{aligned} \tag{460}$$

Hence, one finally finds [7]

$$\begin{aligned}
\hat{\mathcal{V}}_C &= \mathcal{N} \left( \hat{\mathcal{V}}_C \right) + \hat{\mathcal{M}}_C \\
&= \hat{\mathcal{U}}_C^{(0)} + \hat{\mathcal{M}}_C^{(0)} + \mathcal{N} \left( \hat{\mathcal{U}}_C^{(+)} \right) + \hat{\mathcal{M}}_C^{(+)} + \mathcal{N} \left( \hat{\mathcal{U}}_C^{(-)} \right) + \hat{\mathcal{M}}_C^{(-)} + \hat{\mathcal{U}}_C^{(+, +)} + \hat{\mathcal{U}}_C^{(-, -)}
\end{aligned} \tag{461}$$

For the Coulomb interaction contribution.

For solving the homogeneous part of the second order differential equation it is convenient to reexpress the particle number conserving contributions by the creation and annihilation operators of the Dirac modes, because these survive remain in the limit  $s \rightarrow \infty$

Using (433) one finds for the particle number conserving contribution  $\hat{\mathcal{M}}_C^{(0)}$  of the Coulomb self energy [7]

$$\hat{\mathcal{M}}_C^{(0)} = \sum_{\mu, \mu'} \left\{ \begin{aligned} &\sum_{K, k} \int d^3r \sum_{\mu} \langle U_K | \mathbf{r}, \mu \rangle \langle \mathbf{r}, \mu | \left( \frac{q_e^2}{2\epsilon_0} \int \frac{d^3q}{(2\pi)^3} \frac{1}{|\mathbf{q}|^2} e^{-iq_a \cdot \hat{\mathbf{x}}_a} (\mathbf{p}^{(+)} - \mathbf{p}^{(-)}) \circ e^{iq_a \cdot \hat{\mathbf{x}}_a} \right) \int d^3r' \sum_{\mu'} |\mathbf{r}', \mu' \rangle \langle \mathbf{r}', \mu' | U_k \rangle \hat{c}_K^\dagger \hat{c}_k \\ & - \sum_{K', k'} \int d^3r \sum_{\mu} \langle V_{k'} | \mathbf{r}, \mu \rangle \langle \mathbf{r}, \mu | \left( \frac{q_e^2}{2\epsilon_0} \int \frac{d^3q}{(2\pi)^3} \frac{1}{|\mathbf{q}|^2} e^{-iq_a \cdot \hat{\mathbf{x}}_a} (\mathbf{p}^{(+)} - \mathbf{p}^{(-)}) \circ e^{iq_a \cdot \hat{\mathbf{x}}_a} \right) \int d^3r' \sum_{\mu'} |\mathbf{r}', \mu' \rangle \langle \mathbf{r}', \mu' | V_{K'} \rangle \hat{b}_{K'}^\dagger \hat{b}_{k'} \end{aligned} \right\} \tag{462}$$

Now with  $\int d^3r \sum_{\mu} |\mathbf{r}, \mu \rangle \langle \mathbf{r}, \mu| = \mathbf{1}_{4 \times 4}$  there follows [7]

$$\begin{aligned}
\hat{\mathcal{M}}_C^{(0)} &= \hat{\mathcal{M}}_C^{(e)} + \hat{\mathcal{M}}_C^{(p)} \\
\hat{\mathcal{M}}_C^{(e)} &= \sum_{K,k} \left( \frac{q_e^2}{2\varepsilon_0} \right) \int \frac{d^3q}{(2\pi)^3} \frac{1}{|\mathbf{q}|^2} \langle U_K | e^{-iq_a \cdot \hat{x}_a} \left( \mathbf{P}^{(+)} - \mathbf{P}^{(-)} \right) \circ e^{iq_a \cdot \hat{x}_a} | U_k \rangle \hat{c}_K^\dagger \hat{c}_k \\
\hat{\mathcal{M}}_C^{(p)} &= \sum_{K',k'} \left( -\frac{q_e^2}{2\varepsilon_0} \right) \int \frac{d^3q}{(2\pi)^3} \frac{1}{|\mathbf{q}|^2} \langle V_{k'} | e^{-iq_a \cdot \hat{x}_a} \left( \mathbf{P}^{(+)} - \mathbf{P}^{(-)} \right) \circ e^{iq_a \cdot \hat{x}_a} | V_{K'} \rangle \hat{b}_{\tilde{K}'}^\dagger \hat{b}_{\tilde{k}'}
\end{aligned} \tag{463}$$

For the particle number conserving part of the coupling to the external Coulomb potential  $\hat{\mathcal{V}}_{ext}^{(0)}$  one finds by using (433) [7]

$$\begin{aligned}
\hat{\mathcal{V}}_{ext}^{(0)} &= \frac{Z|q_e|}{4\pi\varepsilon_0} \int \frac{d^3q}{(2\pi)^3} \frac{e^{i\mathbf{q}\cdot\mathbf{R}}}{|\mathbf{q}|^2} \tilde{\rho}_0(\mathbf{q}) \\
&= -\frac{Zq_e^2}{4\pi\varepsilon_0} \left\{ \begin{aligned} &\sum_{K,k} \int \frac{d^3q}{(2\pi)^3} \frac{e^{i\mathbf{q}\cdot\mathbf{R}}}{|\mathbf{q}|^2} \langle U_K | e^{-iq_a x_a} \left( \int d^3r \sum_\mu |\mathbf{r}, \mu\rangle \langle \mathbf{r}, \mu| \right) | U_k \rangle \hat{c}_K^\dagger \hat{c}_k \\ & - \sum_{K,k} \int \frac{d^3q}{(2\pi)^3} \frac{e^{i\mathbf{q}\cdot\mathbf{R}}}{|\mathbf{q}|^2} \langle V_k | e^{-iq_a x_a} \left( \int d^3r \sum_\mu |\mathbf{r}, \mu\rangle \langle \mathbf{r}, \mu| \right) | V_K \rangle \hat{b}_{\tilde{K}}^\dagger \hat{b}_{\tilde{k}} \end{aligned} \right.
\end{aligned} \tag{464}$$

yielding [7]

$$\begin{aligned}
\hat{\mathcal{V}}_{ext}^{(0)} &= \hat{\mathcal{V}}_{ext}^{(e)} + \hat{\mathcal{V}}_{ext}^{(p)} \\
\hat{\mathcal{V}}_{ext}^{(e)} &= -\frac{Zq_e^2}{4\pi\varepsilon_0} \sum_{K,k} \int \frac{d^3q}{(2\pi)^3} \frac{e^{i\mathbf{q}\cdot\mathbf{R}}}{|\mathbf{q}|^2} \langle U_K | e^{-iq_a x_a} | U_k \rangle \hat{c}_K^\dagger \hat{c}_k \\
\hat{\mathcal{V}}_{ext}^{(p)} &= +\frac{Zq_e^2}{4\pi\varepsilon_0} \sum_{K,k} \int \frac{d^3q}{(2\pi)^3} \frac{e^{i\mathbf{q}\cdot\mathbf{R}}}{|\mathbf{q}|^2} \langle V_k | e^{-iq_a x_a} | V_K \rangle \hat{b}_{\tilde{K}}^\dagger \hat{b}_{\tilde{k}}
\end{aligned} \tag{465}$$

Finally, by inserting (433) into the particle number conserving part of the normally ordered QED Coulomb interaction between the fermions  $\mathcal{N}(\hat{\mathcal{V}}_C^{(0)})$  [7]

$$\mathcal{N}(\hat{\mathcal{V}}_C^{(0)}) = \frac{q_e^2}{2\varepsilon_0} \int \frac{d^3q}{(2\pi)^3} \frac{1}{|\mathbf{q}|^2} \sum_{K,k} \sum_{K',k'} \left( \begin{aligned} &\langle U_K | e^{-iq_a x_a} | U_k \rangle \langle U_{K'} | e^{iq_a x_a} | U_{k'} \rangle \hat{c}_K^\dagger \hat{c}_{K'}^\dagger \hat{c}_k \hat{c}_{k'} \\ & + \langle V_k | e^{-iq_a x_a} | V_K \rangle \langle V_{k'} | e^{iq_a x_a} | V_{K'} \rangle \hat{b}_{\tilde{K}}^\dagger \hat{b}_{\tilde{K}'}^\dagger \hat{b}_{\tilde{k}} \hat{b}_{\tilde{k}'} \\ & - 2 \langle U_K | e^{-iq_a x_a} | U_k \rangle \langle V_{k'} | e^{iq_a x_a} | V_{K'} \rangle \hat{c}_K^\dagger \hat{c}_k \hat{b}_{\tilde{K}'}^\dagger \hat{b}_{\tilde{k}'} \\ & + 2 \langle U_K | e^{-iq_a x_a} | V_k \rangle \langle V_{k'} | e^{iq_a x_a} | U_{K'} \rangle \hat{c}_K^\dagger \hat{b}_{\tilde{k}}^\dagger \hat{b}_{\tilde{k}'} \hat{c}_{K'} \end{aligned} \right) \tag{466}$$



## H Complement to the Inhomogeneous Solution

$$\hat{H}^{(2,i)}(s)$$

Here, first, the special solution to the inhomogeneous differential equation of the second order perturbation expansion.

Then it is shown by means of the example of the eigenvalue relation of the kernel  $\hat{J}^{(\pm,\pm)}(s, s')$  that the relations (485) being a part of the solution are valid.

Then it is proven that in the limit  $s \rightarrow \infty$  all contributions that violate the particle number in the inhomogeneous solution of the second order differential equation solution (476) vanish exponentially.

Finally the evaluation of the effective transversal potentials is presented.

### Construction of the special solution

For the construction of the special solution  $\hat{H}^{(2,i)}(s)$  to the inhomogeneous differential equation (122) with initial value  $\hat{H}^{(2,i)}(0) = 0$  inhomogeneity  $\hat{I}(s)$  is decomposed into terms which conserve the particle number, and such ones that do not. Then the solution to the differential equation is presented, proven, and show by the help of an example term why it is indeed a solution.

Rewriting the inhomogeneous differential equation (122) according to [7]

$$\begin{aligned} \frac{d}{ds} \hat{H}^{(2,i)}(s) &= \left\{ \begin{array}{l} - \left[ \hat{H}^{(0)}, \left[ \hat{H}^{(0)}, \left( \left[ N_I, \left[ N_I, \hat{H}^{(2,i)}(s) \right] \right) + \left[ N_{II}, \left[ N_{II}, \hat{H}^{(2,i)}(s) \right] \right] \right] \right] \\ + I^{(0)}(s) + I^{(+)}(s) + I^{(-)}(s) + I^{(+,+)}(s) + I^{(-,-)}(s) \end{array} \right\} \\ \hat{H}^{(2,i)}(0) &= \hat{0} \end{aligned} \tag{467}$$

gives the inhomogeneity according to [7]

$$\begin{aligned} \hat{I}(s) &= \hat{I}^{(0)}(s) + \hat{I}^{(+)}(s) + \hat{I}^{(-)}(s) + \hat{I}^{(+,+)}(s) + \hat{I}^{(-,-)}(s) \\ &= - \left\{ \begin{array}{l} \left[ \left[ \hat{H}^{(0)}, \hat{H}^{(1)}(s) \right], \left( \left[ \hat{N}_I, \left[ \hat{N}_I, \hat{H}^{(1)}(s) \right] \right) + \left[ \hat{N}_{II}, \left[ \hat{N}_{II}, \hat{H}^{(1)}(s) \right] \right] \right] \\ + 2 \left[ \hat{H}^{(1)}(s), \left( \left[ \hat{H}^{(0)}, \left( \left[ \hat{N}_I, \left[ \hat{N}_I, \hat{H}^{(1)}(s) \right] \right) + \left[ \hat{N}_{II}, \left[ \hat{N}_{II}, \hat{H}^{(1)}(s) \right] \right] \right] \right) \right] \right] \end{array} \right\} \end{aligned} \tag{468}$$

Here use has been made of the rule

$$[X, [Y, Z]] = [[X, Y], Z] + [Y, [X, Z]] \quad (469)$$

for any operators  $X, Y$  and  $Z$ .

This decomposition (468) follows from the solution  $\hat{H}^{(1)}(s)$  [7]

$$\hat{H}^{(1)}(s) = \hat{H}^{(1,0)}(s) + \hat{H}^{(1,+)}(s) + \hat{H}^{(1,-)}(s) \quad (470)$$

where  $\hat{H}^{(1,0)}(s)$  is given in (105),  $\hat{H}^{(1,+)}(s)$  is given in (107) and  $\hat{H}^{(1,-)}(s)$  is given in (108)

Hence,  $\hat{I}^{(0)}(s)$  is the part of all commutators with  $\hat{H}^{(1)}(s)$  in (468) which altogether conserves the particle number [7]:

$$\hat{I}^{(0)}(s) = - \left\{ \begin{array}{l} \left[ \left[ \hat{H}^{(0)}, \hat{H}^{(1,0)}(s) \right], \left( \left[ \hat{N}_I, \left[ \hat{N}_I, \hat{H}^{(1,0)}(s) \right] \right] + \left[ \hat{N}_{II}, \left[ \hat{N}_{II}, \hat{H}^{(1,0)}(s) \right] \right] \right) \right] \\ + 2 \left[ \hat{H}^{(1,0)}(s), \left( \left[ \hat{H}^{(0)}, \left( \left[ \hat{N}_I, \left[ \hat{N}_I, \hat{H}^{(1,0)}(s) \right] \right] + \left[ \hat{N}_{II}, \left[ \hat{N}_{II}, \hat{H}^{(1,0)}(s) \right] \right] \right) \right) \right] \right] \\ + \left[ \left[ \hat{H}^{(0)}, \hat{H}^{(1,+)}(s) \right], \left( \left[ \hat{N}_I, \left[ \hat{N}_I, \hat{H}^{(1,-)}(s) \right] \right] + \left[ \hat{N}_{II}, \left[ \hat{N}_{II}, \hat{H}^{(1,-)}(s) \right] \right] \right) \right] \\ + 2 \left[ \hat{H}^{(1,+)}(s), \left[ \hat{H}^{(0)}, \left( \left[ \hat{N}_I, \left[ \hat{N}_I, \hat{H}^{(1,-)}(s) \right] \right] + \left[ \hat{N}_{II}, \left[ \hat{N}_{II}, \hat{H}^{(1,-)}(s) \right] \right] \right) \right] \right] \\ + \left[ \left[ \hat{H}^{(0)}, \hat{H}^{(1,-)}(s) \right], \left( \left[ \hat{N}_I, \left[ \hat{N}_I, \hat{H}^{(1,+)}(s) \right] \right] + \left[ \hat{N}_{II}, \left[ \hat{N}_{II}, \hat{H}^{(1,+)}(s) \right] \right] \right) \right] \\ + 2 \left[ \hat{H}^{(1,-)}(s), \left[ \hat{H}^{(0)}, \left( \left[ \hat{N}_I, \left[ \hat{N}_I, \hat{H}^{(1,+)}(s) \right] \right] + \left[ \hat{N}_{II}, \left[ \hat{N}_{II}, \hat{H}^{(1,+)}(s) \right] \right] \right) \right] \right] \end{array} \right\} \quad (471)$$

Now  $\hat{I}^{(+)}(s)$  is the part which contains all commutators describing the creation of one matter–antimatter pair as [7]

$$\hat{I}^{(+)}(s) = - \left\{ \begin{array}{l} \left[ \left[ \hat{H}^{(0)}, \hat{H}^{(1,0)}(s) \right], \left( \left[ \hat{N}_I, \left[ \hat{N}_I, \hat{H}^{(1,+)}(s) \right] \right] + \left[ \hat{N}_{II}, \left[ \hat{N}_{II}, \hat{H}^{(1,+)}(s) \right] \right] \right) \right] \\ + 2 \left[ \hat{H}^{(1,0)}(s), \left[ \hat{H}^{(0)}, \left( \left[ \hat{N}_I, \left[ \hat{N}_I, \hat{H}^{(1,+)}(s) \right] \right] + \left[ \hat{N}_{II}, \left[ \hat{N}_{II}, \hat{H}^{(1,+)}(s) \right] \right] \right) \right] \right] \\ + \left[ \left[ \hat{H}^{(0)}, \hat{H}^{(1,+)}(s) \right], \left( \left[ \hat{N}_I, \left[ \hat{N}_I, \hat{H}^{(1,0)}(s) \right] \right] + \left[ \hat{N}_{II}, \left[ \hat{N}_{II}, \hat{H}^{(1,0)}(s) \right] \right] \right) \right] \\ + 2 \left[ \hat{H}^{(1,+)}(s), \left[ \hat{H}^{(0)}, \left( \left[ \hat{N}_I, \left[ \hat{N}_I, \hat{H}^{(1,0)}(s) \right] \right] + \left[ \hat{N}_{II}, \left[ \hat{N}_{II}, \hat{H}^{(1,0)}(s) \right] \right] \right) \right] \right] \end{array} \right\} \quad (472)$$

Finally,  $\hat{I}^{(+,+)}(s)$  is the part of the inhomogeneity (468) which contains all commutators describing the creation of two matter–antimatter pairs [7]:

$$\hat{I}^{(+,+)}(s) = - \left\{ \left[ \left[ \hat{H}^{(0)}, \hat{H}^{(1,+)}(s) \right], \left( \left[ \hat{N}_I, \left[ \hat{N}_I, \hat{H}^{(1,+)}(s) \right] \right] + \left[ \hat{N}_{II}, \left[ \hat{N}_{II}, \hat{H}^{(1,+)}(s) \right] \right] \right) \right] \right. \\ \left. + 2 \left[ \hat{H}^{(1,+)}(s), \left[ \hat{H}^{(0)}, \left( \left[ \hat{N}_I, \left[ \hat{N}_I, \hat{H}^{(1,+)}(s) \right] \right] + \left[ \hat{N}_{II}, \left[ \hat{N}_{II}, \hat{H}^{(1,+)}(s) \right] \right] \right) \right] \right] \right\} \quad (473)$$

The hermitian conjugates are then given by [7]

$$\begin{aligned} \hat{I}^{(-)}(s) &= \left[ \hat{I}^{(+)}(s) \right]^\dagger \\ \hat{I}^{(-,-)}(s) &= \left[ \hat{I}^{(+,+)}(s) \right]^\dagger \end{aligned} \quad (474)$$

Note that with  $\hat{N}_I$  given in (84) there holds [7]

$$\begin{aligned} \left[ \hat{N}_I, \hat{I}^{(0)}(s) \right] &= \hat{0} \\ \left[ \hat{N}_I, \hat{I}^{(\pm)}(s) \right] &= \pm 2 \hat{I}^{(\pm)}(s) \\ \left[ \hat{N}_I, \hat{I}^{(\pm,\pm)}(s) \right] &= \pm 4 \hat{I}^{(\pm,\pm)}(s) \end{aligned} \quad (475)$$

Now in the following it will be shown that the ansatz [7]

$$\hat{H}^{(2,i)}(s) = \begin{cases} \int_0^s ds' J^{(0)}(s, s') \\ + \int_0^s ds' J^{(+)}(s, s') + \int_0^s ds' J^{(-)}(s, s') \\ + \int_0^s ds' J^{(+,+)}(s, s') + \int_0^s ds' J^{(-,-)}(s, s') \end{cases} \quad (476)$$

solves the inhomogeneous differential equation (122). First note that  $\hat{H}^{(2,i)}(s=0) = \hat{0}$  as it should be.

The integral kernels  $\hat{J}^{(0)}(s, s')$ ,  $\hat{J}^{(\pm)}(s, s')$  and  $\hat{J}^{(\pm,\pm)}(s, s')$  are defined as [7]

$$\begin{aligned} \hat{j}^{(0)}(s, s') &= \hat{j}^{(0,0)}(s, s') + \hat{j}^{(0,+)}(s, s') + \hat{j}^{(0,-)}(s, s') \\ \hat{J}^{(0,0)}(s, s') &= \hat{J}_1^{(0,0)}(s, s') + J_2^{(0,0)}(s, s') \\ \hat{J}^{(0,+)}(s, s') &= \hat{J}_1^{(0,+)}(s, s') + J_2^{(0,+)}(s, s') \\ \hat{J}^{(0,-)}(s, s') &= \left[ \hat{J}^{(0,+)}(s, s') \right]^\dagger \end{aligned} \quad (477)$$

with [7]

$$\begin{aligned}
\hat{j}_1^{(0,0)}(s, s') = & - \left( \frac{q_e}{m_0 c} \right)^2 \sum_{k, k'} \sum_{K, K'} \frac{1}{V} \sum_{q, q'} \sum_{b, b'} \mathcal{A}_b(q) \mathcal{A}_{b'}(q') \times \\
& \left( \begin{aligned}
& + \langle U_k | \alpha_b e^{iq_a x_a} | U_{k'} \rangle \langle U_{K'} | \alpha_{b'} e^{-iq'_a x_a} | U_K \rangle e^{-\kappa_q s' (\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)^2} e^{-\kappa_{q'} s' (\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2} \times \\
& \quad \times \left( \tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q + 2 \left( \tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'} \right) \right) \kappa_{q'} \times \\
& \quad \times e^{-(s-s')(-\kappa_q + \kappa_{q'})^2 (\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q + \tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2} \left[ \hat{c}_k^\dagger \hat{c}_{k'} \hat{a}_q, \hat{c}_K^\dagger \hat{c}_{K'} \hat{a}_{q'}^\dagger \right] \\
& - \langle U_k | \alpha_b e^{iq_a x_a} | U_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{-iq'_a x_a} | V_K \rangle e^{-\kappa_q s' (\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)^2} e^{-\kappa_{q'} s' (\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'})^2} \times \\
& \quad \times \left( \tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q + 2 \left( \tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'} \right) \right) \kappa_{q'} \times \\
& \quad \times e^{-(s-s')(-\kappa_q + \kappa_{q'})^2 (\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q + \tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'})^2} \left[ \hat{c}_k^\dagger \hat{c}_{k'} \hat{a}_q, \hat{b}_{\tilde{K}}^\dagger \hat{b}_{\tilde{K}'} \hat{a}_{q'}^\dagger \right] \\
& - \langle V_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle U_{K'} | \alpha_{b'} e^{-iq'_a x_a} | U_K \rangle e^{-\kappa_q s' (\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q)^2} e^{-\kappa_{q'} s' (\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2} \times \\
& \quad \times \left( \tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q + 2 \left( \tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'} \right) \right) \kappa_{q'} \times \\
& \quad \times e^{-(s-s')(-\kappa_q + \kappa_{q'})^2 (\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q + \tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2} \left[ \hat{b}_{k'}^\dagger \hat{b}_{\tilde{k}} \hat{a}_q, \hat{c}_K^\dagger \hat{c}_{K'} \hat{a}_{q'}^\dagger \right] \\
& + \langle V_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{-iq'_a x_a} | V_K \rangle e^{-\kappa_q s' (\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q)^2} e^{-\kappa_{q'} s' (\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'})^2} \times \\
& \quad \times \left( \tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q + 2 \left( \tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'} \right) \right) \kappa_{q'} \times \\
& \quad \times e^{-(s-s')(-\kappa_q + \kappa_{q'})^2 (\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q + \tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'})^2} \left[ \hat{b}_{k'}^\dagger \hat{b}_{\tilde{k}} \hat{a}_q, \hat{b}_{\tilde{K}}^\dagger \hat{b}_{\tilde{K}'} \hat{a}_{q'}^\dagger \right] \\
& \times \\
& + \langle U_{k'} | \alpha_b e^{-iq_a x_a} | U_k \rangle \langle U_K | \alpha_{b'} e^{iq'_a x_a} | U_{K'} \rangle e^{-\kappa_q s' (\tilde{E}_{k'} - \tilde{E}_k + \tilde{\omega}_q)^2} e^{-\kappa_{q'} s' (\tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_{q'})^2} \times \\
& \quad \times \left( \tilde{E}_{k'} - \tilde{E}_k + \tilde{\omega}_q + 2 \left( \tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_{q'} \right) \right) \kappa_{q'} \times \\
& \quad \times e^{-(s-s')(\kappa_q - \kappa_{q'})^2 (\tilde{E}_{k'} - \tilde{E}_k + \tilde{\omega}_q + \tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_{q'})^2} \left[ \hat{c}_k^\dagger \hat{c}_{k'} \hat{a}_q^\dagger, \hat{c}_K^\dagger \hat{c}_{K'} \hat{a}_{q'} \right] \\
& - \langle U_{k'} | \alpha_b e^{-iq_a x_a} | U_k \rangle \langle V_K | \alpha_{b'} e^{iq'_a x_a} | V_{K'} \rangle e^{-\kappa_q s' (\tilde{E}_{k'} - \tilde{E}_k + \tilde{\omega}_q)^2} e^{-\kappa_{q'} s' (\tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})^2} \times \\
& \quad \times \left( \tilde{E}_{k'} - \tilde{E}_k + \tilde{\omega}_q + 2 \left( \tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'} \right) \right) \kappa_{q'} \times \\
& \quad \times e^{-(s-s')(\kappa_q - \kappa_{q'})^2 (\tilde{E}_{k'} - \tilde{E}_k + \tilde{\omega}_q + \tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})^2} \left[ \hat{c}_k^\dagger \hat{c}_{k'} \hat{a}_q^\dagger, \hat{b}_{\tilde{K}}^\dagger \hat{b}_{\tilde{K}'} \hat{a}_{q'} \right] \\
& - \langle V_{k'} | \alpha_b e^{-iq_a x_a} | V_k \rangle \langle U_K | \alpha_{b'} e^{iq'_a x_a} | U_{K'} \rangle e^{-\kappa_q s' (\tilde{E}_k - \tilde{E}_{k'} + \tilde{\omega}_q)^2} e^{-\kappa_{q'} s' (\tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_{q'})^2} \times \\
& \quad \times \left( \tilde{E}_k - \tilde{E}_{k'} + \tilde{\omega}_q + 2 \left( \tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_{q'} \right) \right) \kappa_{q'} \times \\
& \quad \times e^{-(s-s')(\kappa_q - \kappa_{q'})^2 (\tilde{E}_k - \tilde{E}_{k'} + \tilde{\omega}_q + \tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_{q'})^2} \left[ \hat{b}_k^\dagger \hat{b}_{\tilde{k}'} \hat{a}_q^\dagger, \hat{c}_K^\dagger \hat{c}_{K'} \hat{a}_{q'} \right] \\
& + \langle V_{k'} | \alpha_b e^{-iq_a x_a} | V_k \rangle \langle V_K | \alpha_{b'} e^{iq'_a x_a} | V_{K'} \rangle e^{-\kappa_q s' (\tilde{E}_k - \tilde{E}_{k'} + \tilde{\omega}_q)^2} e^{-\kappa_{q'} s' (\tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})^2} \times \\
& \quad \times \left( \tilde{E}_k - \tilde{E}_{k'} + \tilde{\omega}_q + 2 \left( \tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'} \right) \right) \kappa_{q'} \times \\
& \quad \times e^{-(s-s')(\kappa_q - \kappa_{q'})^2 (\tilde{E}_k - \tilde{E}_{k'} + \tilde{\omega}_q + \tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})^2} \left[ \hat{b}_k^\dagger \hat{b}_{\tilde{k}'} \hat{a}_q^\dagger, \hat{b}_{\tilde{K}}^\dagger \hat{b}_{\tilde{K}'} \hat{a}_{q'} \right]
\end{aligned} \right) \tag{478}
\end{aligned}$$

$$\begin{aligned}
\hat{j}_2^{(0,0)}(s, s') = & - \left( \frac{q_e}{m_0 c} \right)^2 \sum_{k, k'} \sum_{K, K'} \frac{1}{V} \sum_{q, q'} \sum_{b, b'} \mathcal{A}_b(q) \mathcal{A}_{b'}(q') \times \\
& \left( \begin{aligned}
& + \langle U_k | \alpha_b e^{iq_a x_a} | U_{k'} \rangle \langle U_K | \alpha_{b'} e^{iq'_a x_a} | U_{K'} \rangle e^{-\kappa_q s' (\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)^2} e^{-\kappa_{q'} s' (\tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_{q'})^2} \times \\
& \quad \times \left( \tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q + 2 \left( \tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_{q'} \right) \right) \kappa_{q'} \times \\
& \quad \times e^{-(s-s')(-\kappa_q - \kappa_{q'})^2 (\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q + \tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_{q'})^2} \left[ \hat{c}_k^\dagger \hat{c}_{k'} \hat{a}_q, \hat{c}_K^\dagger \hat{c}_{K'} \hat{a}_{q'} \right] \\
& + \langle V_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle V_K | \alpha_{b'} e^{iq'_a x_a} | V_{K'} \rangle e^{-\kappa_q s' (\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q)^2} e^{-\kappa_{q'} s' (\tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})^2} \times \\
& \quad \times \left( \tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q + 2 \left( \tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'} \right) \right) \kappa_{q'} \times \\
& \quad \times e^{-(s-s')(-\kappa_q - \kappa_{q'})^2 (\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q + \tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})^2} \left[ \hat{b}_{k'}^\dagger \hat{b}_k \hat{a}_q, \hat{b}_{K'}^\dagger \hat{b}_K \hat{a}_{q'} \right] \\
& \times \\
& + \langle U_{k'} | \alpha_b e^{-iq_a x_a} | U_k \rangle \langle U_{K'} | \alpha_{b'} e^{-iq'_a x_a} | U_K \rangle e^{-\kappa_q s' (\tilde{E}_{k'} - \tilde{E}_k + \tilde{\omega}_q)^2} e^{-\kappa_{q'} s' (\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2} \times \\
& \quad \times \left( \tilde{E}_{k'} - \tilde{E}_k + \tilde{\omega}_q + 2 \left( \tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'} \right) \right) \kappa_{q'} \times \\
& \quad \times e^{-(s-s')(\kappa_q + \kappa_{q'})^2 (\tilde{E}_{k'} - \tilde{E}_k + \tilde{\omega}_q + \tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2} \left[ \hat{c}_{k'}^\dagger \hat{c}_k \hat{a}_q^\dagger, \hat{c}_{K'}^\dagger \hat{c}_K \hat{a}_{q'}^\dagger \right] \\
& + \langle V_{k'} | \alpha_b e^{-iq_a x_a} | V_k \rangle \langle V_{K'} | \alpha_{b'} e^{-iq'_a x_a} | V_K \rangle e^{-\kappa_q s' (\tilde{E}_k - \tilde{E}_{k'} + \tilde{\omega}_q)^2} e^{-\kappa_{q'} s' (\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'})^2} \times \\
& \quad \times \left( \tilde{E}_k - \tilde{E}_{k'} + \tilde{\omega}_q + 2 \left( \tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'} \right) \right) \kappa_{q'} \times \\
& \quad \times e^{-(s-s')(\kappa_q + \kappa_{q'})^2 (\tilde{E}_k - \tilde{E}_{k'} + \tilde{\omega}_q + \tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'})^2} \left[ \hat{b}_k^\dagger \hat{b}_{k'} \hat{a}_q^\dagger, \hat{b}_K^\dagger \hat{b}_{K'} \hat{a}_{q'}^\dagger \right]
\end{aligned} \right) \quad (479)
\end{aligned}$$

$$\begin{aligned}
\hat{j}_1^{(0,+)}(s, s') = & - \left( \frac{q_e}{m_0 c} \right)^2 \sum_{k, k'} \sum_{K, K'} \frac{1}{V} \sum_{q, q'} \sum_{b, b'} \mathcal{A}_b(q) \mathcal{A}_{b'}(q') \times \\
& \left( \begin{aligned}
& \langle U_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{-iq'_a x_a} | U_K \rangle e^{-(4+\kappa_q)s' (\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q)^2} e^{-(4+\kappa_{q'})s' (-\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2} \times \\
& \quad \times \left( \tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q + 2 \left( -\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'} \right) \right) (4 + \kappa_{q'}) \times \\
& \quad \times e^{-(s-s')(-\kappa_q + \kappa_{q'})^2 (\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q - \tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2} \left[ \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q, \hat{b}_{K'} \hat{c}_K \hat{a}_{q'}^\dagger \right] \\
& \times \\
& + \langle U_k | \alpha_b e^{-iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{iq'_a x_a} | U_K \rangle e^{-(4+\kappa_q)s' (\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q)^2} e^{-(4+\kappa_{q'})s' (-\tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})^2} \times \\
& \quad \times \left( \tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q + 2 \left( -\tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'} \right) \right) (4 + \kappa_{q'}) \times \\
& \quad \times e^{-(s-s')(\kappa_q - \kappa_{q'})^2 (\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q - \tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})^2} \left[ \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q^\dagger, \hat{b}_{K'} \hat{c}_K \hat{a}_{q'} \right]
\end{aligned} \right) \quad (480)
\end{aligned}$$

$$\begin{aligned}
\hat{j}_2^{(0,+)}(s, s') = & - \left( \frac{q_e}{m_0 c} \right)^2 \sum_{k, k'} \sum_{K, K'} \frac{1}{V} \sum_{q, q'} \sum_{b, b'} \mathcal{A}_b(q) \mathcal{A}_{b'}(q') \times \\
& \left( \begin{aligned}
& + \langle U_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{iq'_a x_a} | U_K \rangle e^{-(4+\kappa_q)s' (\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q)^2} e^{-(4+\kappa_{q'})s' (-\tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})^2} \times \\
& \quad \times \left( \tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q + 2 \left( -\tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_{q'} \right) \right) (4 + \kappa_{q'}) \times \\
& \quad \times e^{-(s-s')(-\kappa_q - \kappa_{q'})^2 (\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q - \tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})^2} \left[ \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q, \hat{b}_{K'} \hat{c}_K \hat{a}_{q'} \right] \\
& \times \\
& + \langle U_k | \alpha_b e^{-iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{-iq'_a x_a} | U_K \rangle e^{-(4+\kappa_q)s' (\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q)^2} e^{-(4+\kappa_{q'})s' (-\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2} \times \\
& \quad \times \left( \tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q + 2 \left( -\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'} \right) \right) (4 + \kappa_{q'}) \times \\
& \quad \times e^{-(s-s')(\kappa_q + \kappa_{q'})^2 (\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q - \tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2} \left[ \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q^\dagger, \hat{b}_{K'} \hat{c}_K \hat{a}_{q'}^\dagger \right]
\end{aligned} \right) \quad (481)
\end{aligned}$$



$$\begin{aligned}
\hat{J}^{(+,+)}(s, s') = & - \left( \frac{q_e}{m_0 c} \right)^2 \sum_{k, k'} \sum_{K, K'} \frac{1}{V} \sum_{q, q'} \sum_{b, b'} \mathcal{A}_b(q) \mathcal{A}_{b'}(q') \times \\
& \left( \begin{aligned}
& \langle U_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle U_K | \alpha_{b'} e^{iq'_a x_a} | V_{K'} \rangle e^{-(4+\kappa_q)s'} (\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q)^2 e^{-(4+\kappa_{q'})s'} (\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'})^2 \times \\
& \quad \times \left( (\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q) + 2(\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'}) \right) (4 + \kappa_{q'}) \times \\
& \quad \times e^{-(s-s') (16 + (-\kappa_q - \kappa_{q'})^2)} (\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q + \tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'})^2 \left[ \hat{c}_k^\dagger \hat{b}_k^\dagger \hat{a}_q, \hat{c}_K^\dagger \hat{b}_K^\dagger \hat{a}_{q'} \right] \\
& + \langle U_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle U_K | \alpha_{b'} e^{-iq'_a x_a} | V_{K'} \rangle e^{-(4+\kappa_q)s'} (\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q)^2 e^{-(4+\kappa_{q'})s'} (\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'})^2 \times \\
& \quad \times \left( \tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q + 2(\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'}) \right) (4 + \kappa_{q'}) \times \\
& \quad \times e^{-(s-s') (16 + (-\kappa_q + \kappa_{q'})^2)} (\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q + \tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'})^2 \left[ \hat{c}_k^\dagger \hat{b}_k^\dagger \hat{a}_q, \hat{c}_K^\dagger \hat{b}_K^\dagger \hat{a}_{q'} \right] \\
& \times \\
& \langle U_k | \alpha_b e^{-iq_a x_a} | V_{k'} \rangle \langle U_K | \alpha_{b'} e^{iq'_a x_a} | V_{K'} \rangle e^{-(4+\kappa_q)s'} (\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q)^2 e^{-(4+\kappa_{q'})s'} (\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'})^2 \times \\
& \quad \times \left( \tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q + 2(\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'}) \right) (4 + \kappa_{q'}) \times \\
& \quad \times e^{-(s-s') (16 + (\kappa_q - \kappa_{q'})^2)} (\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q + \tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'})^2 \left[ \hat{c}_k^\dagger \hat{b}_k^\dagger \hat{a}_q, \hat{c}_K^\dagger \hat{b}_K^\dagger \hat{a}_{q'} \right] \\
& + \langle U_k | \alpha_b e^{-iq_a x_a} | V_{k'} \rangle \langle U_K | \alpha_{b'} e^{-iq'_a x_a} | V_{K'} \rangle e^{-(4+\kappa_q)s'} (\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q)^2 e^{-(4+\kappa_{q'})s'} (\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'})^2 \times \\
& \quad \times \left( \tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q + 2(\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'}) \right) (4 + \kappa_{q'}) \times \\
& \quad \times e^{-(s-s') (16 + (\kappa_q + \kappa_{q'})^2)} (\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q + \tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'})^2 \left[ \hat{c}_k^\dagger \hat{b}_k^\dagger \hat{a}_q, \hat{c}_K^\dagger \hat{b}_K^\dagger \hat{a}_{q'} \right]
\end{aligned} \right) \tag{483}
\end{aligned}$$

$$\text{and } \hat{J}^{(-,-)}(s, s') = \left[ \hat{J}^{(+,+)}(s, s') \right]^\dagger.$$

Now the relation between the kernels  $\hat{J}^{(\cdot)}(s, s')$  and the terms  $\hat{I}^{(\cdot)}(s)$  is given by [7]

$$\begin{aligned}
\lim_{s' \rightarrow s} \hat{J}^{(0)}(s, s') &= \hat{I}^{(0)}(s) \\
\lim_{s' \rightarrow s} \hat{J}^{(\pm)}(s, s') &= \hat{I}^{(\pm)}(s) \\
\lim_{s' \rightarrow s} \hat{J}^{(\pm, \pm)}(s, s') &= \hat{I}^{(\pm, \pm)}(s)
\end{aligned} \tag{484}$$

(for showing this one has to further decompose the inhomogeneous terms  $\hat{I}^{(\cdot)}(s)$  as has been done for the kernels  $\hat{J}^{(-,-)}(s, s')$  above).

For proving the ansatz (476) one needs the following eigenvalue relations [7]

$$\begin{aligned}
\frac{d}{ds} \hat{J}^{(0)}(s, s') &= - \left[ \hat{H}^{(0)}, \left[ \hat{H}^{(0)}, \left( \left[ N_I, \left[ N_I, \hat{J}^{(0)}(s, s') \right] \right) + \left[ N_{II}, \left[ N_{II}, \hat{J}^{(0)}(s, s') \right] \right] \right] \right] \\
\frac{d}{ds} \hat{J}^{(\pm)}(s, s') &= - \left[ \hat{H}^{(0)}, \left[ \hat{H}^{(0)}, \left( \left[ N_I, \left[ N_I, \hat{J}^{(\pm)}(s, s') \right] \right) + \left[ N_{II}, \left[ N_{II}, \hat{J}^{(\pm)}(s, s') \right] \right] \right] \right] \\
\frac{d}{ds} \hat{J}^{(\pm, \pm)}(s, s') &= - \left[ \hat{H}^{(0)}, \left[ \hat{H}^{(0)}, \left( \left[ N_I, \left[ N_I, \hat{J}^{(\pm, \pm)}(s, s') \right] \right) + \left[ N_{II}, \left[ N_{II}, \hat{J}^{(\pm, \pm)}(s, s') \right] \right] \right] \right]
\end{aligned} \tag{485}$$

Below the validation of the third line in (485) is shown explicitly, as an example.

Now differentiating the ansatz (476) with respect to  $s$  one finds [7]

$$\begin{aligned}
\frac{d}{ds} \hat{H}^{(2,i)}(s) &= \frac{d}{ds} \int_0^s ds' \left( J^{(0)}(s, s') + J^{(+)}(s, s') + J^{(-)}(s, s') + J^{(+,+)}(s, s') + J^{(-,-)}(s, s') \right) \\
&= \left\{ \begin{aligned} &J^{(0)}(s, s) + J^{(+)}(s, s) + J^{(-)}(s, s) + J^{(+,+)}(s, s) + J^{(-,-)}(s, s) \\ &+ \int_0^s ds' \left( \frac{d}{ds} J^{(0)}(s, s') + \frac{d}{ds} J^{(+)}(s, s') + \frac{d}{ds} J^{(-)}(s, s') + \frac{d}{ds} J^{(+,+)}(s, s') + \frac{d}{ds} J^{(-,-)}(s, s') \right) \end{aligned} \right\} \\
&= \left\{ \begin{aligned} &J^{(0)}(s, s) + J^{(+)}(s, s) + J^{(-)}(s, s) + J^{(+,+)}(s, s) + J^{(-,-)}(s, s) \\ &+ \int_0^s ds' \left( \frac{d}{ds} J^{(0)}(s, s') + \frac{d}{ds} J^{(+)}(s, s') + \frac{d}{ds} J^{(-)}(s, s') + \frac{d}{ds} J^{(+,+)}(s, s') + \frac{d}{ds} J^{(-,-)}(s, s') \right) \end{aligned} \right\} \\
&= \left\{ \begin{aligned} &I^{(0)}(s) + I^{(+)}(s) + I^{(-)}(s) + I^{(+,+)}(s) + I^{(-,-)}(s) \\ &- \int_0^s ds' \left[ \hat{H}^{(0)}, \left[ \hat{H}^{(0)}, \left( [N_I, [N_I, J^{(0)}(s, s')]] + [N_{II}, [N_{II}, J^{(0)}(s, s')]] \right) \right] \right] \\ &- \int_0^s ds' \left[ \hat{H}^{(0)}, \left[ \hat{H}^{(0)}, \left( [N_I, [N_I, J^{(+)}(s, s')]] + [N_{II}, [N_{II}, J^{(+)}(s, s')]] \right) \right] \right] \\ &- \int_0^s ds' \left[ \hat{H}^{(0)}, \left[ \hat{H}^{(0)}, \left( [N_I, [N_I, J^{(-)}(s, s')]] + [N_{II}, [N_{II}, J^{(-)}(s, s')]] \right) \right] \right] \\ &- \int_0^s ds' \left[ \hat{H}^{(0)}, \left[ \hat{H}^{(0)}, \left( [N_I, [N_I, J^{(+,+)}(s, s')]] + [N_{II}, [N_{II}, J^{(+,+)}(s, s')]] \right) \right] \right] \\ &- \int_0^s ds' \left[ \hat{H}^{(0)}, \left[ \hat{H}^{(0)}, \left( [N_I, [N_I, J^{(-,-)}(s, s')]] + [N_{II}, [N_{II}, J^{(-,-)}(s, s')]] \right) \right] \right] \end{aligned} \right\} \quad (486)
\end{aligned}$$

Using (485) there follows for (486) [7]

$$\begin{aligned}
\frac{d}{ds} \hat{H}^{(2,i)}(s) &= \left\{ \begin{aligned} &I^{(0)}(s) + I^{(+)}(s) + I^{(-)}(s) + I^{(+,+)}(s) + I^{(-,-)}(s) \\ &- \left[ \hat{H}^{(0)}, \left[ \hat{H}^{(0)}, \left( \begin{aligned} &[N_I, [N_I, \int_0^s ds' (J^{(0)}(s, s') + J^{(+)}(s, s') + J^{(-)}(s, s') + J^{(+,+)}(s, s') + J^{(-,-)}(s, s'))]] + \\ &+ [N_{II}, [N_{II}, \int_0^s ds' (J^{(0)}(s, s') + J^{(+)}(s, s') + J^{(-)}(s, s') + J^{(+,+)}(s, s') + J^{(-,-)}(s, s'))]] \end{aligned} \right) \right] \right] \end{aligned} \right\} \\
&= \left\{ \begin{aligned} &+I^{(0)}(s) + I^{(+)}(s) + I^{(-)}(s) + I^{(+,+)}(s) + I^{(-,-)}(s) \\ &- \left[ \hat{H}^{(0)}, \left[ \hat{H}^{(0)}, \left( [N_I, [N_I, \hat{H}^{(2,i)}(s)]] + [N_{II}, [N_{II}, \hat{H}^{(2,i)}(s)]] \right) \right] \right] \end{aligned} \right\} \\
&= - \left[ \hat{H}^{(0)}, \left[ \hat{H}^{(0)}, \left( [N_I, [N_I, \hat{H}^{(2,i)}(s)]] + [N_{II}, [N_{II}, \hat{H}^{(2,i)}(s)]] \right) \right] \right] + \hat{I}(s) \quad (487)
\end{aligned}$$

As it should be!

In the following, after it has been shown by the example  $\hat{J}^{(\pm,\pm)}(s, s')$  how the eigenvalue relations (485) can be proven, the limit  $s \rightarrow \infty$  of the solution  $\hat{H}^{(2,i)}(s)$  is evaluated. This is done below, where the integrals are calculated. With that it will also be proven that all terms that violate the particle number vanish exponentially, again provided that one first takes the limit  $V \rightarrow \infty$  such that the mode indices  $k, k', K, K', q, q'$  lie dense in the Volume  $V$  and that their discrete summation can be converted into integral.



## Eigenvalue relation of the kernel $\hat{J}^{(\pm,\pm)}(s, s')$

The third line in (485) is given by [7]

$$\frac{d}{ds} \hat{J}^{(\pm,\pm)}(s, s') = - \left[ \hat{H}^{(0)}, \left[ \hat{H}^{(0)}, \left( \left[ N_I, \left[ N_I, \hat{J}^{(\pm,\pm)}(s, s') \right] \right) + \left[ N_{II}, \left[ N_{II}, \hat{J}^{(\pm,\pm)}(s, s') \right] \right] \right] \right] \quad (488)$$

For showing the equivalence one has to differentiate the kernel with respect to  $s$  and on the other hand evaluate the multiple commutator on the right side of (488). For the latter the following considerations are useful.

As a reminder note that [7]

$$\begin{aligned} \hat{H}^{(0)} &= \hat{H}_D + \hat{H}_{rad} \\ \hat{H}_{rad} &= \sum_q \tilde{\omega}_q \left( \hat{a}_q^\dagger \hat{a}_q + \frac{1}{2} \hat{1} \right) \\ \hat{H}_D &= \sum_k \tilde{E}_k \left( c_k^\dagger c_k + b_k^\dagger b_k \right) \\ N_I &= \sum_{k''} \left( c_{k''}^\dagger c_{k''} + b_{k''}^\dagger b_{k''} \right) \\ \hat{N}_{II} &= \sum_q \kappa_q \hat{a}_q^\dagger \hat{a}_q \end{aligned} \quad (489)$$

For the following the identity

$$[AB, CD] = A \{B, C\} D - B \{D, A\} C - ACBD + CADB \quad (490)$$

which can be found in [14], will be very useful.

Starting simply yields [7]

$$\left[ \hat{N}_I, \hat{c}_{k'}^\dagger \hat{c}_k \right] = 0 = \left[ \hat{N}_I, \hat{b}_k^\dagger \hat{b}_{k'} \right] \quad (491)$$

However, for pair creation terms holds [7]

$$\begin{aligned}
\left[ \hat{N}_I, \hat{c}_k^\dagger \hat{b}_{\tilde{k}'}^\dagger \right] &= \left[ \sum_{k''} \left( c_{k''}^\dagger c_{k''} + b_{\tilde{k}''}^\dagger b_{\tilde{k}''} \right), \hat{c}_k^\dagger \hat{b}_{\tilde{k}'}^\dagger \right] \\
&= \sum_{k''} \left( \left[ c_{k''}^\dagger c_{k''}, \hat{c}_k^\dagger \hat{b}_{\tilde{k}'}^\dagger \right] + \left[ b_{\tilde{k}''}^\dagger b_{\tilde{k}''}, \hat{c}_k^\dagger \hat{b}_{\tilde{k}'}^\dagger \right] \right) \\
&= \sum_{k''} \left( \left[ c_{k''}^\dagger c_{k''}, \hat{c}_k^\dagger \hat{b}_{\tilde{k}'}^\dagger \right] + \left[ b_{\tilde{k}''}^\dagger b_{\tilde{k}''}, \hat{c}_k^\dagger \hat{b}_{\tilde{k}'}^\dagger \right] \right) \\
&= \sum_{k''} \begin{pmatrix} c_{k''}^\dagger \left\{ c_{k''}, \hat{c}_k^\dagger \right\} \hat{b}_{\tilde{k}'}^\dagger \\ -b_{\tilde{k}''}^\dagger \left\{ b_{\tilde{k}''}, \hat{b}_{\tilde{k}'}^\dagger \right\} \hat{c}_k^\dagger \end{pmatrix} \\
&= \sum_{k''} \left( c_{k''}^\dagger \hat{b}_{\tilde{k}'}^\dagger \delta_{k'',k} - b_{\tilde{k}''}^\dagger \hat{c}_k^\dagger \delta_{\tilde{k}'',\tilde{k}'} \right) \\
&= 2c_k^\dagger \hat{b}_{\tilde{k}'}^\dagger
\end{aligned} \tag{492}$$

where (490) and the fundamental commutation algebra for the fermions (15) has been used.

This implies at once [7]

$$\left[ \hat{N}_I, \left[ \hat{N}_I, \hat{c}_k^\dagger \hat{b}_{\tilde{k}'}^\dagger \right] \right] = 4c_k^\dagger \hat{b}_{\tilde{k}'}^\dagger \tag{493}$$

On the other hand [7]

$$\begin{aligned}
\left[ \hat{N}_I, \hat{b}_{\tilde{k}'} \hat{c}_k \right] &= \left[ \sum_{k''} \left( c_{k''}^\dagger c_{k''} + b_{\tilde{k}''}^\dagger b_{\tilde{k}''} \right), \hat{b}_{\tilde{k}'} \hat{c}_k \right] \\
&= \sum_{k''} \left( \left[ c_{k''}^\dagger c_{k''}, \hat{b}_{\tilde{k}'} \hat{c}_k \right] + \left[ b_{\tilde{k}''}^\dagger b_{\tilde{k}''}, \hat{b}_{\tilde{k}'} \hat{c}_k \right] \right) \\
&= \sum_{k''} \left( -\hat{b}_{\tilde{k}'} \left\{ \hat{c}_k, c_{k''}^\dagger \right\} c_{k''} + \hat{c}_k b_{\tilde{k}''} \left\{ \hat{b}_{\tilde{k}'}^\dagger, b_{\tilde{k}''}^\dagger \right\} \right) \\
&= -2\hat{b}_{\tilde{k}'} c_k \\
\left[ \hat{N}_I, \left[ \hat{N}_I, \hat{b}_{\tilde{k}'} \hat{c}_k \right] \right] &= -4\hat{b}_{\tilde{k}'} c_k
\end{aligned} \tag{494}$$

Implying at once that  $\left[ \hat{N}_I, \left[ \hat{c}_k^\dagger \hat{b}_{\tilde{k}'}^\dagger, \hat{b}_{\tilde{K}'} \hat{c}_K \right] \right] = \hat{0}!$

Now what about pairs of pair creators? [7]

$$\begin{aligned}
\left[ \hat{N}_I, \left[ \hat{c}_k^\dagger \hat{b}_{\tilde{k}'}^\dagger, \hat{c}_K^\dagger \hat{b}_{\tilde{K}'}^\dagger \right] \right] &= \left[ \hat{N}_I, \hat{c}_k^\dagger \hat{b}_{\tilde{k}'}^\dagger \hat{c}_K^\dagger \hat{b}_{\tilde{K}'}^\dagger \right] - \left[ \hat{N}_I, \hat{c}_K^\dagger \hat{b}_{\tilde{K}'}^\dagger \hat{c}_k^\dagger \hat{b}_{\tilde{k}'}^\dagger \right] \\
&= \begin{cases} \left[ \hat{N}_I, \hat{c}_k^\dagger \hat{b}_{\tilde{k}'}^\dagger \right] \hat{c}_K^\dagger \hat{b}_{\tilde{K}'}^\dagger \\ + \hat{c}_k^\dagger \hat{b}_{\tilde{k}'}^\dagger \left[ \hat{N}_I, \hat{c}_K^\dagger \hat{b}_{\tilde{K}'}^\dagger \right] \\ - \left[ \hat{N}_I, \hat{c}_K^\dagger \hat{b}_{\tilde{K}'}^\dagger \right] \hat{c}_k^\dagger \hat{b}_{\tilde{k}'}^\dagger \\ - \hat{c}_K^\dagger \hat{b}_{\tilde{K}'}^\dagger \left[ \hat{N}_I, \hat{c}_k^\dagger \hat{b}_{\tilde{k}'}^\dagger \right] \end{cases} \\
&= \begin{cases} 2\hat{c}_k^\dagger \hat{b}_{\tilde{k}'}^\dagger \hat{c}_K^\dagger \hat{b}_{\tilde{K}'}^\dagger \\ + 2\hat{c}_k^\dagger \hat{b}_{\tilde{k}'}^\dagger \hat{c}_K^\dagger \hat{b}_{\tilde{K}'}^\dagger \\ - 2\hat{c}_K^\dagger \hat{b}_{\tilde{K}'}^\dagger \hat{c}_k^\dagger \hat{b}_{\tilde{k}'}^\dagger \\ - 2\hat{c}_K^\dagger \hat{b}_{\tilde{K}'}^\dagger \hat{c}_k^\dagger \hat{b}_{\tilde{k}'}^\dagger \end{cases} \\
&= 4 \left[ \hat{c}_k^\dagger \hat{b}_{\tilde{k}'}^\dagger \hat{c}_K^\dagger \hat{b}_{\tilde{K}'}^\dagger - \hat{c}_K^\dagger \hat{b}_{\tilde{K}'}^\dagger \hat{c}_k^\dagger \hat{b}_{\tilde{k}'}^\dagger \right] \\
&= 4 \left[ \hat{c}_k^\dagger \hat{b}_{\tilde{k}'}^\dagger, \hat{c}_K^\dagger \hat{b}_{\tilde{K}'}^\dagger \right]
\end{aligned} \tag{495}$$

Therefore [7]

$$\left[ \hat{N}_I, \left[ \hat{N}_I, \left[ \hat{c}_k^\dagger \hat{b}_{\tilde{k}'}^\dagger, \hat{c}_K^\dagger \hat{b}_{\tilde{K}'}^\dagger \right] \right] \right] = 16 \left[ \hat{c}_k^\dagger \hat{b}_{\tilde{k}'}^\dagger, \hat{c}_K^\dagger \hat{b}_{\tilde{K}'}^\dagger \right] \tag{496}$$

Now for the photonic commutators [7]

$$\begin{aligned}
\left[ \hat{N}_{II}, \hat{a}_{q'}^\dagger \right] &= \left[ \sum_q \kappa_q \hat{a}_q^\dagger \hat{a}_q, \hat{a}_{q'}^\dagger \right] \\
&= \sum_q \kappa_q \left[ \hat{a}_q^\dagger \hat{a}_q, \hat{a}_{q'}^\dagger \right] \\
&= \sum_q \kappa_q \left( \hat{a}_q^\dagger \left[ \hat{a}_q, \hat{a}_{q'}^\dagger \right] + \left[ \hat{a}_q^\dagger, \hat{a}_{q'}^\dagger \right] \hat{a}_q \right) \\
&= \sum_q \kappa_q \left( \hat{a}_q^\dagger \delta_{q,q'} \right) \\
&= \kappa_q \hat{a}_q^\dagger
\end{aligned} \tag{497}$$

where the fundamental commutation algebra for the photons (27) has been used.

Then readily [7]

$$\begin{aligned}
[\hat{N}_{II}, \hat{a}_{q'}] &= \left[ \sum_q \kappa_q \hat{a}_q^\dagger \hat{a}_q, \hat{a}_{q'} \right] \\
&= \sum_q \kappa_q (\hat{a}_q^\dagger [\hat{a}_q, \hat{a}_{q'}] + [\hat{a}_q^\dagger, \hat{a}_{q'}] \hat{a}_q) \\
&= -\kappa_q \hat{a}_q
\end{aligned} \tag{498}$$

Note that  $\kappa_q^2 = \kappa_q$ .

Based on these equations there follows for example, since fermionic and photonic creators and annihilators always commute [7],

$$\begin{aligned}
[\hat{N}_I, [\hat{N}_I, \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q^\dagger]] + [\hat{N}_{II}, [\hat{N}_{II}, \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q^\dagger]] &= (4 + \kappa_q^2) \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q^\dagger \\
[\hat{N}_I, [\hat{N}_I, \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q]] + [\hat{N}_{II}, [\hat{N}_{II}, \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q]] &= (4 + \kappa_q^2) \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q \\
[\hat{N}_I, [\hat{N}_I, \hat{b}_{k'} \hat{c}_k \hat{a}_q^\dagger]] + [\hat{N}_{II}, [\hat{N}_{II}, \hat{b}_{k'} \hat{c}_k \hat{a}_q^\dagger]] &= (4 + \kappa_q^2) \hat{b}_{k'} \hat{c}_k \hat{a}_q^\dagger \\
[\hat{N}_I, [\hat{N}_I, \hat{b}_{k'} \hat{c}_k \hat{a}_q]] + [\hat{N}_{II}, [\hat{N}_{II}, \hat{b}_{k'} \hat{c}_k \hat{a}_q]] &= (4 + \kappa_q^2) \hat{b}_{k'} \hat{c}_k \hat{a}_q
\end{aligned} \tag{499}$$

or [7]

$$\begin{aligned}
[\hat{N}_I, [\hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q, \hat{c}_K^\dagger \hat{b}_{K'}^\dagger \hat{a}_{q'}]] &= 4 [\hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q, \hat{c}_K^\dagger \hat{b}_{K'}^\dagger \hat{a}_{q'}] \\
[\hat{N}_I, [\hat{N}_I, [\hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q, \hat{c}_K^\dagger \hat{b}_{K'}^\dagger \hat{a}_{q'}]]] &= 16 [\hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q, \hat{c}_K^\dagger \hat{b}_{K'}^\dagger \hat{a}_{q'}]
\end{aligned} \tag{500}$$

The commutator with  $\hat{H}^{(0)}$  yields for example [7]

$$\begin{aligned}
[\hat{H}^{(0)}, ([\hat{N}_I, [\hat{N}_I, \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q^\dagger]] + [\hat{N}_{II}, [\hat{N}_{II}, \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q^\dagger]])] &= (\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q) (4 + \kappa_q) \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q^\dagger \\
[\hat{H}^{(0)}, ([\hat{N}_I, [\hat{N}_I, \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q]] + [\hat{N}_{II}, [\hat{N}_{II}, \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q]])] &= (\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q) (4 + \kappa_q) \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q \\
[\hat{H}^{(0)}, ([\hat{N}_I, [\hat{N}_I, \hat{b}_{k'} \hat{c}_k \hat{a}_q^\dagger]] + [\hat{N}_{II}, [\hat{N}_{II}, \hat{b}_{k'} \hat{c}_k \hat{a}_q^\dagger]])] &= (-\tilde{E}_{k'} - \tilde{E}_k + \tilde{\omega}_q) (4 + \kappa_q) \hat{b}_{k'} \hat{c}_k \hat{a}_q^\dagger \\
[\hat{H}^{(0)}, ([\hat{N}_I, [\hat{N}_I, \hat{b}_{k'} \hat{c}_k \hat{a}_q]] + [\hat{N}_{II}, [\hat{N}_{II}, \hat{b}_{k'} \hat{c}_k \hat{a}_q]])] &= (-\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q) (4 + \kappa_q) \hat{b}_{k'} \hat{c}_k \hat{a}_q
\end{aligned} \tag{501}$$

or [7]

$$\begin{aligned}
\left[ \hat{H}^{(0)}, \left( \left[ \hat{N}_I, \left[ \hat{N}_I, \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q^\dagger \right] \right) + \left[ \hat{N}_{II}, \left[ \hat{N}_{II}, \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q^\dagger \right] \right) \right] &= \left( \tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q \right) (4 + \kappa_q) \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q^\dagger \\
\left[ \hat{H}^{(0)}, \left( \left[ \hat{N}_I, \left[ \hat{N}_I, \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q \right] \right) + \left[ \hat{N}_{II}, \left[ \hat{N}_{II}, \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q \right] \right) \right] &= \left( \tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q \right) (4 + \kappa_q) \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q \\
\left[ \hat{H}^{(0)}, \left( \left[ \hat{N}_I, \left[ \hat{N}_I, \hat{b}_{\tilde{k}'} \hat{c}_k \hat{a}_q^\dagger \right] \right) + \left[ \hat{N}_{II}, \left[ \hat{N}_{II}, \hat{b}_{\tilde{k}'} \hat{c}_k \hat{a}_q^\dagger \right] \right) \right] &= \left( -\tilde{E}_{k'} - \tilde{E}_k + \tilde{\omega}_q \right) (4 + \kappa_q) \hat{b}_{\tilde{k}'} \hat{c}_k \hat{a}_q^\dagger \\
\left[ \hat{H}^{(0)}, \left( \left[ \hat{N}_I, \left[ \hat{N}_I, \hat{b}_{\tilde{k}'} \hat{c}_k \hat{a}_q \right] \right) + \left[ \hat{N}_{II}, \left[ \hat{N}_{II}, \hat{b}_{\tilde{k}'} \hat{c}_k \hat{a}_q \right] \right) \right] &= \left( -\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q \right) (4 + \kappa_q) \hat{b}_{\tilde{k}'} \hat{c}_k \hat{a}_q
\end{aligned} \tag{502}$$

or [7]

$$\begin{aligned}
\left[ \hat{N}_I, \left[ \hat{N}_I, \left[ \hat{c}_{k'}^\dagger \hat{c}_k \hat{a}_q^\dagger, \hat{c}_{K'}^\dagger \hat{c}_K \hat{a}_{q'}^\dagger \right] \right] \right] + \left[ \hat{N}_{II}, \left[ \hat{N}_{II}, \left[ \hat{c}_{k'}^\dagger \hat{c}_k \hat{a}_q^\dagger, \hat{c}_{K'}^\dagger \hat{c}_K \hat{a}_{q'}^\dagger \right] \right] \right] &= (\kappa_q + \kappa_{q'})^2 \left[ \hat{c}_{k'}^\dagger \hat{c}_k \hat{a}_q^\dagger, \hat{c}_{K'}^\dagger \hat{c}_K \hat{a}_{q'}^\dagger \right] \\
\left[ \hat{N}_I, \left[ \hat{N}_I, \left[ \hat{c}_k^\dagger \hat{b}_{\tilde{k}'}^\dagger \hat{a}_q, \hat{b}_{\tilde{K}'} \hat{c}_K \hat{a}_{q'}^\dagger \right] \right] \right] + \left[ \hat{N}_{II}, \left[ \hat{N}_{II}, \left[ \hat{c}_k^\dagger \hat{b}_{\tilde{k}'}^\dagger \hat{a}_q, \hat{b}_{\tilde{K}'} \hat{c}_K \hat{a}_{q'}^\dagger \right] \right] \right] &= (-\kappa_q + \kappa_{q'})^2 \left[ \hat{c}_k^\dagger \hat{b}_{\tilde{k}'}^\dagger \hat{a}_q, \hat{b}_{\tilde{K}'} \hat{c}_K \hat{a}_{q'}^\dagger \right] \\
\left[ \hat{N}_I, \left[ \hat{N}_I, \left[ \hat{c}_k^\dagger \hat{b}_{\tilde{k}'}^\dagger \hat{a}_q, \hat{c}_{K'}^\dagger \hat{b}_{\tilde{K}'}^\dagger \hat{a}_{q'}^\dagger \right] \right] \right] + \left[ \hat{N}_{II}, \left[ \hat{N}_{II}, \left[ \hat{c}_k^\dagger \hat{b}_{\tilde{k}'}^\dagger \hat{a}_q, \hat{c}_{K'}^\dagger \hat{b}_{\tilde{K}'}^\dagger \hat{a}_{q'}^\dagger \right] \right] \right] &= \left( 16 + (-\kappa_q + \kappa_{q'})^2 \right) \left[ \hat{c}_k^\dagger \hat{b}_{\tilde{k}'}^\dagger \hat{a}_q, \hat{c}_{K'}^\dagger \hat{b}_{\tilde{K}'}^\dagger \hat{a}_{q'}^\dagger \right]
\end{aligned} \tag{503}$$

With these eigenvalue relations one is prepared for the multiple commutator of the right hand side in (488).

For the inner commutator  $\left[ N_I, \left[ N_I, \hat{J}^{(\pm, \pm)}(s, s') \right] \right] + \left[ N_{II}, \left[ N_{II}, \hat{J}^{(\pm, \pm)}(s, s') \right] \right]$  take a look at the first line. The commutator is of the form [7]

$$\begin{aligned}
&\left[ N_I \left[ N_I, \left[ \hat{c}_k^\dagger \hat{b}_{\tilde{k}'}^\dagger \hat{a}_q, \hat{c}_{K'}^\dagger \hat{b}_{\tilde{K}'}^\dagger \hat{a}_{q'}^\dagger \right] \right] \right] + \left[ N_{II}, \left[ N_{II}, \left[ \hat{c}_k^\dagger \hat{b}_{\tilde{k}'}^\dagger \hat{a}_q, \hat{c}_{K'}^\dagger \hat{b}_{\tilde{K}'}^\dagger \hat{a}_{q'}^\dagger \right] \right] \right] \\
&= \left( 16 + (-\kappa_q - \kappa_{q'})^2 \right) \left[ \hat{c}_k^\dagger \hat{b}_{\tilde{k}'}^\dagger \hat{a}_q, \hat{c}_{K'}^\dagger \hat{b}_{\tilde{K}'}^\dagger \hat{a}_{q'}^\dagger \right]
\end{aligned} \tag{504}$$

Therefore one finds as an interim solution [7]

$$\begin{aligned}
& [N_I, [N_I, \hat{J}^{(\pm, \pm)}(s, s')]] + [N_{II}, [N_{II}, \hat{J}^{(\pm, \pm)}(s, s')]] = - \left( \frac{qe}{m_0 c} \right)^2 \sum_{k, k'} \sum_{K, K'} \frac{1}{V} \sum_{q, q'} \sum_{b, b'} \mathcal{A}_b(q) \mathcal{A}_{b'}(q') \\
& \times \left( \begin{aligned}
& \left( 16 + (-\kappa_q - \kappa_{q'})^2 \right) \langle U_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle U_K | \alpha_{b'} e^{iq'_a x_a} | V_{K'} \rangle e^{-(4+\kappa_q)s'} (\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q)^2 e^{-(4+\kappa_{q'})s'} (\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'})^2 \times \\
& \quad \times \left( (\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q) + 2(\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'}) \right) (4 + \kappa_{q'}) \times \\
& \quad \times e^{-(s-s')} \left( 16 + (-\kappa_q - \kappa_{q'})^2 \right) (\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q + \tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'})^2 \left[ \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q, \hat{c}_K^\dagger \hat{b}_{K'}^\dagger \hat{a}_{q'} \right] \\
& + \left( 16 + (-\kappa_q + \kappa_{q'})^2 \right) \langle U_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle U_K | \alpha_{b'} e^{-iq'_a x_a} | V_{K'} \rangle e^{-(4+\kappa_q)s'} (\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q)^2 e^{-(4+\kappa_{q'})s'} (\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'})^2 \times \\
& \quad \times \left( \tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q + 2(\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'}) \right) (4 + \kappa_{q'}) \times \\
& \quad \times e^{-(s-s')} \left( 16 + (-\kappa_q + \kappa_{q'})^2 \right) (\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q + \tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'})^2 \left[ \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q, \hat{c}_K^\dagger \hat{b}_{K'}^\dagger \hat{a}_{q'} \right] \\
& + \left( 16 + (\kappa_q - \kappa_{q'})^2 \right) \langle U_k | \alpha_b e^{-iq_a x_a} | V_{k'} \rangle \langle U_K | \alpha_{b'} e^{iq'_a x_a} | V_{K'} \rangle e^{-(4+\kappa_q)s'} (\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q)^2 e^{-(4+\kappa_{q'})s'} (\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'})^2 \times \\
& \quad \times \left( \tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q + 2(\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'}) \right) (4 + \kappa_{q'}) \times \\
& \quad \times e^{-(s-s')} \left( 16 + (\kappa_q - \kappa_{q'})^2 \right) (\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q + \tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'})^2 \left[ \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q, \hat{c}_K^\dagger \hat{b}_{K'}^\dagger \hat{a}_{q'} \right] \\
& + \left( 16 + (\kappa_q + \kappa_{q'})^2 \right) \langle U_k | \alpha_b e^{-iq_a x_a} | V_{k'} \rangle \langle U_K | \alpha_{b'} e^{-iq'_a x_a} | V_{K'} \rangle e^{-(4+\kappa_q)s'} (\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q)^2 e^{-(4+\kappa_{q'})s'} (\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'})^2 \times \\
& \quad \times \left( \tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q + 2(\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'}) \right) (4 + \kappa_{q'}) \times \\
& \quad \times e^{-(s-s')} \left( 16 + (\kappa_q + \kappa_{q'})^2 \right) (\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q + \tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'})^2 \left[ \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q, \hat{c}_K^\dagger \hat{b}_{K'}^\dagger \hat{a}_{q'} \right]
\end{aligned} \right) \tag{505}
\end{aligned}$$

Now the commutator with [7]

$$\left[ \hat{H}^{(0)}, \left( \left[ N_I, \left[ N_I, \hat{J}^{(\pm, \pm)}(s, s') \right] \right] + \left[ N_{II}, \left[ N_{II}, \hat{J}^{(\pm, \pm)}(s, s') \right] \right] \right) \right]$$

is therefore of the form [7]

$$\begin{aligned}
& \left[ \hat{H}^{(0)}, \left( \left[ N_I, \left[ N_I, \left[ \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q, \hat{c}_K^\dagger \hat{b}_{K'}^\dagger \hat{a}_{q'} \right] \right] + \left[ N_{II}, \left[ N_{II}, \left[ \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q, \hat{c}_K^\dagger \hat{b}_{K'}^\dagger \hat{a}_{q'} \right] \right] \right) \right] \right] \\
& = \left( \tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q + \tilde{E}_{K'} + \tilde{E}_K - \tilde{\omega}_{q'} \right) \left( 16 + (-\kappa_q + \kappa_{q'})^2 \right) \left[ \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q, \hat{c}_K^\dagger \hat{b}_{K'}^\dagger \hat{a}_{q'} \right] \tag{506}
\end{aligned}$$

see for example (502).

Again commuting (506) with  $\hat{H}^{(0)}$  readily gives another factor

$$\left( \tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q + \tilde{E}_{K'} + \tilde{E}_K - \tilde{\omega}_{q'} \right)^2 \left( 16 + (-\kappa_q + \kappa_{q'})^2 \right) \left[ \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q, \hat{c}_K^\dagger \hat{b}_{K'}^\dagger \hat{a}_{q'} \right].$$

Hence, for the multiple commutator on the right hand side of (488) there follows [7]

$$\begin{aligned}
& [\hat{H}^{(0)}, [\hat{H}^{(0)}, ([N_I, [N_I, j^{(\pm, \pm)}(s, s')]] + [N_{II}, [N_{II}, j^{(\pm, \pm)}(s, s')]])]] \\
&= - \left( \frac{qe}{m_0 c} \right)^2 \sum_{\kappa, \kappa'} \sum_{K, K'} \frac{1}{V} \sum_{q, q'} \sum_{b, b'} \mathcal{A}_b(q) \mathcal{A}_{b'}(q') \times \\
& \quad \times \left( \begin{aligned}
& \left( 16 + (-\kappa_q - \kappa_{q'})^2 \right) \left( \tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q + \tilde{E}_{K'} + \tilde{E}_K - \tilde{\omega}_{q'} \right)^2 \langle U_k | \alpha_b e^{iq_a x_a} | V_{K'} \rangle \langle U_K | \alpha_{b'} e^{iq'_a x_a} | V_{K'} \rangle \\
& \times e^{-(4+\kappa_q)s'} \left( \tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q \right)^2 e^{-(4+\kappa_{q'})s'} \left( \tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'} \right)^2 \left( \left( \tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q \right) + 2 \left( \tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'} \right) \right) \left( 4 + \kappa_{q'} \right) \times \\
& \quad \times e^{-(s-s') \left( 16 + (-\kappa_q - \kappa_{q'})^2 \right)} \left( \tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q + \tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'} \right)^2 \left[ \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q, \hat{c}_K^\dagger \hat{b}_{K'}^\dagger \hat{a}_{q'} \right] \\
& + \left( 16 + (-\kappa_q + \kappa_{q'})^2 \right) \left( \tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q + \tilde{E}_{K'} + \tilde{E}_K + \tilde{\omega}_{q'} \right)^2 \langle U_k | \alpha_b e^{iq_a x_a} | V_{K'} \rangle \langle U_K | \alpha_{b'} e^{-iq'_a x_a} | V_{K'} \rangle \\
& \times e^{-(4+\kappa_q)s'} \left( \tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q \right)^2 e^{-(4+\kappa_{q'})s'} \left( \tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'} \right)^2 \left( \tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q + 2 \left( \tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'} \right) \right) \left( 4 + \kappa_{q'} \right) \times \\
& \quad \times e^{-(s-s') \left( 16 + (-\kappa_q + \kappa_{q'})^2 \right)} \left( \tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q + \tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'} \right)^2 \left[ \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q, \hat{c}_K^\dagger \hat{b}_{K'}^\dagger \hat{a}_{q'} \right] \\
& + \left( 16 + (\kappa_q - \kappa_{q'})^2 \right) \left( \tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q + \tilde{E}_{K'} + \tilde{E}_K - \tilde{\omega}_{q'} \right)^2 \langle U_k | \alpha_b e^{-iq_a x_a} | V_{K'} \rangle \langle U_K | \alpha_{b'} e^{iq'_a x_a} | V_{K'} \rangle \\
& \times e^{-(4+\kappa_q)s'} \left( \tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q \right)^2 e^{-(4+\kappa_{q'})s'} \left( \tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'} \right)^2 \left( \tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q + 2 \left( \tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'} \right) \right) \left( 4 + \kappa_{q'} \right) \times \\
& \quad \times e^{-(s-s') \left( 16 + (\kappa_q - \kappa_{q'})^2 \right)} \left( \tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q + \tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'} \right)^2 \left[ \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q, \hat{c}_K^\dagger \hat{b}_{K'}^\dagger \hat{a}_{q'} \right] \\
& + \left( 16 + (\kappa_q + \kappa_{q'})^2 \right) \left( \tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q + \tilde{E}_{K'} + \tilde{E}_K + \tilde{\omega}_{q'} \right)^2 \langle U_k | \alpha_b e^{-iq_a x_a} | V_{K'} \rangle \langle U_K | \alpha_{b'} e^{-iq'_a x_a} | V_{K'} \rangle \\
& \times e^{-(4+\kappa_q)s'} \left( \tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q \right)^2 e^{-(4+\kappa_{q'})s'} \left( \tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'} \right)^2 \left( \tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q + 2 \left( \tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'} \right) \right) \left( 4 + \kappa_{q'} \right) \times \\
& \quad \times e^{-(s-s') \left( 16 + (\kappa_q + \kappa_{q'})^2 \right)} \left( \tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q + \tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'} \right)^2 \left[ \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q, \hat{c}_K^\dagger \hat{b}_{K'}^\dagger \hat{a}_{q'} \right]
\end{aligned} \right) \tag{507}
\end{aligned}$$

On the other hand, for the derivative with respect to  $s$  of (488) there follows with [7]

$$\begin{aligned}
& \frac{d}{ds} e^{-(s-s') \left( 16 + (-\kappa_q - \kappa_{q'})^2 \right)} \left( \tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q + \tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'} \right)^2 \\
&= \left( 16 + (-\kappa_q - \kappa_{q'})^2 \right) \left( \tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q + \tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'} \right)^2 e^{-(s-s') \left( 16 + (-\kappa_q - \kappa_{q'})^2 \right)} \left( \tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q + \tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'} \right)^2 \\
& \tag{508}
\end{aligned}$$

as an example then [7]

$$\begin{aligned}
\frac{d}{ds} \hat{J}^{(+,+)}(s, s') &= - \left( \frac{q_e}{m_0 c} \right)^2 \sum_{k, k'} \sum_{K, K'} \frac{1}{V} \sum_{q, q'} \sum_{b, b'} \mathcal{A}_b(q) \mathcal{A}_{b'}(q') \times \\
&\left( \begin{aligned}
&\langle U_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle U_K | \alpha_{b'} e^{iq'_a x_a} | V_{K'} \rangle e^{-(4+\kappa_q)s'} (\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q)^2 e^{-(4+\kappa_{q'})s'} (\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'})^2 \times \\
&\quad \times \left( (\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q) + 2(\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'}) \right) (4 + \kappa_{q'}) \times \\
&\quad \times e^{-(s-s') \left( 16 + (-\kappa_q - \kappa_{q'})^2 \right)} (\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q + \tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'})^2 \left[ \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q, \hat{c}_K^\dagger \hat{b}_{K'}^\dagger \hat{a}_{q'} \right] \\
&+ \langle U_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle U_K | \alpha_{b'} e^{-iq'_a x_a} | V_{K'} \rangle e^{-(4+\kappa_q)s'} (\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q)^2 e^{-(4+\kappa_{q'})s'} (\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'})^2 \times \\
&\quad \times \left( \tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q + 2(\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'}) \right) (4 + \kappa_{q'}) \times \\
&\quad \times e^{-(s-s') \left( 16 + (-\kappa_q + \kappa_{q'})^2 \right)} (\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q + \tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'})^2 \left[ \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q, \hat{c}_K^\dagger \hat{b}_{K'}^\dagger \hat{a}_{q'} \right] \\
&+ \langle U_k | \alpha_b e^{-iq_a x_a} | V_{k'} \rangle \langle U_K | \alpha_{b'} e^{iq'_a x_a} | V_{K'} \rangle e^{-(4+\kappa_q)s'} (\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q)^2 e^{-(4+\kappa_{q'})s'} (\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'})^2 \times \\
&\quad \times \left( \tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q + 2(\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'}) \right) (4 + \kappa_{q'}) \times \\
&\quad \times e^{-(s-s') \left( 16 + (\kappa_q - \kappa_{q'})^2 \right)} (\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q + \tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'})^2 \left[ \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q, \hat{c}_K^\dagger \hat{b}_{K'}^\dagger \hat{a}_{q'} \right] \\
&+ \langle U_k | \alpha_b e^{-iq_a x_a} | V_{k'} \rangle \langle U_K | \alpha_{b'} e^{-iq'_a x_a} | V_{K'} \rangle e^{-(4+\kappa_q)s'} (\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q)^2 e^{-(4+\kappa_{q'})s'} (\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'})^2 \times \\
&\quad \times \left( \tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q + 2(\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'}) \right) (4 + \kappa_{q'}) \times \\
&\quad \times e^{-(s-s') \left( 16 + (\kappa_q + \kappa_{q'})^2 \right)} (\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q + \tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'})^2 \left[ \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q, \hat{c}_K^\dagger \hat{b}_{K'}^\dagger \hat{a}_{q'} \right]
\end{aligned} \right) \\
&= - \left( \frac{q_e}{m_0 c} \right)^2 \sum_{k, k'} \sum_{K, K'} \frac{1}{V} \sum_{q, q'} \sum_{b, b'} \mathcal{A}_b(q) \mathcal{A}_{b'}(q') \times \\
&\left( \begin{aligned}
&\left( 16 + (-\kappa_q - \kappa_{q'})^2 \right) (\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q + \tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'})^2 \langle U_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle U_K | \alpha_{b'} e^{iq'_a x_a} | V_{K'} \rangle \\
&\times e^{-(4+\kappa_q)s'} (\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q)^2 e^{-(4+\kappa_{q'})s'} (\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'})^2 \left( (\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q) + 2(\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'}) \right) (4 + \kappa_{q'}) \times \\
&\quad \times e^{-(s-s') \left( 16 + (-\kappa_q - \kappa_{q'})^2 \right)} (\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q + \tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'})^2 \left[ \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q, \hat{c}_K^\dagger \hat{b}_{K'}^\dagger \hat{a}_{q'} \right] \\
&+ \left( 16 + (-\kappa_q + \kappa_{q'})^2 \right) (\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q + \tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'})^2 \langle U_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle U_K | \alpha_{b'} e^{-iq'_a x_a} | V_{K'} \rangle \\
&\times e^{-(4+\kappa_q)s'} (\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q)^2 e^{-(4+\kappa_{q'})s'} (\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'})^2 \left( \tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q + 2(\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'}) \right) (4 + \kappa_{q'}) \times \\
&\quad \times e^{-(s-s') \left( 16 + (-\kappa_q + \kappa_{q'})^2 \right)} (\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q + \tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'})^2 \left[ \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q, \hat{c}_K^\dagger \hat{b}_{K'}^\dagger \hat{a}_{q'} \right] \\
&\times \\
&+ \left( 16 + (\kappa_q - \kappa_{q'})^2 \right) (\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q + \tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'})^2 \langle U_k | \alpha_b e^{-iq_a x_a} | V_{k'} \rangle \langle U_K | \alpha_{b'} e^{iq'_a x_a} | V_{K'} \rangle \\
&\times e^{-(4+\kappa_q)s'} (\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q)^2 e^{-(4+\kappa_{q'})s'} (\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'})^2 \left( \tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q + 2(\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'}) \right) (4 + \kappa_{q'}) \times \\
&\quad \times e^{-(s-s') \left( 16 + (\kappa_q - \kappa_{q'})^2 \right)} (\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q + \tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'})^2 \left[ \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q, \hat{c}_K^\dagger \hat{b}_{K'}^\dagger \hat{a}_{q'} \right] \\
&+ \left( 16 + (\kappa_q + \kappa_{q'})^2 \right) (\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q + \tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'})^2 \langle U_k | \alpha_b e^{-iq_a x_a} | V_{k'} \rangle \langle U_K | \alpha_{b'} e^{-iq'_a x_a} | V_{K'} \rangle \\
&\times e^{-(4+\kappa_q)s'} (\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q)^2 e^{-(4+\kappa_{q'})s'} (\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'})^2 \left( \tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q + 2(\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'}) \right) (4 + \kappa_{q'}) \times \\
&\quad \times e^{-(s-s') \left( 16 + (\kappa_q + \kappa_{q'})^2 \right)} (\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q + \tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'})^2 \left[ \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q, \hat{c}_K^\dagger \hat{b}_{K'}^\dagger \hat{a}_{q'} \right]
\end{aligned} \right) \tag{509}
\end{aligned}$$

which is exactly the same in (507)!

## Evaluation of $\lim_{s \rightarrow \infty} \hat{H}^{(2,i)}(s)$

The integrals  $\int_0^s ds' J^{(+)}(s, s')$  and  $\int_0^s ds' J^{(+,+)}(s, s')$  occurring in the solution (476) are of the following types [7]



$$\begin{aligned}
& f^{(+)}(s, x, y, \kappa_q, \kappa_{q'}) \\
&= (x(4 + \kappa_{q'} - 2\kappa_q) + y(8 + 2\kappa_{q'} - \kappa_q)) \int_0^s ds' e^{-(s-s')\left(4 + (\kappa_q + \kappa_{q'})^2\right)(x+y)^2} e^{-s'(\kappa_q x^2 + (4 + \kappa_{q'})y^2)} \\
&= (x(4 + \kappa_{q'} - 2\kappa_q) + y(8 + 2\kappa_{q'} - \kappa_q)) e^{-s\left(4 + (\kappa_q + \kappa_{q'})^2\right)(x+y)^2} \int_0^s ds' e^{s'\left(\left(4 + (\kappa_q + \kappa_{q'})^2\right)(x+y)^2 - \kappa_q x^2 - (4 + \kappa_{q'})y^2\right)} \\
&= (x(4 + \kappa_{q'} - 2\kappa_q) + y(8 + 2\kappa_{q'} - \kappa_q)) \frac{e^{-s(\kappa_q x^2 + (4 + \kappa_{q'})y^2)} - e^{-s\left(4 + (\kappa_q + \kappa_{q'})^2\right)(x+y)^2}}{\left(4 + (\kappa_q + \kappa_{q'})^2\right)(x+y)^2 - \kappa_q x^2 - (4 + \kappa_{q'})y^2}
\end{aligned} \tag{510}$$

and [7]

$$\begin{aligned}
& f^{(+,+)}(s, x, y, \kappa_q, \kappa_{q'}) \\
&= (x + 2y) \int_0^s ds' e^{-(s-s')\left(16 + (\kappa_q + \kappa_{q'})^2\right)(x+y)^2} e^{-s'\left((4 + \kappa_q)x^2 + (4 + \kappa_{q'})y^2\right)} \\
&= (x + 2y) e^{-s\left(16 + (\kappa_q + \kappa_{q'})^2\right)(x+y)^2} \frac{e^{s\left(\left(16 + (\kappa_q + \kappa_{q'})^2\right)(x+y)^2 - (4 + \kappa_q)x^2 - (4 + \kappa_{q'})y^2\right)} - 1}{\left(16 + (\kappa_q + \kappa_{q'})^2\right)(x+y)^2 - (4 + \kappa_q)x^2 - (4 + \kappa_{q'})y^2} \\
&= (x + 2y) \frac{e^{-s\left((4 + \kappa_q)x^2 + (4 + \kappa_{q'})y^2\right)} - e^{-s\left(16 + (\kappa_q + \kappa_{q'})^2\right)(x+y)^2}}{\left(16 + (\kappa_q + \kappa_{q'})^2\right)(x+y)^2 - (4 + \kappa_q)x^2 - (4 + \kappa_{q'})y^2}
\end{aligned} \tag{511}$$

For  $\kappa_q, \kappa_{q'} \in \{0, 1\}$ ,  $x, y \in \mathbb{R}$  and  $x + y \neq 0$  both integrals vanish in the limit  $s \rightarrow \infty$ .

Contributions of the sums over the mode indices  $k, k', K, K', q, q'$  that relate to the special case  $x + y = 0$  do not vanish in the limit  $s \rightarrow \infty$ . However, these contributions have zero measure, such that we can proceed again such that one first has to take the limit  $V \rightarrow \infty$ , and then take the limit  $s \rightarrow \infty$ .

For sure this argument also holds for the hermitean conjugates. Altogether then [7]

$$\begin{aligned}
& \lim_{s \rightarrow \infty} \lim_{V \rightarrow \infty} \int_0^s ds' J^{(\pm)}(s, s') = \hat{0} \\
& \lim_{s \rightarrow \infty} \lim_{V \rightarrow \infty} \int_0^s ds' J^{(\pm, \pm)}(s, s') = \hat{0}
\end{aligned} \tag{512}$$

Hence, the only contribution of the solution that survives our limiting procedure is given by  $\lim_{s \rightarrow \infty} \lim_{V \rightarrow \infty} \int_0^s ds' J^{(0)}(s, s')$  given by [7]

$$\lim_{s \rightarrow \infty} \lim_{V \rightarrow \infty} \int_0^s ds' J^{(0)}(s, s') = \lim_{s \rightarrow \infty} \lim_{V \rightarrow \infty} \left\{ \begin{array}{l} + \int_0^s ds' \left( \hat{J}_1^{(0,0)}(s, s') + J_2^{(0,0)}(s, s') \right) \\ + \int_0^s ds' \left( \hat{J}_1^{(0,+)}(s, s') + \hat{J}_1^{(0,-)}(s, s') \right) \\ + \int_0^s ds' \left( J_2^{(0,+)}(s, s') + J_2^{(0,-)}(s, s') \right) \end{array} \right. \quad (513)$$

These integrals are now evaluated explicitly in order to show that there do not remain terms that violate the particle number

## Integral 1

$$\begin{aligned}
& \lim_{s \rightarrow \infty} \lim_{V \rightarrow \infty} \int_0^s ds' \hat{J}_1^{(0,0)}(s, s') \\
&= - \left( \frac{q_e}{m_0 c} \right)^2 \lim_{s \rightarrow \infty} \lim_{V \rightarrow \infty} \sum_{k, k'} \sum_{K, K'} \frac{1}{V} \sum_{q, q'} \sum_{b, b'} \mathcal{A}_b(q) \mathcal{A}_{b'}(q') \times \\
& \left( \begin{aligned}
& + \int_0^s ds' \langle U_k | \alpha_b e^{iq_a x_a} | U_{k'} \rangle \langle U_{K'} | \alpha_{b'} e^{-iq'_a x_a} | U_K \rangle e^{-\kappa_q s' (\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)^2} e^{-\kappa_{q'} s' (\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2} \times \\
& \quad \times \left( \tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q + 2 \left( \tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'} \right) \right) \kappa_{q'} \times \\
& \quad \times e^{-(s-s')(-\kappa_q + \kappa_{q'})^2 (\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q + \tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2} \left[ \hat{c}_k^\dagger \hat{c}_{k'} \hat{a}_q, \hat{c}_K^\dagger \hat{c}_{K'} \hat{a}_{q'}^\dagger \right] \\
& - \int_0^s ds' \langle U_k | \alpha_b e^{iq_a x_a} | U_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{-iq'_a x_a} | V_K \rangle e^{-\kappa_q s' (\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)^2} e^{-\kappa_{q'} s' (\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'})^2} \times \\
& \quad \times \left( \tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q + 2 \left( \tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'} \right) \right) \kappa_{q'} \times \\
& \quad \times e^{-(s-s')(-\kappa_q + \kappa_{q'})^2 (\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q + \tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'})^2} \left[ \hat{c}_k^\dagger \hat{c}_{k'} \hat{a}_q, \hat{b}_{\tilde{K}}^\dagger \hat{b}_{\tilde{K}'} \hat{a}_{q'}^\dagger \right] \\
& - \int_0^s ds' \langle V_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle U_{K'} | \alpha_{b'} e^{-iq'_a x_a} | U_K \rangle e^{-\kappa_q s' (\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q)^2} e^{-\kappa_{q'} s' (\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2} \times \\
& \quad \times \left( \tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q + 2 \left( \tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'} \right) \right) \kappa_{q'} \times \\
& \quad \times e^{-(s-s')(-\kappa_q + \kappa_{q'})^2 (\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q + \tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2} \left[ \hat{b}_{\tilde{k}'}^\dagger \hat{b}_{\tilde{k}} \hat{a}_q, \hat{c}_K^\dagger \hat{c}_{K'} \hat{a}_{q'}^\dagger \right] \\
& + \int_0^s ds' \langle V_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{-iq'_a x_a} | V_K \rangle e^{-\kappa_q s' (\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q)^2} e^{-\kappa_{q'} s' (\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'})^2} \times \\
& \quad \times \left( \tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q + 2 \left( \tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'} \right) \right) \kappa_{q'} \times \\
& \quad \times e^{-(s-s')(-\kappa_q + \kappa_{q'})^2 (\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q + \tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'})^2} \left[ \hat{b}_{\tilde{k}'}^\dagger \hat{b}_{\tilde{k}} \hat{a}_q, \hat{b}_{\tilde{K}}^\dagger \hat{b}_{\tilde{K}'} \hat{a}_{q'}^\dagger \right] \\
& \times \\
& + \int_0^s ds' \langle U_{k'} | \alpha_b e^{-iq_a x_a} | U_k \rangle \langle U_K | \alpha_{b'} e^{iq'_a x_a} | U_{K'} \rangle e^{-\kappa_q s' (\tilde{E}_{k'} - \tilde{E}_k + \tilde{\omega}_q)^2} e^{-\kappa_{q'} s' (\tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_{q'})^2} \times \\
& \quad \times \left( \tilde{E}_{k'} - \tilde{E}_k + \tilde{\omega}_q + 2 \left( \tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_{q'} \right) \right) \kappa_{q'} \times \\
& \quad \times e^{-(s-s')(\kappa_q - \kappa_{q'})^2 (\tilde{E}_{k'} - \tilde{E}_k + \tilde{\omega}_q + \tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_{q'})^2} \left[ \hat{c}_k^\dagger \hat{c}_{k'} \hat{a}_q^\dagger, \hat{c}_K^\dagger \hat{c}_{K'} \hat{a}_{q'} \right] \\
& - \int_0^s ds' \langle U_{k'} | \alpha_b e^{-iq_a x_a} | U_k \rangle \langle V_{K'} | \alpha_{b'} e^{iq'_a x_a} | V_K \rangle e^{-\kappa_q s' (\tilde{E}_{k'} - \tilde{E}_k + \tilde{\omega}_q)^2} e^{-\kappa_{q'} s' (\tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})^2} \times \\
& \quad \times \left( \tilde{E}_{k'} - \tilde{E}_k + \tilde{\omega}_q + 2 \left( \tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'} \right) \right) \kappa_{q'} \times \\
& \quad \times e^{-(s-s')(\kappa_q - \kappa_{q'})^2 (\tilde{E}_{k'} - \tilde{E}_k + \tilde{\omega}_q + \tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})^2} \left[ \hat{c}_k^\dagger \hat{c}_{k'} \hat{a}_q^\dagger, \hat{b}_{\tilde{K}'}^\dagger \hat{b}_{\tilde{K}} \hat{a}_{q'} \right] \\
& - \int_0^s ds' \langle V_{k'} | \alpha_b e^{-iq_a x_a} | V_k \rangle \langle U_K | \alpha_{b'} e^{iq'_a x_a} | U_{K'} \rangle e^{-\kappa_q s' (\tilde{E}_k - \tilde{E}_{k'} + \tilde{\omega}_q)^2} e^{-\kappa_{q'} s' (\tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_{q'})^2} \times \\
& \quad \times \left( \tilde{E}_k - \tilde{E}_{k'} + \tilde{\omega}_q + 2 \left( \tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_{q'} \right) \right) \kappa_{q'} \times \\
& \quad \times e^{-(s-s')(\kappa_q - \kappa_{q'})^2 (\tilde{E}_k - \tilde{E}_{k'} + \tilde{\omega}_q + \tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_{q'})^2} \left[ \hat{b}_{\tilde{k}}^\dagger \hat{b}_{\tilde{k}'} \hat{a}_q^\dagger, \hat{c}_K^\dagger \hat{c}_{K'} \hat{a}_{q'} \right] \\
& + \int_0^s ds' \langle V_{k'} | \alpha_b e^{-iq_a x_a} | V_k \rangle \langle V_{K'} | \alpha_{b'} e^{iq'_a x_a} | V_K \rangle e^{-\kappa_q s' (\tilde{E}_k - \tilde{E}_{k'} + \tilde{\omega}_q)^2} e^{-\kappa_{q'} s' (\tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})^2} \times \\
& \quad \times \left( \tilde{E}_k - \tilde{E}_{k'} + \tilde{\omega}_q + 2 \left( \tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'} \right) \right) \kappa_{q'} \times \\
& \quad \times e^{-(s-s')(\kappa_q - \kappa_{q'})^2 (\tilde{E}_k - \tilde{E}_{k'} + \tilde{\omega}_q + \tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})^2} \left[ \hat{b}_{\tilde{k}}^\dagger \hat{b}_{\tilde{k}'} \hat{a}_q^\dagger, \hat{b}_{\tilde{K}'}^\dagger \hat{b}_{\tilde{K}} \hat{a}_{q'} \right]
\end{aligned} \right) \tag{514}
\end{aligned}$$

These integrals are of the type [7]

$$\begin{aligned}
f_1^{(0,0)}(x, y, \kappa_q, \kappa_{q'}) &= (x+2y) \kappa_{q'} \int_0^s ds' e^{-(s-s')(\kappa_q - \kappa_{q'})^2 (x+y)^2} e^{-s'(\kappa_q x^2 + \kappa_{q'} y^2)} \\
&= (x+2y) \kappa_{q'} e^{-s(\kappa_q - \kappa_{q'})^2 (x+y)^2} \int_0^s e^{s' \left( (\kappa_q - \kappa_{q'})^2 (x+y)^2 - \kappa_q x^2 - \kappa_{q'} y^2 \right)} ds' \\
&= (x+2y) \kappa_{q'} e^{-s(\kappa_q - \kappa_{q'})^2 (x+y)^2} \frac{e^{s \left( (\kappa_q - \kappa_{q'})^2 (x+y)^2 - \kappa_q x^2 - \kappa_{q'} y^2 \right)} - 1}{(\kappa_q - \kappa_{q'})^2 (x+y)^2 - \kappa_q x^2 - \kappa_{q'} y^2} \\
&= (x+2y) \kappa_{q'} \frac{e^{-s(\kappa_q x^2 + \kappa_{q'} y^2)} - e^{-s(\kappa_q - \kappa_{q'})^2 (x+y)^2}}{(\kappa_q - \kappa_{q'})^2 (x+y)^2 - \kappa_q x^2 - \kappa_{q'} y^2} \\
&= \begin{cases} 0 & \text{für } \kappa_{q'} = 0 \\ (x+2y) \frac{e^{-s(\kappa_q x^2 + y^2)} - e^{-s(\kappa_q - 1)^2 (x+y)^2}}{(\kappa_q - 1)^2 (x+y)^2 - \kappa_q x^2 - y^2} & \text{für } \kappa_{q'} = 1 \end{cases} \quad (515) \\
&= \begin{cases} 0 & \text{für } \kappa_{q'} = 0 \\ (x+2y) \frac{e^{-sy^2} - e^{-s(x+y)^2}}{(x+y)^2 - y^2} & \text{für } \kappa_{q'} = 1, \kappa_q = 0 \\ (x+2y) \frac{e^{-s(x^2 + y^2)} - 1}{-x^2 - y^2} & \text{für } \kappa_{q'} = 1, \kappa_q = 1 \end{cases} \\
&= \begin{cases} 0 & \text{für } \kappa_{q'} = 0 \\ \frac{e^{-sy^2} - e^{-s(x+y)^2}}{x} & \text{für } \kappa_{q'} = 1, \kappa_q = 0 \\ \frac{x+2y}{x^2 + y^2} (1 - e^{-s(x^2 + y^2)}) & \text{für } \kappa_{q'} = 1, \kappa_q = 1 \end{cases}
\end{aligned}$$

Hence, only the term  $\kappa_{q'} = 1$  and  $\kappa_q = 1$  contribute to the limit  $s \rightarrow \infty$  (besides a contribution of zero measure for  $x + y = 0$ ).

Therefore [7],

$$\begin{aligned}
&\lim_{s \rightarrow \infty} \lim_{V \rightarrow \infty} \int_0^s ds' \hat{J}_1^{(0,0)}(s, s') \\
&= - \left( \frac{q_e}{m_0 c} \right)^2 \sum_{k, k'} \sum_{K, K'} \lim_{V \rightarrow \infty} \frac{1}{V} \sum_{q > q_B} \sum_{q' > q_B} \sum_{b, b'} \mathcal{A}_b(q) \mathcal{A}_{b'}(q') \times \\
&\quad \left( \begin{aligned}
&+ \langle U_k | \alpha_b e^{iq_a x_a} | U_{k'} \rangle \langle U_{K'} | \alpha_{b'} e^{-iq'_a x_a} | U_K \rangle \frac{\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q + 2(\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})}{(\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)^2 + (\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2} \left[ \hat{c}_k^\dagger \hat{c}_{k'} \hat{a}_q, \hat{c}_{K'}^\dagger \hat{c}_K \hat{a}_{q'}^\dagger \right] \\
&- \langle U_k | \alpha_b e^{iq_a x_a} | U_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{-iq'_a x_a} | V_K \rangle \frac{\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q + 2(\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'})}{(\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)^2 + (\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'})^2} \left[ \hat{c}_k^\dagger \hat{c}_{k'} \hat{a}_q, \hat{b}_{\bar{K}}^\dagger \hat{b}_{\bar{K}'} \hat{a}_{q'}^\dagger \right] \\
&- \langle V_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle U_{K'} | \alpha_{b'} e^{-iq'_a x_a} | U_K \rangle \frac{\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q + 2(\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})}{(\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)^2 + (\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2} \left[ \hat{b}_{\bar{k}}^\dagger \hat{b}_{\bar{k}'} \hat{a}_q, \hat{c}_{K'}^\dagger \hat{c}_K \hat{a}_{q'}^\dagger \right] \\
&+ \langle V_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{-iq'_a x_a} | V_K \rangle \frac{\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q + 2(\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'})}{(\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)^2 + (\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'})^2} \left[ \hat{b}_{\bar{k}'}^\dagger \hat{b}_{\bar{k}} \hat{a}_q, \hat{b}_{\bar{K}}^\dagger \hat{b}_{\bar{K}'} \hat{a}_{q'}^\dagger \right] \\
&\times \left( \begin{aligned}
&+ \langle U_{k'} | \alpha_b e^{-iq_a x_a} | U_k \rangle \langle U_K | \alpha_{b'} e^{iq'_a x_a} | U_{K'} \rangle \frac{\tilde{E}_{k'} - \tilde{E}_k + \tilde{\omega}_q + 2(\tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_{q'})}{(\tilde{E}_{k'} - \tilde{E}_k + \tilde{\omega}_q)^2 + (\tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_{q'})^2} \left[ \hat{c}_k^\dagger \hat{c}_{k'} \hat{a}_q^\dagger, \hat{c}_K^\dagger \hat{c}_{K'} \hat{a}_{q'} \right] \\
&- \langle U_{k'} | \alpha_b e^{-iq_a x_a} | U_k \rangle \langle V_K | \alpha_{b'} e^{iq'_a x_a} | V_{K'} \rangle \frac{\tilde{E}_{k'} - \tilde{E}_k + \tilde{\omega}_q + 2(\tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})}{(\tilde{E}_{k'} - \tilde{E}_k + \tilde{\omega}_q)^2 + (\tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})^2} \left[ \hat{c}_k^\dagger \hat{c}_{k'} \hat{a}_q^\dagger, \hat{b}_{\bar{K}}^\dagger \hat{b}_{\bar{K}'} \hat{a}_{q'} \right] \\
&- \langle V_{k'} | \alpha_b e^{-iq_a x_a} | V_k \rangle \langle U_K | \alpha_{b'} e^{iq'_a x_a} | U_{K'} \rangle \frac{\tilde{E}_k - \tilde{E}_{k'} + \tilde{\omega}_q + 2(\tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_{q'})}{(\tilde{E}_k - \tilde{E}_{k'} + \tilde{\omega}_q)^2 + (\tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_{q'})^2} \left[ \hat{b}_{\bar{k}}^\dagger \hat{b}_{\bar{k}'} \hat{a}_q^\dagger, \hat{c}_K^\dagger \hat{c}_{K'} \hat{a}_{q'} \right] \\
&+ \langle V_{k'} | \alpha_b e^{-iq_a x_a} | V_k \rangle \langle V_{K'} | \alpha_{b'} e^{iq'_a x_a} | V_K \rangle \frac{\tilde{E}_k - \tilde{E}_{k'} + \tilde{\omega}_q + 2(\tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})}{(\tilde{E}_k - \tilde{E}_{k'} + \tilde{\omega}_q)^2 + (\tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})^2} \left[ \hat{b}_{\bar{k}}^\dagger \hat{b}_{\bar{k}'} \hat{a}_q^\dagger, \hat{b}_{\bar{K}}^\dagger \hat{b}_{\bar{K}'} \hat{a}_{q'} \right]
\end{aligned} \right)
\end{aligned} \right) \quad (516)
\end{aligned}$$

These terms can be sorted by creation and annihilation operators for matter and antimatter according to [7]

$$\begin{aligned}
& \lim_{s \rightarrow \infty} \lim_{V \rightarrow \infty} \int_0^s ds' \hat{J}_1^{(0,0)}(s, s') \\
&= - \left( \frac{q_e}{m_0 c} \right)^2 \sum_{k, k'} \sum_{K, K'} \lim_{V \rightarrow \infty} \frac{1}{V} \sum_{q > q_B} \sum_{q' > q_B} \sum_{b, b'} \mathcal{A}_b(q) \mathcal{A}_{b'}(q') \times \\
& \quad \times \left( \begin{aligned}
& + \langle U_k | \alpha_b e^{iq_a x_a} | U_{k'} \rangle \langle U_{K'} | \alpha_{b'} e^{-iq'_a x_a} | U_K \rangle \frac{\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q + 2(\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})}{(\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)^2 + (\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2} \left[ \hat{c}_k^\dagger \hat{c}_{k'} \hat{a}_q, \hat{c}_{K'}^\dagger \hat{c}_K \hat{a}_{q'}^\dagger \right] \\
& + \langle U_{k'} | \alpha_b e^{-iq_a x_a} | U_k \rangle \langle U_K | \alpha_{b'} e^{iq'_a x_a} | U_{K'} \rangle \frac{\tilde{E}_{k'} - \tilde{E}_k + \tilde{\omega}_q + 2(\tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_{q'})}{(\tilde{E}_{k'} - \tilde{E}_k + \tilde{\omega}_q)^2 + (\tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_{q'})^2} \left[ \hat{c}_k^\dagger \hat{c}_{k'} \hat{a}_q^\dagger, \hat{c}_{K'}^\dagger \hat{c}_K \hat{a}_{q'} \right] \\
& + \langle V_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{-iq'_a x_a} | V_K \rangle \frac{\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q + 2(\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'})}{(\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q)^2 + (\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'})^2} \left[ \hat{b}_{k'}^\dagger \hat{b}_k \hat{a}_q, \hat{b}_{\tilde{K}}^\dagger \hat{b}_{\tilde{K}'} \hat{a}_{q'}^\dagger \right] \\
& + \langle V_{k'} | \alpha_b e^{-iq_a x_a} | V_k \rangle \langle V_K | \alpha_{b'} e^{iq'_a x_a} | V_{K'} \rangle \frac{\tilde{E}_k - \tilde{E}_{k'} + \tilde{\omega}_q + 2(\tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})}{(\tilde{E}_k - \tilde{E}_{k'} + \tilde{\omega}_q)^2 + (\tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})^2} \left[ \hat{b}_k^\dagger \hat{b}_{k'} \hat{a}_q^\dagger, \hat{b}_{\tilde{K}}^\dagger \hat{b}_{\tilde{K}'} \hat{a}_{q'} \right] \\
& - \langle U_k | \alpha_b e^{iq_a x_a} | U_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{-iq'_a x_a} | V_K \rangle \frac{\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q + 2(\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'})}{(\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)^2 + (\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'})^2} \left[ \hat{c}_k^\dagger \hat{c}_{k'} \hat{a}_q, \hat{b}_{\tilde{K}}^\dagger \hat{b}_{\tilde{K}'} \hat{a}_{q'}^\dagger \right] \\
& - \langle V_{k'} | \alpha_b e^{-iq_a x_a} | V_k \rangle \langle U_K | \alpha_{b'} e^{iq'_a x_a} | U_{K'} \rangle \frac{\tilde{E}_k - \tilde{E}_{k'} + \tilde{\omega}_q + 2(\tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})}{(\tilde{E}_k - \tilde{E}_{k'} + \tilde{\omega}_q)^2 + (\tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})^2} \left[ \hat{b}_k^\dagger \hat{b}_{k'} \hat{a}_q^\dagger, \hat{c}_K^\dagger \hat{c}_{K'} \hat{a}_{q'} \right] \\
& - \langle V_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle U_{K'} | \alpha_{b'} e^{-iq'_a x_a} | U_K \rangle \frac{\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q + 2(\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})}{(\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q)^2 + (\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2} \left[ \hat{b}_{k'}^\dagger \hat{b}_k \hat{a}_q, \hat{c}_{K'}^\dagger \hat{c}_K \hat{a}_{q'}^\dagger \right] \\
& - \langle U_{k'} | \alpha_b e^{-iq_a x_a} | U_k \rangle \langle V_K | \alpha_{b'} e^{iq'_a x_a} | V_{K'} \rangle \frac{\tilde{E}_{k'} - \tilde{E}_k + \tilde{\omega}_q + 2(\tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})}{(\tilde{E}_{k'} - \tilde{E}_k + \tilde{\omega}_q)^2 + (\tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})^2} \left[ \hat{c}_k^\dagger \hat{c}_{k'} \hat{a}_q^\dagger, \hat{b}_{\tilde{K}}^\dagger \hat{b}_{\tilde{K}'} \hat{a}_{q'} \right]
\end{aligned} \right) \tag{517}
\end{aligned}$$

Further rearrangements and renaming of the summation indices according to [7]

$$(k, k', K, K', q, q', b, b') \rightarrow (\underline{K}, \underline{K}', \underline{k}, \underline{k}', \underline{q}', \underline{q}, \underline{b}', \underline{b}) \tag{518}$$

yield [7]

$$\begin{aligned}
& \lim_{s \rightarrow \infty} \lim_{V \rightarrow \infty} \int_0^s ds' \hat{J}_1^{(0,0)}(s, s') \\
&= - \left( \frac{q_e}{m_0 c} \right)^2 \sum_{k, k'} \sum_{K, K'} \lim_{V \rightarrow \infty} \frac{1}{V} \sum_{q > q_B} \sum_{q' > q_B} \sum_{b, b'} \mathcal{A}_b(q) \mathcal{A}_{b'}(q') \times \\
& \left( \begin{aligned}
& + \langle U_k | \alpha_b e^{iq_a x_a} | U_{k'} \rangle \langle U_{K'} | \alpha_{b'} e^{-iq'_a x_a} | U_K \rangle \left( \frac{\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q + 2(\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})}{(\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)^2 + (\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2} - \frac{\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'} + 2(\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)}{(\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2 + (\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)^2} \right) \times \\
& \quad \times \left[ \hat{c}_k^\dagger \hat{c}_{k'} \hat{a}_q, \hat{c}_{K'}^\dagger \hat{c}_K \hat{a}_{q'}^\dagger \right] \\
& + \langle V_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{-iq'_a x_a} | V_K \rangle \left( \frac{\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q + 2(\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'})}{(\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q)^2 + (\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'})^2} - \frac{\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'} + 2(\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q)}{(\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'})^2 + (\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q)^2} \right) \times \\
& \quad \times \left[ \hat{b}_{k'}^\dagger \hat{b}_{\bar{k}} \hat{a}_q, \hat{b}_{\bar{K}}^\dagger \hat{b}_{\bar{K}'} \hat{a}_{q'}^\dagger \right] \\
& - \langle U_k | \alpha_b e^{iq_a x_a} | U_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{-iq'_a x_a} | V_K \rangle \left( \frac{\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q + 2(\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'})}{(\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)^2 + (\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'})^2} - \frac{\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'} + 2(\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)}{(\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'})^2 + (\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)^2} \right) \times \\
& \quad \times \left[ \hat{c}_k^\dagger \hat{c}_{k'} \hat{a}_q, \hat{b}_{\bar{K}}^\dagger \hat{b}_{\bar{K}'} \hat{a}_{q'}^\dagger \right] \\
& - \langle V_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle U_{K'} | \alpha_{b'} e^{-iq'_a x_a} | U_K \rangle \left( \frac{\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q + 2(\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})}{(\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q)^2 + (\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2} - \frac{\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'} + 2(\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q)}{(\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2 + (\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q)^2} \right) \times \\
& \quad \times \left[ \hat{b}_{k'}^\dagger \hat{b}_{\bar{k}} \hat{a}_q, \hat{c}_{K'}^\dagger \hat{c}_K \hat{a}_{q'}^\dagger \right]
\end{aligned} \right) \tag{519}
\end{aligned}$$

Finally, terms with the same denominator can be picked up such that [\[7\]](#)

$$\begin{aligned}
& \lim_{s \rightarrow \infty} \lim_{V \rightarrow \infty} \int_0^s ds' \hat{J}_1^{(0,0)}(s, s') \\
&= - \left( \frac{q_e}{m_0 c} \right)^2 \sum_{k, k'} \sum_{K, K'} \lim_{V \rightarrow \infty} \frac{1}{V} \sum_{q > q_B} \sum_{q' > q_B} \sum_{b, b'} \mathcal{A}_b(q) \mathcal{A}_{b'}(q') \times \\
& \left( \begin{aligned}
& + \langle U_k | \alpha_b e^{iq_a x_a} | U_{k'} \rangle \langle U_{K'} | \alpha_{b'} e^{-iq'_a x_a} | U_K \rangle \frac{(\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'}) - (\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)}{(\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)^2 + (\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2} \left[ \hat{c}_k^\dagger \hat{c}_{k'} \hat{a}_q, \hat{c}_{K'}^\dagger \hat{c}_K \hat{a}_{q'}^\dagger \right] \\
& + \langle V_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{-iq'_a x_a} | V_K \rangle \frac{(\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'}) - (\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q)}{(\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q)^2 + (\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'})^2} \left[ \hat{b}_{k'}^\dagger \hat{b}_{\bar{k}} \hat{a}_q, \hat{b}_{\bar{K}}^\dagger \hat{b}_{\bar{K}'} \hat{a}_{q'}^\dagger \right] \\
& - \langle U_k | \alpha_b e^{iq_a x_a} | U_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{-iq'_a x_a} | V_K \rangle \frac{(\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'}) - (\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)}{(\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)^2 + (\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'})^2} \left[ \hat{c}_k^\dagger \hat{c}_{k'} \hat{a}_q, \hat{b}_{\bar{K}}^\dagger \hat{b}_{\bar{K}'} \hat{a}_{q'}^\dagger \right] \\
& - \langle V_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle U_{K'} | \alpha_{b'} e^{-iq'_a x_a} | U_K \rangle \frac{(\tilde{E}_{k'} - \tilde{E}_k + \tilde{\omega}_{q'}) - (\tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_q)}{(\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q)^2 + (\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2} \left[ \hat{b}_{k'}^\dagger \hat{b}_{\bar{k}} \hat{a}_q, \hat{c}_{K'}^\dagger \hat{c}_K \hat{a}_{q'}^\dagger \right]
\end{aligned} \right) \tag{520}
\end{aligned}$$

Now the multiple commutators in [\(520\)](#) can be evaluated by the help of the following identities:

$$\begin{aligned}
\frac{1}{2} [\hat{f}, \hat{g}] \{\hat{F}, \hat{G}\} + \frac{1}{2} \{\hat{f}, \hat{g}\} [\hat{F}, \hat{G}] &= \frac{1}{2} (\hat{f}\hat{g} - \hat{g}\hat{f}) (\hat{F}\hat{G} + \hat{G}\hat{F}) + \frac{1}{2} (\hat{f}\hat{g} + \hat{g}\hat{f}) (\hat{F}\hat{G} - \hat{G}\hat{F}) \\
&= (\hat{f}\hat{g}\hat{F}\hat{G} - \hat{g}\hat{f}\hat{G}\hat{F}) \\
&= (\hat{f}\hat{F}\hat{g}\hat{G} - \hat{g}\hat{G}\hat{f}\hat{F}) \\
&= [\hat{f}\hat{F}, \hat{g}\hat{G}]
\end{aligned} \tag{521}$$

For operators  $\hat{f}, \hat{g}, \hat{F}, \hat{G}$  with the property  $[\hat{f}, \hat{G}] = \hat{0} = [\hat{g}, \hat{F}]$ .

Furthermore we remind that

$$\begin{aligned}
[\hat{a}_q^\dagger, \hat{a}_{q'}] &= -\delta_{q,q'} \hat{1} \\
[\hat{a}_q, \hat{a}_{q'}^\dagger] &= +\delta_{q,q'} \hat{1} \\
\frac{1}{2} \{\hat{a}_q^\dagger, \hat{a}_{q'}\} &= \hat{a}_q^\dagger \hat{a}_{q'} + \frac{1}{2} \delta_{q,q'} \hat{1} \\
\frac{1}{2} \{\hat{a}_q, \hat{a}_{q'}^\dagger\} &= \hat{a}_{q'}^\dagger \hat{a}_q + \frac{1}{2} \delta_{q,q'} \hat{1}
\end{aligned} \tag{522}$$

From (521) follows for (520) [7]

$$\begin{aligned}
& \lim_{s \rightarrow \infty} \lim_{V \rightarrow \infty} \int_0^s ds' \hat{J}_1^{(0,0)}(s, s') = - \left( \frac{q_e}{m_0 c} \right)^2 \sum_{k, k'} \sum_{K, K'} \lim_{V \rightarrow \infty} \frac{1}{V} \sum_{q > q_B} \sum_{q' > q_B} \sum_{b, b'} \mathcal{A}_b(q) \mathcal{A}_{b'}(q') \times \\
& \left( \begin{aligned}
& + \langle U_k | \alpha_b e^{i q_a x_a} | U_{k'} \rangle \langle U_{K'} | \alpha_{b'} e^{-i q'_a x_a} | U_K \rangle \frac{(\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'}) - (\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)}{(\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)^2 + (\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2} \left( \begin{aligned}
& \frac{1}{2} [\hat{c}_k^\dagger \hat{c}_{k'}, \hat{c}_{K'}^\dagger \hat{c}_K] \left\{ \hat{a}_q, \hat{a}_{q'}^\dagger \right\} \\
& + \frac{1}{2} \left\{ \hat{c}_k^\dagger \hat{c}_{k'}, \hat{c}_{K'}^\dagger \hat{c}_K \right\} \left[ \hat{a}_q, \hat{a}_{q'}^\dagger \right]
\end{aligned} \right) \\
& + \langle V_k | \alpha_b e^{i q_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{-i q'_a x_a} | V_K \rangle \frac{(\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'}) - (\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)}{(\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q)^2 + (\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'})^2} \left( \begin{aligned}
& \frac{1}{2} [\hat{b}_{k'}^\dagger \hat{b}_{\tilde{k}'}, \hat{b}_{\tilde{K}}^\dagger \hat{b}_{\tilde{K}'}] \left\{ \hat{a}_q, \hat{a}_{q'}^\dagger \right\} \\
& + \frac{1}{2} \left\{ \hat{b}_{k'}^\dagger \hat{b}_{\tilde{k}'}, \hat{b}_{\tilde{K}}^\dagger \hat{b}_{\tilde{K}'} \right\} \left[ \hat{a}_q, \hat{a}_{q'}^\dagger \right]
\end{aligned} \right) \\
& - \langle U_k | \alpha_b e^{i q_a x_a} | U_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{-i q'_a x_a} | V_K \rangle \frac{(\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'}) - (\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)}{(\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)^2 + (\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'})^2} \left( \begin{aligned}
& \frac{1}{2} [\hat{c}_k^\dagger \hat{c}_{k'}, \hat{b}_{\tilde{K}}^\dagger \hat{b}_{\tilde{K}'}] \left\{ \hat{a}_q, \hat{a}_{q'}^\dagger \right\} \\
& + \frac{1}{2} \left\{ \hat{c}_k^\dagger \hat{c}_{k'}, \hat{b}_{\tilde{K}}^\dagger \hat{b}_{\tilde{K}'} \right\} \left[ \hat{a}_q, \hat{a}_{q'}^\dagger \right]
\end{aligned} \right) \\
& - \langle V_k | \alpha_b e^{i q_a x_a} | V_{k'} \rangle \langle U_{K'} | \alpha_{b'} e^{-i q'_a x_a} | U_K \rangle \frac{(\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'}) - (\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q)}{(\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q)^2 + (\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2} \left( \begin{aligned}
& \frac{1}{2} [\hat{b}_{k'}^\dagger \hat{b}_{\tilde{k}'}, \hat{c}_{K'}^\dagger \hat{c}_K] \left\{ \hat{a}_q, \hat{a}_{q'}^\dagger \right\} \\
& + \frac{1}{2} \left\{ \hat{b}_{k'}^\dagger \hat{b}_{\tilde{k}'}, \hat{c}_{K'}^\dagger \hat{c}_K \right\} \left[ \hat{a}_q, \hat{a}_{q'}^\dagger \right]
\end{aligned} \right)
\end{aligned} \right) \\
& = - \left( \frac{q_e}{m_0 c} \right)^2 \sum_{k, k'} \sum_{K, K'} \lim_{V \rightarrow \infty} \frac{1}{V} \sum_{q > q_B} \sum_{q' > q_B} \sum_{b, b'} \mathcal{A}_b(q) \mathcal{A}_{b'}(q') \\
& \left( \begin{aligned}
& + \langle U_k | \alpha_b e^{i q_a x_a} | U_{k'} \rangle \langle U_{K'} | \alpha_{b'} e^{-i q'_a x_a} | U_K \rangle \frac{(\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'}) - (\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)}{(\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)^2 + (\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2} \times \\
& \quad \times \left( \begin{aligned}
& (\delta_{k', K'} \hat{c}_k^\dagger \hat{c}_K - \delta_{k, K} \hat{c}_{K'}^\dagger \hat{c}_{k'}) \left( \hat{a}_q^\dagger \hat{a}_q + \frac{1}{2} \delta_{q, q'} \hat{1} \right) \\
& + (\delta_{k', K'} \hat{c}_k^\dagger \hat{c}_K + \delta_{k, K} \hat{c}_{K'}^\dagger \hat{c}_{k'}) \frac{1}{2} \delta_{q, q'}
\end{aligned} \right) \\
& + \langle V_k | \alpha_b e^{i q_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{-i q'_a x_a} | V_K \rangle \frac{(\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'}) - (\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q)}{(\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q)^2 + (\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'})^2} \times \\
& \quad \times \left( \begin{aligned}
& (\delta_{k, K} \hat{b}_{k'}^\dagger \hat{b}_{\tilde{K}'} - \delta_{K', k'} \hat{b}_{\tilde{K}}^\dagger \hat{b}_{\tilde{k}'}) \left( \hat{a}_q^\dagger \hat{a}_q + \frac{1}{2} \delta_{q, q'} \hat{1} \right) \\
& + (\delta_{k, K} \hat{b}_{k'}^\dagger \hat{b}_{\tilde{K}'} + \delta_{K', k'} \hat{b}_{\tilde{K}}^\dagger \hat{b}_{\tilde{k}'}) \frac{1}{2} \delta_{q, q'}
\end{aligned} \right) \\
& - \langle U_k | \alpha_b e^{i q_a x_a} | U_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{-i q'_a x_a} | V_K \rangle \frac{(\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'}) - (\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)}{(\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)^2 + (\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'})^2} \hat{c}_k^\dagger \hat{c}_{k'} \hat{b}_{\tilde{K}}^\dagger \hat{b}_{\tilde{K}'} \delta_{q, q'} \\
& - \langle V_k | \alpha_b e^{i q_a x_a} | V_{k'} \rangle \langle U_{K'} | \alpha_{b'} e^{-i q'_a x_a} | U_K \rangle \frac{(\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'}) - (\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q)}{(\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q)^2 + (\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2} \hat{b}_{k'}^\dagger \hat{b}_{\tilde{k}'} \hat{c}_{K'}^\dagger \hat{c}_K \delta_{q, q'}
\end{aligned} \right) \tag{523}
\end{aligned}$$

In the last line of (523) use has been made of

$$\left[ \hat{c}_k^\dagger \hat{c}_{k'}, \hat{c}_{K'}^\dagger \hat{c}_K \right] = \delta_{k', K'} \hat{c}_k^\dagger \hat{c}_K - \delta_{k, K} \hat{c}_{K'}^\dagger \hat{c}_{k'} \tag{524}$$

$$\left\{ \hat{c}_k^\dagger \hat{c}_{k'}, \hat{c}_{K'}^\dagger \hat{c}_K \right\} = \delta_{k', K'} \hat{c}_k^\dagger \hat{c}_K + \delta_{k, K} \hat{c}_{K'}^\dagger \hat{c}_{k'} + 2 \hat{c}_k^\dagger \hat{c}_{K'}^\dagger \hat{c}_K \hat{c}_{k'} \tag{525}$$

$$\left[ \hat{b}_{k'}^\dagger \hat{b}_{\tilde{k}'}, \hat{b}_{\tilde{K}}^\dagger \hat{b}_{\tilde{K}'} \right] = \delta_{k, K} \hat{b}_{k'}^\dagger \hat{b}_{\tilde{K}'} - \delta_{K', k'} \hat{b}_{\tilde{K}}^\dagger \hat{b}_{\tilde{k}'} \tag{526}$$

$$\left\{ \hat{b}_{k'}^\dagger \hat{b}_{\tilde{k}'}, \hat{b}_{\tilde{K}}^\dagger \hat{b}_{\tilde{K}'} \right\} = \delta_{k, K} \hat{b}_{k'}^\dagger \hat{b}_{\tilde{K}'} + \delta_{K', k'} \hat{b}_{\tilde{K}}^\dagger \hat{b}_{\tilde{k}'} + 2 \hat{b}_{k'}^\dagger \hat{b}_{\tilde{K}}^\dagger \hat{b}_{\tilde{K}'} \hat{b}_{\tilde{k}'} \tag{527}$$



and

$$\frac{1}{2} \left\{ \hat{a}_q, \hat{a}_{q'}^\dagger \right\} = \frac{1}{2} \left( \hat{a}_q \hat{a}_{q'}^\dagger + \hat{a}_{q'}^\dagger \hat{a}_q \right) = \frac{1}{2} \left( 2 \hat{a}_{q'}^\dagger \hat{a}_q + \hat{a}_q \hat{a}_{q'}^\dagger - \hat{a}_{q'}^\dagger \hat{a}_q \right) = \hat{a}_{q'}^\dagger \hat{a}_q + \frac{1}{2} \delta_{q,q'} \hat{1} \quad (528)$$

Several rearrangements lead to [7]

$$\lim_{s \rightarrow \infty} \lim_{V \rightarrow \infty} \int_0^s ds' \hat{J}_1^{(0,0)}(s, s') = + \left( \frac{qe}{m_0 c} \right)^2 \sum_{k, k'} \sum_{K, K'} \times \lim_{V \rightarrow \infty} \left( \begin{aligned} & \frac{1}{V} \sum_{q, q'} \kappa_q \kappa_{q'} \sum_{b, b'} \mathcal{A}_b(q) \mathcal{A}_{b'}(q') \langle U_k | \alpha_b e^{i q a \times a} | U_{k'} \rangle \langle U_{K'} | \alpha_{b'} e^{-i q' a \times a} | U_K \rangle \frac{(\bar{E}_k - \bar{E}_{k'} - \bar{\omega}_q) - (\bar{E}_{K'} - \bar{E}_K + \bar{\omega}_{q'})}{(\bar{E}_k - \bar{E}_{k'} - \bar{\omega}_q)^2 + (\bar{E}_{K'} - \bar{E}_K + \bar{\omega}_{q'})^2} \times \\ & \times \left( \begin{aligned} & (\delta_{k', K'} \hat{c}_k^\dagger \hat{c}_K - \delta_{k, K} \hat{c}_{K'}^\dagger \hat{c}_{k'}) \hat{a}_{q'}^\dagger \hat{a}_q \\ & + \delta_{q, q'} \hat{c}_k^\dagger \hat{c}_{K'}^\dagger \hat{c}_K \hat{c}_{k'} + \delta_{q, q'} \delta_{k', K'} \hat{c}_k^\dagger \hat{c}_K \end{aligned} \right) \\ & + \frac{1}{V} \sum_{q, q'} \kappa_q \kappa_{q'} \sum_{b, b'} \mathcal{A}_b(q) \mathcal{A}_{b'}(q') \langle V_k | \alpha_b e^{i q a \times a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{-i q' a \times a} | V_K \rangle \frac{(\bar{E}_{k'} - \bar{E}_k - \bar{\omega}_q) - (\bar{E}_K - \bar{E}_{K'} + \bar{\omega}_{q'})}{(\bar{E}_{k'} - \bar{E}_k - \bar{\omega}_q)^2 + (\bar{E}_K - \bar{E}_{K'} + \bar{\omega}_{q'})^2} \times \\ & \times \left( \begin{aligned} & (\delta_{k, K} \hat{b}_k^\dagger \hat{b}_{K'} - \delta_{K', k'} \hat{b}_{K'}^\dagger \hat{b}_k) \hat{a}_{q'}^\dagger \hat{a}_q \\ & + \delta_{q, q'} \hat{b}_k^\dagger \hat{b}_{K'}^\dagger \hat{b}_{K'} \hat{b}_k + \delta_{q, q'} \delta_{k, K} \hat{b}_k^\dagger \hat{b}_{K'} \end{aligned} \right) \\ & + \frac{1}{V} \sum_q \kappa_q \sum_{b, b'} \mathcal{A}_b(q) \mathcal{A}_{b'}(q) \langle U_k | \alpha_b e^{i q a \times a} | U_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{-i q a \times a} | V_K \rangle \frac{(\bar{E}_K - \bar{E}_{K'} + \bar{\omega}_q) - (\bar{E}_k - \bar{E}_{k'} - \bar{\omega}_q)}{(\bar{E}_k - \bar{E}_{k'} - \bar{\omega}_q)^2 + (\bar{E}_K - \bar{E}_{K'} + \bar{\omega}_q)^2} \hat{c}_k^\dagger \hat{c}_{k'} \hat{b}_{K'}^\dagger \hat{b}_{K'} \\ & + \frac{1}{V} \sum_q \kappa_q \sum_{b, b'} \mathcal{A}_b(q) \mathcal{A}_{b'}(q) \langle V_k | \alpha_b e^{i q a \times a} | V_{k'} \rangle \langle U_{K'} | \alpha_{b'} e^{-i q a \times a} | U_K \rangle \frac{(\bar{E}_{K'} - \bar{E}_K + \bar{\omega}_q) - (\bar{E}_{k'} - \bar{E}_k - \bar{\omega}_q)}{(\bar{E}_{k'} - \bar{E}_k - \bar{\omega}_q)^2 + (\bar{E}_{K'} - \bar{E}_K + \bar{\omega}_q)^2} \hat{c}_{K'}^\dagger \hat{c}_K \hat{b}_{k'}^\dagger \hat{b}_k \end{aligned} \right) \quad (529)$$

Here we have inserted the definitions of the electromagnetic amplitudes (24), (25), (26), and the polarization vectors (28).

Now with [7]

$$\begin{aligned} \frac{1}{V} \sum_q \kappa_q \mathcal{A}_b(q) \mathcal{A}_{b'}(q) &= \frac{1}{V} \sum_{\mathbf{q}} \kappa_{\mathbf{q}} \sum_{\lambda \in \{I, II\}} \mathcal{A}_b(\mathbf{q}, \lambda) \mathcal{A}_{b'}(\mathbf{q}, \lambda) \\ &= \frac{1}{V} \sum_{\mathbf{q}} \kappa_{\mathbf{q}} \sum_{\lambda \in \{I, II\}} \sqrt{\frac{\hbar}{2\varepsilon_0 \omega(\mathbf{q})}} u_b(\mathbf{q}, \lambda) \sqrt{\frac{\hbar}{2\varepsilon_0 \omega(\mathbf{q})}} u_{b'}(\mathbf{q}, \lambda) \\ &= \frac{1}{V} \sum_{\mathbf{q}} \kappa_{\mathbf{q}} \frac{\hbar}{2\varepsilon_0 \omega(\mathbf{q})} \left( \sum_{\lambda \in \{I, II\}} u_b(\mathbf{q}, \lambda) u_{b'}(\mathbf{q}, \lambda) \right) \\ &= \frac{1}{V} \sum_{\mathbf{q}} \kappa_{\mathbf{q}} \frac{\hbar}{2\varepsilon_0 \omega(\mathbf{q})} \left( \delta_{b, b'} - \frac{q_b q_{b'}}{|\mathbf{q}|^2} \right) \end{aligned} \quad (530)$$

and renaming the summation indices according to  $\{k, k', K, K', b, b', q\} \rightarrow \{\underline{K}', \underline{K}, \underline{k}', \underline{k}, \underline{b}', \underline{b}, -\underline{q}\}$  (minding  $\tilde{\omega}_{-q} = \tilde{\omega}_q$ ) then [7]

$$\begin{aligned}
\lim_{s \rightarrow \infty} \lim_{V \rightarrow \infty} \int_0^s ds' \hat{J}_1^{(0,0)}(s, s') &= + \left( \frac{qe}{m_0 c} \right)^2 \sum_{k, k'} \sum_{K, K'} \times \lim_{V \rightarrow \infty} \\
&\times \left( \begin{aligned}
&\frac{1}{\sqrt{V}} \sum_{q, q'} \kappa_q \kappa_{q'} \sum_{b, b'} \mathcal{A}_b(q) \mathcal{A}_{b'}(q') \langle U_k | \alpha_b e^{iq_a x_a} | U_{k'} \rangle \langle U_{K'} | \alpha_{b'} e^{-iq'_a x_a} | U_K \rangle \frac{(\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q) - (\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})}{(\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)^2 + (\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2} \times \\
&\quad \times \left( \begin{aligned}
&\left( \delta_{k', K'} \hat{c}_k^\dagger \hat{c}_K - \delta_{k, K} \hat{c}_{K'}^\dagger \hat{c}_{k'} \right) \hat{a}_q^\dagger \hat{a}_q \\
&+ \delta_{q, q'} \hat{c}_k^\dagger \hat{c}_K^\dagger \hat{c}_K \hat{c}_{k'} + \delta_{q, q'} \delta_{k', K'} \hat{c}_k^\dagger \hat{c}_K
\end{aligned} \right) \\
&+ \frac{1}{\sqrt{V}} \sum_{q, q'} \kappa_q \kappa_{q'} \sum_{b, b'} \mathcal{A}_b(q) \mathcal{A}_{b'}(q') \langle V_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{-iq'_a x_a} | V_K \rangle \frac{(\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q) - (\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'})}{(\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q)^2 + (\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'})^2} \times \\
&\quad \times \left( \begin{aligned}
&\left( \delta_{k, K} \hat{b}_k^\dagger \hat{b}_{K'} - \delta_{K', k'} \hat{b}_{K'}^\dagger \hat{b}_k \right) \hat{a}_q^\dagger \hat{a}_q \\
&+ \delta_{q, q'} \hat{b}_k^\dagger \hat{b}_{K'}^\dagger \hat{b}_{K'} \hat{b}_k + \delta_{q, q'} \delta_{k, K} \hat{b}_k^\dagger \hat{b}_{K'}
\end{aligned} \right) \\
&+ \frac{1}{\sqrt{V}} \sum_{\mathbf{q}} \kappa_q \frac{\hbar}{2\varepsilon_0 \omega(\mathbf{q})} \left( \delta_{b, b'} - \frac{q_b q_{b'}}{|\mathbf{q}|^2} \right) \langle U_k | \alpha_b e^{iq_a x_a} | U_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{-iq_a x_a} | V_K \rangle \frac{(\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_q) - (\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)}{(\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)^2 + (\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_q)^2} \hat{c}_k^\dagger \hat{c}_{k'} \hat{b}_K^\dagger \hat{b}_{K'} \\
&+ \frac{1}{\sqrt{V}} \sum_{\mathbf{q}} \kappa_q \frac{\hbar}{2\varepsilon_0 \omega(\mathbf{q})} \left( \delta_{b, b'} - \frac{q_b q_{b'}}{|\mathbf{q}|^2} \right) \langle V_{K'} | \alpha_{b'} e^{-iq_a x_a} | V_K \rangle \langle U_k | \alpha_b e^{iq_a x_a} | U_{k'} \rangle \frac{(\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_q) - (\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)}{(\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_q)^2 + (\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)^2} \hat{c}_k^\dagger \hat{c}_{k'} \hat{b}_K^\dagger \hat{b}_{K'}
\end{aligned} \right) \tag{531}
\end{aligned}$$

(531) can last be summarized to [7]

$$\begin{aligned}
\lim_{s \rightarrow \infty} \lim_{V \rightarrow \infty} \int_0^s ds' \hat{J}_1^{(0,0)}(s, s') &= + \left( \frac{qe}{m_0 c} \right)^2 \sum_{k, k'} \sum_{K, K'} \times \lim_{V \rightarrow \infty} \\
&\times \left( \begin{aligned}
&\frac{1}{\sqrt{V}} \sum_{q, q'} \kappa_q \kappa_{q'} \sum_{b, b'} \mathcal{A}_b(q) \mathcal{A}_{b'}(q') \langle U_k | \alpha_b e^{iq_a x_a} | U_{k'} \rangle \langle U_{K'} | \alpha_{b'} e^{-iq'_a x_a} | U_K \rangle \times \\
&\quad \times \frac{(\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q) - (\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})}{(\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)^2 + (\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2} \left( \delta_{k', K'} \hat{c}_k^\dagger \hat{c}_K - \delta_{k, K} \hat{c}_{K'}^\dagger \hat{c}_{k'} \right) \hat{a}_q^\dagger \hat{a}_q \\
&+ \frac{1}{\sqrt{V}} \sum_{q, q'} \kappa_q \kappa_{q'} \sum_{b, b'} \mathcal{A}_b(q) \mathcal{A}_{b'}(q') \langle V_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{-iq'_a x_a} | V_K \rangle \times \\
&\quad \times \frac{(\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q) - (\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'})}{(\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q)^2 + (\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'})^2} \left( \delta_{k, K} \hat{b}_k^\dagger \hat{b}_{K'} - \delta_{K', k'} \hat{b}_{K'}^\dagger \hat{b}_k \right) \hat{a}_q^\dagger \hat{a}_q \\
&+ \frac{1}{\sqrt{V}} \sum_{\mathbf{q}} \kappa_q \frac{\hbar}{2\varepsilon_0 \omega(\mathbf{q})} \sum_{b, b'} \left( \delta_{b, b'} - \frac{q_b q_{b'}}{|\mathbf{q}|^2} \right) \langle U_k | \alpha_b e^{iq_a x_a} | U_{k'} \rangle \langle U_{K'} | \alpha_{b'} e^{-iq_a x_a} | U_K \rangle \times \\
&\quad \times \frac{(\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q) - (\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_q)}{(\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)^2 + (\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_q)^2} \delta_{k', K'} \hat{c}_k^\dagger \hat{c}_K \\
&+ \frac{1}{\sqrt{V}} \sum_{\mathbf{q}} \kappa_q \frac{\hbar}{2\varepsilon_0 \omega(\mathbf{q})} \sum_{b, b'} \left( \delta_{b, b'} - \frac{q_b q_{b'}}{|\mathbf{q}|^2} \right) \langle V_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{-iq_a x_a} | V_K \rangle \times \\
&\quad \times \frac{(\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q) - (\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_q)}{(\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q)^2 + (\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_q)^2} \delta_{k, K} \hat{b}_k^\dagger \hat{b}_{K'} \\
&+ \frac{1}{\sqrt{V}} \sum_{\mathbf{q}} \kappa_q \frac{\hbar}{2\varepsilon_0 \omega(\mathbf{q})} \sum_{b, b'} \left( \delta_{b, b'} - \frac{q_b q_{b'}}{|\mathbf{q}|^2} \right) \langle U_k | \alpha_b e^{iq_a x_a} | U_{k'} \rangle \langle U_{K'} | \alpha_{b'} e^{-iq_a x_a} | U_K \rangle \times \\
&\quad \times \frac{(\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q) - (\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_q)}{(\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)^2 + (\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_q)^2} \hat{c}_k^\dagger \hat{c}_{K'} \hat{c}_K \hat{c}_{k'} \\
&+ \frac{1}{\sqrt{V}} \sum_{\mathbf{q}} \kappa_q \frac{\hbar}{2\varepsilon_0 \omega(\mathbf{q})} \sum_{b, b'} \left( \delta_{b, b'} - \frac{q_b q_{b'}}{|\mathbf{q}|^2} \right) \langle V_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{-iq_a x_a} | V_K \rangle \times \\
&\quad \times \frac{(\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q) - (\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_q)}{(\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q)^2 + (\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_q)^2} \hat{b}_k^\dagger \hat{b}_{K'} \hat{b}_{K'} \hat{b}_k \\
&+ \frac{1}{\sqrt{V}} \sum_{\mathbf{q}} \kappa_q \frac{\hbar}{2\varepsilon_0 \omega(\mathbf{q})} \sum_{b, b'} \left( \delta_{b, b'} - \frac{q_b q_{b'}}{|\mathbf{q}|^2} \right) \langle U_k | \alpha_b e^{iq_a x_a} | U_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{-iq_a x_a} | V_K \rangle \times \\
&\quad \times \left( \frac{(\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q) - (\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_q)}{(\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)^2 + (\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_q)^2} + \frac{(\tilde{E}_k - \tilde{E}_{k'} + \tilde{\omega}_q) - (\tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_q)}{(\tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_q)^2 + (\tilde{E}_k - \tilde{E}_{k'} + \tilde{\omega}_q)^2} \right) \hat{c}_k^\dagger \hat{c}_{k'} \hat{b}_K^\dagger \hat{b}_{K'}
\end{aligned} \right) \tag{532}
\end{aligned}$$

where no particle number violating term occurs!

The terms in the first two lines contribute to the self-energy of the photon  $\hat{Q}_{\perp, ph}$ . The terms in the third and fourth line contribute to the renormalization contributions  $\hat{\mathcal{M}}_{\perp}$  of the fermions, whereas the other

terms contribute to the transversal effective matter–matter interaction  $\hat{\mathcal{V}}_{\perp,ee}$ , the effective positron–positron interaction  $\hat{\mathcal{V}}_{\perp,pp}$  and the effective electron–positron interaction  $\hat{\mathcal{V}}_{\perp,ep}$ .

## Integral 2

The second integral is given by

$$\begin{aligned}
& \lim_{s \rightarrow \infty} \lim_{V \rightarrow \infty} \int_0^s ds' \hat{J}_2^{(0,0)}(s, s') = - \left( \frac{qe}{m_0 c} \right)^2 \lim_{s \rightarrow \infty} \lim_{V \rightarrow \infty} \sum_{k, k'} \sum_{K, K'} \frac{1}{V} \sum_{q, q'} \sum_{b, b'} \mathcal{A}_b(q) \mathcal{A}_{b'}(q') \times \\
& \left( \begin{aligned}
& + \int_0^s ds' \langle U_k | \alpha_b e^{iq_a x_a} | U_{k'} \rangle \langle U_K | \alpha_{b'} e^{iq'_a x_a} | U_{K'} \rangle e^{-\kappa_q s' (\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)^2} e^{-\kappa_{q'} s' (\tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_{q'})^2} \times \\
& \quad \times \left( \tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q + 2 \left( \tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_{q'} \right) \right) \kappa_{q'} \times \\
& \quad \times e^{-(s-s')(-\kappa_q - \kappa_{q'})^2 (\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q + \tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_{q'})^2} \left[ \hat{c}_k^\dagger \hat{c}_k \hat{a}_q, \hat{c}_K^\dagger \hat{c}_K \hat{a}_{q'} \right] \\
& + \int_0^s ds' \langle V_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle V_K | \alpha_{b'} e^{iq'_a x_a} | V_{K'} \rangle e^{-\kappa_q s' (\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q)^2} e^{-\kappa_{q'} s' (\tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})^2} \times \\
& \quad \times \left( \tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q + 2 \left( \tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'} \right) \right) \kappa_{q'} \times \\
& \quad \times e^{-(s-s')(-\kappa_q - \kappa_{q'})^2 (\tilde{E}_{k'} - \tilde{E}_k - \tilde{\omega}_q + \tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})^2} \left[ \hat{b}_{k'}^\dagger \hat{b}_{k'} \hat{a}_q, \hat{b}_{K'}^\dagger \hat{b}_{K'} \hat{a}_{q'} \right] \\
& \times \left( \begin{aligned}
& + \int_0^s ds' \langle U_{k'} | \alpha_b e^{-iq_a x_a} | U_k \rangle \langle U_{K'} | \alpha_{b'} e^{-iq'_a x_a} | U_K \rangle e^{-\kappa_q s' (\tilde{E}_k - \tilde{E}_{k'} + \tilde{\omega}_q)^2} e^{-\kappa_{q'} s' (\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2} \times \\
& \quad \times \left( \tilde{E}_{k'} - \tilde{E}_k + \tilde{\omega}_q + 2 \left( \tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'} \right) \right) \kappa_{q'} \times \\
& \quad \times e^{-(s-s')(\kappa_q + \kappa_{q'})^2 (\tilde{E}_{k'} - \tilde{E}_k + \tilde{\omega}_q + \tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2} \left[ \hat{c}_k^\dagger \hat{c}_k \hat{a}_q^\dagger, \hat{c}_K^\dagger \hat{c}_K \hat{a}_{q'}^\dagger \right] \\
& + \int_0^s ds' \langle V_{k'} | \alpha_b e^{-iq_a x_a} | V_k \rangle \langle V_{K'} | \alpha_{b'} e^{-iq'_a x_a} | V_K \rangle e^{-\kappa_q s' (\tilde{E}_k - \tilde{E}_{k'} + \tilde{\omega}_q)^2} e^{-\kappa_{q'} s' (\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2} \times \\
& \quad \times \left( \tilde{E}_k - \tilde{E}_{k'} + \tilde{\omega}_q + 2 \left( \tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'} \right) \right) \kappa_{q'} \times \\
& \quad \times e^{-(s-s')(\kappa_q + \kappa_{q'})^2 (\tilde{E}_k - \tilde{E}_{k'} + \tilde{\omega}_q + \tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2} \left[ \hat{b}_k^\dagger \hat{b}_k \hat{a}_q^\dagger, \hat{b}_{K'}^\dagger \hat{b}_{K'} \hat{a}_{q'}^\dagger \right]
\end{aligned} \right)
\end{aligned} \right) \quad (533)
\end{aligned}$$

The integrals occuring here are of the type [7]

$$\begin{aligned}
f_2^{(0,0)}(x, y, \kappa_q, \kappa_{q'}) &= (x + 2y) \kappa_{q'} \int_0^s ds' e^{-(s-s')(\kappa_q + \kappa_{q'})^2 (x+y)^2} e^{-s'(\kappa_q x^2 + \kappa_{q'} y^2)} \\
&= (x + 2y) \kappa_{q'} \frac{e^{-s(\kappa_q x^2 + \kappa_{q'} y^2)} - e^{-s(\kappa_q + \kappa_{q'})^2 (x+y)^2}}{(\kappa_q + \kappa_{q'})^2 (x+y)^2 - \kappa_q x^2 - \kappa_{q'} y^2} \\
&= \begin{cases} 0 & \text{für } \kappa_{q'} = 0 \\ (x + 2y) \frac{e^{-s(\kappa_q x^2 + y^2)} - e^{-s(\kappa_q + 1)^2 (x+y)^2}}{(\kappa_q + 1)^2 (x+y)^2 - \kappa_q x^2 - y^2} & \text{für } \kappa_{q'} = 1 \end{cases} \quad (534) \\
&= \begin{cases} 0 & \text{für } \kappa_{q'} = 0 \\ (x + 2y) \frac{e^{-s y^2} - e^{-s(x+y)^2}}{(x+y)^2 - y^2} & \text{für } \kappa_{q'} = 1, \kappa_q = 0 \\ (x + 2y) \frac{e^{-s(x^2 + y^2)} - e^{-4s(x+y)^2}}{4(x+y)^2 - x^2 - y^2} & \text{für } \kappa_{q'} = 1, \kappa_q = 1 \end{cases}
\end{aligned}$$

Hence, all terms for  $\kappa_q, \kappa_{q'} \in \{0, 1\}$  yield the contribution zero in the limit  $s \rightarrow \infty$  (besides a term of zero measure  $x + y = 0$ ) [7]:

$$\lim_{s \rightarrow \infty} \lim_{V \rightarrow \infty} \int_0^s ds' \hat{J}_2^{(0,0)}(s, s') = 0 \quad (535)$$

### Integral 3

The third integral is given by

$$\begin{aligned} & \lim_{s \rightarrow \infty} \lim_{V \rightarrow \infty} \int_0^s ds' \hat{J}_1^{(0,+)}(s, s') \\ &= - \lim_{s \rightarrow \infty} \lim_{V \rightarrow \infty} \left( \frac{q_e}{m_0 c} \right)^2 \sum_{k, k'} \sum_{K, K'} \frac{1}{V} \sum_{q, q'} \sum_{b, b'} \mathcal{A}_b(q) \mathcal{A}_{b'}(q') \times \\ & \times \left( \begin{aligned} & \int_0^s ds' \langle U_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{-iq'_a x_a} | U_K \rangle e^{-(4+\kappa_q)s'} (\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q)^2 e^{-(4+\kappa_{q'})s'} (-\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2 \times \\ & \quad \times \left( \tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q + 2 \left( -\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'} \right) \right) (4 + \kappa_{q'}) \times \\ & \quad \times e^{-(s-s')} (-\kappa_q + \kappa_{q'})^2 (\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q - \tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2 \left[ \hat{c}_k^\dagger \hat{b}_{\tilde{k}'}^\dagger \hat{a}_q, \hat{b}_{\tilde{K}'} \hat{c}_K \hat{a}_{q'}^\dagger \right] \\ & + \int_0^s ds' \langle U_k | \alpha_b e^{-iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{+iq'_a x_a} | U_K \rangle e^{-(4+\kappa_q)s'} (\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q)^2 e^{-(4+\kappa_{q'})s'} (-\tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})^2 \times \\ & \quad \times \left( \tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q + 2 \left( -\tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'} \right) \right) (4 + \kappa_{q'}) \times \\ & \quad \times e^{-(s-s')} (\kappa_q - \kappa_{q'})^2 (\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q - \tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})^2 \left[ \hat{c}_k^\dagger \hat{b}_{\tilde{k}'}^\dagger \hat{a}_q, \hat{b}_{\tilde{K}'} \hat{c}_K \hat{a}_{q'}^\dagger \right] \end{aligned} \right) \quad (536) \end{aligned}$$

The occuring integrals are of the type [7]

$$\begin{aligned} f_1^{(0,+)}(x, y, \kappa_q, \kappa_{q'}) &= (x + 2y) (4 + \kappa_{q'}) \int_0^s ds' e^{-(s-s')(\kappa_q - \kappa_{q'})^2 (x+y)^2} e^{-s'((4+\kappa_q)x^2 + (4+\kappa_{q'})y^2)} \\ &= (x + 2y) (4 + \kappa_{q'}) e^{-s(\kappa_q - \kappa_{q'})^2 (x+y)^2} \int_0^s ds' e^{s'((\kappa_q - \kappa_{q'})^2 (x+y)^2 - (4+\kappa_q)x^2 - (4+\kappa_{q'})y^2)} \\ &= (x + 2y) (4 + \kappa_{q'}) \frac{e^{-s((4+\kappa_q)x^2 + (4+\kappa_{q'})y^2)} - e^{-s(\kappa_q - \kappa_{q'})^2 (x+y)^2}}{(\kappa_q - \kappa_{q'})^2 (x+y)^2 - (4 + \kappa_q)x^2 - (4 + \kappa_{q'})y^2} \\ &= \begin{cases} \frac{x+2y}{x^2+y^2} \left( 1 - e^{-s(4x^2+4y^2)} \right) & \text{für } \kappa_{q'} = 0, \kappa_q = 0 \\ \frac{(x+2y)5}{(x+y)^2 - 4x^2 - 5y^2} \left( e^{-s(4x^2+5y^2)} - e^{-s(x+y)^2} \right) & \text{für } \kappa_{q'} = 1, \kappa_q = 0 \\ \frac{(x+2y)4}{(x+y)^2 - 5x^2 - 4y^2} \left( e^{-s(5x^2+4y^2)} - e^{-s(x+y)^2} \right) & \text{für } \kappa_{q'} = 0, \kappa_q = 1 \\ \frac{x+2y}{x^2+y^2} \left( 1 - e^{-s(5x^2+5y^2)} \right) & \text{für } \kappa_{q'} = 1, \kappa_q = 1 \end{cases} \quad (537) \end{aligned}$$

In the limit  $s \rightarrow \infty$  the term with  $\kappa_{q'} = 1$  and  $\kappa_q = 0$ , as well as the term with  $\kappa_{q'} = 0$  and  $\kappa_q = 1$  do not contribute (besides the zero measure contribution  $x + y = 0$ ). The contributions of the terms  $\kappa_{q'} = 1$  and  $\kappa_q = 1$ , as well as  $\kappa_{q'} = 0$  and  $\kappa_q = 0$  are the same.

Therefore one finds for (536) [7]

$$\begin{aligned}
& \lim_{s \rightarrow \infty} \lim_{V \rightarrow \infty} \int_0^s ds' \hat{J}_1^{(0,+)}(s, s') \\
&= - \lim_{s \rightarrow \infty} \lim_{V \rightarrow \infty} \left( \frac{qe}{m_0 c} \right)^2 \sum_{k, k'} \sum_{K, K'} \frac{1}{V} \sum_{q, q'} \sum_{b, b'} \mathcal{A}_b(q) \mathcal{A}_{b'}(q') \times \\
& \times \left( \begin{aligned} & \langle U_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{-iq'_a x_a} | U_K \rangle \frac{(\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q) + 2(-\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'})}{(\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q)^2 + (-\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2} \left[ \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q, \hat{b}_{\tilde{K}'} \hat{c}_K \hat{a}_{q'}^\dagger \right] \\ & + \langle U_k | \alpha_b e^{-iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{+iq'_a x_a} | U_K \rangle \frac{(\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q) + 2(-\tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})}{(\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q)^2 + (-\tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})^2} \left[ \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q^\dagger, \hat{b}_{\tilde{K}'} \hat{c}_K \hat{a}_{q'} \right] \end{aligned} \right) \quad (538)
\end{aligned}$$

Now with the relations (521) one can write [7]

$$\begin{aligned}
& \lim_{s \rightarrow \infty} \lim_{V \rightarrow \infty} \int_0^s ds' \hat{J}_1^{(0,+)}(s, s') \\
&= - \lim_{s \rightarrow \infty} \lim_{V \rightarrow \infty} \left( \frac{qe}{m_0 c} \right)^2 \sum_{k, k'} \sum_{K, K'} \frac{1}{V} \sum_{q, q'} \sum_{b, b'} \mathcal{A}_b(q) \mathcal{A}_{b'}(q') \times \\
& \times \left( \begin{aligned} & \langle U_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{-iq'_a x_a} | U_K \rangle \frac{(\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q) + 2(-\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'})}{(\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q)^2 + (-\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2} \left( \begin{aligned} & \frac{1}{2} \left[ \hat{c}_k^\dagger \hat{b}_{k'}^\dagger, \hat{b}_{\tilde{K}'} \hat{c}_K \right] \left\{ \hat{a}_q, \hat{a}_{q'}^\dagger \right\} \\ & + \frac{1}{2} \left\{ \hat{c}_k^\dagger \hat{b}_{k'}^\dagger, \hat{b}_{\tilde{K}'} \hat{c}_K \right\} \left[ \hat{a}_q, \hat{a}_{q'}^\dagger \right] \end{aligned} \right) \\ & + \langle U_k | \alpha_b e^{-iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{+iq'_a x_a} | U_K \rangle \frac{(\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q) + 2(-\tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})}{(\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q)^2 + (-\tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})^2} \left( \begin{aligned} & \frac{1}{2} \left[ \hat{c}_k^\dagger \hat{b}_{k'}^\dagger, \hat{b}_{\tilde{K}'} \hat{c}_K \right] \left\{ \hat{a}_q^\dagger, \hat{a}_{q'} \right\} \\ & + \frac{1}{2} \left\{ \hat{c}_k^\dagger \hat{b}_{k'}^\dagger, \hat{b}_{\tilde{K}'} \hat{c}_K \right\} \left[ \hat{a}_q^\dagger, \hat{a}_{q'} \right] \end{aligned} \right) \end{aligned} \right) \quad (539)
\end{aligned}$$

(539) can be evaluated according to [7]

$$\begin{aligned}
& \lim_{s \rightarrow \infty} \lim_{V \rightarrow \infty} \int_0^s ds' \hat{J}_1^{(0,+)}(s, s') \\
&= - \left( \frac{qe}{m_0 c} \right)^2 \sum_{k, k'} \sum_{K, K'} \lim_{V \rightarrow \infty} \frac{1}{V} \left( \sum_{q > q_B} \sum_{q' > q_B} + \sum_{q < q_B} \sum_{q' < q_B} \right) \sum_{b, b'} \mathcal{A}_b(q) \mathcal{A}_{b'}(q') \times \\
& \times \left( \begin{aligned} & \langle U_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{-iq'_a x_a} | U_K \rangle \frac{(\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q) + 2(-\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'})}{(\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q)^2 + (-\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2} \times \\ & \times \left( (-\delta_{K', k'} \delta_{K, k} \hat{1} + \delta_{K, k} \hat{b}_{k'}^\dagger \hat{b}_{\tilde{K}'} + \delta_{K', k'} \hat{c}_k^\dagger \hat{c}_K) \hat{a}_q^\dagger \hat{a}_q + \delta_{q, q'} \hat{c}_k^\dagger \hat{c}_K \hat{b}_{k'}^\dagger \hat{b}_{\tilde{K}'} \right) \\ & + \langle U_k | \alpha_b e^{-iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{+iq'_a x_a} | U_K \rangle \frac{(\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q) + 2(-\tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})}{(\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q)^2 + (-\tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})^2} \times \\ & \times \left( (-\delta_{K', k'} \delta_{K, k} \hat{1} + \delta_{K, k} \hat{b}_{k'}^\dagger \hat{b}_{\tilde{K}'} + \delta_{K', k'} \hat{c}_k^\dagger \hat{c}_K) \hat{a}_q^\dagger \hat{a}_{q'} - \delta_{q, q'} \hat{c}_k^\dagger \hat{c}_K \hat{b}_{k'}^\dagger \hat{b}_{\tilde{K}'} \right) \\ & + \left( \frac{1}{2} + \frac{1}{2} \right) \delta_{q, q'} \left( -\delta_{K', k'} \delta_{K, k} \hat{1} + \delta_{K, k} \hat{b}_{k'}^\dagger \hat{b}_{\tilde{K}'} + \delta_{K', k'} \hat{c}_k^\dagger \hat{c}_K \right) \end{aligned} \right) \quad (540)
\end{aligned}$$

where use has been made of

$$\left[ \hat{c}_k^\dagger \hat{b}_{k'}^\dagger, \hat{b}_{\tilde{K}'} \hat{c}_K \right] = -\delta_{K', k'} \delta_{K, k} \hat{1} + \delta_{K, k} \hat{b}_{k'}^\dagger \hat{b}_{\tilde{K}'} + \delta_{K', k'} \hat{c}_k^\dagger \hat{c}_K \quad (541)$$

$$\left\{ \hat{c}_k^\dagger \hat{b}_{k'}^\dagger, \hat{b}_{\tilde{K}'} \hat{c}_K \right\} = \delta_{K', k'} \delta_{K, k} \hat{1} - \delta_{K, k} \hat{b}_{k'}^\dagger \hat{b}_{\tilde{K}'} - \delta_{K', k'} \hat{c}_k^\dagger \hat{c}_K + 2 \hat{c}_k^\dagger \hat{c}_K \hat{b}_{k'}^\dagger \hat{b}_{\tilde{K}'} \quad (542)$$

and the identity (528).

Decomposing (540) into contributions with and without photons there follows [7]

$$\begin{aligned}
\lim_{s \rightarrow \infty} \lim_{V \rightarrow \infty} \int_0^s ds' J_1^{(0,+)}(s, s') = & - \left( \frac{qe}{m_0 c} \right)^2 \sum_{k, k'} \sum_{K, K'} \lim_{V \rightarrow \infty} \frac{1}{V} \left( \sum_{q > q_B} \sum_{q' > q_B} + \sum_{q < q_B} \sum_{q' < q_B} \right) \sum_{b, b'} \mathcal{A}_b(q) \mathcal{A}_{b'}(q') \times \\
& \times \left( \begin{aligned}
& \langle U_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{-iq'_a x_a} | U_K \rangle \frac{(\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q) + 2(-\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'})}{(\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q)^2 + (-\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2} \times \\
& \quad \times \left( -\delta_{K', k'} \delta_{K, k} \hat{1} + \delta_{K, k} \hat{b}_{\tilde{k}}^\dagger \hat{b}_{\tilde{K}'} + \delta_{K', k'} \hat{c}_k^\dagger \hat{c}_K \right) \hat{a}_q^\dagger \hat{a}_q \\
& + \langle U_k | \alpha_b e^{-iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{+iq'_a x_a} | U_K \rangle \frac{(\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q) + 2(-\tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})}{(\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q)^2 + (-\tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})^2} \times \\
& \quad \times \left( -\delta_{K', k'} \delta_{K, k} \hat{1} + \delta_{K, k} \hat{b}_{\tilde{k}}^\dagger \hat{b}_{\tilde{K}'} + \delta_{K', k'} \hat{c}_k^\dagger \hat{c}_K \right) \hat{a}_q^\dagger \hat{a}_q \\
& + \langle U_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{-iq'_a x_a} | U_K \rangle \frac{(\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q) + 2(-\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'})}{(\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q)^2 + (-\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2} \delta_{q, q'} \hat{c}_k^\dagger \hat{c}_K \hat{b}_{\tilde{k}}^\dagger \hat{b}_{\tilde{K}'} \\
& - \langle U_k | \alpha_b e^{-iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{+iq'_a x_a} | U_K \rangle \frac{(\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q) + 2(-\tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})}{(\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q)^2 + (-\tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})^2} \delta_{q, q'} \hat{c}_k^\dagger \hat{c}_K \hat{b}_{\tilde{k}}^\dagger \hat{b}_{\tilde{K}'} \\
& + \langle U_k | \alpha_b e^{-iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{+iq'_a x_a} | U_K \rangle \frac{(\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q) + 2(-\tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})}{(\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q)^2 + (-\tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})^2} \times \\
& \quad \times \delta_{q, q'} \left( -\delta_{K', k'} \delta_{K, k} \hat{1} + \delta_{K, k} \hat{b}_{\tilde{k}}^\dagger \hat{b}_{\tilde{K}'} + \delta_{K', k'} \hat{c}_k^\dagger \hat{c}_K \right)
\end{aligned} \right) \tag{543}
\end{aligned}$$

In the terms with  $\delta_{q, q'}$  the definitions of the electromagnetic amplitudes (24), (25), (26), and the polarization vectors (28) are inserted [7]:

$$\begin{aligned}
& \frac{1}{V} \left( \sum_{q > q_B} \sum_{q' > q_B} + \sum_{q < q_B} \sum_{q' < q_B} \right) \mathcal{A}_b(q) \mathcal{A}_{b'}(q') \delta_{q, q'} F(q, q') \\
& = \frac{1}{V} \sum_{\mathbf{q}, \lambda} \mathcal{A}_b(\mathbf{q}, \lambda) \mathcal{A}_{b'}(\mathbf{q}, \lambda) F(q, q) \\
& = \frac{1}{V} \sum_{\mathbf{q}} \frac{\hbar}{2\varepsilon_0 \omega(\mathbf{q})} \left( \sum_{\lambda \in \{I, II\}} u_b(\mathbf{q}, \lambda) u_{b'}(\mathbf{q}, \lambda) \right) F(q, q) \\
& = \frac{1}{V} \sum_{\mathbf{q}} \frac{\hbar}{2\varepsilon_0 \omega(\mathbf{q})} \left( \delta_{b, b'} - \frac{q_b q_{b'}}{|\mathbf{q}|^2} \right) F(q, q)
\end{aligned} \tag{544}$$

which leads to [7]

$$\begin{aligned}
& \lim_{s \rightarrow \infty} \lim_{V \rightarrow \infty} \int_0^s ds' \hat{J}_1^{(0,+)}(s, s') = - \left( \frac{qe}{m_0 c} \right)^2 \sum_{k, k'} \sum_{K, K'} \lim_{V \rightarrow \infty} \times \\
& \left( \begin{aligned}
& \frac{1}{V} \left( \sum_{q > q_B} \sum_{q' > q_B} + \sum_{q < q_B} \sum_{q' < q_B} \right) \sum_{b, b'} \mathcal{A}_b(q) \mathcal{A}_{b'}(q') \langle U_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{-iq'_a x_a} | U_K \rangle \times \\
& \quad \times \frac{(\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q) + 2(-\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'})}{(\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q)^2 + (-\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_{q'})^2} \left( -\delta_{K', k'} \delta_{K, k} \hat{1} + \delta_{K, k} \hat{b}_{\tilde{k}}^\dagger \hat{b}_{\tilde{K}'} + \delta_{K', k'} \hat{c}_k^\dagger \hat{c}_K \right) \hat{a}_q^\dagger \hat{a}_{q'} \\
& + \frac{1}{V} \left( \sum_{q > q_B} \sum_{q' > q_B} + \sum_{q < q_B} \sum_{q' < q_B} \right) \sum_{b, b'} \mathcal{A}_b(q) \mathcal{A}_{b'}(q') \langle U_k | \alpha_b e^{-iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{+iq'_a x_a} | U_K \rangle \times \\
& \quad \times \frac{(\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q) + 2(-\tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_{q'})}{(\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q)^2 + (-\tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_{q'})^2} \left( -\delta_{K', k'} \delta_{K, k} \hat{1} + \delta_{K, k} \hat{b}_{\tilde{k}}^\dagger \hat{b}_{\tilde{K}'} + \delta_{K', k'} \hat{c}_k^\dagger \hat{c}_K \right) \hat{a}_q^\dagger \hat{a}_{q'} \\
& + \frac{1}{V} \sum_{\mathbf{q}} \frac{\hbar}{2\varepsilon_0 \omega(\mathbf{q})} \left( \delta_{b, b'} - \frac{q_b q_{b'}}{|\mathbf{q}|^2} \right) \langle U_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{-iq'_a x_a} | U_K \rangle \frac{(\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q) + 2(-\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_q)}{(\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q)^2 + (-\tilde{E}_K - \tilde{E}_{K'} + \tilde{\omega}_q)^2} \hat{c}_k^\dagger \hat{c}_K \hat{b}_{\tilde{k}}^\dagger \hat{b}_{\tilde{K}'} \\
& - \frac{1}{V} \sum_{\mathbf{q}} \frac{\hbar}{2\varepsilon_0 \omega(\mathbf{q})} \left( \delta_{b, b'} - \frac{q_b q_{b'}}{|\mathbf{q}|^2} \right) \langle U_k | \alpha_b e^{-iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{+iq'_a x_a} | U_K \rangle \frac{(\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q) + 2(-\tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_q)}{(\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q)^2 + (-\tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_q)^2} \hat{c}_k^\dagger \hat{c}_K \hat{b}_{\tilde{k}}^\dagger \hat{b}_{\tilde{K}'} \\
& + \frac{1}{V} \sum_{\mathbf{q}} \frac{\hbar}{2\varepsilon_0 \omega(\mathbf{q})} \left( \delta_{b, b'} - \frac{q_b q_{b'}}{|\mathbf{q}|^2} \right) \langle U_k | \alpha_b e^{-iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{+iq'_a x_a} | U_K \rangle \frac{(\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q) + 2(-\tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_q)}{(\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q)^2 + (-\tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_q)^2} \times \\
& \quad \times \left( -\delta_{K', k'} \delta_{K, k} \hat{1} + \delta_{K, k} \hat{b}_{\tilde{k}}^\dagger \hat{b}_{\tilde{K}'} + \delta_{K', k'} \hat{c}_k^\dagger \hat{c}_K \right)
\end{aligned} \right) \quad (545)
\end{aligned}$$

Adding the hermetian conjugate  $\hat{J}_1^{(0,-)}(s, s')$  yields after some rearrangements [7]

$$\begin{aligned}
& \lim_{s \rightarrow \infty} \lim_{V \rightarrow \infty} \int_0^s ds' \left( \hat{J}_1^{(0,+)}(s, s') + \hat{J}_1^{(0,-)}(s, s') \right) = + \left( \frac{qe}{m_0 c} \right)^2 \sum_{k, k'} \sum_{K, K'} \lim_{V \rightarrow \infty} \times \\
& \left( \begin{aligned}
& \frac{1}{V} \left( \sum_{q > q_B} \sum_{q' > q_B} + \sum_{q < q_B} \sum_{q' < q_B} \right) \sum_{b, b'} \mathcal{A}_b(q) \mathcal{A}_{b'}(q') \langle U_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{-iq'_a x_a} | U_K \rangle \times \\
& \quad \times \frac{(\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q) + (\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'})}{(\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q)^2 + (\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'})^2} \left( -\delta_{k', K'} \delta_{k, K} \hat{1} + \delta_{k, K} \hat{b}_{\tilde{k}}^\dagger \hat{b}_{\tilde{K}'} + \delta_{k', K'} \hat{c}_k^\dagger \hat{c}_K \right) \hat{a}_q^\dagger \hat{a}_{q'} \\
& + \frac{1}{V} \left( \sum_{q > q_B} \sum_{q' > q_B} + \sum_{q < q_B} \sum_{q' < q_B} \right) \sum_{b, b'} \mathcal{A}_b(q) \mathcal{A}_{b'}(q') \langle U_k | \alpha_b e^{-iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{+iq'_a x_a} | U_K \rangle \times \\
& \quad \times \frac{(\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q) + (\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'})}{(\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q)^2 + (\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'})^2} \left( -\delta_{k', k'} \delta_{K, k} \hat{1} + \delta_{K, k} \hat{b}_{\tilde{k}}^\dagger \hat{b}_{\tilde{K}'} + \delta_{k', k'} \hat{c}_k^\dagger \hat{c}_K \right) \hat{a}_q^\dagger \hat{a}_{q'} \\
& + \frac{1}{V} \sum_{\mathbf{q}} \frac{\hbar}{2\varepsilon_0 \omega(\mathbf{q})} \left( \delta_{b, b'} - \frac{q_b q_{b'}}{|\mathbf{q}|^2} \right) \sum_{b, b'} \langle U_k | \alpha_b e^{-iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{+iq_a x_a} | U_K \rangle \times \\
& \quad \times \left( \frac{(\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q) + (\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_q)}{(\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q)^2 + (\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_q)^2} - \frac{(\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q) + (\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_q)}{(\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q)^2 + (\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_q)^2} \right) \hat{c}_k^\dagger \hat{c}_K \hat{b}_{\tilde{k}}^\dagger \hat{b}_{\tilde{K}'} \\
& + \frac{1}{V} \sum_{\mathbf{q}} \frac{\hbar}{2\varepsilon_0 \omega(\mathbf{q})} \left( \delta_{b, b'} - \frac{q_b q_{b'}}{|\mathbf{q}|^2} \right) \sum_{b, b'} \langle U_k | \alpha_b e^{-iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{+iq_a x_a} | U_K \rangle \times \\
& \quad \times \frac{(\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q) + (\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_q)}{(\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q)^2 + (\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_q)^2} \left( -\delta_{k', K'} \delta_{k, K} \hat{1} + \delta_{k, K} \hat{b}_{\tilde{k}}^\dagger \hat{b}_{\tilde{K}'} + \delta_{k', K'} \hat{c}_k^\dagger \hat{c}_K \right)
\end{aligned} \right) \quad (546)
\end{aligned}$$

(546) can be finally rewritte according to [7]

$$\begin{aligned}
& \lim_{s \rightarrow \infty} \lim_{V \rightarrow \infty} \int_0^s ds' \left( \hat{J}_1^{(0,+)}(s, s') + \hat{J}_1^{(0,-)}(s, s') \right) \\
& = \left( \frac{q_e}{m_0 c} \right)^2 \lim_{V \rightarrow \infty} \left( \begin{aligned}
& -\frac{1}{V} \left( \sum_{q > q_B} \sum_{q' > q_B} + \sum_{q < q_B} \sum_{q' < q_B} \right) \sum_{b, b'} \mathcal{A}_b(q) \mathcal{A}_{b'}(q') \times \\
& \times \sum_{K, K'} \langle U_K | \alpha_b e^{iq_a x_a} | V_{K'} \rangle \langle V_{K'} | \alpha_{b'} e^{-iq'_a x_a} | U_K \rangle \frac{(\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_q) + (\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'})}{(\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_q)^2 + (\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'})^2} \hat{a}_q^\dagger \hat{a}_{q'} \\
& -\frac{1}{V} \left( \sum_{q > q_B} \sum_{q' > q_B} + \sum_{q < q_B} \sum_{q' < q_B} \right) \sum_{b, b'} \mathcal{A}_b(q) \mathcal{A}_{b'}(q') \times \\
& \times \sum_{K, K'} \langle U_K | \alpha_b e^{-iq_a x_a} | V_{K'} \rangle \langle V_{K'} | \alpha_{b'} e^{iq'_a x_a} | U_K \rangle \frac{(\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_q) + (\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'})}{(\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_q)^2 + (\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'})^2} \hat{a}_q^\dagger \hat{a}_{q'} \\
& + \frac{1}{V} \left( \sum_{q > q_B} \sum_{q' > q_B} + \sum_{q < q_B} \sum_{q' < q_B} \right) \sum_{b, b'} \mathcal{A}_b(q) \mathcal{A}_{b'}(q') \times \\
& \times \sum_{k, k'} \sum_{K, K'} \langle U_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle V_{k'} | \alpha_{b'} e^{-iq'_a x_a} | U_K \rangle \frac{(\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q) + (\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_{q'})}{(\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q)^2 + (\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_{q'})^2} \times \\
& \quad \times \left( \delta_{k, K} \hat{b}_{\tilde{k}}^\dagger \hat{b}_{\tilde{K}'} + \delta_{k', K'} \hat{c}_k^\dagger \hat{c}_K \right) \hat{a}_q^\dagger \hat{a}_{q'} \\
& + \frac{1}{V} \left( \sum_{q > q_B} \sum_{q' > q_B} + \sum_{q < q_B} \sum_{q' < q_B} \right) \sum_{b, b'} \mathcal{A}_b(q) \mathcal{A}_{b'}(q') \times \\
& \times \sum_{k, k'} \sum_{K, K'} \langle U_k | \alpha_b e^{-iq_a x_a} | V_{k'} \rangle \langle V_{k'} | \alpha_{b'} e^{iq'_a x_a} | U_K \rangle \frac{(\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q) + (\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_{q'})}{(\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q)^2 + (\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_{q'})^2} \\
& \quad \times \left( \delta_{K, k} \hat{b}_{\tilde{k}}^\dagger \hat{b}_{\tilde{K}'} + \delta_{K', k'} \hat{c}_k^\dagger \hat{c}_K \right) \hat{a}_q^\dagger \hat{a}_{q'} \\
& + \sum_{k, k'} \sum_{K, K'} \frac{1}{V} \sum_{\mathbf{q}} \frac{\hbar}{2\varepsilon_0 \omega(\mathbf{q})} \sum_{b, b'} \left( \delta_{b, b'} - \frac{q_b q_{b'}}{|\mathbf{q}|^2} \right) \langle U_k | \alpha_b e^{-iq_a x_a} | V_{k'} \rangle \langle V_{k'} | \alpha_{b'} e^{iq_a x_a} | U_K \rangle \times \\
& \quad \times \left( \frac{(\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q) + (\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_q)}{(\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q)^2 + (\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_q)^2} - \frac{(\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q) + (\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_q)}{(\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q)^2 + (\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_q)^2} \right) \hat{c}_k^\dagger \hat{c}_K \hat{b}_{\tilde{k}}^\dagger \hat{b}_{\tilde{K}'} \\
& + \sum_k \sum_{K, K'} \frac{1}{V} \sum_{\mathbf{q}} \frac{\hbar}{2\varepsilon_0 \omega(\mathbf{q})} \sum_{b, b'} \left( \delta_{b, b'} - \frac{q_b q_{b'}}{|\mathbf{q}|^2} \right) \langle U_k | \alpha_b e^{-iq_a x_a} | V_{K'} \rangle \langle V_{K'} | \alpha_{b'} e^{iq_a x_a} | U_K \rangle \times \\
& \quad \times \frac{(\tilde{E}_k + \tilde{E}_{K'} + \tilde{\omega}_q) + (\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_q)}{(\tilde{E}_k + \tilde{E}_{K'} + \tilde{\omega}_q)^2 + (\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_q)^2} \hat{c}_k^\dagger \hat{c}_K \\
& + \sum_{k'} \sum_{K, K'} \frac{1}{V} \sum_{\mathbf{q}} \frac{\hbar}{2\varepsilon_0 \omega(\mathbf{q})} \sum_{b, b'} \left( \delta_{b, b'} - \frac{q_b q_{b'}}{|\mathbf{q}|^2} \right) \langle U_K | \alpha_b e^{-iq_a x_a} | V_{k'} \rangle \langle V_{k'} | \alpha_{b'} e^{iq_a x_a} | U_K \rangle \times \\
& \quad \times \frac{(\tilde{E}_K + \tilde{E}_{k'} + \tilde{\omega}_q) + (\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_q)}{(\tilde{E}_K + \tilde{E}_{k'} + \tilde{\omega}_q)^2 + (\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_q)^2} \hat{b}_{\tilde{k}'}^\dagger \hat{b}_{\tilde{K}'} \\
& - \frac{1}{V} \sum_{\mathbf{q}} \frac{\hbar}{2\varepsilon_0 \omega(\mathbf{q})} \sum_{b, b'} \left( \delta_{b, b'} - \frac{q_b q_{b'}}{|\mathbf{q}|^2} \right) \times \\
& \quad \times \sum_{K, K'} \langle U_K | \alpha_b e^{-iq_a x_a} | V_{K'} \rangle \langle V_{K'} | \alpha_{b'} e^{iq_a x_a} | U_K \rangle \frac{(\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_q) + (\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_q)}{(\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_q)^2 + (\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_q)^2} \hat{1}
\end{aligned} \right) \tag{547}
\end{aligned}$$

These integrals comprise the constant spectral shift  $\mathcal{C}_\perp \hat{1}$ , contributions to the transversal renormalization  $\hat{\mathcal{M}}_\perp$ , to the effective electron-positron interaction  $\hat{\mathcal{V}}_{\perp, ep}$  and to the photon renormalization term  $\hat{\mathcal{Q}}_{\perp, ph}$ .

#### Integral 4

The fourth integral is given by



$$\begin{aligned}
\lim_{s \rightarrow \infty} \lim_{V \rightarrow \infty} \int_0^s ds' \hat{J}_2^{(0,+)}(s, s') &= - \lim_{s \rightarrow \infty} \lim_{V \rightarrow \infty} \left( \frac{q_e}{m_0 c} \right)^2 \sum_{k, k'} \sum_{K, K'} \frac{1}{V} \sum_{q, q'} \sum_{b, b'} \mathcal{A}_b(q) \mathcal{A}_{b'}(q') \times \\
&\times \left( \begin{aligned}
&+ \int_0^s ds' \langle U_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{iq'_a x_a} | U_K \rangle e^{-(4+\kappa_q)s'} (\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q)^2 e^{-(4+\kappa_{q'})s'} (-\tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})^2 \times \\
&\quad \times \left( \tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q + 2 \left( -\tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_{q'} \right) \right) (4 + \kappa_{q'}) \times \\
&\quad \times e^{-(s-s')(-\kappa_q - \kappa_{q'})^2 (\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q - \tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})^2} \left[ \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q, \hat{b}_{K'} \hat{c}_K \hat{a}_{q'} \right] \\
&+ \int_0^s ds' \langle U_k | \alpha_b e^{-iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{-iq'_a x_a} | U_K \rangle e^{-(4+\kappa_q)s'} (\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q)^2 e^{-(4+\kappa_{q'})s'} (-\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2 \times \\
&\quad \times \left( \tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q + 2 \left( -\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'} \right) \right) (4 + \kappa_{q'}) \times \\
&\quad \times e^{-(s-s')(\kappa_q + \kappa_{q'})^2 (\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q - \tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2} \left[ \hat{c}_k^\dagger \hat{b}_{k'}^\dagger \hat{a}_q^\dagger, \hat{b}_{K'} \hat{c}_K \hat{a}_{q'}^\dagger \right]
\end{aligned} \right) \quad (548)
\end{aligned}$$

The occuring integrals are of the type [7]

$$\begin{aligned}
&f_2^{(0,+)}(x, y, \kappa_q, \kappa_{q'}) \\
&= (x + 2y) (4 + \kappa_{q'}) \int_0^s ds' e^{-(s-s')(\kappa_q + \kappa_{q'})^2 (x+y)^2} e^{-s'((4+\kappa_q)x^2 + (4+\kappa_{q'})y^2)} \\
&(x + 2y) (4 + \kappa_{q'}) e^{-s(\kappa_q + \kappa_{q'})^2 (x+y)^2} \int_0^s ds' e^{s'((\kappa_q + \kappa_{q'})^2 (x+y)^2 - (4+\kappa_q)x^2 - (4+\kappa_{q'})y^2)} \\
&(x + 2y) (4 + \kappa_{q'}) \frac{e^{-s((4+\kappa_q)x^2 + (4+\kappa_{q'})y^2)} - e^{-s(\kappa_q + \kappa_{q'})^2 (x+y)^2}}{(\kappa_q + \kappa_{q'})^2 (x + y)^2 - (4 + \kappa_q) x^2 - (4 + \kappa_{q'}) y^2} \\
&= \begin{cases} \frac{x+2y}{x^2+y^2} \left( 1 - e^{-s(4x^2+4y^2)} \right) & \text{für } \kappa_{q'} = 0, \kappa_q = 0 \\ \frac{(x+2y)5}{(x+y)^2 - 4x^2 - 5y^2} \left( e^{-s(4x^2+5y^2)} - e^{-s(x+y)^2} \right) & \text{für } \kappa_{q'} = 1, \kappa_q = 0 \\ \frac{(x+2y)4}{(x+y)^2 - 5x^2 - 4y^2} \left( e^{-s(5x^2+4y^2)} - e^{-s(x+y)^2} \right) & \text{für } \kappa_{q'} = 0, \kappa_q = 1 \\ \frac{(x+2y)5}{4(x+y)^2 - 5x^2 - 5y^2} \left( e^{-5s(x^2+y^2)} - e^{-4s(x+y)^2} \right) & \text{für } \kappa_{q'} = 1, \kappa_q = 1 \end{cases} \quad (549)
\end{aligned}$$

Only the term  $\kappa_{q'} = 0, \kappa_q = 0$  contributes in the limit  $s \rightarrow \infty$ . The other terms vanish besides one being of zero measure for  $x + y = 0$ . Hence we get by applying (521) [7]

$$\begin{aligned}
& \lim_{s \rightarrow \infty} \lim_{V \rightarrow \infty} \int_0^s ds' \hat{J}_2^{(0,+)}(s, s') \\
&= - \left( \frac{q_e}{m_0 c} \right)^2 \sum_{k, k'} \sum_{K, K'} \lim_{V \rightarrow \infty} \frac{1}{V} \sum_{q < q_B} \sum_{q' < q_B} \sum_{b, b'} \mathcal{A}_b(q) \mathcal{A}_{b'}(q') \times \\
& \times \left( \begin{aligned}
& \langle U_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{iq'_a x_a} | U_K \rangle \frac{\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q + 2(-\tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_{q'})}{(\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q)^2 + (-\tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})^2} \left[ \hat{c}_k^\dagger \hat{b}_{k'}^\dagger, \hat{b}_{\tilde{K}'} \hat{c}_K \right] \hat{a}_q \hat{a}_{q'} \\
& + \langle U_k | \alpha_b e^{-iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{-iq'_a x_a} | U_K \rangle \frac{\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q + 2(-\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})}{(\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q)^2 + (-\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2} \left[ \hat{c}_k^\dagger \hat{b}_{k'}^\dagger, \hat{b}_{\tilde{K}'} \hat{c}_K \right] \hat{a}_{q'}^\dagger \hat{a}_q^\dagger
\end{aligned} \right) \quad (550)
\end{aligned}$$

By evaluating

$$\left[ \hat{c}_k^\dagger \hat{b}_{k'}^\dagger, \hat{b}_{\tilde{K}'} \hat{c}_K \right] = -\delta_{K', k'} \delta_{K, k} \hat{1} + \delta_{K, k} \hat{b}_{k'}^\dagger \hat{b}_{\tilde{K}'} + \delta_{K', k'} \hat{c}_k^\dagger \hat{c}_K \quad (551)$$

there follows for (550) [7]

$$\begin{aligned}
& \lim_{s \rightarrow \infty} \lim_{V \rightarrow \infty} \int_0^s ds' \hat{J}_2^{(0,+)}(s, s') \\
&= - \left( \frac{q_e}{m_0 c} \right)^2 \sum_{k, k'} \sum_{K, K'} \lim_{V \rightarrow \infty} \frac{1}{V} \sum_{q < q_B} \sum_{q' < q_B} \sum_{b, b'} \mathcal{A}_b(q) \mathcal{A}_{b'}(q') \times \\
& \times \left( \begin{aligned}
& \langle U_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{iq'_a x_a} | U_K \rangle \frac{\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q + 2(-\tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_{q'})}{(\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q)^2 + (-\tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})^2} \times \\
& \quad \times \left( -\delta_{K', k'} \delta_{K, k} \hat{1} + \delta_{K, k} \hat{b}_{k'}^\dagger \hat{b}_{\tilde{K}'} + \delta_{K', k'} \hat{c}_k^\dagger \hat{c}_K \right) \hat{a}_q \hat{a}_{q'} \\
& + \langle U_k | \alpha_b e^{-iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{-iq'_a x_a} | U_K \rangle \frac{\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q + 2(-\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})}{(\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q)^2 + (-\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2} \times \\
& \quad \times \left( -\delta_{K', k'} \delta_{K, k} \hat{1} + \delta_{K, k} \hat{b}_{k'}^\dagger \hat{b}_{\tilde{K}'} + \delta_{K', k'} \hat{c}_k^\dagger \hat{c}_K \right) \hat{a}_{q'}^\dagger \hat{a}_q^\dagger
\end{aligned} \right) \quad (552)
\end{aligned}$$

Adding the hermetian conjugate  $\hat{J}_2^{(0,-)}(s, s')$  then [7]

$$\begin{aligned}
& \lim_{s \rightarrow \infty} \lim_{V \rightarrow \infty} \int_0^s ds' \hat{J}_2^{\hat{\gamma}(0,+)}(s, s') \\
&= - \left( \frac{q_e}{m_0 c} \right)^2 \sum_{k, k'} \sum_{K, K'} \lim_{V \rightarrow \infty} \frac{1}{V} \sum_{q < q_B} \sum_{q' < q_B} \sum_{b, b'} \mathcal{A}_b(q) \mathcal{A}_{b'}(q') \times \\
& \times \left( \begin{aligned}
& \langle U_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{iq'_a x_a} | U_K \rangle \frac{\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q + 2(-\tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_{q'})}{(\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q)^2 + (-\tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})^2} \times \\
& \quad \times \left( -\delta_{K', k'} \delta_{K, k} \hat{1} + \delta_{K, k} \hat{b}_{\tilde{k}'}^\dagger \hat{b}_{\tilde{K}'} + \delta_{K', k'} \hat{c}_k^\dagger \hat{c}_K \right) \hat{a}_q \hat{a}_{q'} \\
& + \langle V_{k'} | \alpha_b e^{iq_a x_a} | U_k \rangle \langle U_K | \alpha_{b'} e^{iq'_a x_a} | V_{K'} \rangle \frac{\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q + 2(-\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})}{(\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q)^2 + (-\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2} \times \\
& \quad \times \left( -\delta_{K', k'} \delta_{K, k} \hat{1} + \delta_{K, k} \hat{b}_{\tilde{k}'}^\dagger \hat{b}_{\tilde{K}'} + \delta_{K', k'} \hat{c}_K^\dagger \hat{c}_k \right) \hat{a}_q \hat{a}_{q'} \\
& + \langle V_{k'} | \alpha_b e^{-iq_a x_a} | U_k \rangle \langle U_K | \alpha_{b'} e^{-iq'_a x_a} | V_{K'} \rangle \frac{\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q + 2(-\tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_{q'})}{(\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q)^2 + (-\tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})^2} \times \\
& \quad \times \left( -\delta_{K', k'} \delta_{K, k} \hat{1} + \delta_{K, k} \hat{b}_{\tilde{k}'}^\dagger \hat{b}_{\tilde{K}'} + \delta_{K', k'} \hat{c}_K^\dagger \hat{c}_k \right) \hat{a}_q^\dagger \hat{a}_{q'}^\dagger \\
& + \langle U_k | \alpha_b e^{-iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{-iq'_a x_a} | U_K \rangle \frac{\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q + 2(-\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})}{(\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q)^2 + (-\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2} \times \\
& \quad \times \left( -\delta_{K', k'} \delta_{K, k} \hat{1} + \delta_{K, k} \hat{b}_{\tilde{k}'}^\dagger \hat{b}_{\tilde{K}'} + \delta_{K', k'} \hat{c}_k^\dagger \hat{c}_K \right) \hat{a}_q^\dagger \hat{a}_{q'}^\dagger
\end{aligned} \right) \tag{553}
\end{aligned}$$

Again substituting the indices  $(k, k', K, K', q, q', b, b') \rightarrow (K, K', k, k', q', q, b', b)$  we find [7]

$$\begin{aligned}
& \lim_{s \rightarrow \infty} \lim_{V \rightarrow \infty} \int_0^s ds' \hat{J}_2^{(0,+)}(s, s') \\
&= - \left( \frac{q_e}{m_0 c} \right)^2 \sum_{k, k'} \sum_{K, K'} \lim_{V \rightarrow \infty} \frac{1}{V} \sum_{q < q_B} \sum_{q' < q_B} \sum_{b, b'} \mathcal{A}_b(q) \mathcal{A}_{b'}(q') \times \\
& \times \left( \begin{aligned}
& \langle U_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{+iq'_a x_a} | U_K \rangle \frac{\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q + 2(-\tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_{q'})}{(\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q)^2 + (-\tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})^2} \times \\
& \quad \times \left( -\delta_{K', k'} \delta_{K, k} \hat{1} + \delta_{K, k} \hat{b}_{k'}^\dagger \hat{b}_{\tilde{K}'} + \delta_{K', k'} \hat{c}_k^\dagger \hat{c}_K \right) \hat{a}_q \hat{a}_{q'} \\
& + \langle V_{K'} | \alpha_{b'} e^{+iq'_a x_a} | U_K \rangle \langle U_k | \alpha_b e^{+iq_a x_a} | V_{k'} \rangle \frac{\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'} + 2(-\tilde{E}_{k'} - \tilde{E}_k + \tilde{\omega}_q)}{(\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'})^2 + (-\tilde{E}_{k'} - \tilde{E}_k + \tilde{\omega}_q)^2} \times \\
& \quad \times \left( -\delta_{K', k'} \delta_{K, k} \hat{1} + \delta_{K, k} \hat{b}_{k'}^\dagger \hat{b}_{\tilde{K}'} + \delta_{K', k'} \hat{c}_k^\dagger \hat{c}_K \right) \hat{a}_{q'} \hat{a}_q \\
& + \langle V_{K'} | \alpha_{b'} e^{-iq'_a x_a} | U_K \rangle \langle U_k | \alpha_b e^{-iq_a x_a} | V_{k'} \rangle \frac{\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'} + 2(-\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)}{(\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'})^2 + (-\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)^2} \times \\
& \quad \times \left( -\delta_{K', k'} \delta_{K, k} \hat{1} + \delta_{K, k} \hat{b}_{k'}^\dagger \hat{b}_{\tilde{K}'} + \delta_{K', k'} \hat{c}_k^\dagger \hat{c}_K \right) \hat{a}_q^\dagger \hat{a}_{q'}^\dagger \\
& + \langle U_k | \alpha_b e^{-iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{-iq'_a x_a} | U_K \rangle \frac{\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q + 2(-\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})}{(\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q)^2 + (-\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2} \times \\
& \quad \times \left( -\delta_{K', k'} \delta_{K, k} \hat{1} + \delta_{K, k} \hat{b}_{k'}^\dagger \hat{b}_{\tilde{K}'} + \delta_{K', k'} \hat{c}_k^\dagger \hat{c}_K \right) \hat{a}_{q'}^\dagger \hat{a}_q^\dagger
\end{aligned} \right) \tag{554}
\end{aligned}$$

Since  $[\hat{a}_{q'}, \hat{a}_q] = \hat{0} = [\hat{a}_{q'}^\dagger, \hat{a}_q^\dagger]$  further rearrangements can be done [7]

$$\begin{aligned}
& \lim_{s \rightarrow \infty} \lim_{V \rightarrow \infty} \int_0^s ds' \hat{J}_2^{(0,+)}(s, s') \\
&= - \left( \frac{q_e}{m_0 c} \right)^2 \sum_{k, k'} \sum_{K, K'} \lim_{V \rightarrow \infty} \frac{1}{V} \sum_{q < q_B} \sum_{q' < q_B} \sum_{b, b'} \mathcal{A}_b(q) \mathcal{A}_{b'}(q') \times \\
& \times \left( \begin{aligned}
& \langle U_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle V_{K'} | \alpha_{b'} e^{+iq'_a x_a} | U_K \rangle \left( \frac{\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q + 2(-\tilde{E}_K - \tilde{E}_{K'} - \tilde{\omega}_{q'})}{(\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q)^2 + (-\tilde{E}_{K'} - \tilde{E}_K - \tilde{\omega}_{q'})^2} + \frac{\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'} + 2(-\tilde{E}_{k'} - \tilde{E}_k + \tilde{\omega}_q)}{(\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'})^2 + (-\tilde{E}_{k'} - \tilde{E}_k + \tilde{\omega}_q)^2} \right) \times \\
& \quad \times \left( -\delta_{K', k'} \delta_{K, k} \hat{1} + \delta_{K, k} \hat{b}_{k'}^\dagger \hat{b}_{\tilde{K}'} + \delta_{K', k'} \hat{c}_k^\dagger \hat{c}_K \right) \hat{a}_q \hat{a}_{q'} \\
& + \langle V_{K'} | \alpha_{b'} e^{-iq'_a x_a} | U_K \rangle \langle U_k | \alpha_b e^{-iq_a x_a} | V_{k'} \rangle \left( \frac{\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'} + 2(-\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)}{(\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'})^2 + (-\tilde{E}_k - \tilde{E}_{k'} - \tilde{\omega}_q)^2} + \frac{\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q + 2(-\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})}{(\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q)^2 + (-\tilde{E}_{K'} - \tilde{E}_K + \tilde{\omega}_{q'})^2} \right) \times \\
& \quad \times \left( -\delta_{K', k'} \delta_{K, k} \hat{1} + \delta_{K, k} \hat{b}_{k'}^\dagger \hat{b}_{\tilde{K}'} + \delta_{K', k'} \hat{c}_k^\dagger \hat{c}_K \right) \hat{a}_{q'}^\dagger \hat{a}_q^\dagger
\end{aligned} \right) \tag{555}
\end{aligned}$$

Which finally gives, by adding the conjugate  $\hat{J}_2^{(0,-)}(s, s')$  the expression [7]

$$\begin{aligned}
& \lim_{s \rightarrow \infty} \lim_{V \rightarrow \infty} \int_0^s ds' (\hat{J}_2^{(0,+)}(s, s') + \hat{J}_2^{(0,-)}(s, s')) \\
&= - \left( \frac{q_e}{m_0 c} \right)^2 \sum_{k, k'} \sum_{K, K'} \lim_{V \rightarrow \infty} \frac{1}{V} \sum_{q < q_B} \sum_{q' < q_B} \sum_{b, b'} \mathcal{A}_b(q) \mathcal{A}_{b'}(q') \times \\
& \times \left( \begin{aligned}
& - \langle U_K | \alpha_b e^{iq_a x_a} | V_{K'} \rangle \langle V_{K'} | \alpha_{b'} e^{+iq'_a x_a} | U_K \rangle \frac{(\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'}) + (\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_q)}{(\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'})^2 + (\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_q)^2} \hat{a}_{q'} \hat{a}_q \\
& - \langle V_{K'} | \alpha_{b'} e^{-iq'_a x_a} | U_K \rangle \langle U_K | \alpha_b e^{-iq_a x_a} | V_{K'} \rangle \frac{(\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'}) + (\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_q)}{(\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'})^2 + (\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_q)^2} \hat{a}_{q'}^\dagger \hat{a}_q^\dagger \\
& + \langle U_k | \alpha_b e^{iq_a x_a} | V_{k'} \rangle \langle V_{k'} | \alpha_{b'} e^{+iq'_a x_a} | U_K \rangle \frac{(\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'}) + (\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q)}{(\tilde{E}_K + \tilde{E}_{K'} + \tilde{\omega}_{q'})^2 + (\tilde{E}_k + \tilde{E}_{k'} - \tilde{\omega}_q)^2} \times \\
& \quad \times \left( \delta_{K, k} \hat{b}_{k'}^\dagger \hat{b}_{\bar{K}'} + \delta_{K', k'} \hat{c}_k^\dagger \hat{c}_K \right) \hat{a}_{q'} \hat{a}_q \\
& + \langle V_{K'} | \alpha_{b'} e^{-iq'_a x_a} | U_K \rangle \langle U_K | \alpha_b e^{-iq_a x_a} | V_{k'} \rangle \frac{(\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'}) + (\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q)}{(\tilde{E}_K + \tilde{E}_{K'} - \tilde{\omega}_{q'})^2 + (\tilde{E}_k + \tilde{E}_{k'} + \tilde{\omega}_q)^2} \times \\
& \quad \times \left( \delta_{K, k} \hat{b}_{k'}^\dagger \hat{b}_{\bar{K}'} + \delta_{K', k'} \hat{c}_k^\dagger \hat{c}_K \right) \hat{a}_{q'}^\dagger \hat{a}_q^\dagger
\end{aligned} \right) \quad (556)
\end{aligned}$$

This integral contributes to the effective fermion–photon interactions  $\hat{\mathcal{H}}_{e,ph}$  and  $\hat{\mathcal{H}}_{p,ph}$ . It describes absorption and emission processes of two photons. Since  $|\mathbf{q}| < q_B$  these are low–energy photons. Discussing only one electromagnetic mode (meaning  $\mathbf{q}' = \mathbf{q}$ ), Avan et al. argue that these terms are of fourth order [45].

### Evaluation of the Effective Potentials $V_{a,b}^{(o,o)}(\mathbf{r})$ , $V_{a,b}^{(sp,sp)}(\mathbf{r})$ and $V_b^{(osp,o)}(\mathbf{r})$

In this section the effective potentials potentials are evaluated [7].

$$\begin{aligned}
V_{a,b}^{(o,o)}(\mathbf{r}) &= \left( -\frac{q_e^2}{\varepsilon_0} \right) \int \frac{d^3 q}{(2\pi)^3} \frac{1}{|\mathbf{q}|^2} e^{i\mathbf{q}\cdot\mathbf{r}} \left( \delta_{a,b} - \frac{q_a q_b}{|\mathbf{q}|^2} \right) \\
V_{a,b}^{(sp,sp)}(\mathbf{r}) &= \left( -\frac{q_e^2}{\varepsilon_0} \right) \frac{1}{4} \left( \frac{\hbar}{m_0 c} \right)^2 \int \frac{d^3 q}{(2\pi)^3} e^{i\mathbf{q}\cdot\mathbf{r}} \left( \delta_{a,b} - \frac{q_a q_b}{|\mathbf{q}|^2} \right) \quad (557) \\
V_b^{(osp,o)}(\mathbf{r}) &= \left( -\frac{q_e^2}{\varepsilon_0} \right) \int \frac{d^3 q}{(2\pi)^3} \frac{1}{|\mathbf{q}|^2} e^{i\mathbf{q}\cdot\mathbf{r}} \left( \frac{i}{2} \frac{\hbar q_b}{m_0 c} \right)
\end{aligned}$$

It is not possible to assume from the beginning that  $\mathbf{q}$  is aligned along the direction of  $\mathbf{r}$ , and the scalar product  $\mathbf{q} \cdot \mathbf{r}$  in spheric coordinates gives an exhausting integral.

However, one lay the  $z$ -axis parallel to  $|\mathbf{r}|$ , such that all other components have to be rotated accordingly:

$$\sum_b [\mathcal{R}^T(\vartheta, \varphi)]_{ab} r_b = |\mathbf{r}| \delta_{a,z} \quad (558)$$

For that purpose one writes in spheric coordinates

$$\begin{aligned}\mathbf{r} &= |\mathbf{r}| \cos(\varphi) \sin(\vartheta) \mathbf{e}^{(x)} + |\mathbf{r}| \sin(\varphi) \sin(\vartheta) \mathbf{e}^{(y)} + |\mathbf{r}| \cos(\vartheta) \mathbf{e}^{(z)} \\ &= \begin{pmatrix} |\mathbf{r}| \cos(\varphi) \sin(\vartheta) \\ |\mathbf{r}| \sin(\varphi) \sin(\vartheta) \\ |\mathbf{r}| \cos(\vartheta) \end{pmatrix}\end{aligned}\tag{559}$$

where  $\{\mathbf{e}^{(x)}, \mathbf{e}^{(y)}, \mathbf{e}^{(z)}\}$  are the cartesian basic vectors,  $|\mathbf{r}|$  is a fixed distance as well as the angles  $\varphi$  and  $\vartheta$ .

Likewise for the vector  $\mathbf{q}'$  then

$$\begin{aligned}\mathbf{q}' &= |\mathbf{q}'| \cos(\varphi') \sin(\vartheta') \mathbf{e}^{(x)} + |\mathbf{q}'| \sin(\varphi') \sin(\vartheta') \mathbf{e}^{(y)} + |\mathbf{q}'| \cos(\vartheta') \mathbf{e}^{(z)} \\ &= \begin{pmatrix} |\mathbf{q}'| \cos(\varphi) \sin(\vartheta) \\ |\mathbf{q}'| \sin(\varphi) \sin(\vartheta) \\ |\mathbf{q}'| \cos(\vartheta) \end{pmatrix}\end{aligned}\tag{560}$$

For the scalar product  $\mathbf{q} \cdot \mathbf{r}$  one finds by inserting the transformation (560)

$$\mathbf{q} \cdot \mathbf{r} = |\mathbf{r}| |\mathbf{q}'| \cos(\vartheta')\tag{561}$$

In this form the integral in spheric coordinates is simple because the scalar product only depends on  $|\mathbf{r}|$ ,  $|\mathbf{q}'|$  and the angle  $\vartheta'$ .

The rotational matrix  $\mathcal{R}(\vartheta, \varphi)$  is given by

$$\mathcal{R} \equiv \mathcal{R}(\vartheta, \varphi) = \begin{pmatrix} \cos(\varphi) & , & -\sin(\varphi) & , & 0 \\ \sin(\varphi) & , & \cos(\varphi) & , & 0 \\ 0 & , & 0 & , & 1 \end{pmatrix} \circ \begin{pmatrix} \cos(\vartheta) & , & 0 & , & \sin(\vartheta) \\ 0 & , & 1 & , & 0 \\ -\sin(\vartheta) & , & 0 & , & \cos(\vartheta) \end{pmatrix}\tag{562}$$

As a rotational matrix is has the following properties:

$$\begin{aligned}\mathcal{R}(\vartheta, \varphi) \circ \mathcal{R}^T(\vartheta, \varphi) &= 1_{3 \times 3} = \mathcal{R}^T(\vartheta, \varphi) \circ \mathcal{R}(\vartheta, \varphi) \\ \det \mathcal{R}(\vartheta, \varphi) &= 1 \\ |\mathbf{q}| &= |\mathcal{R}(\vartheta, \varphi) \mathbf{q}'| = |\mathbf{q}'|\end{aligned}\tag{563}$$

For example

$$\begin{aligned}
\mathcal{R}^T \mathbf{r} &= \begin{pmatrix} \cos(\vartheta) & , 0 & , -\sin(\vartheta) \\ 0 & , 1 & , 0 \\ \sin(\vartheta) & , 0 & , \cos(\vartheta) \end{pmatrix} \circ \begin{pmatrix} \cos(\varphi) & , \sin(\varphi) & , 0 \\ -\sin(\varphi) & , \cos(\varphi) & , 0 \\ 0 & , 0 & , 1 \end{pmatrix} \begin{pmatrix} |\mathbf{r}| \cos(\varphi) \sin(\vartheta) \\ |\mathbf{r}| \sin(\varphi) \sin(\vartheta) \\ |\mathbf{r}| \cos(\vartheta) \end{pmatrix} \\
&= \begin{pmatrix} 0 \\ 0 \\ |\mathbf{r}| \end{pmatrix} \equiv |\mathbf{r}| \mathbf{e}^{(z)}
\end{aligned} \tag{564}$$

Such that  $\mathcal{R}^T \frac{\mathbf{r}}{|\mathbf{r}|} = \mathbf{e}^{(z)}$  On the other hand  $\mathcal{R} \mathbf{e}^{(z)} = \frac{\mathbf{r}}{|\mathbf{r}|}$ ,  $\mathcal{R}_{b,z} = \frac{r_b}{r}$ .

With that one can evaluate the integral for  $V_{a,b}^{(o,o)}(\mathbf{r})$  according to

$$\begin{aligned}
V_{a,b}^{(o,o)}(\mathbf{r}) &= \left( -\frac{q_e^2}{\varepsilon_0} \right) \int \frac{d^3 q'}{(2\pi)^3 |\mathbf{q}'|^2} e^{i(\mathcal{R}\mathbf{q}') \cdot \mathbf{r}} \left( \delta_{a,b} - \frac{(\mathcal{R}\mathbf{q}')_a (\mathcal{R}\mathbf{q}')_b}{|\mathbf{q}'|^2} \right) \\
&= \left( -\frac{q_e^2}{\varepsilon_0} \right) \frac{1}{(2\pi)^3} \int_0^\infty dq' q'^2 \int_0^\pi d\vartheta' \sin(\vartheta') \int_0^{2\pi} d\varphi' \frac{1}{q'^2} e^{irq' \cos(\vartheta')} \sum_{m,n} \mathcal{R}_{a,m} \left( \delta_{m,n} - \frac{q'_m q'_n}{q'^2} \right) \mathcal{R}_{n,b}^T \\
&= \left( -\frac{q_e^2}{\varepsilon_0} \right) \frac{1}{(2\pi)^2} \int_0^\infty dq' q'^2 \int_0^\pi d\vartheta' \sin(\vartheta') \frac{1}{q'^2} e^{irq' \cos(\vartheta')} \sum_{m,n} \mathcal{R}_{a,m} \frac{1}{2\pi} \int_0^{2\pi} d\varphi' \left( \delta_{m,n} - \frac{q'_m q'_n}{q'^2} \right) \mathcal{R}_{n,b}^T
\end{aligned} \tag{565}$$

The integral of the angle  $\varphi'$  is given by

$$\begin{aligned}
&\frac{1}{2\pi} \int_0^{2\pi} d\varphi' \left( \delta_{m,n} - \frac{q'_m q'_n}{q'^2} \right) \\
&= \begin{pmatrix} 1 - \sin^2(\vartheta') \frac{1}{2\pi} \int_0^{2\pi} d\varphi' \cos^2(\varphi') & , 0 & , 0 \\ 0 & , 1 - \sin^2(\vartheta') \frac{1}{2\pi} \int_0^{2\pi} d\varphi' \sin^2(\varphi') & , 0 \\ 0 & , 0 & , 1 - \cos^2(\vartheta') \end{pmatrix}_{m,n} \\
&= \begin{pmatrix} 1 - \frac{\sin^2(\vartheta')}{2} & , 0 & , 0 \\ 0 & , 1 - \frac{\sin^2(\vartheta')}{2} & , 0 \\ 0 & , 0 & , 1 - \cos^2(\vartheta') \end{pmatrix}_{m,n} \\
&= \begin{pmatrix} \frac{1+\cos^2(\vartheta')}{2} & , 0 & , 0 \\ 0 & , \frac{1+\cos^2(\vartheta')}{2} & , 0 \\ 0 & , 0 & , 1 - \cos^2(\vartheta') \end{pmatrix}_{m,n} \\
&= \frac{1 + \cos^2(\vartheta')}{2} \begin{pmatrix} 1 & , 0 & , 0 \\ 0 & , 1 & , 0 \\ 0 & , 0 & , 1 \end{pmatrix}_{m,n} + \frac{1 - 3\cos^2(\vartheta')}{2} \begin{pmatrix} 0 & , 0 & , 0 \\ 0 & , 0 & , 0 \\ 0 & , 0 & , 1 \end{pmatrix}_{m,n}
\end{aligned} \tag{566}$$

which can be brought to the form

$$\begin{aligned}
& \sum_{m,n} \mathcal{R}_{a,m} \frac{1}{2\pi} \int_0^{2\pi} d\varphi' \left( \delta_{m,n} - \frac{q'_m q'_n}{q'^2} \right) \mathcal{R}_{n,b}^T \\
&= \frac{1+\cos^2(\vartheta')}{2} \mathcal{R} \begin{pmatrix} 1 & , 0 & , 0 \\ 0 & , 1 & , 0 \\ 0 & , 0 & , 1 \end{pmatrix} \mathcal{R}^T + \frac{1-3\cos^2(\vartheta')}{2} \mathcal{R} \circ \begin{pmatrix} 0 & , 0 & , 0 \\ 0 & , 0 & , 0 \\ 0 & , 0 & , 1 \end{pmatrix} \circ \mathcal{R}^T \\
&= \frac{1+\cos^2(\vartheta')}{2} \mathbf{1}_{3 \times 3} + \frac{1-3\cos^2(\vartheta')}{2} \mathcal{R} \left( \mathbf{e}^{(z)} \otimes \left[ \mathbf{e}^{(z)} \right]^T \right) \mathcal{R}^T \\
&= \frac{1+\cos^2(\vartheta')}{2} \mathbf{1}_{3 \times 3} + \frac{1-3\cos^2(\vartheta')}{2} \left( \mathcal{R} \mathbf{e}^{(z)} \otimes \left[ \mathcal{R} \mathbf{e}^{(z)} \right]^T \right) \\
&= \frac{1+\cos^2(\vartheta')}{2} \mathbf{1}_{3 \times 3} + \frac{1-3\cos^2(\vartheta')}{2} \left( \frac{\mathbf{r} \otimes \mathbf{r}^T}{|\mathbf{r}|^2} \right)
\end{aligned} \tag{567}$$

Altogether now

$$V_{a,b}^{(o,o)}(\mathbf{r}) = \left( -\frac{q_e^2}{\varepsilon_0} \right) \frac{1}{(2\pi)^2} \int_0^\infty dq' q'^2 \int_0^\pi d\vartheta' \sin(\vartheta') \frac{1}{q'^2} e^{irq' \cos(\vartheta')} \left( \frac{1+\cos^2(\vartheta')}{2} \delta_{a,b} + \frac{1-3\cos^2(\vartheta')}{2} \frac{r_a r_b}{r^2} \right) \tag{568}$$

Substituting  $t = \cos(\vartheta')$  and  $rq' = x$  then

$$V_{a,b}^{(o,o)}(\mathbf{r}) = \left( -\frac{q_e^2}{\varepsilon_0} \right) \frac{1}{(2\pi)^2} \frac{1}{r} \int_0^\infty dx \int_{-1}^1 dt e^{ixt} \left( \frac{1+t^2}{2} \delta_{a,b} + \frac{1-3t^2}{2} \frac{r_a r_b}{r^2} \right) \tag{569}$$

The remaining integrals are

$$\begin{aligned}
\int_{-1}^1 dt \frac{e^{ixt}}{2} &= \frac{\sin(x)}{x} \\
\int_{-1}^1 dt \frac{e^{ixt}}{2} t^2 &= \frac{2}{x^2} \cos(x) + \left( 1 - \frac{2}{x^2} \right) \frac{\sin(x)}{x}
\end{aligned} \tag{570}$$

Such that

$$V_{a,b}^{(o,o)}(\mathbf{r}) = \left( -\frac{q_e^2}{\varepsilon_0} \right) \frac{1}{(2\pi)^2} \frac{1}{r} \int_{-\infty}^\infty dx \left( \begin{aligned} & \left( \frac{1}{x^2} \cos(x) + \left( 1 - \frac{1}{x^2} \right) \frac{\sin(x)}{x} \right) \delta_{a,b} + \\ & - \left( \frac{\sin(x)}{x} + \frac{3}{x^2} \left( \cos(x) - \frac{\sin(x)}{x} \right) \right) \frac{r_a r_b}{r^2} \end{aligned} \right) \tag{571}$$



Hence,

$$V_{a,b}^{(o,o)}(\mathbf{r}) = \left( -\frac{q_e^2}{4\pi\epsilon_0} \right) \frac{1}{2} \left( \frac{\delta_{a,b}}{r} + \frac{r_a r_b}{r^3} \right) \quad (572)$$

Here it has been used that

$$\begin{aligned} I_1 &\equiv \int_{-\infty}^{\infty} dx \frac{\sin(x)}{x} = \pi \\ I_2 &\equiv \int_{-\infty}^{\infty} dx \left( \frac{\sin(x)}{x^3} - \frac{\cos(x)}{x^2} \right) = \frac{\pi}{2} \end{aligned} \quad (573)$$

Following from the residue theorem.

For the integral of the dipole-dipole potential  $V_{a,b}^{(sp,sp)}(\mathbf{r})$  follows by observing that

$$\begin{aligned} V_{a,b}^{(sp,sp)}(\mathbf{r}) &= \left( -\frac{q_e^2}{\epsilon_0} \right) \frac{1}{4} \left( \frac{\hbar}{m_0 c} \right)^2 \int \frac{d^3 q}{(2\pi)^3} e^{i\mathbf{q}\cdot\mathbf{r}} \left( \delta_{a,b} - \frac{q_a q_b}{|\mathbf{q}|^2} \right) \\ &= \left( -\frac{q_e^2}{\epsilon_0} \right) \frac{1}{4} \left( \frac{\hbar}{m_0 c} \right)^2 \int \frac{d^3 q}{(2\pi)^3} e^{i\mathbf{q}\cdot\mathbf{r}} \left( \delta_{a,b} - \frac{q_a q_b}{|\mathbf{q}|^2} \right) \\ &= \left( -\frac{q_e^2}{\epsilon_0} \right) \frac{1}{4} \left( \frac{\hbar}{m_0 c} \right)^2 \left( \int \frac{d^3 q}{(2\pi)^3} e^{i\mathbf{q}\cdot\mathbf{r}} \delta_{a,b} + \nabla_a \nabla_b \int \frac{d^3 q}{(2\pi)^3} \frac{e^{i\mathbf{q}\cdot\mathbf{r}}}{|\mathbf{q}|^2} \right) \\ &= \left( -\frac{q_e^2}{\epsilon_0} \right) \frac{1}{4} \left( \frac{\hbar}{m_0 c} \right)^2 \left( \delta^{(3)}(\mathbf{r}) \delta_{a,b} + \nabla_a \nabla_b \frac{1}{4\pi|\mathbf{r}|} \right) \end{aligned} \quad (574)$$

and with

$$\begin{aligned} -\nabla^2 \frac{1}{|\mathbf{r}|} &= 4\pi \delta^{(3)}(\mathbf{r}) \\ \nabla_a \nabla_b \frac{1}{|\mathbf{r}|} &= -\frac{4\pi}{3} \delta^{(3)}(\mathbf{r}) \delta_{a,b} + \frac{3r_a r_b - 3|\mathbf{r}|^2 \delta_{a,b}}{|\mathbf{r}|^5} \\ \frac{1}{4\pi|\mathbf{r}|} &= \int \frac{d^3 q}{(2\pi)^3} \frac{e^{i\mathbf{q}\cdot\mathbf{r}}}{|\mathbf{q}|^2} \end{aligned} \quad (575)$$

then

$$\begin{aligned} V_{a,b}^{(sp,sp)}(\mathbf{r}) &= \left( -\frac{q_e^2}{\epsilon_0} \right) \frac{1}{4} \left( \frac{\hbar}{m_0 c} \right)^2 \left( \frac{2}{3} \delta^{(3)}(\mathbf{r}) \delta_{a,b} + \frac{3r_a r_b - 3|\mathbf{r}|^2 \delta_{a,b}}{4\pi|\mathbf{r}|^5} \right) \\ &= \left( -\frac{q_e^2}{4\pi\epsilon_0} \right) \frac{1}{4} \left( \frac{\hbar}{m_0 c} \right)^2 \left( \frac{8}{3} \pi \delta^{(3)}(\mathbf{r}) \delta_{a,b} + \frac{3r_a r_b - 3|\mathbf{r}|^2 \delta_{a,b}}{|\mathbf{r}|^5} \right) \end{aligned} \quad (576)$$

Finally the potential of the spin–other orbit interaction  $V_b^{(osp,o)}(\mathbf{r})$  is evaluated. Here one can again make use of the transformation (558) and find

$$\begin{aligned}
V_b^{(osp,o)}(\mathbf{r}) &= \left(-\frac{q_e^2}{\varepsilon_0}\right) \int \frac{d^3q}{(2\pi)^3} \frac{1}{|\mathbf{q}|^2} e^{i\mathbf{q}\cdot\mathbf{r}} \left(\frac{i}{2} \frac{\hbar q_b}{m_0 c}\right) \\
&= \left(-\frac{q_e^2}{\varepsilon_0}\right) \frac{i}{2} \frac{\hbar}{m_0 c} \int \frac{d^3q}{(2\pi)^3} \frac{(\mathcal{R}\mathbf{q}')_b}{|\mathbf{q}'|^2} e^{i(\mathcal{R}\mathbf{q}')\cdot\mathbf{r}} \\
&= \left(-\frac{q_e^2}{\varepsilon_0}\right) \frac{i}{2} \frac{\hbar}{m_0 c} \frac{1}{(2\pi)^2} \int_0^\infty dq' q'^2 \int_0^\pi d\vartheta' \sin(\vartheta') \frac{1}{2\pi} \int_0^{2\pi} d\varphi \frac{\mathcal{R}_{b,m} q'_m}{q'^2} e^{irq' \cos(\vartheta')} \\
&= \left(-\frac{q_e^2}{\varepsilon_0}\right) \frac{i}{2} \frac{\hbar}{m_0 c} \frac{1}{(2\pi)^2} \int_0^\infty dq' q'^2 \int_0^\pi d\vartheta' \sin(\vartheta') \frac{\mathcal{R}_{b,z} q' \cos(\vartheta')}{q'^2} e^{irq' \cos(\vartheta')} \\
&= \left(-\frac{q_e^2}{\varepsilon_0}\right) \frac{i}{2} \frac{\hbar}{m_0 c} \mathcal{R}_{b,z} \frac{1}{(2\pi)^2} \int_0^\infty dq' q' \int_{-1}^1 dt t e^{irq't} \\
&= \left(-\frac{q_e^2}{\varepsilon_0}\right) \frac{1}{2} \frac{\hbar}{m_0 c} \mathcal{R}_{b,z} \frac{1}{(2\pi)^2} \underbrace{\left(\frac{-1}{r^2}\right) \int_{-\infty}^\infty dx \frac{\sin(x)}{x}}_{=\pi}
\end{aligned} \tag{577}$$

Applying  $\mathcal{R}_{b,z} = \frac{r_b}{r}$  then

$$\begin{aligned}
V_b^{(osp,o)}(\mathbf{r}) &= \left(-\frac{q_e^2}{\varepsilon_0}\right) \frac{1}{2} \frac{\hbar}{m_0 c} \frac{1}{4\pi} \frac{-r_b}{r^3} \\
&= \frac{1}{2} \frac{\hbar}{m_0 c} \frac{q_e^2}{4\pi\varepsilon_0} \frac{r_b}{r^3}
\end{aligned} \tag{578}$$

# I Complement to the Evaluation of $\hat{\mathcal{M}}_{\perp}^{(e)}$

**Proof of Identity (196)**

Consider a power series with matrix valued coefficients  $F_n$  according to

$$F(w) = \sum_{n=0}^{\infty} F_n \cdot w^n \quad (579)$$

With the projection operators  $P^{(\pm)}$  follows [7]

$$\begin{aligned} F \left[ z \left( P^{(+)} - P^{(-)} \right) \right] &= \sum_{n=0}^{\infty} F_n \cdot \left( z \left( P^{(+)} - P^{(-)} \right) \right)^n \\ &= \sum_{j=0}^{\infty} F_{2j} \cdot \left( z \left( P^{(+)} - P^{(-)} \right) \right)^{2j} + \sum_{j=0}^{\infty} F_{2j+1} \cdot \left( z \left( P^{(+)} - P^{(-)} \right) \right)^{2j+1} \\ &= \sum_{j=0}^{\infty} F_{2j} \cdot z^{2j} \left( P^{(+)} - P^{(-)} \right)^{2j} + \sum_{j=0}^{\infty} F_{2j+1} \cdot z^{2j+1} \left( P^{(+)} - P^{(-)} \right)^{2j+1} \end{aligned} \quad (580)$$

Now [7]

$$\begin{aligned} \left( P^{(+)} - P^{(-)} \right)^{2j} &= \left( \left( P^{(+)} - P^{(-)} \right)^2 \right)^j = P^{(+)} + P^{(-)} = \mathbf{1} \\ \left( P^{(+)} - P^{(-)} \right)^{2j+1} &= \left( P^{(+)} - P^{(-)} \right)^{2j} \left( P^{(+)} - P^{(-)} \right) = P^{(+)} - P^{(-)} \end{aligned} \quad (581)$$

Therefore one finds for (580) [7]

$$F \left[ z \left( P^{(+)} - P^{(-)} \right) \right] = \left( \sum_{j=0}^{\infty} F_{2j} \cdot z^{2j} \right) \left( P^{(+)} + P^{(-)} \right) + \left( \sum_{j=0}^{\infty} F_{2j+1} \cdot z^{2j+1} \right) \left( P^{(+)} - P^{(-)} \right) \quad (582)$$

On the other hand there holds [7]

$$\begin{aligned} \sum_{j=0}^{\infty} F_{2j} \cdot z^{2j} &= \frac{1}{2} (F(z) + F(-z)) \\ \sum_{j=0}^{\infty} F_{2j+1} \cdot z^{2j+1} &= \frac{1}{2} (F(z) - F(-z)) \end{aligned} \quad (583)$$

Inserting (583) to (582) finally yields [7]

$$\begin{aligned} F \left[ z \left( P^{(+)} - P^{(-)} \right) \right] &= \frac{1}{2} (F(z) + F(-z)) \left( P^{(+)} + P^{(-)} \right) + \frac{1}{2} (F(z) - F(-z)) \left( P^{(+)} - P^{(-)} \right) \\ &= F(z) P^{(+)} + F(-z) P^{(-)} \end{aligned} \quad (584)$$

End of the proof.

### Evaluation of $\hat{\mathcal{M}}_{\perp}^{(e)}$

Here it is shown how one can come to the final result (203) for the transversal renormalization contribution. For this the operator  $e^{-iq_a \hat{x}_a} \circ$

$\frac{Z - \frac{\tilde{E}_{K'} + \tilde{E}_{K'}}{2} \mathbf{1}_{4 \times 4}}{Z^2 - \left( \frac{\tilde{E}_{K'} + \tilde{E}_{K'}}{2} \right)^2 \mathbf{1}_{4 \times 4}} \circ e^{iq_a \hat{x}_a}$  and the operator  $e^{-iq_a \hat{x}_a} \circ \mathbb{C}_q \circ e^{iq_a \hat{x}_a}$  have to be further evaluated.

Recalling

$$\begin{aligned} \tilde{\mathbb{H}}^{(D)} &= \beta + \alpha_a \frac{\Pi_a}{m_0 c} \\ \tilde{\mathbb{H}}^{(D)} \circ \tilde{\mathbb{H}}^{(D)} &= \mathbf{1}_{4 \times 4} + \frac{2}{m_0 c^2} \mathbb{H}_{4 \times 4}^{(P,0)} \\ \mathbb{H}_{4 \times 4}^{(P,0)} &= \frac{\Pi_b \Pi_b}{2m_0} \mathbf{1}_{4 \times 4} - \frac{q_e \hbar}{2m_0} B_b^{(ext)} \sigma_b \end{aligned}$$

one finds for  $Z^2$  [7]

$$\begin{aligned} Z^2 &= (1 + \tilde{\omega}_q^2) \mathbf{1}_{4 \times 4} + \frac{2}{m_0 c^2} \left( \frac{\Pi_b \Pi_b}{2m_0} \mathbf{1}_{4 \times 4} - \frac{q_e \hbar}{2m_0} B_b^{(ext)} \sigma_b \right) \\ &\quad + 2\tilde{\omega}_q \cdot \sqrt{\mathbf{1}_{4 \times 4} + \frac{2}{m_0 c^2} \left( \frac{\Pi_b \Pi_b}{2m_0} \mathbf{1}_{4 \times 4} - \frac{q_e \hbar}{2m_0} B_b^{(ext)} \sigma_b \right)} \end{aligned}$$

From the BCH expansion, see also below (629), one finds [7]

$$e^{-iq_a \cdot \hat{x}_a} \circ \Pi_b \circ e^{iq_a \cdot \hat{x}_a} = \Pi_b + \sum_{j=1}^{\infty} \frac{1}{j!} [-iq_a \cdot \hat{x}_a, \Pi_b]^{(j)} = \Pi_b + \hbar q_b \quad (585)$$

which is valid for any potency  $n$  according to [7]

$$e^{-iq_a \cdot \hat{x}_a} \circ (\Pi_b)^n \circ e^{iq_a \cdot \hat{x}_a} = \left( e^{-iq_a \cdot \hat{x}_a} \circ (\Pi_b) \circ e^{iq_a \cdot \hat{x}_a} \right)^n = (\Pi_b + \hbar q_b)^n \quad (586)$$

and for any function being representable as a power series  $F(z) = \sum_n F_n z^n$  [7]

$$\begin{aligned}
e^{-iq_a \cdot \hat{x}_a} \circ F(\Pi_b) \circ e^{iq_a \cdot \hat{x}_a} &= \sum_n F_n \cdot e^{-iq_a \cdot \hat{x}_a} \circ (\Pi_b)^n \circ e^{iq_a \cdot \hat{x}_a} \\
&= \sum_n F_n \cdot (\Pi_b + \hbar q_b)^n \\
&= F(\Pi_b + \hbar q_b)
\end{aligned} \tag{587}$$

From this readily follows for the Dirac Hamiltonian  $\tilde{H}^{(D)}$  [7]

$$\begin{aligned}
e^{-iq_a \cdot \hat{x}_a} \circ \tilde{H}^{(D)} \circ e^{iq_a \cdot \hat{x}_a} &= \tilde{H}^{(D)} + \alpha_a \frac{\hbar q_a}{m_0 c} \\
&= \beta + \alpha_a \frac{\Pi_a}{m_0 c} + \alpha_a \frac{\hbar q_a}{m_0 c}
\end{aligned} \tag{588}$$

and for its square [7]

$$\begin{aligned}
e^{-iq_a \cdot \hat{x}_a} \circ \sqrt{\tilde{H}^{(D)} \circ \tilde{H}^{(D)}} \circ e^{iq_a \cdot \hat{x}_a} &= e^{-iq_a \cdot \hat{x}_a} \circ \sqrt{\mathbf{1}_{4 \times 4} + \frac{2}{m_0 c^2} \mathbf{H}_{4 \times 4}^{(P,0)}} \circ e^{iq_a \cdot \hat{x}_a} \\
&= \sqrt{\mathbf{1}_{4 \times 4} + \frac{2}{m_0 c^2} \left( e^{-iq_a \cdot \hat{x}_a} \circ \mathbf{H}_{4 \times 4}^{(P,0)} \circ e^{iq_a \cdot \hat{x}_a} \right)} \\
&= \sqrt{\left( 1 + \left| \frac{\hbar \mathbf{q}}{m_0 c} \right|^2 \right) \mathbf{1}_{4 \times 4} + 2 \left( \frac{\hbar q_b}{m_0 c} \frac{\Pi_b}{m_0 c} \mathbf{1}_{4 \times 4} + \frac{\mathbf{H}_{4 \times 4}^{(P,0)}}{m_0 c^2} \right)}
\end{aligned} \tag{589}$$

Please recognize that in the nonrelativistic subspace of the QED Hamiltonian the following inequality holds for **any** wavenumber  $|\mathbf{q}|$  of the photons [7]

$$\left( 1 + \left| \frac{\hbar \mathbf{q}}{m_0 c} \right|^2 \right) \mathbf{1}_{4 \times 4} \gg 2 \left( \frac{\hbar q_b}{m_0 c} \frac{\Pi_b}{m_0 c} \mathbf{1}_{4 \times 4} + \frac{\mathbf{H}_{4 \times 4}^{(P,0)}}{m_0 c^2} \right) \tag{590}$$

iff the operators  $\frac{\Pi_b}{m_0 c}$  and  $\frac{\mathbf{H}_{4 \times 4}^{(P,0)}}{m_0 c^2}$  are being applied to nonrelativistic wave functions. This is because the latter vary slowly on the Compton wavelength  $\lambda_C$  compared to the Bohr lengthscale  $a_B$ .

Therefore one may assume that the contributions generated by  $\frac{\hbar q_b}{m_0 c} \frac{\Pi_b}{m_0 c}$  are of first order, and the contributions generated by  $\frac{\mathbf{H}_{4 \times 4}^{(P,0)}}{m_0 c^2}$  are of second

order with respect to the leading term  $1 + \left(\frac{\hbar|\mathbf{q}|}{m_0c}\right)^2$ . This is important where the renormalizing corrections are transformed to the Newton–Wigner representation.

Introducing the abbreviations [7]

$$\begin{aligned} \left|\frac{\hbar\mathbf{q}}{m_0c}\right| &= \tilde{\omega}_q \\ \sqrt{1 + \left|\frac{\hbar\mathbf{q}}{m_0c}\right|^2} &= \sqrt{1 + \tilde{\omega}_q^2} \end{aligned} \tag{591}$$

and using the Taylor expansions

$$\begin{aligned} \sqrt{1 + 2(X\varepsilon + Y\varepsilon^2)} &= 1 + X\varepsilon + \left(Y - \frac{1}{2}X^2\right)\varepsilon^2 + O(\varepsilon^3) \\ \frac{1}{\sqrt{1 + 2(X\varepsilon + Y\varepsilon^2)}} &= 1 - X\varepsilon + \left(\frac{3}{2}X^2 - Y\right)\varepsilon^2 + O(\varepsilon^3) \\ (1 + X\varepsilon + Y\varepsilon^2)^{-1} &= 1 - X\varepsilon + (X^2 - Y)\varepsilon^2 + O(\varepsilon^3) \end{aligned} \tag{592}$$

one can now evaluate the operator in (202) according to [7]

$$\begin{aligned}
& e^{-iq_a \hat{x}_a} \frac{z \pm \frac{\tilde{E}_k + \tilde{E}_K}{2} \mathbf{1}_{4 \times 4}}{z^2 - \left( \frac{\tilde{E}_k + \tilde{E}_K}{2} \right)^2} e^{+iq_a \hat{x}_a} \\
&= e^{-iq_a \hat{x}_a} \left( \frac{\pm \frac{\tilde{E}_k + \tilde{E}_K}{2} \mathbf{1}_{4 \times 4} + \left( \beta + \alpha_a \frac{\Pi_a}{m_0 c} \right) \left( \mathbf{1}_{4 \times 4} + \frac{\tilde{\omega}_q}{\sqrt{\mathbf{1}_{4 \times 4} + \frac{2}{m_0 c^2} \left( \frac{\Pi_b \Pi_b}{2 m_0} \mathbf{1}_{4 \times 4} - \frac{q_e \hbar}{2 m_0} B_b^{(ext)} \sigma_b \right)}} \right)}{\left( (1 + \tilde{\omega}_q^2) \mathbf{1}_{4 \times 4} + \frac{2}{m_0 c^2} \left( \frac{\Pi_b \Pi_b}{2 m_0} \mathbf{1}_{4 \times 4} - \frac{q_e \hbar}{2 m_0} B_b^{(ext)} \sigma_b \right) + 2 \tilde{\omega}_q \cdot \sqrt{\mathbf{1}_{4 \times 4} + \frac{2}{m_0 c^2} \left( \frac{\Pi_b \Pi_b}{2 m_0} \mathbf{1}_{4 \times 4} - \frac{q_e \hbar}{2 m_0} B_b^{(ext)} \sigma_b \right)} - \left( \frac{\tilde{E}_k + \tilde{E}_K}{2} \right)^2 \right)} \right) e^{+iq_a \hat{x}_a} \\
&= \frac{\pm \frac{\tilde{E}_k + \tilde{E}_K}{2} \mathbf{1}_{4 \times 4} + \left( \beta + \alpha_a \frac{(\Pi_a + \hbar q_a)}{m_0 c} \right) \left( \mathbf{1}_{4 \times 4} + \frac{\tilde{\omega}_q}{\sqrt{\mathbf{1}_{4 \times 4} + \frac{2}{m_0 c^2} \left( \frac{(\Pi_b + \hbar q_b)(\Pi_b + \hbar q_b)}{2 m_0} \mathbf{1}_{4 \times 4} - \frac{q_e \hbar}{2 m_0} B_b^{(ext)} \sigma_b \right)}} \right)}{\tilde{\omega}_q^2 \mathbf{1}_{4 \times 4} + \frac{2}{m_0 c^2} \left( \frac{(\Pi_b + \hbar q_b)(\Pi_b + \hbar q_b)}{2 m_0} \mathbf{1}_{4 \times 4} - \frac{q_e \hbar}{2 m_0} B_b^{(ext)} \sigma_b \right) + 2 \tilde{\omega}_q \cdot \sqrt{\mathbf{1}_{4 \times 4} + \frac{2}{m_0 c^2} \left( \frac{(\Pi_b + \hbar q_b)(\Pi_b + \hbar q_b)}{2 m_0} \mathbf{1}_{4 \times 4} - \frac{q_e \hbar}{2 m_0} B_b^{(ext)} \sigma_b \right)} + \left( 1 - \left( \frac{\tilde{E}_k + \tilde{E}_K}{2} \right)^2 \right) \mathbf{1}_{4 \times 4}} \\
&= \frac{\pm \frac{\tilde{E}_k + \tilde{E}_K}{2} \mathbf{1}_{4 \times 4} + \left( \beta + \alpha_a \frac{(\Pi_a + \hbar q_a)}{m_0 c} \right) \left( \mathbf{1}_{4 \times 4} + \frac{\tilde{\omega}_q}{\sqrt{\left( 1 + \left| \frac{\hbar \mathbf{q}}{m_0 c} \right|^2 \right) \mathbf{1}_{4 \times 4} + 2 \left( \frac{\hbar q_b}{m_0 c} \frac{\Pi_b}{m_0 c} \mathbf{1}_{4 \times 4} + \frac{H_{4 \times 4}^{(P,0)}}{m_0 c^2} \right)}} \right)}{\tilde{\omega}_q^2 \mathbf{1}_{4 \times 4} + \left| \frac{\hbar \mathbf{q}}{m_0 c} \right|^2 \mathbf{1}_{4 \times 4} + 2 \left( \frac{\hbar q_b}{m_0 c} \frac{\Pi_b}{m_0 c} \mathbf{1}_{4 \times 4} + \frac{H_{4 \times 4}^{(P,0)}}{m_0 c^2} \right) + 2 \tilde{\omega}_q \cdot \sqrt{\left( 1 + \left| \frac{\hbar \mathbf{q}}{m_0 c} \right|^2 \right) \mathbf{1}_{4 \times 4} + 2 \left( \frac{\hbar q_b}{m_0 c} \frac{\Pi_b}{m_0 c} \mathbf{1}_{4 \times 4} + \frac{H_{4 \times 4}^{(P,0)}}{m_0 c^2} \right)} + \left( 1 - \left( \frac{\tilde{E}_k + \tilde{E}_K}{2} \right)^2 \right) \mathbf{1}_{4 \times 4}} \\
&= \frac{\pm \frac{\tilde{E}_k + \tilde{E}_K}{2} \mathbf{1}_{4 \times 4} + \left( \beta + \alpha_a \frac{\hbar q_a}{m_0 c} + \alpha_a \frac{\Pi_a}{m_0 c} \right) \left( \mathbf{1}_{4 \times 4} + \frac{\tilde{\omega}_q}{\sqrt{\left( 1 + \tilde{\omega}_q^2 \right) \mathbf{1}_{4 \times 4} + 2 \left( \frac{\hbar q_b}{m_0 c} \frac{\Pi_b}{m_0 c} \mathbf{1}_{4 \times 4} + \frac{H_{4 \times 4}^{(P,0)}}{m_0 c^2} \right)}} \right)}{2 \tilde{\omega}_q^2 \mathbf{1}_{4 \times 4} + 2 \left( \frac{\hbar q_b}{m_0 c} \frac{\Pi_b}{m_0 c} \mathbf{1}_{4 \times 4} + \frac{H_{4 \times 4}^{(P,0)}}{m_0 c^2} \right) + 2 \tilde{\omega}_q \cdot \sqrt{\left( 1 + \tilde{\omega}_q^2 \right) \mathbf{1}_{4 \times 4} + 2 \left( \frac{\hbar q_b}{m_0 c} \frac{\Pi_b}{m_0 c} \mathbf{1}_{4 \times 4} + \frac{H_{4 \times 4}^{(P,0)}}{m_0 c^2} \right)} + \left( 1 - \left( \frac{\tilde{E}_k + \tilde{E}_K}{2} \right)^2 \right) \mathbf{1}_{4 \times 4}} \\
&\equiv \frac{1}{2G_q} \circ F_q^{(\pm)}
\end{aligned} \tag{593}$$

Here has been defined [7]

$$\begin{aligned}
F_q^{(\pm)} &= \left( \pm \frac{\tilde{E}_k + \tilde{E}_K}{2} + \beta + \alpha_a \frac{\hbar q_a}{m_0 c} + \alpha_a \frac{\Pi_a}{m_0 c} \right) \mathbf{1}_{4 \times 4} + \tilde{\omega}_q \mathbf{R}_q \\
\mathbf{R}_q &= \frac{\beta + \alpha_a \frac{\hbar q_a}{m_0 c} + \alpha_a \frac{\Pi_a}{m_0 c}}{\sqrt{\left( 1 + \tilde{\omega}_q^2 \right) \mathbf{1}_{4 \times 4} + 2 \left( \frac{\hbar q_b}{m_0 c} \frac{\Pi_b}{m_0 c} \mathbf{1}_{4 \times 4} + \frac{H_{4 \times 4}^{(P,0)}}{m_0 c^2} \right)}} \\
&= e^{-iq_a \cdot \hat{x}_a} \circ \frac{\tilde{\mathbf{H}}^{(D)}}{\sqrt{\tilde{\mathbf{H}}^{(D)} \circ \tilde{\mathbf{H}}^{(D)}}} \circ e^{iq_a \cdot \hat{x}_a}
\end{aligned} \tag{594}$$

and [7]

$$G_q = \begin{cases} \tilde{\omega}_q^2 \mathbf{1}_{4 \times 4} + \left( \frac{\hbar q_b}{m_0 c} \frac{\Pi_b}{m_0 c} \mathbf{1}_{4 \times 4} + \frac{H_{4 \times 4}^{(P,0)}}{m_0 c^2} \right) + \tilde{\omega}_q \cdot \sqrt{\left( 1 + \tilde{\omega}_q^2 \right) \mathbf{1}_{4 \times 4} + 2 \left( \frac{\hbar q_b}{m_0 c} \frac{\Pi_b}{m_0 c} \mathbf{1}_{4 \times 4} + \frac{H_{4 \times 4}^{(P,0)}}{m_0 c^2} \right)} \\ + \frac{1 - \left( \frac{\tilde{E}_k + \tilde{E}_K}{2} \right)^2}{2} \mathbf{1}_{4 \times 4} \end{cases} \tag{595}$$

Further abbreviations for the purpose of clarity according to [7]

$$\begin{aligned}\xi &\equiv \tilde{\omega}_q \\ w &\equiv \sqrt{1 + \tilde{\omega}_q^2} = w(\xi)\end{aligned}\tag{596}$$

lead to the representation of the inverse of  $\mathbf{G}_q$  [7]

$$\frac{1}{\mathbf{G}_q} = \left( \begin{aligned} &\underbrace{\left( \frac{w}{\xi} - 1 \right) \mathbf{1}_{4 \times 4}}_{=O(1)} \\ &+ \underbrace{\frac{\hbar q_a}{m_0 c} \frac{\Pi_a}{m_0 c} \left( \frac{w}{\xi} - \frac{\xi}{w} - \frac{1}{\xi^2} \right) \mathbf{1}_{4 \times 4}}_{=O(\alpha_{FS})} \\ &+ \left( \begin{aligned} &+ \frac{\hbar q_a}{m_0 c} \frac{\Pi_a}{m_0 c} \frac{\hbar q_{a'}}{m_0 c} \frac{\Pi_{a'}}{m_0 c} \left( -\frac{w}{2\xi} + \frac{\xi}{2w} + \frac{\xi}{2w^3} + \frac{w}{\xi^3} - \frac{1}{\xi^2} \right) \mathbf{1}_{4 \times 4} \\ &+ \left( \frac{w}{\xi} - \frac{\xi}{w} - \frac{1}{\xi^2} \right) \frac{\mathbf{H}_{4 \times 4}^{(P,0)}}{m_0 c^2} \\ &+ \left( 1 - \left( \frac{\tilde{E}_k + \tilde{E}_K}{2} \right)^2 \right) \left( \frac{w}{\xi} - 1 - \frac{1}{2\xi^2} \right) \mathbf{1}_{4 \times 4} \end{aligned} \right) \\ &\underbrace{\hspace{10em}}_{=O(\alpha_{FS}^2)} \\ &+ O(\alpha_{FS}^3) \end{aligned} \right)\tag{597}$$

Now the operators  $\mathbf{F}_q^{(\pm)}$  are expanded. The expansion of the inverse of the square root (592) is given by [7]

$$\begin{aligned}&\frac{1}{\sqrt{(1 + \tilde{\omega}_q^2) \mathbf{1}_{4 \times 4} + 2 \left( \frac{\hbar q_b}{m_0 c} \frac{\Pi_b}{m_0 c} \mathbf{1}_{4 \times 4} + \frac{\mathbf{H}_{4 \times 4}^{(P,0)}}{m_0 c^2} \right)}} \\ &= \frac{1}{w} - \frac{1}{w^3} \frac{\hbar q_b}{m_0 c} \frac{\Pi_b}{m_0 c} + \frac{3}{2w^5} \left( \frac{\hbar q_b}{m_0 c} \frac{\Pi_b}{m_0 c} \right)^2 - \frac{1}{w^3} \frac{\mathbf{H}_{4 \times 4}^{(P,0)}}{m_0 c^2} + O(\alpha_{FS}^3)\end{aligned}\tag{598}$$

Since  $\alpha_a$  and  $\frac{\mathbf{H}_{4 \times 4}^{(P,0)}}{m_0 c^2}$  do not commute for a given magnetic induction field  $B_b^{(ext)} \neq 0$  one has to symmetrize the operators  $\mathbf{R}_q$  and  $\mathbf{F}_q^{(\pm)}$  [7]:



$$\begin{aligned}
R_q &= \frac{\beta + \alpha_a \frac{\hbar q_a}{m_0 c} + \alpha_a \frac{\Pi_a}{m_0 c}}{\sqrt{\left(1 + \tilde{\omega}_q^2\right) 1_{4 \times 4} + 2 \left( \frac{\hbar q_b}{m_0 c} \frac{\Pi_b}{m_0 c} 1_{4 \times 4} + \frac{H_{4 \times 4}^{(P,0)}}{m_0 c^2} \right)}} \\
&= \frac{1}{2} \left[ \left( \underbrace{\beta + \alpha_a \frac{\hbar q_a}{m_0 c}}_{=O(1)} + \underbrace{\alpha_a \frac{\Pi_a}{m_0 c}}_{=O(\alpha_{FS})} \right) \left( \underbrace{\frac{1}{w}}_{=O(1)} - \underbrace{\frac{1}{w^3} \frac{\hbar q_b}{m_0 c} \frac{\Pi_b}{m_0 c}}_{=O(\alpha_{FS})} + \underbrace{\frac{3}{2w^5} \left( \frac{\hbar q_b}{m_0 c} \frac{\Pi_b}{m_0 c} \right)^2}_{=O(\alpha_{FS}^2)} - \underbrace{\frac{1}{w^3} \frac{H_{4 \times 4}^{(P,0)}}{m_0 c^2}}_{=O(\alpha_{FS}^2)} + O(\alpha_{FS}^3) \right) \right. \\
&\quad \left. + \left( \underbrace{\frac{1}{w}}_{=O(1)} - \underbrace{\frac{1}{w^3} \frac{\hbar q_b}{m_0 c} \frac{\Pi_b}{m_0 c}}_{=O(\alpha_{FS})} + \underbrace{\frac{3}{2w^5} \left( \frac{\hbar q_b}{m_0 c} \frac{\Pi_b}{m_0 c} \right)^2}_{=O(\alpha_{FS}^2)} - \underbrace{\frac{1}{w^3} \frac{H_{4 \times 4}^{(P,0)}}{m_0 c^2}}_{=O(\alpha_{FS}^2)} + O(\alpha_{FS}^3) \right) \left( \underbrace{\beta + \alpha_a \frac{\hbar q_a}{m_0 c}}_{=O(1)} + \underbrace{\alpha_a \frac{\Pi_a}{m_0 c}}_{=O(\alpha_{FS})} \right) \right] \\
&= \left[ \underbrace{\left( \beta + \alpha_a \frac{\hbar q_a}{m_0 c} \right) \frac{1}{w}}_{=O(1)} \right. \\
&\quad \left. + \underbrace{\alpha_a \frac{\Pi_a}{m_0 c} \frac{1}{w} - \left( \beta + \alpha_a \frac{\hbar q_a}{m_0 c} \right) \frac{\hbar q_b}{m_0 c} \frac{\Pi_b}{m_0 c} \frac{1}{w^3}}_{O(\alpha_{FS})} \right] \\
&\quad + \left( \underbrace{-\frac{1}{w^3} \frac{H_{4 \times 4}^{(P,0)}}{m_0 c^2} \beta - \frac{1}{2w^3} \left( \frac{H_{4 \times 4}^{(P,0)}}{m_0 c^2} \alpha_a \frac{\hbar q_a}{m_0 c} + \alpha_a \frac{\hbar q_a}{m_0 c} \frac{H_{4 \times 4}^{(P,0)}}{m_0 c^2} \right)}_{=O(\alpha_{FS}^2)} \right. \\
&\quad \left. - \frac{1}{w^3} \frac{\hbar q_b}{m_0 c} \frac{\Pi_b}{m_0 c} \alpha_a \frac{\Pi_a}{m_0 c} \right)
\end{aligned}$$

(599)

And altogether [7]

$$\begin{aligned}
e^{-iq_a \bar{\lambda}_a} \frac{Z \pm \frac{\tilde{E}_k + \tilde{E}_K}{2} 1_{4 \times 4}}{Z^2 - \left( \frac{\tilde{E}_k + \tilde{E}_K}{2} \right)^2} e^{+iq_a \bar{\lambda}_a} &\equiv \frac{1}{2G_q} \circ F_q^{(\pm)} = \frac{1}{2} \left( \frac{1}{2G_q} F_q^{(\pm)} + F_q^{(\pm)} \frac{1}{2G_q} \right) \\
&\left( \underbrace{\left( \frac{w}{\xi} - 1 \right) 1_{4 \times 4}}_{O(1)} \underbrace{\left( \pm \frac{\tilde{E}_k + \tilde{E}_K}{2} 1_{4 \times 4} + \left( \beta + \alpha_a \frac{\hbar q_a}{m_0 c} \right) \left( 1 + \frac{\xi}{w} \right) \right)}_{O(1)} \right) \\
&+ \underbrace{\left( \frac{w}{\xi} - 1 \right) 1_{4 \times 4}}_{O(1)} \left( \underbrace{\left( \left( 1 + \frac{\xi}{w} \right) \frac{\Pi_a}{m_0 c} - \frac{\xi}{w^3} \frac{\hbar q_a}{m_0 c} \frac{\hbar q_b}{m_0 c} \frac{\Pi_b}{m_0 c} \right) \alpha_a - \frac{\xi}{w^3} \frac{\hbar q_b}{m_0 c} \frac{\Pi_b}{m_0 c}}_{O(\alpha_{FS})} \beta \right) \\
&+ \underbrace{\frac{\hbar q_{a'}}{m_0 c} \frac{\Pi_{a'}}{m_0 c}}_{O(\alpha_{FS})} \underbrace{\left( \frac{w}{\xi} - \frac{\xi}{w} - \frac{1}{\xi^2} \right) 1_{4 \times 4}}_{O(\alpha_{FS})} \cdot \underbrace{\left( \pm \frac{\tilde{E}_k + \tilde{E}_K}{2} 1_{4 \times 4} + \left( \beta + \alpha_a \frac{\hbar q_a}{m_0 c} \right) \left( 1 + \frac{\xi}{w} \right) \right)}_{O(1)} \\
&+ \underbrace{\left( \frac{w}{\xi} - 1 \right) 1_{4 \times 4}}_{O(1)} \left( \underbrace{\left( \begin{aligned} &\left( \frac{3\xi}{2w^5} \left( \frac{\hbar q_b}{m_0 c} \frac{\Pi_b}{m_0 c} \right)^2 - \frac{\xi}{w^3} \frac{H_{4 \times 4}^{(P,0)}}{m_0 c^2} \right) \beta \\ &\left( \frac{3\xi}{2w^5} \frac{\hbar q_a}{m_0 c} \left( \frac{\hbar q_b}{m_0 c} \frac{\Pi_b}{m_0 c} \right)^2 - \frac{\xi}{w^3} \frac{\hbar q_b}{m_0 c} \frac{\Pi_b}{m_0 c} \frac{\Pi_a}{m_0 c} \right) \alpha_a \\ &- \frac{\xi}{2w^3} \left( \frac{H_{4 \times 4}^{(P,0)}}{m_0 c^2} \alpha_a \frac{\hbar q_a}{m_0 c} + \alpha_a \frac{\hbar q_a}{m_0 c} \frac{H_{4 \times 4}^{(P,0)}}{m_0 c^2} \right) \end{aligned} \right)}_{=O(\alpha_{FS}^2)} \right) \\
&= \frac{1}{2} + \underbrace{\frac{\hbar q_{a'}}{m_0 c} \frac{\Pi_{a'}}{m_0 c}}_{O(\alpha_{FS})} \underbrace{\left( \frac{w}{\xi} - \frac{\xi}{w} - \frac{1}{\xi^2} \right) 1_{4 \times 4}}_{O(\alpha_{FS})} \cdot \underbrace{\left( \left( \left( 1 + \frac{\xi}{w} \right) \frac{\Pi_a}{m_0 c} - \frac{\xi}{w^3} \frac{\hbar q_a}{m_0 c} \frac{\hbar q_b}{m_0 c} \frac{\Pi_b}{m_0 c} \right) \alpha_a - \frac{\xi}{w^3} \frac{\hbar q_b}{m_0 c} \frac{\Pi_b}{m_0 c} \right)}_{O(\alpha_{FS})} \beta \\
&+ \frac{1}{2} \left( \underbrace{\left( \begin{aligned} &+ \frac{\hbar q_a}{m_0 c} \frac{\Pi_a}{m_0 c} \frac{\hbar q_{a'}}{m_0 c} \frac{\Pi_{a'}}{m_0 c} \left( -\frac{w}{2\xi} + \frac{\xi}{2w} + \frac{\xi}{2w^3} + \frac{w}{\xi^3} - \frac{1}{\xi^2} \right) 1_{4 \times 4} \\ &+ \left( \frac{w}{\xi} - \frac{\xi}{w} - \frac{1}{\xi^2} \right) \frac{H_{4 \times 4}^{(P,0)}}{m_0 c^2} \\ &+ \left( 1 - \left( \frac{\tilde{E}_k + \tilde{E}_K}{2} \right)^2 \right) \left( \frac{w}{\xi} - 1 - \frac{1}{2\xi^2} \right) 1_{4 \times 4} \end{aligned} \right)}_{=O(\alpha_{FS}^2)} \cdot \underbrace{\left( \pm \frac{\tilde{E}_k + \tilde{E}_K}{2} 1_{4 \times 4} + \left( \beta + \alpha_a \frac{\hbar q_a}{m_0 c} \right) \left( 1 + \frac{\xi}{w} \right) \right)}_{O(1)} \\
&+ \frac{1}{2} \underbrace{\left( \pm \frac{\tilde{E}_k + \tilde{E}_K}{2} 1_{4 \times 4} + \left( \beta + \alpha_a \frac{\hbar q_a}{m_0 c} \right) \left( 1 + \frac{\xi}{w} \right) \right)}_{O(1)} \left( \underbrace{\left( \begin{aligned} &+ \frac{\hbar q_a}{m_0 c} \frac{\Pi_a}{m_0 c} \frac{\hbar q_{a'}}{m_0 c} \frac{\Pi_{a'}}{m_0 c} \left( -\frac{w}{2\xi} + \frac{\xi}{2w} + \frac{\xi}{2w^3} + \frac{w}{\xi^3} - \frac{1}{\xi^2} \right) 1_{4 \times 4} \\ &+ \left( \frac{w}{\xi} - \frac{\xi}{w} - \frac{1}{\xi^2} \right) \frac{H_{4 \times 4}^{(P,0)}}{m_0 c^2} \\ &+ \left( 1 - \left( \frac{\tilde{E}_k + \tilde{E}_K}{2} \right)^2 \right) \left( \frac{w}{\xi} - 1 - \frac{1}{2\xi^2} \right) 1_{4 \times 4} \end{aligned} \right)}_{=O(\alpha_{FS}^2)} \right) \\
&\quad + O(\alpha_{FS}^3)
\end{aligned} \tag{600}$$

Next the  $q$ -shift of the operator  $C_q$  evaluated [7]:

$$\begin{aligned}
\mathbf{K}_q &\equiv e^{-iq_a \hat{x}_a} \circ \mathbf{C}_q \circ e^{iq_a \hat{x}_a} \\
&= e^{-iq_a \hat{x}_a} \circ \Theta_H \left[ \left( 2\tilde{\Omega}_{max} - \tilde{\omega}_q \right) \mathbf{1}_{4 \times 4} - \sqrt{\tilde{\mathbf{H}}(D) \circ \tilde{\mathbf{H}}(D)} \right] \circ e^{iq_a \hat{x}_a} \\
&= \Theta_H \left[ \left( 2\tilde{\Omega}_{max} - \tilde{\omega}_q \right) \mathbf{1}_{4 \times 4} - e^{-iq_a \hat{x}_a} \circ \sqrt{\tilde{\mathbf{H}}(D) \circ \tilde{\mathbf{H}}(D)} \circ e^{iq_a \hat{x}_a} \right] \\
&= \Theta_H \left[ \left( 2\tilde{\Omega}_{max} - \tilde{\omega}_q \right) \mathbf{1}_{4 \times 4} - \sqrt{\left( 1 + \tilde{\omega}_q^2 \right) \mathbf{1}_{4 \times 4} + 2 \left( \frac{\hbar q_b}{m_0 c} \frac{\Pi_b}{m_0 c} \mathbf{1}_{4 \times 4} + \frac{\mathbf{H}_{4 \times 4}^{(P,0)}}{m_0 c^2} \right)} \right] \\
&= \Theta_H \left[ \left( 2\tilde{\Omega}_{max} - \xi \right) \mathbf{1}_{4 \times 4} - w \cdot \sqrt{\mathbf{1}_{4 \times 4} + \frac{2}{w^2} \left( \xi \hat{q}_b \frac{\Pi_b}{m_0 c} \mathbf{1}_{4 \times 4} + \frac{\mathbf{H}_{4 \times 4}^{(P,0)}}{m_0 c^2} \right)} \right] \\
&= \Theta_H \left[ \left( 2\tilde{\Omega}_{max} - \xi - w \right) \mathbf{1}_{4 \times 4} - \frac{\xi}{w} \hat{q}_b \frac{\Pi_b}{m_0 c} \mathbf{1}_{4 \times 4} + O\left(\frac{1}{\xi}\right) \right] \\
&= \Theta_H \left[ \left( 2\tilde{\Omega}_{max} - 2\xi - \frac{1}{w+\xi} \right) \mathbf{1}_{4 \times 4} - \frac{\xi}{w} \hat{q}_b \frac{\Pi_b}{m_0 c} \mathbf{1}_{4 \times 4} + O\left(\frac{1}{\xi}\right) \right] \\
&= \Theta_H \left[ \left( 2\tilde{\Omega}_{max} - 2\xi \right) \mathbf{1}_{4 \times 4} - \hat{q}_b \frac{\Pi_b}{m_0 c} \mathbf{1}_{4 \times 4} + O\left(\frac{1}{\xi}\right) \right]
\end{aligned} \tag{601}$$

Since for the cut-off it has been assumed  $\tilde{\Omega}_{max} \gg 1$  contributions of the order  $O\left(\frac{1}{\xi}\right)$  and smaller do not contribute in the arguments of  $\mathbf{K}_q$  for  $\xi > \tilde{\Omega}_{max}$ . Hence one can neglect them, their contribution is smaller like  $O\left(\frac{1}{\tilde{\Omega}_{max}}\right)$ .

For the identity  $\Theta_H(2x) \equiv \Theta_H(x)$  one can write [7]

$$\frac{\mathbf{K}_q + \mathbf{K}_{-q}}{2} = \Theta_H\left(\tilde{\Omega}_{max} - \xi\right) + \left( \frac{\Theta_H\left[\left(\tilde{\Omega}_{max} - \xi\right) - \frac{1}{2} \hat{q}_b \frac{\Pi_b}{m_0 c}\right] - \Theta_H\left(\tilde{\Omega}_{max} - \xi\right)}{2} \right. \\
\left. \frac{\Theta_H\left[\left(\tilde{\Omega}_{max} - \xi\right) + \frac{1}{2} \hat{q}_b \frac{\Pi_b}{m_0 c}\right] - \Theta_H\left(\tilde{\Omega}_{max} - \xi\right)}{2} \right) \tag{602}$$

for the symmetric part of  $\mathbf{K}_q$ , and [7]

$$\frac{\mathbf{K}_q - \mathbf{K}_{-q}}{2} = \frac{\Theta_H\left[\left(\tilde{\Omega}_{max} - \xi\right) - \frac{1}{2} \hat{q}_b \frac{\Pi_b}{m_0 c}\right] - \Theta_H\left[\left(\tilde{\Omega}_{max} - \xi\right) + \frac{1}{2} \hat{q}_b \frac{\Pi_b}{m_0 c}\right]}{2} \tag{603}$$

for the antisymmetric part of  $\mathbf{K}_q$ .

As will be shown now, the symmetric part  $\frac{\mathsf{K}_q + \mathsf{K}_{-q}}{2}$  yields the main contribution to the integral, whereas the antisymmetric part  $\frac{\mathsf{K}_q - \mathsf{K}_{-q}}{2}$  yields a tiny, however important correction.

This can be seen by expanding the theta function for  $x \ll a$  according to [7]

$$\begin{aligned}\Theta_H[a+x] &= \Theta_H(a) + x\Theta'_H(a) + \frac{x^2}{2}\Theta''_H(a) + \dots \\ \Theta'_H(x) &= \delta(x) \\ \Theta''_H(x) &= \delta'(x)\end{aligned}\tag{604}$$

Now for the symmetric part (602), in case that  $\tilde{\Omega}_{max} \gg 1$ , the main contribution to the integral is given by  $\Theta_H(\tilde{\Omega}_{max} - \xi)$  because the first order contributions cancel due to the different signs in the expansion (604). This contribution corresponds to the cut-off procedure suggested by Cohen–Tannoudji et al. who only truncate the photon energy and do not consider the kinetic energy of the fermions in the cut-off [50].

One can therefore set [7]

$$\frac{\mathsf{K}_q + \mathsf{K}_{-q}}{2} = \Theta_H(\tilde{\Omega}_{max} - \xi)\tag{605}$$

For the antisymmetric part (603) there survives for  $\tilde{\Omega}_{max} \gg 1$  a small correction term  $-\hat{q}_b \frac{\Pi_b}{m_0 c} \delta(\tilde{\Omega}_{max} - \xi)$  because in that case the first order contribution of the expansion (604) does not cancel due to to sign! As is shown in subsection 6.3, this small correction will be crucial for a consistent renormalization of the bare electron mass  $m_e$ .

Inserting  $e^{-iq_a \hat{x}_a} \frac{Z_{\pm} \frac{\tilde{E}_k + \tilde{E}_K}{2} \mathbf{1}_{4 \times 4}}{Z^2 - \left(\frac{\tilde{E}_k + \tilde{E}_K}{2}\right)^2} e^{iq_a \hat{x}_a} \equiv \frac{1}{2G_q} \circ \mathsf{F}_q^{(\pm)}$  and  $e^{-iq_a \hat{x}_a} \circ \mathsf{C}_q \circ e^{iq_a \hat{x}_a} \equiv \mathsf{K}_q$  in (201) one finds [7]

$$\tilde{\mathsf{M}}_{k,K}^{(\perp, e, high)} = - \left(\frac{q_e^2}{2\varepsilon_0}\right) \left(\frac{\hbar}{m_0 c}\right)^2 \frac{1}{V} \sum_{\mathbf{q}} \frac{1}{\tilde{\omega}_q} \sum_{b,b'} \left(\delta_{b,b'} - \frac{q_b q_{b'}}{|\mathbf{q}|^2}\right) \langle U_k | \alpha_b \left(\mathsf{K}_q \circ \frac{1}{2G_q} \circ \mathsf{F}_q^{(+)}\right) \alpha_{b'} | U_K \rangle\tag{606}$$

and the symmetrization yields, under the substitution  $q_b \rightarrow -q_b$  [7],

$$\begin{aligned}
\tilde{M}_{k,K}^{(\perp,e)} = & - \left( \frac{q_e^2}{2\varepsilon_0} \right) \left( \frac{\hbar}{m_0 c} \right)^2 \frac{1}{V} \sum_{\mathbf{q}} \frac{1}{\tilde{\omega}_q} \sum_{b,b'} \left( \delta_{b,b'} - \frac{q_b q_{b'}}{|\mathbf{q}|^2} \right) \\
& \times \langle U_k | \alpha_b \left( \begin{array}{c} \frac{\mathbf{K}_q + \mathbf{K}_{-q}}{4} \circ \left( \frac{1}{2\mathbf{G}_q} \circ \mathbf{F}_q^{(+)} + \frac{1}{2\mathbf{G}_{-q}} \circ \mathbf{F}_{-q}^{(+)} \right) \\ + \frac{\mathbf{K}_q - \mathbf{K}_{-q}}{4} \circ \left( \frac{1}{2\mathbf{G}_q} \circ \mathbf{F}_q^{(+)} - \frac{1}{2\mathbf{G}_{-q}} \circ \mathbf{F}_{-q}^{(+)} \right) \end{array} \right) \alpha_{b'} | U_K \rangle
\end{aligned} \tag{607}$$

In the following evaluation of the term  $\left( \frac{1}{2\mathbf{G}_q} \circ \mathbf{F}_q^{(\pm)} + \frac{1}{2\mathbf{G}_{-q}} \circ \mathbf{F}_{-q}^{(\pm)} \right)$  of even parity with respect to  $q_b$  as well as the evaluation of the term  $\left( \frac{1}{2\mathbf{G}_q} \circ \mathbf{F}_q^{(-)} - \frac{1}{2\mathbf{G}_{-q}} \circ \mathbf{F}_{-q}^{(-)} \right)$  of odd parity with respect to  $q_b$  is presented.

The goal is to only keep corrections of the order  $\frac{1}{\Omega_{max}}$  and in the final result of the renormalization. Hence, all terms yielding corrections of the order  $O(\frac{1}{\Omega_{max}^2})$  are neglected.

Starting with the contribution of even parity with respect to  $q_a \rightarrow -q_a$ , one finds, by inserting the shift identity (587) [7]

$$\begin{aligned}
& \frac{1}{2\mathbf{G}_q} \circ \mathbf{F}_q^{(\pm)} + \frac{1}{2\mathbf{G}_{-q}} \circ \mathbf{F}_{-q}^{(\pm)} \\
& = \left( \begin{aligned}
& \left( \frac{w}{\xi} - 1 \right) \left( 1 + \frac{\xi}{w} \right) \beta \\
& + \left( \frac{w}{\xi} - 1 \right) \left( \pm \frac{\tilde{E}_k + \tilde{E}_K}{2} \mathbf{1}_{4 \times 4} \right) \\
& + \left( \begin{aligned}
& \left( \frac{w}{\xi} - 1 \right) \left( 1 + \frac{\xi}{w} \right) \delta_{a,a'} \\
& + \left( \left( \frac{w}{\xi} - \frac{\xi}{w} - \frac{1}{\xi^2} \right) \left( 1 + \frac{\xi}{w} \right) - \left( \frac{w}{\xi} - 1 \right) \frac{\xi}{w^3} \right) \frac{\hbar q_a \hbar q_{a'}}{m_0 c m_0 c} \end{aligned} \right) \frac{\Pi_{a'}}{m_0 c} \alpha_a \\
& + \left( \left( \frac{w}{\xi} - \frac{\xi}{w} - \frac{1}{\xi^2} \right) \left( 1 + \frac{\xi}{w} \right) - \left( \frac{w}{\xi} - 1 \right) \frac{\xi}{w^3} \right) \beta \frac{H_{4 \times 4}^{(P,0)}}{m_0 c^2} \\
& + \left( \begin{aligned}
& \left( \frac{w}{\xi} - 1 \right) \frac{3\xi}{2w^5} \\
& - \left( \frac{w}{\xi} - \frac{\xi}{w} - \frac{1}{\xi^2} \right) \frac{\xi}{w^3} \\
& + \left( -\frac{w}{2\xi} + \frac{\xi}{2w} + \frac{\xi}{2w^3} + \frac{w}{\xi^3} - \frac{1}{\xi^2} \right) \left( 1 + \frac{\xi}{w} \right) \end{aligned} \right) \frac{\hbar q_a \Pi_a \hbar q_{a'} \Pi_{a'}}{m_0 c m_0 c m_0 c m_0 c} \beta \\
& + \beta \left( 1 - \left( \frac{\tilde{E}_k + \tilde{E}_K}{2} \right)^2 \right) \left( \frac{w}{\xi} - 1 - \frac{1}{2\xi^2} \right) \left( 1 + \frac{\xi}{w} \right) \\
& + \left( \begin{aligned}
& + \frac{\hbar q_a \Pi_a \hbar q_{a'} \Pi_{a'}}{m_0 c m_0 c m_0 c m_0 c} \left( -\frac{w}{2\xi} + \frac{\xi}{2w} + \frac{\xi}{2w^3} + \frac{w}{\xi^3} - \frac{1}{\xi^2} \right) \mathbf{1}_{4 \times 4} \\
& + \left( \frac{w}{\xi} - \frac{\xi}{w} - \frac{1}{\xi^2} \right) \frac{H_{4 \times 4}^{(P,0)}}{m_0 c^2} \\
& + \left( 1 - \left( \frac{\tilde{E}_k + \tilde{E}_K}{2} \right)^2 \right) \left( \frac{w}{\xi} - 1 - \frac{1}{2\xi^2} \right) \mathbf{1}_{4 \times 4} \end{aligned} \right) \left( \pm \frac{\tilde{E}_k + \tilde{E}_K}{2} \mathbf{1}_{4 \times 4} \right) \\
& + O(\alpha_{FS}^3)
\end{aligned} \right) \quad (608)
\end{aligned}$$

Hence, under even parity, all contributions with a uneven number of wavenumber  $q_b$  drop.

With the abbreviations  $\frac{q_b}{|\mathbf{q}|} = \hat{q}_b$ ,  $\hat{q}_b \hat{q}_b = \hat{q}_x \hat{q}_x + \hat{q}_y \hat{q}_y + \hat{q}_z \hat{q}_z = 1$  and  $\frac{\hbar q_a}{m_0 c} = \tilde{\omega}_q \hat{q}_a \equiv \xi \hat{q}_a$  one yields, with further rearrangements [7],

$$\begin{aligned}
& \frac{1}{2\mathbf{G}_q} \circ \mathbf{F}_q^{(\pm)} + \frac{1}{2\mathbf{G}_{-q}} \circ \mathbf{F}_{-q}^{(\pm)} \\
& = \left( \begin{aligned}
& \left( \frac{w}{\xi} - 1 \right) \left( 1 + \frac{\xi}{w} \right) \beta \\
& + \left( \begin{aligned}
& \left( \frac{w}{\xi} - 1 \right) \left( 1 + \frac{\xi}{w} \right) \delta_{a,a'} \\
& + \left( \left( \frac{w}{\xi} - \frac{\xi}{w} - \frac{1}{\xi^2} \right) \left( 1 + \frac{\xi}{w} \right) - \left( \frac{w}{\xi} - 1 \right) \frac{\xi}{w^3} \right) \xi^2 \hat{q}_a \hat{q}_{a'} \end{aligned} \right) \frac{\Pi_{a'}}{m_0 c} \alpha_a \\
& \quad + \left( \left( \frac{w}{\xi} - \frac{\xi}{w} - \frac{1}{\xi^2} \right) \left( 1 + \frac{\xi}{w} \right) - \left( \frac{w}{\xi} - 1 \right) \frac{\xi}{w^3} \right) \frac{\mathbf{H}_{4 \times 4}^{(P,0)}}{m_0 c^2} \beta \\
& + \left( \begin{aligned}
& \left( \frac{w}{\xi} - 1 \right) \frac{3\xi}{2w^5} \\
& - \left( \frac{w}{\xi} - \frac{\xi}{w} - \frac{1}{\xi^2} \right) \frac{\xi}{w^3} \\
& + \left( -\frac{w}{2\xi} + \frac{\xi}{2w} + \frac{\xi}{2w^3} + \frac{w}{\xi^3} - \frac{1}{\xi^2} \right) \left( 1 + \frac{\xi}{w} \right) \end{aligned} \right) \xi^2 \hat{q}_a \hat{q}_{a'} \frac{\Pi_a \Pi_{a'}}{m_0 c m_0 c} \beta \\
& + \left( \begin{aligned}
& \left( -\frac{w}{2\xi} + \frac{\xi}{2w} + \frac{\xi}{2w^3} + \frac{w}{\xi^3} - \frac{1}{\xi^2} \right) \xi^2 \hat{q}_a \hat{q}_{a'} \frac{\Pi_a \Pi_{a'}}{m_0 c m_0 c} \\
& \quad + \left( \frac{w}{\xi} - \frac{\xi}{w} - \frac{1}{\xi^2} \right) \frac{\mathbf{H}_{4 \times 4}^{(P,0)}}{m_0 c^2} \\
& \quad + \left( \frac{w}{\xi} - 1 - \frac{1}{2\xi^2} \right) \left( 1 - \left( \frac{\tilde{E}_k + \tilde{E}_K}{2} \right)^2 \right) \\
& \quad \quad + \left( \frac{w}{\xi} - 1 \right) \end{aligned} \right) \left( \pm \frac{\tilde{E}_k + \tilde{E}_K}{2} \mathbf{1}_{4 \times 4} \right) \\
& \quad + \left( \frac{w}{\xi} - 1 - \frac{1}{2\xi^2} \right) \left( 1 + \frac{\xi}{w} \right) \left( 1 - \left( \frac{\tilde{E}_k + \tilde{E}_K}{2} \right)^2 \right) \beta \\
& \quad \quad + O(\alpha_{FS}^3)
\end{aligned} \right) \tag{609}
\end{aligned}$$

For the terms with  $\xi$  and  $w$  there holds [7]

$$\begin{aligned}
& \left(\frac{w}{\xi} - 1\right) \left(1 + \frac{\xi}{w}\right) = \frac{w}{\xi} - \frac{\xi}{w} = O\left(\frac{1}{\xi^2}\right) \\
& \left(\left(\frac{w}{\xi} - \frac{\xi}{w} - \frac{1}{\xi^2}\right) \left(1 + \frac{\xi}{w}\right) - \left(\frac{w}{\xi} - 1\right) \frac{\xi}{w^3}\right) \xi^2 = -1 + \frac{\xi^3}{w^3} = O\left(-\frac{3}{2\xi^2}\right) \\
& \left(\frac{w}{\xi} - \frac{\xi}{w} - \frac{1}{\xi^2}\right) \left(1 + \frac{\xi}{w}\right) - \left(\frac{w}{\xi} - 1\right) \frac{\xi}{w^3} = -\frac{1}{\xi^2} + \frac{\xi}{w^3} = O\left(-\frac{3}{2\xi^4}\right) \\
& \left( \begin{aligned} & \left(1 + \frac{\xi}{w}\right) \left(-\frac{w}{2\xi} + \frac{\xi}{2w} + \frac{\xi}{2w^3} + \frac{w}{\xi^3} - \frac{1}{\xi^2}\right) \\ & + \left(\frac{w}{\xi} - 1\right) \frac{3\xi}{2w^5} \\ & - \left(\frac{w}{\xi} - \frac{\xi}{w} - \frac{1}{\xi^2}\right) \frac{\xi}{w^3} \end{aligned} \right) \xi^2 = \frac{w}{\xi} - \frac{\xi}{w} - \frac{\xi}{w^3} + \frac{3\xi}{2w^5} = \frac{2+5\xi^2}{2\xi w^5} = O\left(\frac{5}{2\xi^4}\right) \\
& \left(-\frac{w}{2\xi} + \frac{\xi}{2w} + \frac{\xi}{2w^3} + \frac{w}{\xi^3} - \frac{1}{\xi^2}\right) \xi^2 = -1 + \frac{w}{\xi} - \frac{\xi}{2w^3} = O\left(\frac{5}{8\xi^4}\right) \\
& \left(\frac{w}{\xi} - 1 - \frac{1}{2\xi^2}\right) \left(1 + \frac{\xi}{w}\right) = -\frac{1}{2\xi^2} - \frac{\xi}{2w} + \frac{w}{2\xi} = O\left(-\frac{1}{4\xi^4}\right)
\end{aligned} \tag{610}$$

These terms behave for large  $\xi$  like  $O(\cdot)$ . However, there are two reasons for not neglecting contributions smaller than the order  $\frac{1}{\xi^2}$  at this point: first, when combining the terms with the antisymmetric part, the weights change further. Second, as will be shown a few lines below, the integration measure of the transversal renormalization contribution provides another  $\xi$  of the radial integral component.

Inserting the identities (610) finally gives [7]



$$\begin{aligned}
& \frac{1}{2\mathbf{G}_q} \circ \mathbf{F}_q^{(\pm)} + \frac{1}{2\mathbf{G}_{-q}} \circ \mathbf{F}_{-q}^{(\pm)} \\
& \left( \begin{aligned}
& \left( \frac{w}{\xi} - \frac{\xi}{w} \right) \beta \\
& + \left( \left( \frac{w}{\xi} - \frac{\xi}{w} \right) \delta_{a,a'} + \left( -1 + \frac{\xi^3}{w^3} \right) \hat{q}_a \hat{q}_{a'} \right) \frac{\Pi_{a'}}{m_0 c} \alpha_a \\
& + \left( -\frac{1}{\xi^2} + \frac{\xi}{w^3} \right) \frac{\mathbf{H}_{4 \times 4}^{(P,0)}}{m_0 c^2} \beta \\
& + \frac{2+5\xi^2}{2\xi w^5} \hat{q}_a \hat{q}_{a'} \frac{\Pi_a}{m_0 c} \frac{\Pi_{a'}}{m_0 c} \beta \\
& + \left( \begin{aligned}
& \left( -1 + \frac{w}{\xi} - \frac{\xi}{2w^3} \right) \hat{q}_a \hat{q}_{a'} \frac{\Pi_a}{m_0 c} \frac{\Pi_{a'}}{m_0 c} \\
& + \left( \frac{w}{\xi} - \frac{\xi}{w} - \frac{1}{\xi^2} \right) \frac{\mathbf{H}_{4 \times 4}^{(P,0)}}{m_0 c^2} \\
& + \left( \frac{w}{\xi} - 1 - \frac{1}{2\xi^2} \right) \left( 1 - \left( \frac{\tilde{E}_k + \tilde{E}_K}{2} \right)^2 \right) \\
& + \left( \frac{w}{\xi} - 1 \right)
\end{aligned} \right) \left( \pm \frac{\tilde{E}_k + \tilde{E}_K}{2} \mathbf{1}_{4 \times 4} \right) \\
& + \left( -\frac{1}{2\xi^2} - \frac{\xi}{2w} + \frac{w}{2\xi} \right) \left( 1 - \left( \frac{\tilde{E}_k + \tilde{E}_K}{2} \right)^2 \right) \beta \\
& + O(\alpha_{FS}^3)
\end{aligned} \right) \tag{611}
\end{aligned}$$

For the contribution with odd parity with respect to  $q_a \rightarrow -q_a$ , by again inserting the shift identity (587), there follows [7]

$$\begin{aligned}
& \frac{1}{2\mathbf{G}_q} \circ \mathbf{F}_q^{(\pm)} - \frac{1}{2\mathbf{G}_{-q}} \circ \mathbf{F}_{-q}^{(\pm)} \\
& = \left( \begin{aligned}
& \left( \frac{w}{\xi} - 1 \right) \left( 1 + \frac{\xi}{w} \right) \left( \alpha_a \frac{\hbar q_a}{m_0 c} \right) \\
& + \left( \frac{w}{\xi} - 1 \right) \left( -\frac{\xi}{w^3} \frac{\hbar q_a}{m_0 c} \frac{\Pi_a}{m_0 c} \beta \right) \\
& + \frac{\hbar q_{a'}}{m_0 c} \frac{\Pi_{a'}}{m_0 c} \left( \frac{w}{\xi} - \frac{\xi}{w} - \frac{1}{\xi^2} \right) \cdot \left( \pm \frac{\tilde{E}_k + \tilde{E}_K}{2} \mathbf{1}_{4 \times 4} + \beta \left( 1 + \frac{\xi}{w} \right) \right) \\
& + \left( \frac{w}{\xi} - 1 \right) \left( \left( \frac{3\xi}{2w^5} \frac{\hbar q_a}{m_0 c} \left( \frac{\hbar q_{a''}}{m_0 c} \frac{\Pi_{a''}}{m_0 c} \frac{\hbar q_{a'}}{m_0 c} \frac{\Pi_{a'}}{m_0 c} \right) - \frac{\xi}{w^3} \frac{\hbar q_{a'}}{m_0 c} \frac{\Pi_{a'}}{m_0 c} \frac{\Pi_a}{m_0 c} \right) \alpha_a \right) \\
& \quad - \frac{\xi}{2w^3} \left( \mathbf{H}_{4 \times 4}^{(P,0)} \alpha_a + \alpha_a \mathbf{H}_{4 \times 4}^{(P,0)} \right) \frac{\hbar q_a}{m_0 c} \\
& + \frac{\hbar q_{a''}}{m_0 c} \frac{\Pi_{a''}}{m_0 c} \left( \frac{w}{\xi} - \frac{\xi}{w} - \frac{1}{\xi^2} \right) \cdot \left( \left( 1 + \frac{\xi}{w} \right) \frac{\Pi_a}{m_0 c} - \frac{\xi}{w^3} \frac{\hbar q_a}{m_0 c} \frac{\hbar q_{a'}}{m_0 c} \frac{\Pi_{a'}}{m_0 c} \right) \alpha_a \\
& + \left( \begin{aligned}
& + \frac{\hbar q_{a''}}{m_0 c} \frac{\Pi_{a''}}{m_0 c} \frac{\hbar q_{a'}}{m_0 c} \frac{\Pi_{a'}}{m_0 c} \left( -\frac{w}{2\xi} + \frac{\xi}{2w} + \frac{\xi}{2w^3} + \frac{w}{\xi^3} - \frac{1}{\xi^2} \right) \cdot \left( 1 + \frac{\xi}{w} \right) \alpha_a \frac{\hbar q_a}{m_0 c} \\
& + \left( \frac{w}{\xi} - \frac{\xi}{w} - \frac{1}{\xi^2} \right) \cdot \left( 1 + \frac{\xi}{w} \right) \frac{1}{2} \left( \mathbf{H}_{4 \times 4}^{(P,0)} \alpha_a + \alpha_a \mathbf{H}_{4 \times 4}^{(P,0)} \right) \frac{\hbar q_a}{m_0 c} \\
& + \left( 1 - \left( \frac{\tilde{E}_k + \tilde{E}_K}{2} \right)^2 \right) \left( \frac{w}{\xi} - 1 - \frac{1}{2\xi^2} \right) \cdot \left( 1 + \frac{\xi}{w} \right) \alpha_a \frac{\hbar q_a}{m_0 c}
\end{aligned} \right) \\
& \quad + O(\alpha_{FS}^3)
\end{aligned} \right) \tag{612}
\end{aligned}$$

Hence, all contributions with an even number of wavenumbers  $q_b$  drop!

Going on then [7]

$$\begin{aligned}
& \frac{1}{2G_q} \circ F_q^{(\pm)} - \frac{1}{2G_{-q}} \circ F_{-q}^{(\pm)} \\
& = \left( \begin{array}{l} \left( \begin{array}{l} \left( \frac{w}{\xi} - 1 \right) \left( 1 + \frac{\xi}{w} \right) \xi \\ + \left( 1 - \left( \frac{\tilde{E}_k + \tilde{E}_K}{2} \right)^2 \right) \left( \frac{w}{\xi} - 1 - \frac{1}{2\xi^2} \right) \left( 1 + \frac{\xi}{w} \right) \xi \end{array} \right) \hat{q}_a \alpha_a \\ \\ \left( \begin{array}{l} \left( \begin{array}{l} \xi^2 \left( -\frac{w}{2\xi} + \frac{\xi}{2w} + \frac{\xi}{2w^3} + \frac{w}{\xi^3} - \frac{1}{\xi^2} \right) \left( 1 + \frac{\xi}{w} \right) \xi \\ + \left( \frac{w}{\xi} - 1 \right) \frac{3\xi^4}{2w^5} - \left( \frac{w}{\xi} - \frac{\xi}{w} - \frac{1}{\xi^2} \right) \frac{\xi^4}{w^3} \end{array} \right) \hat{q}_a \hat{q}_{a'} \hat{q}_{a''} \\ + \left( \xi \left( \frac{w}{\xi} - \frac{\xi}{w} - \frac{1}{\xi^2} \right) \cdot \left( 1 + \frac{\xi}{w} \right) - \left( \frac{w}{\xi} - 1 \right) \frac{\xi^2}{w^3} \right) \hat{q}_{a''} \delta_{a,a'} \end{array} \right) \frac{\Pi_{a''} \Pi_{a'}}{m_0 c m_0 c} \alpha_a \\ \\ + \left( - \left( \frac{w}{\xi} - 1 \right) \frac{\xi^2}{w^3} + \xi \left( \frac{w}{\xi} - \frac{\xi}{w} - \frac{1}{\xi^2} \right) \left( 1 + \frac{\xi}{w} \right) \right) \hat{q}_a \frac{\Pi_a}{m_0 c} \beta \\ \\ + \xi \left( \frac{w}{\xi} - \frac{\xi}{w} - \frac{1}{\xi^2} \right) \cdot \left( \pm \frac{\tilde{E}_k + \tilde{E}_K}{2} \mathbf{1}_{4 \times 4} \right) \hat{q}_a \frac{\Pi_a}{m_0 c} \\ \\ + \left( \left( \frac{w}{\xi} - \frac{\xi}{w} - \frac{1}{\xi^2} \right) \cdot \left( 1 + \frac{\xi}{w} \right) \xi - \left( \frac{w}{\xi} - 1 \right) \frac{\xi^2}{w^3} \right) \hat{q}_a \frac{1}{2} \left( \frac{\mathbf{H}_{4 \times 4}^{(P,0)}}{m_0 c^2} \alpha_a + \alpha_a \frac{\mathbf{H}_{4 \times 4}^{(P,0)}}{m_0 c^2} \right) \\ \\ + O(\alpha_{FS}^3) \end{array} \right) \quad (613)
\end{aligned}$$

Inserting the following identities [7]

$$\begin{aligned}
& \left( \frac{w}{\xi} - 1 \right) \left( 1 + \frac{\xi}{w} \right) \xi = \frac{1}{w} \\
& \left( \frac{w}{\xi} - 1 - \frac{1}{2\xi^2} \right) \left( 1 + \frac{\xi}{w} \right) \xi = \frac{1}{2} \left( \frac{1}{w} - \frac{1}{\xi} \right) \\
& \left( \begin{array}{l} \xi^3 \left( -\frac{w}{2\xi} + \frac{\xi}{2w} + \frac{\xi}{2w^3} + \frac{w}{\xi^3} - \frac{1}{\xi^2} \right) \left( 1 + \frac{\xi}{w} \right) \\ + \left( \frac{w}{\xi} - 1 \right) \frac{3\xi^4}{2w^5} - \left( \frac{w}{\xi} - \frac{\xi}{w} - \frac{1}{\xi^2} \right) \frac{\xi^4}{w^3} \end{array} \right) = \frac{5}{2w^3} - \frac{3}{2w^5} \\
& \xi \left( \frac{w}{\xi} - \frac{\xi}{w} - \frac{1}{\xi^2} \right) \cdot \left( 1 + \frac{\xi}{w} \right) - \left( \frac{w}{\xi} - 1 \right) \frac{\xi^2}{w^3} = \frac{1}{w} - \frac{1}{\xi} - \frac{1}{w^3} \\
& - \left( \frac{w}{\xi} - 1 \right) \frac{\xi^2}{w^3} + \xi \left( \frac{w}{\xi} - \frac{\xi}{w} - \frac{1}{\xi^2} \right) \left( 1 + \frac{\xi}{w} \right) = \frac{1}{w} - \frac{1}{\xi} - \frac{1}{w^3} \\
& \xi \left( \frac{w}{\xi} - \frac{\xi}{w} - \frac{1}{\xi^2} \right) = \frac{1}{w} - \frac{1}{\xi} \\
& \left( \frac{w}{\xi} - \frac{\xi}{w} - \frac{1}{\xi^2} \right) \left( 1 + \frac{\xi}{w} \right) \xi - \left( \frac{w}{\xi} - 1 \right) \frac{\xi^2}{w^3} = \frac{1}{w} - \frac{1}{\xi} - \frac{1}{w^3}
\end{aligned} \quad (614)$$

One finally finds [7]

$$\begin{aligned}
& \frac{1}{2G_q} \circ \mathbf{F}_q^{(\pm)} - \frac{1}{2G_{-q}} \circ \mathbf{F}_{-q}^{(\pm)} \\
& = \left( \begin{aligned}
& \left( \frac{1}{w} + \left( 1 - \left( \frac{\tilde{E}_k + \tilde{E}_K}{2} \right)^2 \right) \underbrace{\frac{1}{2} \left( \frac{1}{w} - \frac{1}{\xi} \right)}_{=O\left(-\frac{1}{4\xi^3}\right)} \right) \hat{q}_a \alpha_a \\
& \left( \underbrace{\left( \frac{5}{2w^3} - \frac{3}{2w^5} \right)}_{=O\left(\frac{5}{2\xi^3}\right)} \hat{q}_a \hat{q}_{a'} \hat{q}_{a''} + \underbrace{\left( \frac{1}{w} - \frac{1}{\xi} - \frac{1}{w^3} \right)}_{=O\left(-\frac{3}{2\xi^3}\right)} \hat{q}_{a'} \delta_{a,a'} \right) \frac{\Pi_{a''} \Pi_{a'}}{m_0 c m_0 c} \alpha_a \\
& + \underbrace{\left( \frac{1}{w} - \frac{1}{\xi} - \frac{1}{w^3} \right)}_{=O\left(-\frac{3}{2\xi^3}\right)} \hat{q}_a \frac{\Pi_a}{m_0 c} \beta \\
& + \underbrace{\left( \frac{1}{w} - \frac{1}{\xi} \right)}_{=O\left(-\frac{1}{2\xi^3}\right)} \left( \pm \frac{\tilde{E}_k + \tilde{E}_K}{2} \mathbf{1}_{4 \times 4} \right) \hat{q}_a \frac{\Pi_a}{m_0 c} \\
& + \underbrace{\left( \frac{1}{w} - \frac{1}{\xi} - \frac{1}{w^3} \right)}_{=O\left(-\frac{3}{2\xi^3}\right)} \frac{1}{2} \left( \frac{H_{4 \times 4}^{(P,0)}}{m_0 c^2} \alpha_a + \alpha_a \frac{H_{4 \times 4}^{(P,0)}}{m_0 c^2} \right) \hat{q}_a \\
& + O(\alpha_{FS}^3)
\end{aligned} \right) \tag{615}
\end{aligned}$$

From (615) one can see that only the contribution in the first line being proportional to  $\frac{1}{w}$  contributes to the integral. This is because together with the  $\xi$  stemming from the integration measure this term give a correction of the order  $O(1)$  in the cut-off, whereas the other contributions are at least of the order  $O\left(\tilde{\Omega}_{max}^{-3}\right)$ .

Hence, one can set [7]

$$\frac{K_q - K_{-q}}{4} \left( \frac{1}{2G_q} \circ \mathbf{F}_q^{(\pm)} - \frac{1}{2G_{-q}} \circ \mathbf{F}_{-q}^{(\pm)} \right) = \frac{K_q - K_{-q}}{4} \left( \frac{1}{w} \hat{q}_a \alpha_a + O\left(\tilde{\Omega}_{max}^{-3}\right) \right) \tag{616}$$

Before putting the results together one has to convert the sum over the continuously varying wavenumbers  $q_b$  of the photons, which lie dense in the large volume  $V$ , to an integral. For  $V \rightarrow \infty$  the error vanishes. Hence,

$$\begin{aligned}
& \left( \frac{q_e^2}{2\varepsilon_0} \right) \left( \frac{\hbar}{m_0 c} \right)^2 \frac{1}{V} \sum_{\mathbf{q}} \frac{1}{\tilde{\omega}_q} \left( \delta_{b,b'} - \frac{q_b q_{b'}}{|\mathbf{q}|^2} \right) f \left( \frac{\hbar}{m_0 c} \mathbf{q} \right) \\
& \rightarrow \left( \frac{q_e^2}{2\varepsilon_0} \right) \left( \frac{\hbar}{m_0 c} \right)^2 \int \frac{d^3 q}{(2\pi)^3} \frac{1}{\tilde{\omega}_q} \left( \delta_{b,b'} - \frac{q_b q_{b'}}{|\mathbf{q}|^2} \right) f \left( \frac{\hbar}{m_0 c} \mathbf{q} \right) \quad (617) \\
& = m_0 c^2 \frac{\alpha_{FS}}{\pi} \int_0^\infty d\xi \xi \int \frac{d\Omega_{\hat{\mathbf{q}}}}{4\pi} (\delta_{b,b'} - \hat{q}_b \hat{q}_{b'}) f(\xi \hat{\mathbf{q}})
\end{aligned}$$

Putting the results (602), (611) and (616) together, and replacing the sum according to (617) one finds for the renormalization due to the high energy photons [7]

$$\begin{aligned}
\tilde{M}_{k,K}^{(\perp,e,high)} &= -m_0 c^2 \frac{\alpha_{FS}}{\pi} \int_0^\infty d\xi \xi \int \frac{d\Omega_{\hat{\mathbf{q}}}}{4\pi} (\delta_{b,b'} - \hat{q}_b \hat{q}_{b'}) \\
& \times \langle U_k | \alpha_b \left( \begin{array}{c} \frac{\Theta_H(\tilde{\Omega}_{max}-\xi)}{2} \left( \frac{1}{2G_q} \circ F_q^{(+)} + \frac{1}{2G_{-q}} \circ F_{-q}^{(+)} \right) \\ + \frac{\Theta_H[(\tilde{\Omega}_{max}-\xi) - \frac{\hat{q}_b \Pi_b}{2 m_0 c}] - \Theta_H[(\tilde{\Omega}_{max}-\xi) + \frac{\hat{q}_b \Pi_b}{2 m_0 c}]}{4} \left( \frac{1}{w} \hat{q}_a \alpha_a \right) \end{array} \right) \alpha_{b'} | U_K \rangle \\
& = -m_0 c^2 \frac{\alpha_{FS}}{\pi} \int_0^\infty d\xi \xi \int \frac{d\Omega_{\hat{\mathbf{q}}}}{4\pi} (\delta_{b,b'} - \hat{q}_b \hat{q}_{b'}) \\
& \times \langle U_k | \left( \begin{array}{c} \frac{\Theta_H(\tilde{\Omega}_{max}-\xi)}{2} \left( \frac{w}{\xi} - \frac{\xi}{w} \right) \alpha_b \beta \alpha_{b'} \\ + \frac{\Theta_H(\tilde{\Omega}_{max}-\xi)}{2} \left( \left( \frac{w}{\xi} - \frac{\xi}{w} \right) \delta_{a,a'} + \left( -1 + \frac{\xi^3}{w^3} \right) \hat{q}_a \hat{q}_{a'} \right) \frac{\Pi_{a'}}{m_0 c} \alpha_b \alpha_a \alpha_{b'} \\ + \frac{\Theta_H(\tilde{\Omega}_{max}-\xi)}{2} \left( -\frac{1}{\xi^2} + \frac{\xi}{w^3} \right) \alpha_b \frac{H_{4 \times 4}^{(P,0)}}{m_0 c^2} \beta \alpha_{b'} \\ + \frac{\Theta_H(\tilde{\Omega}_{max}-\xi)}{2} \frac{2+5\xi^2}{2\xi w^5} \hat{q}_a \hat{q}_{a'} \frac{\Pi_a}{m_0 c} \frac{\Pi_{a'}}{m_0 c} \alpha_b \beta \alpha_{b'} \\ + \frac{\Theta_H(\tilde{\Omega}_{max}-\xi)}{2} \left( \begin{array}{c} \left( -1 + \frac{w}{\xi} - \frac{\xi}{2w^3} \right) \hat{q}_a \hat{q}_{a'} \frac{\Pi_a}{m_0 c} \frac{\Pi_{a'}}{m_0 c} \alpha_b \alpha_{b'} \\ + \left( \frac{w}{\xi} - \frac{\xi}{w} - \frac{1}{\xi^2} \right) \alpha_b \frac{H_{4 \times 4}^{(P,0)}}{m_0 c^2} \alpha_{b'} \\ + \left( \frac{w}{\xi} - 1 - \frac{1}{2\xi^2} \right) \left( 1 - \left( \frac{\tilde{E}_k + \tilde{E}_K}{2} \right)^2 \right) \alpha_b \alpha_{b'} \\ + \left( \frac{w}{\xi} - 1 \right) \alpha_b \alpha_{b'} \end{array} \right) \frac{\tilde{E}_k + \tilde{E}_K}{2} | U_K \rangle \\ + \frac{\Theta_H(\tilde{\Omega}_{max}-\xi)}{2} \left( -\frac{1}{2\xi^2} - \frac{\xi}{2w} + \frac{w}{2\xi} \right) \left( 1 - \left( \frac{\tilde{E}_k + \tilde{E}_K}{2} \right)^2 \right) \alpha_b \beta \alpha_{b'} \\ + \frac{\Theta_H[(\tilde{\Omega}_{max}-\xi) - \frac{\hat{q}_b \Pi_b}{2 m_0 c}] - \Theta_H[(\tilde{\Omega}_{max}-\xi) + \frac{\hat{q}_b \Pi_b}{2 m_0 c}]}{4} \alpha_b \left( \frac{1}{w} \hat{q}_a \alpha_a \right) \alpha_{b'} \end{array} \right) \\
& \quad + O(\alpha_{FS}^3)
\end{array} \quad (618)$$

For the further evaluation one needs the following relations. From the properties of the Dirac matrices

$$\begin{aligned}
\alpha_b \beta &= -\beta \alpha_b \\
\alpha_b \alpha_{b'} &= \delta_{b',b} \mathbf{1}_{4 \times 4} + i \sum_{b''} \varepsilon_{bb'b''} \sigma_{b''} = \sigma_b \sigma_{b'} \\
\alpha_b \sigma_a \alpha_{b'} &= \sigma_b \sigma_a \sigma_{b'} \\
\sigma_b \beta &= \beta \sigma_b \\
a, b, b' &\in \{x, y, z\}
\end{aligned} \tag{619}$$

there follows [7]

$$\begin{aligned}
(\delta_{b,b'} - \hat{q}_b \hat{q}_{b'}) \alpha_b \alpha_{b'} &= (\delta_{b,b'} - \hat{q}_b \hat{q}_{b'}) (\delta_{b',b} \mathbf{1}_{4 \times 4} + i \varepsilon_{bb'b''} \sigma_{b''}) \\
&= \left( \underbrace{\delta_{b,b}}_{=3} - \underbrace{\hat{q}_b \hat{q}_b}_{=1} \right) \mathbf{1}_{4 \times 4} = 2 \cdot \mathbf{1}_{4 \times 4} \\
(\delta_{b,b'} - \hat{q}_b \hat{q}_{b'}) \sigma_b \sigma_{b'} &= 2 \cdot \mathbf{1}_{4 \times 4} \\
(\delta_{b,b'} - \hat{q}_b \hat{q}_{b'}) \alpha_b \alpha_a \alpha_{b'} &= (\delta_{b,b'} - \hat{q}_b \hat{q}_{b'}) (\alpha_b \alpha_a + \alpha_a \alpha_b - \alpha_a \alpha_b) \alpha_{b'} = -2 \hat{q}_a \hat{q}_{b'} \alpha_{b'} \\
(\delta_{b,b'} - \hat{q}_b \hat{q}_{b'}) \alpha_b \sigma_a \alpha_{b'} &= (\delta_{b,b'} - \hat{q}_b \hat{q}_{b'}) \sigma_b \sigma_a \sigma_{b'} = -2 \hat{q}_a \hat{q}_{b'} \sigma_{b'} \\
(\delta_{b,b'} - \hat{q}_b \hat{q}_{b'}) \alpha_b \alpha_a \alpha_{b'} \hat{q}_a &= -2 \hat{q}_a \hat{q}_{b'} \alpha_{b'} \hat{q}_a = -2 \alpha_{b'} \hat{q}_{b'} \\
(\delta_{b,b'} - \hat{q}_b \hat{q}_{b'}) \alpha_b \frac{H_{4 \times 4}^{(P,0)}}{m_0 c^2} \alpha_{b'} &= \frac{1}{m_0 c^2} (\delta_{b,b'} - \hat{q}_b \hat{q}_{b'}) \alpha_b \left( \frac{\Pi_a \Pi_a}{2m_0} \mathbf{1}_{4 \times 4} - \frac{q_e \hbar}{2m_0} B_a^{(ext)} \sigma_a \right) \alpha_{b'} \\
&= \frac{2}{m_0 c^2} \left( \frac{\Pi_a \Pi_a}{2m_0} \mathbf{1}_{4 \times 4} + \hat{q}_a \hat{q}_{b'} \sigma_{b'} \left( \frac{q_e \hbar}{2m_0} \right) B_a^{(ext)} \right)
\end{aligned} \tag{620}$$

With this there follows for (618) [7]

$$\begin{aligned}
\tilde{M}_{k,K}^{(\perp, e, high)} &= -m_0 c^2 \frac{\alpha_{FS}}{\pi} \int_0^\infty d\xi \xi \int \frac{d\Omega_{\hat{q}}}{4\pi} (\delta_{b,b'} - \hat{q}_b \hat{q}_{b'}) \\
&\times \langle U_k | \left( \begin{aligned} &\frac{\Theta_H(\tilde{\Omega}_{max} - \xi)}{2} \left( \frac{w}{\xi} - \frac{\xi}{w} \right) \alpha_b \beta \alpha_{b'} \\ &+ \frac{\Theta_H(\tilde{\Omega}_{max} - \xi)}{2} \left( \left( \frac{w}{\xi} - \frac{\xi}{w} \right) \delta_{a,a'} + \left( -1 + \frac{\xi^3}{w^3} \right) \hat{q}_a \hat{q}_{a'} \right) \frac{\Pi_{a'}}{m_0 c} \alpha_b \alpha_a \alpha_{b'} \\ &\quad + \frac{\Theta_H(\tilde{\Omega}_{max} - \xi)}{2} \left( -\frac{1}{\xi^2} + \frac{\xi}{w^3} \right) \alpha_b \frac{H_{4 \times 4}^{(P,0)}}{m_0 c^2} \beta \alpha_{b'} \\ &\quad + \frac{\Theta_H(\tilde{\Omega}_{max} - \xi)}{2} \frac{2+5\xi^2}{2\xi w^5} \hat{q}_a \hat{q}_{a'} \frac{\Pi_a}{m_0 c} \frac{\Pi_{a'}}{m_0 c} \alpha_b \beta \alpha_{b'} \\ &+ \frac{\Theta_H(\tilde{\Omega}_{max} - \xi)}{2} \left( \begin{aligned} &\left( -1 + \frac{w}{\xi} - \frac{\xi}{2w^3} \right) \hat{q}_a \hat{q}_{a'} \frac{\Pi_a}{m_0 c} \frac{\Pi_{a'}}{m_0 c} \alpha_b \alpha_{b'} \\ &\quad + \left( \frac{w}{\xi} - \frac{\xi}{w} - \frac{1}{\xi^2} \right) \alpha_b \frac{H_{4 \times 4}^{(P,0)}}{m_0 c^2} \alpha_{b'} \\ &\quad + \left( \frac{w}{\xi} - 1 - \frac{1}{2\xi^2} \right) \left( 1 - \left( \frac{\tilde{E}_k + \tilde{E}_K}{2} \right)^2 \right) \alpha_b \alpha_{b'} \\ &\quad + \left( \frac{w}{\xi} - 1 \right) \alpha_b \alpha_{b'} \end{aligned} \right) \frac{\tilde{E}_k + \tilde{E}_K}{2} |U_K \rangle \\ &\quad + \frac{\Theta_H(\tilde{\Omega}_{max} - \xi)}{2} \left( -\frac{1}{2\xi^2} - \frac{\xi}{2w} + \frac{w}{2\xi} \right) \left( 1 - \left( \frac{\tilde{E}_k + \tilde{E}_K}{2} \right)^2 \right) \alpha_b \beta \alpha_{b'} \\ &\quad + \frac{\Theta_H \left[ (\tilde{\Omega}_{max} - \xi) - \frac{\hat{q}_b}{2} \frac{\Pi_b}{m_0 c} \right] - \Theta_H \left[ (\tilde{\Omega}_{max} - \xi) + \frac{\hat{q}_b}{2} \frac{\Pi_b}{m_0 c} \right]}{4} \alpha_b \left( \frac{1}{w} \hat{q}_a \alpha_a \right) \alpha_{b'} \\ &\quad + O(\alpha_{FS}^3) \end{aligned} \right) \\
&= -m_0 c^2 \frac{\alpha_{FS}}{\pi} \int_0^\infty d\xi \xi \int \frac{d\Omega_{\hat{q}}}{4\pi} \\
&\times \langle U_k | \left( \begin{aligned} &\frac{\Theta_H(\tilde{\Omega}_{max} - \xi)}{2} \left( \frac{w}{\xi} - \frac{\xi}{w} \right) \underbrace{(\delta_{b,b'} - \hat{q}_b \hat{q}_{b'})}_{=-2\beta} \alpha_b \beta \alpha_{b'} \\ &+ \frac{\Theta_H(\tilde{\Omega}_{max} - \xi)}{2} \left( \left( \frac{w}{\xi} - \frac{\xi}{w} \right) \delta_{a,a'} + \left( -1 + \frac{\xi^3}{w^3} \right) \hat{q}_a \hat{q}_{a'} \right) \frac{\Pi_{a'}}{m_0 c} \underbrace{(\delta_{b,b'} - \hat{q}_b \hat{q}_{b'})}_{=-2\hat{q}_a \hat{q}_{b'} \alpha_{b'}} \alpha_b \alpha_a \alpha_{b'} \\ &\quad + \frac{\Theta_H(\tilde{\Omega}_{max} - \xi)}{2} \left( -\frac{1}{\xi^2} + \frac{\xi}{w^3} \right) \times \underbrace{(\delta_{b,b'} - \hat{q}_b \hat{q}_{b'})}_{=-\frac{2}{m_0 c^2} \beta \left( \frac{\Pi_a \Pi_a}{2m_0} 1_{4 \times 4} + \hat{q}_a \hat{q}_{b'} \sigma_{b'} \right) \left( \frac{q_e \hbar}{2m_0} \right) B_a^{(ext)}} \alpha_b \frac{H_{4 \times 4}^{(P,0)}}{m_0 c^2} \beta \alpha_{b'} \\ &\quad + \frac{\Theta_H(\tilde{\Omega}_{max} - \xi)}{2} \frac{2+5\xi^2}{2\xi w^5} \hat{q}_a \hat{q}_{a'} \frac{\Pi_a}{m_0 c} \frac{\Pi_{a'}}{m_0 c} \underbrace{(\delta_{b,b'} - \hat{q}_b \hat{q}_{b'})}_{=-2\beta} \alpha_b \beta \alpha_{b'} \\ &+ \frac{\Theta_H(\tilde{\Omega}_{max} - \xi)}{2} \left( \begin{aligned} &\left( -1 + \frac{w}{\xi} - \frac{\xi}{2w^3} \right) \hat{q}_a \hat{q}_{a'} \frac{\Pi_a}{m_0 c} \frac{\Pi_{a'}}{m_0 c} \underbrace{(\delta_{b,b'} - \hat{q}_b \hat{q}_{b'})}_{=-2} \alpha_b \alpha_{b'} \\ &\quad + \left( \frac{w}{\xi} - \frac{\xi}{w} - \frac{1}{\xi^2} \right) \underbrace{(\delta_{b,b'} - \hat{q}_b \hat{q}_{b'})}_{=\frac{2}{m_0 c^2} \left( \frac{\Pi_a \Pi_a}{2m_0} 1_{4 \times 4} + \hat{q}_a \hat{q}_{b'} \sigma_{b'} \right) \left( \frac{q_e \hbar}{2m_0} \right) B_a^{(ext)}} \alpha_b \frac{H_{4 \times 4}^{(P,0)}}{m_0 c^2} \alpha_{b'} \\ &\quad + \left( 1 - \left( \frac{\tilde{E}_k + \tilde{E}_K}{2} \right)^2 \right) \left( \frac{w}{\xi} - 1 - \frac{1}{2\xi^2} \right) \underbrace{(\delta_{b,b'} - \hat{q}_b \hat{q}_{b'})}_{=2} \alpha_b \alpha_{b'} \\ &\quad + \left( \frac{w}{\xi} - 1 \right) \underbrace{(\delta_{b,b'} - \hat{q}_b \hat{q}_{b'})}_{=2} \alpha_b \alpha_{b'} \end{aligned} \right) \frac{\tilde{E}_k + \tilde{E}_K}{2} |U_K \rangle \\ &\quad + \frac{\Theta_H(\tilde{\Omega}_{max} - \xi)}{2} \left( -\frac{1}{2\xi^2} - \frac{\xi}{2w} + \frac{w}{2\xi} \right) \left( 1 - \left( \frac{\tilde{E}_k + \tilde{E}_K}{2} \right)^2 \right) \underbrace{(\delta_{b,b'} - \hat{q}_b \hat{q}_{b'})}_{=-2\beta} \alpha_b \beta \alpha_{b'} \\ &\quad + \frac{\Theta_H \left[ (\tilde{\Omega}_{max} - \xi) - \frac{\hat{q}_b}{2} \frac{\Pi_b}{m_0 c} \right] - \Theta_H \left[ (\tilde{\Omega}_{max} - \xi) + \frac{\hat{q}_b}{2} \frac{\Pi_b}{m_0 c} \right]}{4} \frac{1}{w} \hat{q}_a \underbrace{(\delta_{b,b'} - \hat{q}_b \hat{q}_{b'})}_{=-2\hat{q}_{b'} \alpha_{b'}} \alpha_b \alpha_a \alpha_{b'} \\ &\quad + O(\alpha_{FS}^3) \end{aligned} \right) \tag{621}
\end{aligned}$$

For the correction term of the last line we use (604) such that [7]

$$\Theta_H \left[ \left( \tilde{\Omega}_{max} - \xi \right) - \frac{\hat{q}_b}{2} \frac{\Pi_b}{m_0 c} \right] - \Theta_H \left[ \left( \tilde{\Omega}_{max} - \xi \right) + \frac{\hat{q}_b}{2} \frac{\Pi_b}{m_0 c} \right] = -\hat{q}_b \frac{\Pi_b}{m_0 c} \delta \left( \tilde{\Omega}_{max} - \xi \right) + .. \quad (622)$$

Hence [7],

$$\begin{aligned} \tilde{M}_{k,K}^{(\perp, e, high)} = & -m_0 c^2 \frac{\alpha_{FS}}{\pi} \int_0^{\tilde{\Omega}_{max}} d\xi \xi \int \frac{d\Omega_{\hat{\mathbf{q}}}}{4\pi} \\ & \times \left\langle U_k \left| \begin{aligned} & - \left( \frac{w}{\xi} - \frac{\xi}{w} \right) \beta \\ & - \left( \left( \frac{w}{\xi} - \frac{\xi}{w} \right) \delta_{a,a'} \hat{q}_a \hat{q}_{b'} + \left( -1 + \frac{\xi^3}{w^3} \right) \underbrace{\hat{q}_a \hat{q}_a}_{=1} \hat{q}_{a'} \hat{q}_{b'} \right) \frac{\Pi_{a'}}{m_0 c} \alpha_{b'} \\ & - \frac{1}{m_0 c^2} \left( -\frac{1}{\xi^2} + \frac{\xi}{w^3} \right) \left( \frac{\Pi_a \Pi_a}{2m_0} \mathbf{1}_{4 \times 4} + \hat{q}_a \hat{q}_{b'} \sigma_{b'} \left( \frac{q_e \hbar}{2m_0} \right) B_a^{(ext)} \right) \beta \\ & - \frac{2+5\xi^2}{2\xi w^5} \hat{q}_a \hat{q}_{a'} \frac{\Pi_a}{m_0 c} \frac{\Pi_{a'}}{m_0 c} \beta \\ & + \left( +\frac{1}{m_0 c^2} \left( \frac{w}{\xi} - \frac{\xi}{w} - \frac{1}{\xi^2} \right) \left( \frac{\Pi_a \Pi_a}{2m_0} \mathbf{1}_{4 \times 4} + \hat{q}_a \hat{q}_{b'} \sigma_{b'} \left( \frac{q_e \hbar}{2m_0} \right) B_a^{(ext)} \right) \right) \frac{\tilde{E}_k + \tilde{E}_K}{2} \\ & + \left( \frac{w}{\xi} - 1 - \frac{1}{2\xi^2} \right) \left( 1 - \left( \frac{\tilde{E}_k + \tilde{E}_K}{2} \right)^2 \right) \frac{\tilde{E}_k + \tilde{E}_K}{2} \\ & + \left( \frac{w}{\xi} - 1 \right) \frac{\tilde{E}_k + \tilde{E}_K}{2} \\ & - \left( -\frac{1}{2\xi^2} - \frac{\xi}{2w} + \frac{w}{2\xi} \right) \left( 1 - \left( \frac{\tilde{E}_k + \tilde{E}_K}{2} \right)^2 \right) \beta \\ & + O(\alpha_{FS}^3) \end{aligned} \right\rangle |U_K\rangle \\ & + \langle U_k | \int_0^\infty d\xi \xi \int \frac{d\Omega_{\hat{\mathbf{q}}}}{4\pi} \frac{1}{4} \left( -\hat{q}_b \frac{\Pi_b}{m_0 c} \delta \left( \tilde{\Omega}_{max} - \xi \right) \right) \frac{1}{w} (-2\hat{q}_{b'} \alpha_{b'}) |U_K\rangle \end{aligned} \quad (623)$$

One has to first evaluate the term  $(\delta_{b,b'} - \hat{q}_b \hat{q}_{b'})$  which yields  $\hat{q}_a \hat{q}_a = 1$ . The occurring angle integrals are thus given by  $\int \frac{d\Omega_{\hat{\mathbf{q}}}}{4\pi} 1 = 1$  and  $\int \frac{d\Omega_{\hat{\mathbf{q}}}}{4\pi} \hat{q}_b \hat{q}_{b'} = \frac{1}{3} \delta_{b,b'}$ . This gives [7]



$$\begin{aligned}
\tilde{M}_{k,K}^{(\perp, e, high)} &= -m_0 c^2 \frac{\alpha_{FS}}{\pi} \times \\
&\times \left( \langle U_k | \int_0^{\tilde{\Omega}_{max}} d\xi \xi \left( \begin{aligned} & - \left( \frac{w}{\xi} - \frac{\xi}{w} \right) \beta \\ & - \frac{1}{3} \left( \left( \frac{w}{\xi} - \frac{\xi}{w} \right) + \left( -1 + \frac{\xi^3}{w^3} \right) \right) \frac{\Pi_a}{m_0 c} \alpha_a \\ & - \frac{1}{m_0 c^2} \left( -\frac{1}{\xi^2} + \frac{\xi}{w^3} \right) \left( \frac{\Pi_a \Pi_a}{2m_0} \mathbf{1}_{4 \times 4} + \frac{1}{3} \left( \frac{q_e \hbar}{2m_0} \right) B_a^{(ext)} \sigma_a \right) \beta \\ & - \frac{2+5\xi^2}{2\xi w^5} \frac{1}{3} \frac{\Pi_a}{m_0 c} \frac{\Pi_a}{m_0 c} \beta \\ & + \left( \begin{aligned} & \left( -1 + \frac{w}{\xi} - \frac{\xi}{2w^3} \right) \frac{1}{3} \frac{\Pi_a}{m_0 c} \frac{\Pi_a}{m_0 c} \\ & + \frac{1}{m_0 c^2} \left( \frac{w}{\xi} - \frac{\xi}{w} - \frac{1}{\xi^2} \right) \left( \frac{\Pi_a \Pi_a}{2m_0} \mathbf{1}_{4 \times 4} + \frac{1}{3} \left( \frac{q_e \hbar}{2m_0} \right) B_a^{(ext)} \sigma_a \right) \end{aligned} \right) \frac{\tilde{E}_k + \tilde{E}_K}{2} \right. \\ & \left. + \left( \begin{aligned} & \left( \frac{w}{\xi} - 1 - \frac{1}{2\xi^2} \right) \left( 1 - \left( \frac{\tilde{E}_k + \tilde{E}_K}{2} \right)^2 \right) \frac{\tilde{E}_k + \tilde{E}_K}{2} \\ & + \left( \frac{w}{\xi} - 1 \right) \frac{\tilde{E}_k + \tilde{E}_K}{2} \\ & - \left( -\frac{1}{2\xi^2} - \frac{\xi}{2w} + \frac{w}{2\xi} \right) \left( 1 - \left( \frac{\tilde{E}_k + \tilde{E}_K}{2} \right)^2 \right) \beta \end{aligned} \right) \right) |U_K \rangle \\ & + \underbrace{\frac{\tilde{\Omega}_{max}}{\sqrt{1 + \tilde{\Omega}_{max}^2}}}_{=1+O(\tilde{\Omega}_{max}^{-2})} \langle U_k | \frac{1}{6} \frac{\Pi_b}{m_0 c} \alpha_b |U_K \rangle + O(\alpha_{FS}^3) \end{aligned} \right) \quad (624)
\end{aligned}$$

Making use of the identities [7]

$$\langle U_k | \frac{\tilde{E}_k + \tilde{E}_K}{2} |U_K \rangle = \langle U_k | \tilde{\mathbf{H}}^{(D)} |U_K \rangle \quad (625)$$

$$\begin{aligned}
\langle U_k | \left( 1 - \left( \frac{\tilde{E}_k + \tilde{E}_K}{2} \right)^2 \right) \beta |U_K \rangle &= \langle U_k | \left( 1 - \frac{\tilde{E}_k^2}{4} - \frac{1}{2} \tilde{E}_k \tilde{E}_K - \frac{\tilde{E}_K^2}{4} \right) \beta |U_K \rangle \\ &= \langle U_k | \beta - \frac{\tilde{\mathbf{H}}^{(D)} \tilde{\mathbf{H}}^{(D)}}{4} \beta - \frac{1}{2} \tilde{\mathbf{H}}^{(D)} \beta \tilde{\mathbf{H}}^{(D)} - \beta \frac{\tilde{\mathbf{H}}^{(D)} \tilde{\mathbf{H}}^{(D)}}{4} |U_K \rangle \\ &= \langle U_k | \left( -\frac{\Pi_a}{m_0 c} \alpha_a \right) |U_K \rangle \quad (626)
\end{aligned}$$

$$\begin{aligned}
\langle U_k | \left( 1 - \left( \frac{\tilde{E}_k + \tilde{E}_K}{2} \right)^2 \right) \frac{\tilde{E}_k + \tilde{E}_K}{2} |U_K \rangle &= \langle U_k | \left( \mathbf{1}_{4 \times 4} - \tilde{\mathbf{H}}^{(D)} \tilde{\mathbf{H}}^{(D)} \right) \tilde{\mathbf{H}}^{(D)} |U_K \rangle \\ &= \langle U_k | \left( -\frac{2}{m_0 c^2} \tilde{\mathbf{H}}_{4 \times 4}^{(P)} \right) \tilde{\mathbf{H}}^{(D)} |U_K \rangle \quad (627)
\end{aligned}$$

and inserting for  $\frac{q_e \hbar}{2m_0} B_a^{(ext)} \sigma_a = \frac{\Pi_a \Pi_a}{2m_0} \mathbf{1}_{4 \times 4} - \mathbf{H}_{4 \times 4}^{(P,0)}$  there follows for (624) [7]

$$\begin{aligned}
\tilde{M}_{k,K}^{(\perp, e, high)} &= -m_0 c^2 \frac{\alpha_{FS}}{\pi} \times \\
&\times \left( \langle U_k | \int_0^{\tilde{\Omega}^{max}} d\xi \xi \left( \begin{aligned} & \left( \frac{\xi}{w} - 1 \right) \beta \\ & \left( -\frac{1}{3} \left( \left( \frac{w}{\xi} - \frac{\xi}{w} \right) + \left( -1 + \frac{\xi^3}{w^3} \right) \right) \right. \right. \\ & \quad \left. \left. + \left( \frac{w}{\xi} - 1 \right) \right) \frac{\Pi_a}{m_0 c} \alpha_a \right. \right. \\ & \quad \left. \left. + \left( -\frac{1}{2\xi^2} - \frac{\xi}{2w} + \frac{w}{2\xi} \right) \right. \right. \\ & \quad \left. \left. + \frac{1}{m_0 c^2} \left( -\frac{1}{\xi^2} + \frac{\xi}{w^3} \right) \frac{1}{3} \tilde{H}_{4 \times 4}^{(P)} \beta \right. \right. \\ & \quad \left. \left. - \frac{1}{m_0 c^2} \left( 2 \left( -\frac{1}{\xi^2} + \frac{\xi}{w^3} \right) + \frac{2+5\xi^2}{2\xi w^5} \right) \frac{2}{3} \frac{\Pi_a \Pi_a}{2m_0} \beta \right. \right. \\ & \quad \left. \left. + \frac{1}{m_0 c^2} \left( \left( \left( -1 + \frac{w}{\xi} - \frac{\xi}{2w^3} \right) + 2 \left( \frac{w}{\xi} - \frac{\xi}{w} - \frac{1}{\xi^2} \right) \right) \frac{2}{3} \left( \frac{\Pi_a \Pi_a}{2m_0} \frac{\tilde{H}^{(D)}}{2} + \frac{\tilde{H}^{(D)}}{2} \frac{\Pi_a \Pi_a}{2m_0} \right) \right. \right. \right. \\ & \quad \left. \left. - \left( \frac{w}{\xi} - \frac{\xi}{w} - \frac{1}{\xi^2} \right) \frac{1}{3} \left( \tilde{H}_{4 \times 4}^{(P)} \frac{\tilde{H}^{(D)}}{2} + \frac{\tilde{H}^{(D)}}{2} \tilde{H}_{4 \times 4}^{(P)} \right) \right. \right. \\ & \quad \left. \left. + \left( \frac{w}{\xi} - 1 - \frac{1}{2\xi^2} \right) \left( -\frac{2}{m_0 c^2} \tilde{H}_{4 \times 4}^{(P)} \right) \tilde{H}^{(D)} \right. \right. \\ & \quad \left. \left. + O(\alpha_{FS}^3) \right. \right. \\ & \quad \left. \left. + \langle U_k | \frac{1}{6} \frac{\Pi_b}{m_0 c} \alpha_b | U_K \rangle \right) \right) |U_K\rangle
\end{aligned} \tag{628}$$

The representation (628) of the transversal renormalization contribution is further evaluated in section 6.1.

### The Baker–Campbell Hausdorff Formula

The BCH formula assumes the following guise [57]

$$\exp(xA) B \exp(-xA) = \sum_{n=0}^{\infty} \frac{x^n}{n!} [A, B]^n \tag{629}$$

where  $A, B$  are operators and  $x$  is a parameter. The symbol  $[A, B]^n$  means to operate as

$$[A, \dots [A, B]] \tag{630}$$

$n$  times.

The initial value for  $n = 0$  is defined as  $[A, B]^0 \equiv B$ .

## J Operator Valued Maxwell Equations

In this part of the appendix it is shown that the operator valued electromagnetic fields obey to the Maxwell equations [6].

For this one has to make use of the Heisenberg equation of motion.

For an operator  $\hat{X}(\mathbf{r})$  of QED in the Heisenberg picture ( $\hat{\mathcal{H}}_{QED}$  being time independant)

$$\hat{X}(\mathbf{r}, t) = \exp\left(i\frac{t}{\hbar}\hat{\mathcal{H}}_{QED}\right) \hat{X}(\mathbf{r}) \exp\left(-i\frac{t}{\hbar}\hat{\mathcal{H}}_{QED}\right) \quad (631)$$

the related Heisenberg equation of motion is given by

$$i\hbar\frac{\partial\hat{X}(\mathbf{r}, t)}{\partial t} = \left[\hat{X}(\mathbf{r}, t), \hat{\mathcal{H}}_{QED}\right] \quad (632)$$

Hence, for the photon vector field  $\hat{A}_a^{(T)}(\mathbf{r}, t)$  as defined in (24) follows for the Heisenberg equation of motion

$$\begin{aligned} i\hbar\frac{\partial\hat{A}_a^{(T)}(\mathbf{r}, t)}{\partial t} &= \left[\hat{A}_a^{(T)}(\mathbf{r}, t), \hat{\mathcal{H}}_{QED}\right] \\ &= \exp\left(i\frac{t}{\hbar}\hat{\mathcal{H}}_{QED}\right) \left[\hat{A}_a^{(T)}(\mathbf{r}), \hat{\mathcal{H}}_{rad}\right] \exp\left(-i\frac{t}{\hbar}\hat{\mathcal{H}}_{QED}\right) \\ &= \exp\left(i\frac{t}{\hbar}\hat{\mathcal{H}}_{QED}\right) \left[\hat{A}_a^{(T)}(\mathbf{r}), \frac{\varepsilon_0}{2} \int d^3r' \sum_{b\in\{x,y,z\}} \left(\hat{E}_b^{(T)}(\mathbf{r}') \hat{E}_b^{(T)}(\mathbf{r}')\right)\right] \exp\left(-i\frac{t}{\hbar}\hat{\mathcal{H}}_{QED}\right) \\ &= \exp\left(i\frac{t}{\hbar}\hat{\mathcal{H}}_{QED}\right) \left(\frac{\hbar}{i} \int d^3r' \sum_{b\in\{x,y,z\}} \delta_{ab}^{(T)}(\mathbf{r}-\mathbf{r}') \hat{E}_b^{(T)}(\mathbf{r}')\right) \exp\left(-i\frac{t}{\hbar}\hat{\mathcal{H}}_{QED}\right) \\ &= \frac{\hbar}{i} \exp\left(i\frac{t}{\hbar}\hat{\mathcal{H}}_{QED}\right) \hat{E}_a^{(T)}(\mathbf{r}) \exp\left(-i\frac{t}{\hbar}\hat{\mathcal{H}}_{QED}\right) \\ &= -i\hbar\hat{E}_a^{(T)}(\mathbf{r}, t) \end{aligned} \quad (633)$$

Now since  $\hat{B}_a^{(T)}(\mathbf{r}, t) = \text{rot}\hat{A}_a^{(T)}(\mathbf{r}, t)$  the Faraday induction law is valid for operator valued electromagnetic fields

$$\frac{\partial\hat{B}_a^{(T)}(\mathbf{r}, t)}{\partial t} + \left(\text{rot}\hat{E}^{(T)}(\mathbf{r}, t)\right)_a = \hat{0} \quad (634)$$

On the other hand there follows for  $\hat{E}_a^{(T)}(\mathbf{r}, t)$  the Heisenberg equation of motion according to

$$\begin{aligned}
i\hbar \frac{\partial \hat{E}_a^{(T)}(\mathbf{r}, t)}{\partial t} &= [\hat{E}_a^{(T)}(\mathbf{r}, t), \hat{\mathcal{H}}_{QED}] \\
&= \exp\left(i\frac{t}{\hbar} \hat{\mathcal{H}}_{QED}\right) [\hat{E}_a^{(T)}(\mathbf{r}), \hat{\mathcal{H}}^{(QED)}] \exp\left(-i\frac{t}{\hbar} \hat{\mathcal{H}}_{QED}\right) \\
&= e^{i\frac{t}{\hbar} \hat{\mathcal{H}}_{QED}} \int d^3r' \left( \begin{array}{l} -[\hat{E}_a^{(T)}(\mathbf{r}), \hat{A}_b^{(T)}(\mathbf{r}')] \hat{j}_b(\mathbf{r}') \\ +\frac{1}{2\mu_0} [\hat{E}_a^{(T)}(\mathbf{r}), \hat{B}_b(\mathbf{r}') \hat{B}_b(\mathbf{r}')] \end{array} \right) e^{-i\frac{t}{\hbar} \hat{\mathcal{H}}_{QED}} \\
&= e^{i\frac{t}{\hbar} \hat{\mathcal{H}}_{QED}} \int d^3r' \left( \begin{array}{l} \frac{q}{\varepsilon_0} \frac{\hbar}{i} \delta_{ab}^{(T)}(\mathbf{r}' - \mathbf{r}) \hat{j}_b(\mathbf{r}') \\ +\frac{1}{2\mu_0} [\hat{E}_a^{(T)}(\mathbf{r}), \hat{B}_b(\mathbf{r}') \hat{B}_b(\mathbf{r}')] \end{array} \right) e^{-i\frac{t}{\hbar} \hat{\mathcal{H}}_{QED}} \\
&= \exp\left(i\frac{t}{\hbar} \hat{\mathcal{H}}_{QED}\right) \left( \begin{array}{l} -i\hbar \frac{1}{\varepsilon_0} \int d^3r' \sum_{b \in \{x,y,z\}} \delta_{ab}^{(T)}(\mathbf{r} - \mathbf{r}') \hat{j}_b(\mathbf{r}') \\ +\frac{i\hbar}{\varepsilon_0 \mu_0} (\text{rot} \hat{\mathbf{B}}(\mathbf{r}'))_a \end{array} \right) \exp\left(-i\frac{t}{\hbar} \hat{\mathcal{H}}_{QED}\right) \tag{635}
\end{aligned}$$

In the last line use has been made of the commutation relations (29) and the relation

$$\begin{aligned}
&\frac{1}{2\mu_0} \int d^3r' \sum_{b \in \{x,y,z\}} [\hat{E}_a^{(T)}(\mathbf{r}), \hat{B}_b(\mathbf{r}') \hat{B}_b(\mathbf{r}')] \\
&= \frac{1}{2\mu_0} \int d^3r' \sum_{b \in \{x,y,z\}} [\hat{E}_a^{(T)}(\mathbf{r}), (\text{rot} \hat{\mathbf{A}}^{(T)}(\mathbf{r}'))_b (\text{rot} \hat{\mathbf{A}}^{(T)}(\mathbf{r}'))_b] \\
&= \frac{1}{2\mu_0} \int d^3r' \sum_{b,c,c' \in \{x,y,z\}} \left( \begin{array}{l} \frac{1}{\varepsilon_0} \frac{\hbar}{i} \delta_{ca}^{(T)}(\mathbf{r}' - \mathbf{r}) \left( \varepsilon_{bc'c} \frac{\partial}{\partial r'_{c'}} \hat{B}_b(\mathbf{r}') \right) \\ + \left( \varepsilon_{bc'c} \frac{\partial}{\partial r'_{c'}} \hat{B}_b(\mathbf{r}') \right) \frac{1}{\varepsilon_0} \frac{\hbar}{i} \delta_{ca}^{(T)}(\mathbf{r}' - \mathbf{r}) \end{array} \right) \tag{636} \\
&= \frac{1}{\varepsilon_0 \mu_0} \frac{\hbar}{i} \int d^3r' \sum_{b,c,c' \in \{x,y,z\}} \delta_{ac}^{(T)}(\mathbf{r} - \mathbf{r}') \left( -\varepsilon_{cc'b} \frac{\partial}{\partial r'_{c'}} \hat{B}_b(\mathbf{r}') \right) \\
&= \frac{i\hbar}{\varepsilon_0 \mu_0} \int d^3r' \sum_{c \in \{x,y,z\}} \delta_{ac}^{(T)}(\mathbf{r} - \mathbf{r}') (\text{rot} \hat{\mathbf{B}}(\mathbf{r}'))_c \\
&= \frac{i\hbar}{\varepsilon_0 \mu_0} (\text{rot} \hat{\mathbf{B}}(\mathbf{r}))_a
\end{aligned}$$

Here,  $\hat{j}_b(\mathbf{r})$  is the relativistic current density operator and ‘p.I.’ stands for partial integration. Decomposing it into longitudinal and transversal parts according to

$$\begin{aligned}
\hat{j}_a^{(T)}(\mathbf{r}) &= \int d^3r' \sum_{b \in \{x,y,z\}} \delta_{ab}^{(T)}(\mathbf{r} - \mathbf{r}') \hat{j}_b(\mathbf{r}') \\
\hat{j}_a^{(L)}(\mathbf{r}) &= \int d^3r' \sum_{b \in \{x,y,z\}} \delta_{ab}^{(L)}(\mathbf{r} - \mathbf{r}') \hat{j}_b(\mathbf{r}') \tag{637} \\
\hat{j}_a(\mathbf{r}) &= \hat{j}_a^{(L)}(\mathbf{r}) + \hat{j}_a^{(T)}(\mathbf{r})
\end{aligned}$$

there follows for the Heisenberg equation of motion (635)

$$\left(\text{rot}\hat{\mathbf{B}}(\mathbf{r}, t)\right)_a = \varepsilon_0\mu_0 \frac{\partial \hat{E}_a^{(T)}(\mathbf{r}, t)}{\partial t} + \mu_0 \hat{j}_a^{(T)}(\mathbf{r}, t) \quad (638)$$

which is the Maxwell equation of the displacement current.

Now, the decomposition of the current density into transversal and longitudinal parts according to (637) is not invariant under Lorentz transformations. However, one can complete equation (638) by adding the equation of motion of the longitudinal current density operator which is closely related to the QED continuity equation. The latter follows from the Heisenberg equation of motion of the charge density operator  $\hat{\rho}(\mathbf{r}, t)$ :

$$\begin{aligned} i\hbar \frac{\partial \hat{\rho}(\mathbf{r}, t)}{\partial t} &= \left[ \hat{\rho}(\mathbf{r}, t), \hat{\mathcal{H}}_{QED} \right] \\ &= \exp\left(i\frac{t}{\hbar} \hat{\mathcal{H}}_{QED}\right) \left[ \hat{\rho}(\mathbf{r}), \hat{\mathcal{H}}_{QED} \right] \exp\left(-i\frac{t}{\hbar} \hat{\mathcal{H}}_{QED}\right) \end{aligned} \quad (639)$$

The commutator can be evaluated according to

$$\begin{aligned} \left[ \hat{\rho}(\mathbf{r}), \hat{\mathcal{H}}_{QED} \right] &= \left[ \hat{\rho}(\mathbf{r}), \hat{\mathcal{H}}_D + \hat{\mathcal{H}}_{rad} + \hat{\mathcal{H}}_A + \hat{V}_C \right] \\ &= \left[ \hat{\rho}(\mathbf{r}), \hat{\mathcal{H}}_D \right] \\ &= \left[ q_0 \sum_{\mu} \hat{\Psi}_{\mu}^{\dagger}(\mathbf{r}) \hat{\Psi}_{\mu}(\mathbf{r}), \int d^3r' \sum_{\mu', \mu''} \hat{\Psi}_{\mu'}^{\dagger}(\mathbf{r}') H_{\mu', \mu''}^{(D)}(\mathbf{r}') \hat{\Psi}_{\mu''}(\mathbf{r}') \right] \\ &= q_0 \int d^3r' \lim_{\mathbf{R}' \rightarrow \mathbf{r}'} \sum_{\mu', \mu''} H_{\mu', \mu''}^{(D)}(\mathbf{r}') \left[ \hat{\Psi}_{\mu}^{\dagger}(\mathbf{r}) \hat{\Psi}_{\mu}(\mathbf{r}), \hat{\Psi}_{\mu'}^{\dagger}(\mathbf{R}') \hat{\Psi}_{\mu''}(\mathbf{r}') \right] \\ &= q_0 \int d^3r' \lim_{\mathbf{R}' \rightarrow \mathbf{r}'} \sum_{\mu', \mu''} H_{\mu', \mu''}^{(D)}(\mathbf{r}') \left\{ \begin{aligned} &\hat{\Psi}_{\mu}^{\dagger}(\mathbf{r}) \left\{ \hat{\Psi}_{\mu}(\mathbf{r}), \hat{\Psi}_{\mu'}^{\dagger}(\mathbf{R}') \right\} \hat{\Psi}_{\mu''}(\mathbf{r}') \\ &- \hat{\Psi}_{\mu'}^{\dagger}(\mathbf{R}') \left\{ \hat{\Psi}_{\mu''}(\mathbf{r}'), \hat{\Psi}_{\mu}^{\dagger}(\mathbf{r}) \right\} \hat{\Psi}_{\mu}(\mathbf{r}) \end{aligned} \right\} \\ &= q_0 \int d^3r' \lim_{\mathbf{R}' \rightarrow \mathbf{r}'} \sum_{\mu', \mu''} H_{\mu', \mu''}^{(D)}(\mathbf{r}') \left\{ \begin{aligned} &\delta^{(3)}(\mathbf{r} - \mathbf{R}') \hat{\Psi}_{\mu'}^{\dagger}(\mathbf{r}) \hat{\Psi}_{\mu''}(\mathbf{r}') \\ &- \delta^{(3)}(\mathbf{r} - \mathbf{r}') \hat{\Psi}_{\mu'}^{\dagger}(\mathbf{R}') \hat{\Psi}_{\mu''}(\mathbf{r}) \end{aligned} \right\} \end{aligned} \quad (640)$$

Partial integration and inserting the single-particle Dirac Hamiltonian  $H_{\mu', \mu''}^{(D)}$  given in (10) yields

$$\begin{aligned}
\left[ \hat{\rho}(\mathbf{r}), \hat{\mathcal{H}}_{QED} \right] &= q_0 \int d^3 r' \delta^{(3)}(\mathbf{r} - \mathbf{r}') \sum_{\mu', \mu''} \left\{ \hat{\Psi}_{\mu'}^\dagger(\mathbf{r}) \left( h_{\mu', \mu''}^{(D)}(\mathbf{r}') \hat{\Psi}_{\mu''}(\mathbf{r}') \right) \right. \\
&\quad \left. - \left( h_{\mu', \mu''}^{*(D)}(\mathbf{r}') \hat{\Psi}_{\mu'}^\dagger(\mathbf{r}') \right) \hat{\Psi}_{\mu''}(\mathbf{r}') \right\} \\
&= q_0 \sum_{\mu', \mu''} \left\{ \hat{\Psi}_{\mu'}^\dagger(\mathbf{r}) \left( h_{\mu', \mu''}^{(D)}(\mathbf{r}) \hat{\Psi}_{\mu''}(\mathbf{r}) \right) \right. \\
&\quad \left. - \left( h_{\mu', \mu''}^{*(D)}(\mathbf{r}) \hat{\Psi}_{\mu'}^\dagger(\mathbf{r}) \right) \hat{\Psi}_{\mu''}(\mathbf{r}) \right\} \\
&= q_0 \sum_{\mu', \mu''} \sum_{b \in \{x, y, z\}} (c\alpha_b)_{\mu', \mu''} \left\{ \hat{\Psi}_{\mu'}^\dagger(\mathbf{r}) \left( \frac{\hbar}{i} \frac{\partial}{\partial r_b} \hat{\Psi}_{\mu''}(\mathbf{r}) \right) \right. \\
&\quad \left. - \left( -\frac{\hbar}{i} \frac{\partial}{\partial r_b} \hat{\Psi}_{\mu'}^\dagger(\mathbf{r}) \right) \hat{\Psi}_{\mu''}(\mathbf{r}) \right\} \\
&= \frac{\hbar}{i} \sum_{b \in \{x, y, z\}} \frac{\partial}{\partial r_b} \left( \hat{\Psi}_{\mu'}^\dagger(\mathbf{r}) (c\alpha_b)_{\mu', \mu''} \hat{\Psi}_{\mu''}(\mathbf{r}) \right) \\
&= -i\hbar \sum_{b \in \{x, y, z\}} \frac{\partial}{\partial r_b} \hat{j}_b(\mathbf{r})
\end{aligned} \tag{641}$$

Hence there follows for the QED continuity equation

$$\frac{\partial \hat{\rho}(\mathbf{r}, t)}{\partial t} + \sum_{b \in \{x, y, z\}} \frac{\partial}{\partial r_b} \hat{j}_b(\mathbf{r}, t) = \hat{0} \tag{642}$$

The longitudinal electric field is defined as

$$\begin{aligned}
\hat{E}_a^{(L)}(\mathbf{r}, t) &= -\frac{\partial}{\partial r_a} \hat{\Phi}(\mathbf{r}, t) \\
\hat{\Phi}(\mathbf{r}, t) &= \int d^3 r' \frac{\hat{\rho}(\mathbf{r}', t)}{4\pi\epsilon_0 |\mathbf{r} - \mathbf{r}'|} \\
\text{div} \hat{\mathbf{E}}^{(L)}(\mathbf{r}, t) &= \frac{\hat{\rho}(\mathbf{r}, t)}{\epsilon_0}
\end{aligned} \tag{643}$$

Using the continuity equation (642) for the temporal derivative of the electric field operator  $\hat{E}_a^{(L)}(\mathbf{r}, t)$  then

$$\begin{aligned}
\frac{\partial \hat{E}_a^{(L)}(\mathbf{r}, t)}{\partial t} &= \frac{\partial}{\partial t} \left( -\frac{\partial}{\partial r_a} \hat{\Phi}(\mathbf{r}, t) \right) \\
&= -\frac{\partial}{\partial r_a} \int d^3 r' \frac{\frac{\partial \hat{\rho}(\mathbf{r}', t)}{\partial t}}{4\pi\epsilon_0 |\mathbf{r} - \mathbf{r}'|} \\
&= \frac{\partial}{\partial r_a} \int d^3 r' \frac{\sum_{b \in \{x, y, z\}} \frac{\partial}{\partial r'_b} \hat{j}_b(\mathbf{r}', t)}{4\pi\epsilon_0 |\mathbf{r} - \mathbf{r}'|} \\
&= \frac{\partial}{\partial r_a} \int d^3 r' \sum_{b \in \{x, y, z\}} \left( \frac{\partial}{\partial r'_b} \left( \frac{\hat{j}_b(\mathbf{r}', t)}{4\pi\epsilon_0 |\mathbf{r} - \mathbf{r}'|} \right) - \hat{j}_b(\mathbf{r}', t) \frac{\partial}{\partial r'_b} \frac{1}{4\pi\epsilon_0 |\mathbf{r} - \mathbf{r}'|} \right) \\
&= \frac{\partial}{\partial r_a} \int d^3 r' \sum_{b \in \{x, y, z\}} \left( \frac{\partial}{\partial r'_b} \left( \frac{\hat{j}_b(\mathbf{r}', t)}{4\pi\epsilon_0 |\mathbf{r} - \mathbf{r}'|} \right) + \left( \frac{\partial}{\partial r_b} \frac{1}{4\pi\epsilon_0 |\mathbf{r} - \mathbf{r}'|} \right) \hat{j}_b(\mathbf{r}', t) \right) \\
&= \left( \frac{\partial}{\partial r_a} \int d^3 r' \sum_{b \in \{x, y, z\}} n_{b'} \frac{\hat{j}_b(\mathbf{r}', t)}{4\pi\epsilon_0 |\mathbf{r} - \mathbf{r}'|} \right) + \frac{1}{\epsilon_0} \int d^3 r' \sum_{b \in \{x, y, z\}} \frac{\partial^2}{\partial r_a \partial r_b} \frac{1}{4\pi |\mathbf{r} - \mathbf{r}'|} \hat{j}_b(\mathbf{r}', t) \\
&\quad \text{(Oberflächenterm verschwindet)}
\end{aligned} \tag{644}$$

Using the representation of the longitudinal delta function (31) there follows

$$\begin{aligned}
\frac{\partial \hat{E}_a^{(L)}(\mathbf{r}, t)}{\partial t} &= -\frac{1}{\epsilon_0} \int d^3 r' \delta_{ab}^{(L)}(\mathbf{r} - \mathbf{r}') \hat{j}_b(\mathbf{r}', t) \\
&= -\frac{1}{\epsilon_0} \hat{j}_a^{(L)}(\mathbf{r}, t)
\end{aligned} \tag{645}$$

With that one finds

$$\epsilon_0 \mu_0 \frac{\partial \hat{E}_a^{(L)}(\mathbf{r}, t)}{\partial t} + \mu_0 \hat{j}_a^{(L)}(\mathbf{r}, t) = \hat{0} \tag{646}$$

The divergence of (646) yields with  $\sum_{a \in \{x, y, z\}} \frac{\partial}{\partial r_a} \hat{E}_a^{(L)}(\mathbf{r}, t) = \text{div} \hat{E}^{(L)}(\mathbf{r}, t) = \frac{1}{\epsilon_0} \hat{\rho}(\mathbf{r}, t)$  the continuity equation.

Adding (646) and (638) now gives the complete Maxwell equation of the operator valued electromagnetic fields as

$$\left( \text{rot} \hat{\mathbf{B}}(\mathbf{r}, t) \right)_a = \epsilon_0 \mu_0 \frac{\partial \hat{E}_a(\mathbf{r}, t)}{\partial t} + \mu_0 \hat{j}_a(\mathbf{r}, t) \tag{647}$$

One can also derive wave equations by differentiating again with respect to time.

$$\begin{aligned} \text{rot} \frac{\partial}{\partial t} \hat{\mathbf{B}}(\mathbf{r}, t) &\stackrel{(634)}{=} -\text{rot} \text{rot} \hat{\mathbf{E}}(\mathbf{r}, t) \\ &= \varepsilon_0 \mu_0 \frac{\partial^2 \hat{\mathbf{E}}(\mathbf{r}, t)}{\partial t^2} + \mu_0 \frac{\partial}{\partial t} \hat{\mathbf{j}}(\mathbf{r}, t) \end{aligned} \quad (648)$$

or

$$\text{rot} \text{rot} \hat{\mathbf{E}}(\mathbf{r}, t) + \frac{1}{c^2} \frac{\partial^2 \hat{\mathbf{E}}(\mathbf{r}, t)}{\partial t^2} = -\mu_0 \frac{\partial}{\partial t} \hat{\mathbf{j}}(\mathbf{r}, t) \quad (649)$$

where  $c = \frac{1}{\sqrt{\varepsilon_0 \mu_0}}$ .

The analogue of equation 649 for the photon field  $\hat{\mathbf{A}}^{(T)}(\mathbf{r}, t)$  follows with 633 and  $\hat{B}_a^{(T)}(\mathbf{r}, t) = \text{rot} \hat{A}_a^{(T)}(\mathbf{r}, t)$  is thus given by

$$\text{rot} \text{rot} \hat{\mathbf{A}}^{(T)}(\mathbf{r}, t) + \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \hat{\mathbf{A}}^{(T)}(\mathbf{r}, t) = \mu_0 \hat{\mathbf{j}}^{(T)}(\mathbf{r}, t) \quad (650)$$

Using

$$\begin{aligned} \text{rot} \text{rot} \hat{\mathbf{A}}^{(T)}(\mathbf{r}, t) &= \nabla \left( \text{div} \hat{\mathbf{A}}^{(T)}(\mathbf{r}, t) \right) - \nabla^2 \hat{\mathbf{A}}^{(T)}(\mathbf{r}, t) \\ \text{div} \hat{\mathbf{A}}^{(T)}(\mathbf{r}, t) &= 0 \end{aligned} \quad (651)$$

there follows

$$\left( \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \nabla^2 \right) \hat{\mathbf{A}}^{(T)}(\mathbf{r}, t) = \mu_0 \hat{\mathbf{j}}^{(T)}(\mathbf{r}, t) \quad (652)$$

whose derivative with respect to the time (in the Heisenberg picture) is identical to the wave equation 649.

Assuming there is no matter to which the photons couple the homogeneous wave equation arises.

In that case one can write for the time dependence of the vector potential (24) and the electric field (25) [7]

$$\begin{aligned} \hat{A}_b^{(T,0)}(\mathbf{r}, t) &= e^{\frac{i}{\hbar} t \hat{\mathcal{H}}_{rad}} \hat{A}_b^{(0)}(\mathbf{r}) e^{-\frac{i}{\hbar} t \hat{\mathcal{H}}_{rad}} \\ \hat{E}_a^{(T,0)}(\mathbf{r}, t) &= e^{\frac{i}{\hbar} t \hat{\mathcal{H}}_{rad}} \hat{E}_a^{(T,0)}(\mathbf{r}) e^{-\frac{i}{\hbar} t \hat{\mathcal{H}}_{rad}} \end{aligned} \quad (653)$$



where  $\hat{A}_b^{(0)}(\mathbf{r})$  and  $\hat{E}_a^{(T,0)}(\mathbf{r})$  are the solutions to the homogenous wave equation (the right hand side of 649 and 652 equals zero).

Now using the BCH formula (see section I) there follows [7]

$$\begin{aligned} e^{\frac{i}{\hbar}t\hat{\mathcal{H}}_{rad}}\hat{a}_{\mathbf{q},\lambda}e^{-\frac{i}{\hbar}t\hat{\mathcal{H}}_{rad}} &= e^{-i\omega_{\mathbf{q}}t}\hat{a}_{\mathbf{q},\lambda} \\ e^{\frac{i}{\hbar}t\hat{\mathcal{H}}_{rad}}\hat{a}_{\mathbf{q},\lambda}^\dagger e^{-\frac{i}{\hbar}t\hat{\mathcal{H}}_{rad}} &= e^{i\omega_{\mathbf{q}}t}\hat{a}_{\mathbf{q},\lambda}^\dagger \end{aligned} \quad (654)$$

which gives for (654) [7]

$$\begin{aligned} \hat{A}_b^{(T,0)}(\mathbf{r}, t) &= \frac{1}{\sqrt{V}} \sum_{\mathbf{q}} \sum_{\lambda \in \{I, II\}} \sqrt{\frac{\hbar}{2\varepsilon_0\omega(\mathbf{q})}} \left( e^{i(\mathbf{q}\cdot\mathbf{r}-\omega_{\mathbf{q}}t)}\hat{a}_{\mathbf{q},\lambda} + e^{-i(\mathbf{q}\cdot\mathbf{r}-\omega_{\mathbf{q}}t)}\hat{a}_{\mathbf{q},\lambda}^\dagger \right) u_b(\mathbf{q}, \lambda) \\ \hat{E}_b^{(T,0)}(\mathbf{r}, t) &= \frac{i}{\sqrt{V}} \sum_{\mathbf{q}} \sum_{\lambda \in \{I, II\}} \sqrt{\frac{\hbar\omega(\mathbf{q})}{2\varepsilon_0}} \left( e^{i(\mathbf{q}\cdot\mathbf{r}-\omega_{\mathbf{q}}t)}\hat{a}_{\mathbf{q},\lambda} - e^{-i(\mathbf{q}\cdot\mathbf{r}-\omega_{\mathbf{q}}t)}\hat{a}_{\mathbf{q},\lambda}^\dagger \right) u_b(\mathbf{q}, \lambda) \end{aligned} \quad (655)$$

The condition  $\omega_{\mathbf{q}} = c|\mathbf{q}|$  leads then to the vacuum wave equations or homogeneous wave equations [7]

$$\begin{aligned} \left( \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \nabla^2 \right) \hat{\mathbf{A}}^{(T,0)}(\mathbf{r}, t) &= 0 \\ \left( \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \nabla^2 \right) \hat{\mathbf{E}}^{(T,0)}(\mathbf{r}, t) &= 0 \end{aligned} \quad (656)$$

It has to be emphasized that the solutions  $\hat{\mathbf{A}}^{(T,0)}(\mathbf{r}, t)$  and  $\hat{\mathbf{E}}^{(T,0)}(\mathbf{r}, t)$  to the homogeneous wave equations cannot be zero (in sharp contrast to classical electromagnetic fields), because otherwise their fundamental commutation relation [7]

$$\left[ \hat{A}_a^{(T,0)}(\mathbf{r}), \hat{E}_b^{(T,0)}(\mathbf{r}') \right] = \frac{1}{\varepsilon_0} \frac{\hbar}{i} \delta_{ab}^{(T)}(\mathbf{r} - \mathbf{r}') \hat{1} \quad (657)$$

would not be satisfied. This means that there is always a electromagnetic vacuum quantum field leading to the so-called vacuum fluctuations  $\langle Vac | \hat{E}_a^{(T,0)}(\mathbf{r}, t) \hat{E}_a^{(T,0)}(\mathbf{r}, t) | Vac \rangle \neq 0$ .

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