
Pair Creation by Strong Laser Fields

Johannes Mattis Nissen-Meyer



München 2018

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Johannes Mattis Nissen-Meyer

Dissertation
an der Fakultät für Mathematik, Informatik und Statistik
der Ludwig-Maximilians-Universität
München

vorgelegt von
Johannes Mattis Nissen-Meyer
aus Gräfelfing

München, den 18. April 2018

Erstgutachter: Prof. Dr. Peter Pickl

Zweitgutachter: Prof. Dr. Felix Finster

Drittgutachter: Prof. Dr. Horia Cornean

Tag der mündlichen Prüfung: 16.07.2018

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Abstract

The goal of my Ph.D. thesis is to achieve a better understanding of the process of pair creation in strong laser fields. Due to the advance in laser technology the currently attainable field strengths start to approach the predicted limit where positron-electron pair production could appear. The available theoretical results so far are based on work done by Schwinger (1951) and Brezin & Itzykson (1970). It is questionable, though, whether these results are applicable to electromagnetic waves at all. Hence, we believe there is a need for a rigorous treatment of this process. We start with a different ansatz and develop an adiabatic perturbation theory with respect to Hilbert-Schmidt norm which is applicable to electromagnetic waves. We implement this into the Fock space formalism of external field QED and rigorously derive estimates on the transition amplitudes from the vacuum state into every (n, m) -particle-antiparticle state for finite times. An order of magnitude estimate, using these results, shows for common laser parameters that the necessary field strengths most likely have to be at least a couple of orders of magnitude higher than what has been suggested so far. In the adiabatic limit of vanishing frequencies there is no pair creation at all.

Zusammenfassung (Translation of Abstract)

Das Ziel der vorliegenden Arbeit ist es, ein besseres Verständnis der Paarerzeugung in starken Laserfeldern zu etablieren. Durch den Fortschritt in der Lasertechnologie werden die verfügbaren Feldstärken in absehbarer Zeit die notwendige Grenzen erreichen werden, die für diesen Prozess vorhergesagt wurde. Die bisher verfügbaren Resultat hierzu basieren hauptsächlich auf zwei Arbeiten von Schwinger (1951) und Brezin & Itzykson (1970). Es ist jedoch fragwürdig ob die Ergebnisse dieser beiden Arbeiten korrekterweise auf elektromagnetische Wellen angewandt werden können. Daher glauben wir, dass eine rigorose Behandlung dieses Prozesses notwendig ist. Wir verfolgen einen anderen Ansatz und entwickeln eine adiabatische Störungstheorie bzgl. der Hilbert-Schmidt Norm, die auf elektromagnetische Wellen anwendbar ist. Wir implementieren diese im Anschluss in den Fockraum Formalismus der externen Feld QED und leiten, in mathematisch rigoroser Form, Abschätzungen für die Übergangsamplituden vom Vakuum in jeden (n, m) -Teilchen-Antiteilchen Zustand ab. Mithilfe dieser Ergebnisse führen wir eine Größenordnungsabschätzung für übliche Laserparameter durch. Diese zeigt bereits, dass die notwendigen Feldstärken sehr wahrscheinlich mehrere Größenordnungen höher sein müssen als bisher vorhergesagt. Im adiabatischen Limes von verschwindenden Frequenzen ist die Paarerzeugungsrate identisch null.

Acknowledgements

I would like to express my very great appreciation to Prof. Dr. Peter Pickl for being my supervisor. Being an outstanding scientist and teacher, his skills as an advisor are exemplary on a professional as well as on the personal level.

I want to thank Prof. Dr. Detlef Dürr who taught me to believe in mathematics and physics being a path towards a true understanding of nature opposed to the so widespread “Shut up and calculate”.

I also want to thank Dr. Dirk-André Deckert for the helpful discussions on external field QED.

I would like to express my gratitude to Prof. Dr. Felix Finster and Prof. Dr. Horia Cornean for being the co-supervisors of this thesis.

I thank my father Sven Nissen-Meyer for his careful proof-reading of my manuscript.

I want to thank my office mate Martin Oelker for many and valuable discussion on- and off-topic. Finally, I would like to thank the whole Kinderzimmer group for great company during the last years.

The funding and support of the Studienstiftung des deutschen Volkes is greatly appreciated.

Preface

Pair creation is a feature of quantum electrodynamics (QED) which has thrilled physicists since the discovery of the Dirac equation 90 years ago. Numerous experiments and theoretical studies have been carried out to investigate this phenomenon. Whereas in high energy physics pair creation is a well established and understood effect this cannot be truly said about strong field QED. In this region, where the electromagnetic fields are of low energy but high intensity, we still lack experimental verification of many theoretical predictions. The necessary field strengths are simply too high to have been produced in the laboratory up to now.

Since the 1960's high intensity lasers have been suggested as a possible source of strong electrical fields to produce electron-positron pairs in the vacuum. While the necessary field strengths of around $10^{18} \frac{\text{V}}{\text{m}}$ have been out of reach for the last decades, current technological progress in laser technology starts to approach this limit. The ELI-NP facility¹ in Romania reaches field strengths of $10^{15} \frac{\text{V}}{\text{m}}$ and the fourth ELI Pillar currently in the development stage will add one more order of magnitude. Hence, at least the next generation laser facility should bring this side of QED into the realm of experimental verification. Almost all available theoretical studies (see [MP77], [AHR⁺01], [Pop01], [Rin01], [NBMP04], [BPR⁺06], [BET⁺10]) concerning this topic are based on a computation by Schwinger [Sch51] from 1951. In that paper Schwinger computes the pair-creation capability of a static, homogenous electrical field. Such a field, however, describes approximately the situation in a plate capacitor but is certainly qualitatively different than an electromagnetic wave. Because of this theoretical ambiguity and the upcoming possibility of experimental verification, we feel the need of a thorough analysis of the current state of research and a rigorous treatment of the process of pair creation by strong laser fields. This effort will prove to be a challenging theoretical exercise, touching various fields of mathematical physics and hopefully helps to shed a little bit more light onto the process of pair creation by strong fields in QED in general.

The intuitive picture we have in mind is Dirac's hole theory which is common in strong field QED (see e.g. [GMR85]). Heuristically speaking, pair creation happens if a negative electron from the Dirac sea is lifted to positive energies. In principle, there are two processes which could be responsible for such a behavior. Either the electromagnetic field creates bound states in the mass gap which wander from the negative energy continuum to the positive over the course of time. Given this, it has been proven by Pickl [Pic05] that pair creation actually exists. This is usually referred to as *spontaneous* or *adiabatic pair creation*. However, analyzing the spectrum of the Dirac operator corresponding to an electromagnetic wave reveals that no eigenstates exist in the gap at any time (see Chapter 3). Hence, this is ruled out. The remaining second possibility of crossing the mass gap would be due to a tunneling process. An electromagnetic field generally

¹www.eli-laser.eu

changes the spectral subspaces. Thus, if the field is time-dependent the negative and positive spectral subspace can rotate into each other which in turn could result in a production of an electron-positron pair. To control such a behavior we observe that usual lasers in the range of $\lambda = 1\text{nm} - 1\mu\text{m}$ vary a thousand to a million times slower with respect to time than solutions of the Dirac equation. We can therefore employ adiabatic perturbation theory to control the time evolution of a solution to the Dirac equation.

The major difficulty hereby is that we have to control the time evolution for any electron in the Dirac sea, i.e. for the whole negative energy spectral subspace. It turns out that the most challenging obstacle for a rigorous proof of adiabatic behavior is to show the regularity of the spectral projections onto this subspace. The usual method which employs Cauchy-Riesz integral formula only works if the spectral subspace corresponds to an isolated part of the spectrum. This is certainly not the case for the complete negative energy subspace. Hence, we have to develop a new method to prove the differentiability of the spectral projections in dependence of the external field.

To establish this method we have to switch to generalized Fourier space for the Dirac operator. For the theory of generalized Fourier transform for the Schrödinger operator one needs a result from Kato concerning the behavior of solutions to the Schrödinger equation at infinity. There exists no comparable result for the Dirac operator. Therefore, we prove in Chapter 2 a similar result (Theorem 2.6) for the Dirac equation. Chapter 3 is then devoted to develop the theory of eigenfunction expansion for the Dirac operator with vector potential together with certain regularity properties of the generalized eigenfunctions. In Chapter 4 we introduce the spectral projections onto positive and negative subspaces. Due to the influence of the external field they will be explicitly time-dependent. Furthermore, we explain how electrons with negative energy are connected to positive energy particles with positive charge.

We go on and use this preliminary work to develop our method for the regularity of the spectral projections with respect to time-derivatives. This is the content of Chapter 5. We then conclude the first part of this thesis with Chapter 6 and a thorough discussion of the adiabatic theorem. We start off with a detailed heuristic argument and explain how adiabatic behavior arises from negative interference. The two main results are then given in Theorem 6.1 and Theorem 6.3. In the first theorem we use the previous work to prove a first order adiabatic theorem for the negative energy subspace of the Dirac operator with vector potential. We are able to state the error in a concise form. Furthermore, we find that with our method of deriving the time-derivatives of the spectral projections it is easy to extend the adiabatic theorem to Hilbert-Schmidt norm. This is the content of the second theorem and is very important in the context of second quantization. A nice by-product of the second theorem is the Hilbert-Schmidt property of the odd terms of the time evolution, $P_t^\pm U(t, s) P_t^\mp$ for a wide range of vector potentials. This is important for the existence of a time evolution in the second quantized theory. We therefore state it as a single result in Corollary 6.4. We finally also give a rigorous procedure how both theorems can be extended to higher order adiabatic perturbation theory depending solely on the regularity of the external field. We work it out explicitly up to second order including all error estimates.

The second part of this thesis is devoted to the external field model of QED which is the common theory to describe strong field effects in QED (see e.g. [GMR85]). The formulation of our problem in the second quantized context poses some difficulties. Usually, external field QED is stated for one fixed Hilbert space – the Fock space. However, due to Shale and Stinespring’s criterion [SS65] and results of Ruijsenaars [Rui77] we know that the time evolution can only be implemented on Fock space if the vector potential vanishes. Hence, we are not able to describe the time evolution of an electromagnetic wave in external field QED with a time-independent Fock space.

However, this problem can be overcome if one requires the Hilbert space of the second quantized theory to be time-dependent as well. This suggestion was first developed by Deckert et al. [DDMS10] in context of a rigorous formulation of the Dirac sea – called *infinite wedge spaces*. We adopt this idea of *time-dependent* Hilbert spaces and develop a time-dependent Fock space formalism in a constructive way in Chapter 7. We proceed with a motivation and definition of a time evolution on such a family of Fock spaces in Chapter 8. In Theorem 8.6 and Theorem 8.7 we prove the Shale-Stinespring criterion for such a time-dependent Fock space formalism. Together with Corollary 6.4 from before this shows that the time evolution in such a context indeed exists for a wide range of vector potentials as external fields. Furthermore, Theorem 8.6 gives an explicit expression of the time evolution of the vacuum. This state is in general not the vacuum state anymore which is the key difference to the usual time-independent Fock space theory and allows for e.g. pair creation. Moreover, as the time evolution of the creation and annihilation operators is known due to Definition 8.1, one can use Theorem 8.6 to state the explicit form of the time evolution of *any* state in closed form. Chapter 9 closes the second part of the thesis with an application of the previous results to establish what we call “Adiabatic perturbation theory in QED”. Theorem 9.1 combined with the results from Chapter 6 can be used to show an adiabatic behavior for the particle-number subspaces of the Fock space. However, the results from Theorem 9.1 and Theorem 9.4 are more general than adiabatic perturbation theory. They establish an explicit and direct connection between the transitions of the one-particle Dirac equation and the second quantized theory, proving that the intuitive picture of the Dirac sea is indeed correct in terms of the second quantized theory. Furthermore, they can be used to compute the explicit pair creation rates directly from the one-particle transition amplitudes.

In the third part of the thesis we finally analyze the pair creation capabilities of strong laser fields. We start off with Chapter 10 and 11 where we examine the current state of research on this topic. We explain how the Klein paradox and the Schwinger mechanism are connected and how their physical origin can be understood. In Chapter 12 we examine the possibility of testing the Schwinger mechanism with the help of lasers. To this end, we apply the theoretical framework which we developed in the first two parts and formulate the main result of this thesis in Theorem 12.1. This allows one to estimate pair creation probabilities in principle for arbitrary changing electromagnetic fields. Through a first order of magnitude estimate using common laser parameters we find that the necessary field strengths to observe effects of pair creation most likely have to be at least multiple orders higher than what has been proposed so far.

Part I.

One particle equation

1. The Dirac equation

1.1. Introduction

After the discovery of the Schrödinger equation and the rise of quantum mechanics people started to look for a relativistic analog. Due to the correspondence principle of quantum mechanics, where we replace classical quantities with operators, in particular $E \rightarrow i\hbar \frac{\partial}{\partial t}$ and $\mathbf{p} \rightarrow -i\hbar \nabla$, we see that the Schrödinger equation amounts to the non-relativistic energy-momentum relation

$$E = \frac{p^2}{2m} + V.$$

Hence, an equation which stems from the relativistic relation

$$E^2 = c^2 p^2 + m^2 c^4$$

had to be found. The closest guess is probably the Klein-Gordon equation

$$-\hbar^2 \frac{\partial^2}{\partial t^2} \psi = c^2 (-\hbar^2 \nabla^2) \psi + m^2 c^4 \psi,$$

which was actually discovered by Schrödinger before his famous non-relativistic equation. The Klein-Gordon equation certainly fulfills the relativistic energy momentum relation but poses problems if one would like to interpret it as a quantum mechanical evolution equation. For a solid probabilistic interpretation one would like to have a continuity equation for the probability density. The continuity equation corresponding to the Klein-Gordon equation is

$$\nabla \cdot \mathbf{j} + \frac{\partial}{\partial t} \rho = 0 \quad \text{with} \quad \rho = \frac{i\hbar}{2mc^2} (\bar{\psi} \cdot \partial_t \psi - \partial_t \bar{\psi} \cdot \psi).$$

As the Klein-Gordon equation is a second order differential equation we can choose the initial values ψ and $\partial_t \psi$ arbitrarily at some point in time and thus ρ can very well be negative which makes no sense in a probabilistic interpretation. The equation was therefore rejected as a relativistic quantum mechanical evolution equation. Dirac saw that one needs a wave equation which is of first order in time to avoid such problems. His ingenious idea was to linearize the energy-momentum relation

$$E = c \boldsymbol{\alpha} \mathbf{p} + mc^2 \beta,$$

such that its square yields the right result. This is certainly not possible for $\boldsymbol{\alpha}$ and β being plain vectors or scalars as one obtains the following necessary conditions

$$\{\alpha_i, \alpha_j\} = 2\delta_{ij}, \quad \{\alpha_i, \beta\} = 0 \quad \text{and} \quad \beta^2 = 1.$$

It can be shown that in three dimensions these matrices have to be at least 4×4 matrices (see e.g. [Tha92]). Dirac himself introduced a set of matrices which fulfill the relation above and are nowadays called the standard representation,

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix},$$

where σ_i are the well-known Pauli matrices and $\mathbb{1}$ is the 2×2 identity matrix. Following the correspondence principle we arrive at the famous Dirac equation

$$i\hbar \frac{\partial}{\partial t} \psi = -i\hbar c \boldsymbol{\alpha} \nabla \psi + mc^2 \beta \psi. \quad (1.1)$$

We see that ψ is not a complex valued scalar function anymore but instead a four component vector. These extra degrees of freedom can be expected to describe the spin of an electron. Why we end up with a four component object instead of two will be discussed in the next chapters. The associated continuity equation has now a clearly non-negative density

$$\rho = \psi^\dagger \psi = \sum_{j=1}^4 \overline{\psi}_j \psi_j = |\psi|^2,$$

and can therefore be interpreted as a probability density.

In theoretical physics one often sets the physical constants which appear in equations equal to one out of notational convenience. This corresponds to a change of the units we measure the physical quantities with. We can do so explicitly with Dirac equation by dividing it with mc^2 which yields

$$i \frac{\hbar}{mc^2} \frac{\partial}{\partial t} \psi = \left(-i \frac{\hbar}{mc} \boldsymbol{\alpha} \nabla_x + \beta \right) \psi.$$

By choosing new variables of time and space

$$t' = \frac{mc^2}{\hbar} t \quad \text{and} \quad \mathbf{x}' = \frac{mc}{\hbar} \mathbf{x},$$

we get the Dirac equation in natural units

$$i \frac{\partial}{\partial t'} \psi = (-i \boldsymbol{\alpha} \nabla_{\mathbf{x}'} + \beta) \psi.$$

Our choice of units simply means that we measure time and space in quanta of the natural time and the reduced Compton wave length

$$t' = \frac{t}{\tau} \quad \text{and} \quad \mathbf{x}' = \frac{\mathbf{x}}{\lambda_C},$$

with

$$\tau = \frac{\hbar}{mc^2} \quad \text{and} \quad \lambda_C = \frac{\hbar}{mc}.$$

Besides notational simplification there is more to this choice of units. Think of a time dependent plane wave

$$\sin\left(\frac{t}{T} - \frac{x}{2\pi\lambda}\right).$$

The scaling constants T and λ determine the scale on which this plane wave varies significantly. Assume furthermore that this plane wave is a solution to a differential equation. Then the only way these scaling constants can enter the solution is if they were already present in the partial differential equation (PDE) like

$$T \frac{\partial}{\partial t} \psi = -2\pi\lambda \frac{\partial}{\partial x} \psi.$$

The rescaled Dirac equation above is free of any constants. Thus, any solution $\psi(t')$ is a solution of solely t' without any additional scaling constants. Thus, we can deduce that wave functions which are solutions to the Dirac equation “live” on the time scale t' which is measured in terms of the natural time τ . In SI units we have approximately $\tau \approx 1,29 \cdot 10^{-21}$ s. This becomes important when we add a time- dependent external field to the Dirac equation which varies slowly compared to the wave function. This is covered in detail in Chapter 6. For the remainder of this work we will always use natural units unless explicitly stated otherwise.

1.2. Free Dirac equation

We give a brief review of the mathematical basis of the free Dirac equation in this section. A more thorough discussion of the Dirac equation can be found in [Tha92]. To use the Dirac equation in a quantum mechanical context we need a proper Hilbert space to formulate our theory on. In ordinary quantum mechanics this is the space of square integrable functions $L^2(\mathbb{R}^3 \rightarrow \mathbb{C})$. As we have seen in the previous section the Dirac hamiltonian acts on four-component functions. Thus, the natural choice is a four-component function with each entry being square integrable,

$$\mathcal{H} := L^2(\mathbb{R}^3 \rightarrow \mathbb{C}) \otimes \mathbb{C}^4.$$

The canonical inner product on this space is given by

$$\langle \varphi, \psi \rangle = \int_{\mathbb{R}^3} \varphi^\dagger(\mathbf{x}) \psi(\mathbf{x}) d^3x = \int_{\mathbb{R}^3} \sum_{j=1}^4 \bar{\varphi}_j(\mathbf{x}) \psi_j(\mathbf{x}) d^3x.$$

Like in Schrödinger mechanics, we would like the differential operator $D = -i\alpha\nabla + \beta$, which appears in the Dirac equation, to be self-adjoint, so we can formulate a quantum mechanical theory in the usual manner. This is the case as $-i\alpha\nabla + \beta$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3) \times \mathbb{C}^4$. Its closure, which we denote by H_0 , is then self-adjoint and its domain is given by $\mathcal{D}(H_0) = H^1(\mathbb{R}^3) \otimes \mathbb{C}^4$ which is a dense subspace of \mathcal{H} . For a proof of this see e.g. [Tha92, Sec. 1.4.4]. The free Dirac equation on this Hilbert space is then

$$i \frac{\partial}{\partial t} \psi(t) = H_0 \psi(t), \quad (1.2)$$

where $(\psi(t))_{t \in \mathbb{R}}$ is a family of *wave functions* in $\mathcal{D}(H_0)$. Due to Stone's theorem we know that every solution is given by $\psi(t) = \exp(-i H_0 t) \psi$ with initial state $\psi(0) = \psi$. This setup now allows for the usual Born interpretations of quantum mechanics. In particular, $|\langle \varphi, \psi \rangle|^2$ is the probability to find the wave function ψ to be in the state φ and for any self-adjoint operator A

$$\langle \psi, A \psi \rangle \quad \text{for } \psi \in \mathcal{D}(A),$$

is the expectation value of the measurement of the observable A . Furthermore, it follows from Born's general rule that the result of every measurement of the observable A has to be in the spectrum of the operator A (see [Tha92]). The troubles with the one-particle Dirac theory start here. The spectrum of the free Dirac hamiltonian is $\sigma(H_0) = (-\infty, -1] \cup [1, \infty)$ and as the hamiltonian is usually interpreted as the energy operator an electron can be measured to have arbitrary negative energy. This is actually a relativistic effect which also appears in classical mechanics and stems from the energy-momentum relation which has positive and negative solutions. In classical mechanics however we have a sharp distinction between positive and negative energy solutions and the latter ones are simply discarded as unphysical. This is not so easy in a quantum theory. Assume that the electron is coupled to an electromagnetic field which obeys the laws of quantum mechanics. It could then spontaneously emit radiation and thus become a negative energy solution. If the electromagnetic field is not quantized but behaves classically, i.e. if we have an external field such a transition is still possible if this perturbation varies with time. This will be the context of the remainder of this work. Only for a constant electromagnetic field one can distinguish solutions according to their energy which is done e.g. when one applies the Dirac equation to the Hydrogen atom. But even then (or in the free field case), if we restrict the Hilbert space to only positive energies one can show that either the usual concept of localization breaks down, i.e. every electron has a non-vanishing probability to be everywhere in space or particles have non-vanishing probability of superluminal propagation and thus violate the concept of relativity (see [Tha92]). Hence, we can conclude that it is in general not possible to simply neglect the negative energies. In turn, not only does this bring up the obvious question what negative energies are supposed to mean but it would lead to a radiation catastrophe¹ where the electron falls down the energy ladder trying to reach the ground state and thereby radiating an infinite amount of energy. This is a scenario which does not take place in nature. All of this cannot be

¹If the electron is coupled to a radiation field.

really resolved within the framework of the one particle Dirac theory. We will discuss this in the last section of this chapter and finish here our brief survey of the free Dirac equation with the Green's function for the Dirac equation.

The resolvent of the free Dirac hamiltonian is defined as the inverse operator of $H_0 - z$ for all $z \in \mathbb{C} \setminus \sigma(H_0)$. It is a bounded operator on the Hilbert space \mathcal{H} , and has the following integral representation (see e.g [Tha92])

$$(H_0 - z)^{-1} [\psi] (\mathbf{x}) = \int_{\mathbb{R}^3} G_z(\mathbf{x} - \mathbf{y}) \psi(\mathbf{y}) d^3x,$$

with

$$G_z(\mathbf{x}) = \left(i \frac{\boldsymbol{\alpha} \mathbf{x}}{|\mathbf{x}|^2} + k \frac{\boldsymbol{\alpha} \mathbf{x}}{|\mathbf{x}|} + \beta + z \right) \frac{e^{ik(z)|\mathbf{x}|}}{4\pi |\mathbf{x}|} \quad (1.3)$$

where $k(z) = \sqrt{z^2 - 1}$ and the branch of the square root is chosen such that $\Im k(z) \geq 0$. If we allow z to take on any values then G_z is certainly not the resolvent kernel anymore but we can still make sense out of it if we change the function space of the resulting integral operator. Let $f \in L^p_{loc}(\mathbb{R}^3 \rightarrow \mathbb{C}^4)$ for any $1 \leq p \leq \infty$ and let $D - z = -i\boldsymbol{\alpha} \nabla + \beta - z$ be the Dirac differential operator. We would like to find solutions in $L^1_{loc}(\mathbb{R}^3 \rightarrow \mathbb{C}^4)$ to the inhomogeneous partial differential equation (PDE)

$$(D - z) u = f,$$

for some $z \in \mathbb{C}$. A common method to solve such equations is by the fundamental solution which can be understood as the integral kernel of the inverse of the differential operator $D - z$. For then,

$$u_p(\mathbf{x}) = (D - z)^{-1} f(\mathbf{x}) = \int G(\mathbf{x}, \mathbf{y}) f(\mathbf{y}) d^3y,$$

is a particular solution of the PDE and $G(\mathbf{x}, \mathbf{y})$ is the integral kernel of the inverse of $(D - z)$. A general solution is achieved if we add the solution of the homogeneous equation

$$u = u_h(\mathbf{x}) + u_p(\mathbf{x}).$$

To impose any boundary conditions one uses the solution of the homogeneous equation with boundary conditions and requires that $G(\mathbf{x}, \mathbf{y}) = 0$ for \mathbf{x} on the boundary of the domain. Such a $G(\mathbf{x}, \mathbf{y})$ is then called Green's function of the problem. To find the fundamental solution to the free Dirac equation we start with the resolvent kernel as it certainly has the desired properties on L^2 already. Let

$$G_z(\mathbf{x}) = \left(i \frac{\boldsymbol{\alpha} \mathbf{x}}{|\mathbf{x}|^2} + k \frac{\boldsymbol{\alpha} \mathbf{x}}{|\mathbf{x}|} + \beta + z \right) \frac{e^{ik(z)|\mathbf{x}|}}{4\pi |\mathbf{x}|} \quad \text{for all } z \in \mathbb{C},$$

with $k(z)$ as above and $G_z(0) := 0$ for $\mathbf{x} = 0$. An easy computation shows that

$$(D - z) G_z(\mathbf{x}) = 0$$

for $\mathbf{x} \neq 0$. The next lemma proves that this definition is indeed the fundamental solution for the free Dirac equation.

Lemma 1.1. Let $z \in \mathbb{C}$, $f \in L^p_{loc}(\mathbb{R}^3 \rightarrow \mathbb{C}^4)$, and such that

$$\int_{\mathbb{R}^3} G_z(\mathbf{x} - \mathbf{y}) f(\mathbf{y}) d^3 \mathbf{y} \in L^1_{loc}(\mathbb{R}^3, \mathbb{C}^4),$$

for any $1 \leq p \leq \infty$. Then the following holds in a weak sense,

$$[-i\boldsymbol{\alpha}\nabla + \beta - z] \int_{\mathbb{R}^3} G_z(\mathbf{x} - \mathbf{y}) f(\mathbf{y}) d^3 \mathbf{y} = f(\mathbf{x}).$$

Proof. Note first, that

$$\int_{\mathbb{R}^3} \varphi(\mathbf{x}) G_z(\mathbf{x} - \mathbf{y}) d^3 \mathbf{x}, \quad \int_{\mathbb{R}^3} \varphi(\mathbf{x}) G_z(\mathbf{x} - \mathbf{y}) f(\mathbf{y}) d^3 \mathbf{y} d^3 \mathbf{x} \quad \text{and} \quad \int_{\mathbb{R}^3} \varphi(\mathbf{x}) f(\mathbf{x}) d^3 \mathbf{x},$$

are well defined for any $\varphi \in C_0^\infty(\mathbb{R}^3 \rightarrow \mathbb{C}^4)$. Thus, we have for all $\varphi \in C_0^\infty(\mathbb{R}^3 \rightarrow \mathbb{C}^4)$

$$\begin{aligned} & \int_{\mathbb{R}^3} ([-i\boldsymbol{\alpha}\nabla_x + \beta - z] \varphi(\mathbf{x}))^\dagger G_z(\mathbf{x} - \mathbf{y}) d^3 \mathbf{x} = \\ &= \int_{\mathbb{R}^3 \setminus B_\epsilon(\mathbf{y})} ([-i\boldsymbol{\alpha}\nabla_x + \beta - z] \varphi(\mathbf{x}))^\dagger G_z(\mathbf{x} - \mathbf{y}) f(\mathbf{y}) d^3 \mathbf{x} \\ &+ \int_{B_\epsilon(\mathbf{y})} ([-i\boldsymbol{\alpha}\nabla_x + \beta - z] \varphi(\mathbf{x}))^\dagger G_z(\mathbf{x} - \mathbf{y}) d^3 \mathbf{x} = \\ &= I_1^\epsilon(\mathbf{y}) + I_2^\epsilon(\mathbf{y}). \end{aligned}$$

For the first term $I_1^\epsilon(\mathbf{y})$ we get with integration by parts²

$$\begin{aligned} I_1^\epsilon(\mathbf{y}) &= \int_{\partial B_\epsilon(\mathbf{y})} \varphi^\dagger(\mathbf{x}) (-i\boldsymbol{\alpha}) \frac{\mathbf{x} - \mathbf{y}}{|\mathbf{x} - \mathbf{y}|} G_z(\mathbf{x} - \mathbf{y}) d\Omega \\ &+ \int_{\mathbb{R}^3 \setminus B_\epsilon(\mathbf{y})} \varphi^\dagger(\mathbf{x}) (D_x - z) G_z(\mathbf{x} - \mathbf{y}) d^3 \mathbf{x} = \\ &= J_1^\epsilon(\mathbf{y}) + J_2^\epsilon(\mathbf{y}). \end{aligned}$$

The first term is with the definition of the Green's function equivalent to

$$\begin{aligned} J_1^\epsilon(\mathbf{y}) &= \int_{\partial B_\epsilon(0)} \varphi^\dagger(\mathbf{x} + \mathbf{y}) (-i\boldsymbol{\alpha}) \frac{\mathbf{x}}{|\mathbf{x}|} G_z(\mathbf{x}) d\Omega = \\ &= \int_{\partial B_\epsilon(0)} \varphi^\dagger(\mathbf{x} + \mathbf{y}) (-i\boldsymbol{\alpha}) \frac{\mathbf{x}}{|\mathbf{x}|} \left(i \frac{\boldsymbol{\alpha}\mathbf{x}}{|\mathbf{x}|^2} + k(z) \frac{\boldsymbol{\alpha}\mathbf{x}}{|\mathbf{x}|} + \beta + z \right) \frac{e^{ik(z)|\mathbf{x}|}}{4\pi|\mathbf{x}|} d\Omega = \\ &= K_1^\epsilon(\mathbf{y}) + K_2^\epsilon(\mathbf{y}) + K_3^\epsilon(\mathbf{y}) + K_4^\epsilon(\mathbf{y}). \end{aligned}$$

²The outward pointing unit vector \mathbf{n} to the subset $\Omega = \mathbb{R}^3 \setminus B_\epsilon(\mathbf{y})$ is minus the outward pointing unit vector to the sphere $B_\epsilon(\mathbf{y})$, thus $\mathbf{n} = -\frac{\mathbf{x} - \mathbf{y}}{|\mathbf{x} - \mathbf{y}|}$.

Using the anti-commutation relations for the Dirac matrices, $\{\alpha_l, \alpha_k\} = 2\delta_{kl}$, we can evaluate K_1^ε to be

$$\begin{aligned} K_1^\varepsilon(\mathbf{y}) &= \int_{\partial B_\varepsilon(0)} \varphi^\dagger(\mathbf{x} + \mathbf{y}) \frac{|\mathbf{x}|^2}{|\mathbf{x}|^3} \frac{e^{ik(z)|\mathbf{x}|}}{4\pi|\mathbf{x}|} d\Omega = \frac{e^{ik\varepsilon}}{4\pi\varepsilon^2} \int_{\partial B_\varepsilon(0)} \varphi^\dagger(\mathbf{x} + \mathbf{y}) d\Omega = \\ &= \frac{e^{ik\varepsilon}}{4\pi\varepsilon^2} \int_{\partial B_\varepsilon(\mathbf{y})} \varphi^\dagger(\mathbf{x}) d\Omega. \end{aligned}$$

The three terms $K_2^\varepsilon, K_3^\varepsilon, K_4^\varepsilon$ can be easily determined by noting that φ is bounded on \mathbb{R}^3 . Thus we can e.g. estimate K_2^ε by

$$\begin{aligned} |K_2^\varepsilon(\mathbf{y})| &\leq k(z) \int_{\partial B_\varepsilon(0)} |\varphi(\mathbf{x} + \mathbf{y})| \frac{|\mathbf{x}|^2}{|\mathbf{x}|^2} \frac{1}{4\pi|\mathbf{x}|} d\Omega \leq k(z) \sup_{x \in \mathbb{R}^3} |\varphi(\mathbf{x})| \frac{1}{4\pi\varepsilon} \int_{\partial B_\varepsilon(0)} d\Omega = \\ &= k(z) \sup_{x \in \mathbb{R}^3} |\varphi(\mathbf{x})| \varepsilon \end{aligned}$$

where $|\cdot|$ is the usual euclidean norm extended to matrices(also called Frobenius norm). Therefore, we have

$$\lim_{\varepsilon \rightarrow 0} K_2^\varepsilon(\mathbf{y}) = 0.$$

uniformly in \mathbf{y} . The other two terms are treated completely analogous. As $(D_x - z)G_z(\mathbf{x} - \mathbf{y}) = 0$ for $\mathbf{x} \neq \mathbf{y}$ we immediately have $J_2^\varepsilon(\mathbf{y}) = 0$ for all \mathbf{y} and $\varepsilon > 0$. For $I_2^\varepsilon(\mathbf{y})$ we have

$$\begin{aligned} I_2^\varepsilon(\mathbf{y}) &= \int_{B_\varepsilon(\mathbf{y})} ([-i\boldsymbol{\alpha}\nabla_x + \beta - z] \varphi(\mathbf{x}))^\dagger G_z(\mathbf{x} - \mathbf{y}) d^3x = \\ &= \int_{B_\varepsilon(0)} ([-i\boldsymbol{\alpha}\nabla_x + \beta - z] \varphi(\mathbf{x} + \mathbf{y}))^\dagger \left(i \frac{\boldsymbol{\alpha}\mathbf{x}}{|\mathbf{x}|^2} + k(z) \frac{\boldsymbol{\alpha}\mathbf{x}}{|\mathbf{x}|} + \beta + z \right) \frac{e^{ik(z)|\mathbf{x}|}}{4\pi|\mathbf{x}|} d^3x = \\ &= L_1^\varepsilon(\mathbf{y}) + L_2^\varepsilon(\mathbf{y}) + L_3^\varepsilon(\mathbf{y}) + L_4^\varepsilon(\mathbf{y}). \end{aligned}$$

For the first term we get again by noting that φ and $\nabla\varphi$ are bounded

$$\begin{aligned} |L_1^\varepsilon(\mathbf{y})| &\leq C \int_{B_\varepsilon(0)} (|\nabla_x \varphi(\mathbf{x} + \mathbf{y})| + |\beta - z| |\varphi(\mathbf{x} + \mathbf{y})|) \frac{1}{4\pi|\mathbf{x}|^2} d^3x \leq \\ &\leq C \left(\sup_{x \in \mathbb{R}^3} |\nabla_x \varphi(\mathbf{x})| + |\beta - z| \sup_{x \in \mathbb{R}^3} |\varphi(\mathbf{x})| \right) \int_{B_\varepsilon(0)} \frac{1}{4\pi|\mathbf{x}|^2} d^3x = \\ &= C \left(\sup_{x \in \mathbb{R}^3} |\nabla_x \varphi(\mathbf{x})| + |\beta - z| \sup_{x \in \mathbb{R}^3} |\varphi(\mathbf{x})| \right) \varepsilon, \end{aligned}$$

hence

$$\lim_{\varepsilon \rightarrow 0} L_1^\varepsilon(\mathbf{y}) = 0.$$

uniformly in \mathbf{y} . The same argument holds for L_2^ε through L_4^ε . Because all vanishing terms tend to zero uniformly in \mathbf{y} we have

$$\begin{aligned} & \int_{\mathbb{R}^3} ([-i\boldsymbol{\alpha}\nabla_x + \beta - z] \varphi(\mathbf{x}))^\dagger G_z(\mathbf{x} - \mathbf{y}) d^3x = \\ & = \lim_{\varepsilon \rightarrow 0} \frac{e^{ik\varepsilon}}{4\pi\varepsilon^2} \int_{\partial B_\varepsilon(\mathbf{y})} \varphi^\dagger(\mathbf{x}) d\Omega = \varphi^\dagger(\mathbf{y}), \end{aligned}$$

where we used the spherical mean in the last step. This then proves the statement as

$$\int_{\mathbb{R}^3} ([-i\boldsymbol{\alpha}\nabla_x + \beta - z] \varphi(\mathbf{x}))^\dagger \left(\int_{\mathbb{R}^3} G_z(\mathbf{x} - \mathbf{y}) f(\mathbf{y}) d^3y \right) d^3x = \int_{\mathbb{R}^3} \varphi^\dagger(\mathbf{x}) f(\mathbf{x}) d^3x.$$

□

1.3. External fields

In this chapter we will extend the previous discussion on the free Dirac equation to external fields. We denote a possible time dependency of the external field by adding a subscript t to all the entities. In general one has an electric potential ϕ and a magnetic vector potential \mathbf{A} for which the free Dirac equation changes to

$$i \frac{\partial}{\partial t} \psi(t) = (H_0 + \mathbb{A}_t) \psi(t) = H_t \psi(t), \quad (1.4)$$

where \mathbb{A}_t is the operator of multiplication defined by the function $\mathbb{A}(\mathbf{x}, t) = \phi(\mathbf{x}, t) - \boldsymbol{\alpha}\mathbf{A}(\mathbf{x}, t)$. As before we would like to have a unitary operator which gives the time- evolution of any wave function ψ but due to the time dependency of the hamiltonian this cannot be a one-parameter group anymore as the initial state of the hamiltonian is now part of the initial condition. The necessary features of a so called *time evolution* for a time-dependent hamiltonian are captured in the following definition.

Definition 1.2. A time evolution on a Hilbertspace \mathcal{H} is a two-parameter family $U(s, t)$ of operators satisfying

1. $U(s, r)U(r, t) = U(s, t)$ for all $s, r, t \in \mathbb{R}$
2. $U(s, s) = \text{id}_{\mathcal{H}}$ for all $s \in \mathbb{R}$
3. the mapping $(s, t) \rightarrow U(s, t)\psi$ is continuous for all $\psi \in \mathcal{H}$
4. $U(s, t)$ is unitary for all $s, t \in \mathbb{R}$.

To ensure the existence of such a time evolution for our case we need to impose some technical properties on the external field. The next condition is certainly not the most general one but it is nice and simple and will suffice our needs.

Condition A. Let the external field $\phi(\mathbf{x}, t)$ and $\mathbf{A}(\mathbf{x}, t)$ be real valued, continuous in t and such that \mathbb{A}_t is a bounded operator on $L^2(\mathbb{R}^3 \rightarrow \mathbb{C}^4) \otimes \mathbb{C}^4$ for all times $t \in \mathbb{R}$.

In this case it is easy to see that the hamiltonian is self-adjoint on a common domain for all times.

Proposition 1.3. Let the external field fulfill Condition A. Then the operator

$$H_t = H_0 + \mathbb{A}_t \tag{1.5}$$

is self-adjoint on $\mathcal{D}(H_t) = \mathcal{D}(H_0) = H^1(\mathbb{R}^3) \otimes \mathbb{C}^4$ for all $t \in \mathbb{R}$.

Proof. Use Kato-Rellich. □

The next proposition ensures the existence of a time evolution to eq. (1.4).

Proposition 1.4. Let the external field fulfill Condition A. Then there exists a time evolution satisfying

$$\begin{aligned} i \frac{\partial}{\partial t} U(t, s) &= H_t U(t, s) \\ i \frac{\partial}{\partial s} U(t, s) &= -U(t, s) H_s \end{aligned} \tag{1.6}$$

and $\mathcal{D}(H_0) = U(t, s)\mathcal{D}(H_0)$ for all $t, s \in \mathbb{R}$. The solution to eq. (1.4) is given by

$$\psi(t) = U(t, s)\psi \quad \text{with initial conditon} \quad \psi \in \mathcal{H}.$$

Proof. Due to Condition A the prerequisites of [Tha92, Thm 4.10] are fulfilled. Thus, there exists a time evolution and $\psi(t) = U(t, s)\psi$ is a strong solution to eq. (1.4). □

2. Kato's theorem for the Dirac equation

In the subsequent chapter we will introduce the so called eigenfunction expansion of the Dirac operator with external vector potential. An important ingredient in the theory of eigenfunction expansion for the Schrödinger operator is a result of Kato [Kat59] concerning the asymptotic behavior for $|\mathbf{x}| \rightarrow \infty$ of solutions of the stationary Schrödinger equation. No such result exists for the Dirac equation. Hence, we prove a similar theorem for the Dirac equation in this chapter, which is of interest on its own. The important consequences regarding the theory of eigenfunction expansion and the Dirac equation are stated in Corollary 2.7 and Corollary 2.8. We set the electrical potential to zero as this is the setup for electromagnetic waves which we are concerned with later. The stationary Dirac equation, understood as a partial differential equation on $C^1(\mathbb{R}^3 \rightarrow \mathbb{C}^4)$ is

$$0 = (-i\boldsymbol{\alpha}\nabla - \boldsymbol{\alpha}\mathbf{A}(\mathbf{x}) + \beta - E_k) f, \quad (2.1)$$

with $E_k = \pm\sqrt{k^2 + 1}$ and k being a fixed positive number. We are interested in the asymptotic behavior at infinity, hence we investigate the equation on the domain $B(R_0, 0)^C = \mathbb{R}^3 \setminus B(R_0, 0)$ for some radius R_0 . Assume f is a solution to the Dirac equation and $\mathbf{A} \in C^\infty(B(R_0, 0)^C \rightarrow \mathbb{R}^3)$. Then it is well known that f is also smooth (see e.g. [Rud91]). In particular f also satisfies the following equation

$$\begin{aligned} 0 &= (-i\boldsymbol{\alpha}\nabla - \boldsymbol{\alpha}\mathbf{A}(\mathbf{x}) + \beta + E_k) (-i\boldsymbol{\alpha}\nabla - \boldsymbol{\alpha}\mathbf{A}(\mathbf{x}) + \beta - E_k) f = \\ &= (-\Delta + \mathbf{D}(\mathbf{x}) \cdot \nabla + P'(\mathbf{x}) - k^2) f, \end{aligned} \quad (2.2)$$

where $\mathbf{D}(\mathbf{x}) = -2i\boldsymbol{\alpha}\mathbf{A}(\mathbf{x})$ and $P'(\mathbf{x}) = \mathbf{A}^2(\mathbf{x}) + i(\nabla \cdot \mathbf{A}(\mathbf{x})) - \gamma_5 \boldsymbol{\alpha}\mathbf{B}(\mathbf{x})$. If the \mathbf{A} -field is compactly supported, we can choose R_0 big enough such that $\mathbf{D}(\mathbf{x}) = 0$ and $P'(\mathbf{x}) = 0$ for $|\mathbf{x}| > R_0$. Hence, these equations reduce to four independent equations,

$$0 = (\Delta + k^2) f_j,$$

with $j = 1, \dots, 4$. This is just the ordinary free Schrödinger equation to which Kato's result already applies. The task for a non-compactly supported potential is thus to incorporate the first derivative of f which now appears. As ∇f is bounded by f through the Dirac equation and the first derivative is multiplied by the potential \mathbf{D} in eq. (2.2), this contribution to the equation can be made arbitrarily small at infinity if the \mathbf{A} -field decays fast enough. Hence, we expect a similar asymptotic result as for a compactly supported potential. We will therefore use Kato's original proof and massage it appropriately where it is necessary.

Let us start with a brief review of his approach. Kato separates the radial and spherical part of the Schrödinger equation by introducing the Hilbert space of square integrable functions on the

unit sphere, $\mathcal{H} = L^2(\Omega)$. The solutions $f(r, \phi, \theta)$ are then interpreted as vector elements $f(r)$ of this Hilbert space and the variable r is simply a parametrization. The Schrödinger equation

$$\Delta f + (k^2 - p(\mathbf{x})) f = 0$$

can then be rewritten into an ordinary differential equation on this parameter r including linear operators acting on the Hilbert space elements $f(r)$

$$f'' + \frac{2}{r} f' - \frac{1}{r^2} L f(r) + (k^2 - P(r)) f(r) = 0,$$

where L is the negative Laplace-Beltrami operator on the unit sphere

$$L = -\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} - \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2}$$

in spherical coordinates and $P(r)$ is an operator of multiplication on the Hilbert space defined by $p(\mathbf{x})$ for $|\mathbf{x}| = r$. The operator L is independent of r , symmetric on the Hilbert space and non-negative. This is all which Kato uses in his proof regarding L . Using the scaled functions

$$g(r) := r f(r) \quad \text{and} \quad g_m(r) := r^m g(r)$$

the Schrödinger equation turns into

$$g'' - \frac{1}{r^2} L g + (k^2 - P) g = 0,$$

and

$$g_m'' - \frac{2m}{r} g_m' + \frac{1}{r^2} (m(m+1) - L) g_m + (k^2 - P) g_m = 0.$$

Kato then goes on to prove a series of lemmas concerning the growth properties of the function

$$F(m, t, r) := \|g_m'\|^2 + \left(k^2 - \frac{2kt}{r} + \frac{m(m+1)}{r^2} \right) \|g_m\|^2 - \frac{1}{r^2} \langle L g_m, g_m \rangle \quad (2.3)$$

and can conclude his theorem straightforward. Here, $\|\cdot\|$ and $\langle \cdot, \cdot \rangle$ are the norm and inner product on the Hilbert space of square integrable functions on the unit sphere.

We will proceed in a similar way. The Hilbert space \mathcal{H} is now given by four-component square integrable functions on the unit sphere, $\mathcal{H} = L^2(\Omega) \otimes \mathbb{C}^4$ and the inner product is for two functions $f, g \in \mathcal{H}$ given as

$$\langle f, g \rangle = \int_{\Omega} f^\dagger g \sin \theta \, d\theta \, d\varphi = \int_{\Omega} \sum_{i=1}^4 \bar{f}_i g_i \sin \theta \, d\theta \, d\varphi$$

where f_i and g_i are the spinor components.

In the spirit of Kato's notation we define

$$p_k(r) := \sup_{|\mathbf{x}|=r} |A^2(\mathbf{x}) - \gamma_5 \alpha \mathbf{B}(\mathbf{x})| + \sup_{|\mathbf{x}|=r} |A(\mathbf{x})| |\alpha A(\mathbf{x}) - \beta + E_k| + \sup_{|\mathbf{x}|=r} |\nabla \cdot A(\mathbf{x})| ,$$

and

$$\mu := \frac{1}{2k} \limsup_{r \rightarrow \infty} r p_k(r) \quad (2.4)$$

where $|\cdot|$ is the Euclidean or Frobenius norm. We assume the vector potential to fulfill the following condition

Condition B. *Let $A \in C^\infty(B(R_0, 0)^C \rightarrow \mathbb{R}^3)$ and A be such that $\mu < 1$.*

For example, a smooth function which, together with its first derivatives, decays faster than r^{-1} for sufficiently large r yields $\mu = 0$ for any $k > 0$. Hence, e.g. the Gaussian function or any Schwartz function fulfills Condition B.

Rewriting eq. (2.2) yields

$$\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} - \frac{1}{r^2} L - D_r(r) \frac{\partial}{\partial r} - \frac{1}{r} B(r) + (k^2 - P(r)) \right) f = 0 .$$

As before, L is the negative Laplace-Beltrami operator on the unit sphere, $B(r)$ is the differential operator given by

$$B(r) := D_\theta(r) \frac{\partial}{\partial \theta} + D_\varphi(r) \frac{1}{\sin \theta} \frac{\partial}{\partial \varphi} + i (\nabla \cdot A)(r) .$$

and $D_r(r)$, $D_\theta(r)$, $D_\varphi(r)$, $(\nabla \cdot A)(r)$ and $P(r)$ are multiplication operators on \mathcal{H} defined by the spherical components of $\mathbf{D}(\mathbf{x})$ and the functions $\nabla \cdot A(\mathbf{x})$ and $P(\mathbf{x}) = P'(\mathbf{x}) - i (\nabla \cdot A(\mathbf{x}))$ at $|\mathbf{x}| = r$. Introducing the function $g_m(r) = r^{m+1} f(r)$ the equation above turns into

$$g_m'' - \frac{2m}{r} g_m' + \frac{1}{r^2} (m(m+1) - L) g_m + (k^2 - P) g_m - D_r g_m' + D_r \frac{m+1}{r} g_m - \frac{1}{r} B g_m = 0 . \quad (2.5)$$

We now prove the same lemmas on the growth property of $F(m, t, r)$ in eq. (2.3) as Kato. Most parts of his proof can simply be copied. In general we have for any real number s

$$\begin{aligned} \frac{dr^{2s} F(m, t, r)}{dr} &= 2r^{2s} \Re \langle g_m', g_m'' + \left(k^2 - \frac{2kt}{r} + \frac{m(m+1)}{r^2} \right) g_m - \frac{1}{r^2} L g_m \rangle \\ &\quad + 2r^{2s-1} \left\{ s \|g_m'\|^2 + \left(sk^2 - \frac{(2s-1)kt}{r} + (s-1) \frac{m(m+1)}{r^2} \right) \|g_m\|^2 - \frac{(s-1)}{r^2} \langle L g_m, g_m \rangle \right\} \end{aligned}$$

where we have used the symmetry of L . If we substitute g_m'' by the differential equation we get

$$\begin{aligned} \frac{dr^{2s}F(m, t, r)}{dr} &= 2(1-s)r^{2s-3}\langle Lg_m, g_m \rangle + 2r^{2s-1}\left\{ (2m+s)\|g_m'\|^2 + \Re\langle g_m', (rP-2kt)g_m \rangle \right. \\ &\quad \left. + \left(sk^2 - \frac{(2s-1)kt}{r} - (1-s)\frac{m(m+1)}{r^2} \right) \|g_m\|^2 \right\} + 2r^{2s}\Re\langle g_m', D_r(r)g_m' \rangle \\ &\quad + 2r^{2s}\Re\langle g_m', \left(\frac{1}{r}B(r) - \frac{m+1}{r}D_r(r) \right) g_m \rangle. \end{aligned} \quad (2.6)$$

Substituting back

$$g_m = r^{m+1}f \quad \text{and} \quad g_m' = (m+1)r^m f + r^{m+1}f'$$

into the last two terms above yields

$$\begin{aligned} &\Re\langle g_m', D_r(r)g_m' \rangle + \Re\langle g_m', \left(\frac{1}{r}B(r) - \frac{m+1}{r}D_r(r) \right) g_m \rangle = \\ &= r^{m+1}\Re\langle g_m', D_r(r)f' \rangle + r^{m+1}\Re\langle g_m', \frac{1}{r}B(r)f \rangle = \\ &= r^{m+1}\Re \int_{\Omega} (g_m')^\dagger(\mathbf{x}) \left(D_r(\mathbf{x})\frac{\partial}{\partial r} + D_\theta(\mathbf{x})\frac{1}{r}\frac{\partial}{\partial \theta} \right. \\ &\quad \left. + D_\varphi(\mathbf{x})\frac{1}{r\sin\theta}\frac{\partial}{\partial \varphi} + i(\nabla \cdot \mathbf{A}(\mathbf{x})) \right) f(\mathbf{x}) \sin\theta d\theta d\varphi \\ &\quad + r^{m+1}\Re \int_{\Omega} (g_m')^\dagger(\mathbf{x}) (\mathbf{D}(\mathbf{x}) \cdot \nabla + i(\nabla \cdot \mathbf{A}(\mathbf{x}))) f(\mathbf{x}) \sin\theta d\theta d\varphi. \end{aligned} \quad (2.7)$$

Using the Hölder inequality gives

$$\begin{aligned} &\left| \Re\langle g_m', D_r(r)g_m' \rangle + \Re\langle g_m', \left(\frac{1}{r}B(r) - \frac{m+1}{r}D_r(r) \right) g_m \rangle \right| \leq \\ &\leq \sup_{|x|=r} |\nabla \cdot \mathbf{A}(\mathbf{x})| \|g_m'\| \|g_m\| + \|g_m'\| \left(\int_{\Omega} |\mathbf{D}(\mathbf{x})|^2 |r^{m+1}\nabla f(\mathbf{x})|^2 \sin\theta d\theta d\varphi \right)^{\frac{1}{2}}. \end{aligned} \quad (2.8)$$

Remember that f is a solution of the Dirac equation and as such obeys

$$|\nabla f(\mathbf{x})|^2 = |-\mathbf{i}\boldsymbol{\alpha} \cdot \nabla f(\mathbf{x})|^2 = |(\boldsymbol{\alpha}\mathbf{A}(\mathbf{x}) - \beta + E_k) f(\mathbf{x})|^2 \leq |\boldsymbol{\alpha}\mathbf{A}(\mathbf{x}) - \beta + E_k|^2 |f(\mathbf{x})|^2,$$

where we used the sub-multiplicity of the Euclidean norm. Hence, we have

$$\begin{aligned} &\left| \Re\langle g_m', D_r(r)g_m' \rangle + \Re\langle g_m', \left(\frac{1}{r}B(r) - \frac{m+1}{r}D_r(r) \right) g_m \rangle \right| \leq \\ &\leq \left(\sup_{|x|=r} |\nabla \cdot \mathbf{A}(\mathbf{x})| + 2 \sup_{|x|=r} |\mathbf{A}(\mathbf{x})| |\boldsymbol{\alpha}\mathbf{A}(\mathbf{x}) - \beta + E_k| \right) \|g_m'\| \|g_m\|. \end{aligned}$$

If $t \geq 0$ we have

$$|\Re\langle g'_m, (rP(r) - 2kt)g_m \rangle| \leq \left(r \sup_{|x|=r} |P(x)| + 2kt \right) \|g'_m\| \|g_m\| ,$$

and thus

$$\begin{aligned} \Re\langle g'_m, (rP(r) - 2kt)g_m \rangle + r \Re\langle g'_m, D_r(r)g'_m \rangle + r \Re\langle g'_m, \left(\frac{1}{r} B(r) - \frac{m+1}{r} D_r(r) \right) g_m \rangle &\geq \\ &\geq -(rp_k(r) + 2kt) \|g'_m\| \|g_m\| . \end{aligned} \quad (2.9)$$

Provided that $2m + s \geq 0$ and that

$$(rp_k(r) + 2kt)^2 \leq 4(2m + s) \left(sk^2 - \frac{(2s-1)kt}{r} - (1-s) \frac{m(m+1)}{r^2} \right) , \quad (2.10)$$

we get a lower estimate for eq. (2.6)

$$\begin{aligned} \frac{dr^{2s} F(m, t, r)}{dr} &\geq \\ &\geq 2(1-s)r^{2s-3} \langle L g_m, g_m \rangle + \frac{2r^{s-1}}{4(2m+s)} (2(2m+s) \|g'_m\| - (rp_k(r) + 2kt) \|g_m\|)^2 . \end{aligned} \quad (2.11)$$

This is the same lower bound which Kato derives. The only difference in our case is the definition of $p_k(r)$. Nevertheless, it fulfills the same property $\frac{1}{2k} \limsup_{r \rightarrow \infty} rp_k(r) < 1$ by assumption. Hence, the proofs of the following lemmas can either be copied from Kato or only require minor changes.

Lemma 2.1. *Let t_0 be a constant such that $0 < t_0 < kR_0$. Then there exists a constant $m_0 \geq 0$ such that*

$$\frac{dr^2 F(m, t_0, r)}{dr} \geq 0 \quad \text{for all } m \geq m_0, r \geq R_0 .$$

Proof. See [Kat59, Lemma 1]. □

Lemma 2.2. *There are constants $m_1 \geq 0$ and $R_1 \geq R_0$ such that*

$$F(m_0, t_0, r) > 0 \quad \text{for } r \geq R_1 .$$

Proof. See [Kat59, Lemma 2]. □

Lemma 2.3. *Assume that $\|g\|^2$ is not monotone increasing in any semi-infinite interval of the form $r \geq R$. Then there are arbitrarily large values of r for which*

$$F(0, 0, r) > 0 .$$

Proof. See [Kat59, Lemma 3]. □

Lemma 2.4. *For any $\varepsilon > 0$ we have*

$$\lim_{r \rightarrow \infty} r^{2\mu+\varepsilon} (\|g'\|^2 + k^2 \|g\|^2) = \infty .$$

Proof. We can restrict the proof to the case where $\|g\|^2$ is not monotone increasing. The statement is obvious if that is not the case. Hence, we can use Lemma 2.3 in this proof. Set $m = t = 0$ and recall eq. (2.11),

$$\frac{dr^{2s}F(m, t, r)}{dr} \geq 2(1-s)r^{2s-3} \langle Lg, g \rangle + \frac{2r^{s-1}}{4s} (2s \|g'\| - rp_k(r) \|g\|)^2 ,$$

which holds if $s \geq 0$ and if eq. (2.10),

$$(rp_k(r))^2 \leq (2sk)^2 ,$$

is fulfilled. As $\mu < 1$, we can choose an s satisfying $\mu < s \leq 1$. As $\limsup rp_k = 2k\mu < 2ks$ there is an $R_1 \geq R_0$ such that $rp_k < 2ks$ for all $r \geq R_1$. Using $\langle Lg, g \rangle \geq 0$ yields

$$\frac{dr^{2s}F(0, 0, r)}{dr} \geq 0 \quad \text{for } r \geq R_1 .$$

The rest of the proof is identical to Kato. Lemma 2.3 tells us that there is an $R_2 \geq R_1$ such that $F(0, 0, R_2) > 0$. It follows that $r^{2s}F(0, 0, r) \geq c > 0$ for all $r \geq R_2$. $F(0, 0, r)$ is given by

$$F(0, 0, r) = \|g'\|^2 + k^2 \|g\|^2 - \frac{1}{r^2} \langle Lg, g \rangle$$

and as $\langle Lg, g \rangle \geq 0$ we have $\|g'\|^2 + k^2 \|g\|^2 \geq F(0, 0, r)$. If we set $2s = 2\mu + \frac{\varepsilon}{2}$ for any $0 < \varepsilon < 4(1-\mu)$ we end up with

$$r^{2\mu+\varepsilon} \|g'\|^2 + k^2 \|g\|^2 \geq cr^{\frac{\varepsilon}{2}} ,$$

which proves the statement for $0 < \varepsilon < 4(1-\mu)$. It is then, of course, also true for all $\varepsilon > 0$. □

Lemma 2.5. *If*

$$\int_{R_0}^{\infty} p_k(r) dr < \infty \quad \text{we have} \quad \liminf_{r \rightarrow \infty} \|g'\|^2 + k^2 \|g\|^2 > 0 .$$

Proof. Combining eq. (2.6) with $s = m = t = 0$ and the estimate in eq. (2.9) we get

$$\frac{dF(0, 0, r)}{dr} \geq \frac{2}{r^3} \langle Lg, g \rangle - 2p_k(r) \|g'\| \|g\| .$$

Note that

$$2p_k(r) \|g'\| \|g\| \leq 2p_k(r) \|g'\| \|g\| + \frac{1}{k} p_k(r) (\|g'\| - k \|g\|)^2 = \frac{1}{k} p_k(r) (\|g'\|^2 + k \|g\|^2),$$

and thus

$$\frac{dF(0,0,r)}{dr} \geq \frac{2}{r^3} \langle Lg, g \rangle - \frac{1}{k} p_k (\|g'\|^2 + k^2 \|g\|^2).$$

As $F(0,0,r) = \|g'\|^2 + k \|g\|^2 - \frac{1}{r^2} \langle Lg, g \rangle$ we have

$$\frac{dF(0,0,r)}{dr} \geq -\frac{1}{k} p_k F(0,0,r) + \frac{1}{kr^3} \langle Lg, g \rangle (2k - rp_k).$$

Because of eq. (2.4) and $\mu < 1$ there exists an $R_5 \geq R_0$ such that $rp_k < 2k$ and since $\langle Lg, g \rangle \geq 0$ this yields

$$\frac{dF(0,0,r)}{dr} \geq -\frac{1}{k} p(r) F(0,0,r) \quad \text{for } r \geq R_5.$$

The rest is then identical to [Kat59, Lemma 5]. From there we know that the solution of this inequality is

$$F(0,0,r) \geq F(0,0,R) \exp\left(-\frac{1}{k} \int_R^r p_k(r) dr\right) \quad \text{for } r \geq R \geq R_5.$$

We can use Lemma 2.3 again (the statement is obviously fulfilled if the prerequisites of Lemma 2.3 are not met) to choose an $R_6 \geq R_5$ such that $F(0,0,R_6) > 0$. As $p_k(r)$ is integrable by assumption we have

$$F(0,0,r) \geq c = F(0,0,R_6) \exp\left(-\frac{1}{k} \int_{R_6}^{\infty} p_k(r) dr\right) > 0 \quad \text{for } r \geq R_6$$

Note finally that $\|g'\|^2 + k^2 \|g\|^2 \geq F(0,0,r)$ which proves the statement. \square

We can now prove the main theorem of this section.

Theorem 2.6. *Let $f \in C^1(B(R_0,0)^C \rightarrow \mathbb{C}^4)$ be a non-trivial solution to eq. (2.1) on the domain $B(R_0,0)^C$ and let the A-field fulfill Condition B. We then have*

$$\lim_{R \rightarrow \infty} R^{2\mu+\varepsilon} \int_R^{R+\delta} \left(r^2 \int_{|x|=r} |f(\mathbf{x})|^2 \sin \theta d\theta d\varphi \right) dr = \infty \quad (2.12)$$

for any given $\varepsilon, \delta > 0$.

Proof. Like Kato we first compute the following expression

$$\frac{d^2 r^s \|g\|^2}{dr^2} = r^s \left(2 \|g'\|^2 + 2\Re\langle g, g'' \rangle + \frac{4s}{r} \Re\langle g, g' \rangle + \frac{s(s-1)}{r^2} \|g\|^2 \right).$$

Substituting g'' by eq. (2.5) and noting that $\langle g, Lg \rangle \geq 0$ and $\left(\frac{2s}{r} \|g\| - \|g'\|\right)^2 \geq 0$ yields

$$\begin{aligned} \frac{d^2 r^s \|g\|^2}{dr^2} &= r^s \left(2 \|g'\|^2 + \frac{2}{r} \langle g, Lg \rangle - \left(2k^2 - \frac{s(s-1)}{r^2} \right) \|g\|^2 + \frac{4s}{r} \Re\langle g, g' \rangle + 2\Re\langle g, P(r)g \rangle \right) \\ &\quad + 2r^s \left(\Re\langle g, D_r(r)g' \rangle + \frac{1}{r} \Re\langle g, (B(r) - D_r(r))g \rangle \right) \geq \\ &\geq r^s \left(\|g'\|^2 - \left(2k^2 + \frac{s(3s+1)}{r^2} \right) \|g\|^2 \right) \\ &\quad + 2r^s \left(\Re\langle g, P(r)g \rangle + \Re\langle g, D_r(r)g' \rangle + \frac{1}{r} \Re\langle g, (B(r) - D_r(r))g \rangle \right). \end{aligned}$$

If we go back to eq. (2.7), (2.8) and (2.9) with $m = 0$ and $t = 0$ and replace g' in the left slot of the inner product with g we get by the very same argument that

$$\left(\Re\langle g, P(r)g \rangle + \Re\langle g, D_r(r)g' \rangle + \frac{1}{r} \Re\langle g, (B(r) - D_r(r))g \rangle \right) \geq -p_k(r) \|g\|^2$$

and therefore

$$\frac{d^2 r^s \|g\|^2}{dr^2} - r^s \|g'\|^2 + 3k^2 r^s \|g\|^2 \geq r^s \left(k^2 - \frac{s(3s+1)}{r^2} - 2p_k(r) \right) \|g\|^2.$$

As $\frac{s(3s+1)}{r^2} + 2p_k(r) \rightarrow 0$ for $r \rightarrow \infty$, there exists an $R_3 \geq R_0$ such that

$$\frac{d^2 r^s \|g\|^2}{dr^2} - r^s \|g'\|^2 + 3k^2 r^s \|g\|^2 \geq 0 \quad \text{for } r \geq R_3.$$

From Lemma 2.4 we know that

$$r^{2\mu+\varepsilon} (\|g'\|^2 + k^2 \|g\|^2) \geq c > 0,$$

for r sufficiently large. Hence, there exists an $R_4 \geq R_3$ such that

$$\frac{d^2 r^{2\mu+\varepsilon} \|g\|^2}{dr^2} + 4k^2 r^{2\mu+\varepsilon} \|g\|^2 \geq c \quad \text{for } r \geq R_4.$$

According to Kato, the solution of such a differential inequality is given by

$$\int_R^{R+\delta} r^{2\mu+\varepsilon} \|g\|^2 dr \geq hc \quad \text{for } R \geq R_4$$

with $h = h(\delta, k)$ being an R - and ε -independent constant. Note that

$$\|g\|^2 = r^2 \|f\|^2 = r^2 \int_{|\mathbf{x}|=r} |f(\mathbf{x})|^2 \sin \theta \, d\theta d\varphi,$$

which yields

$$\int_R^{R+\delta} r^{2\mu+\varepsilon} \left(r^2 \int_{|\mathbf{x}|=r} |f(\mathbf{x})|^2 \sin \theta \, d\theta d\varphi \right) dr \geq hc^2 \quad \text{for all } \varepsilon > 0 \text{ and } R \geq R_4.$$

Trivially, it follows that this inequality also holds for $\frac{\varepsilon}{2}$

$$\int_R^{R+\delta} r^{2\mu+\frac{\varepsilon}{2}} \left(r^2 \int_{|\mathbf{x}|=r} |f(\mathbf{x})|^2 \sin \theta \, d\theta d\varphi \right) dr \geq hc^2$$

and thus

$$(R + \delta)^{2\mu+\frac{\varepsilon}{2}} \int_R^{R+\delta} \left(r^2 \int_{|\mathbf{x}|=r} |f(\mathbf{x})|^2 \sin \theta \, d\theta d\varphi \right) dr \geq hc^2.$$

Multiplying with $R^{\frac{\varepsilon}{2}}$ yields

$$R^{2\mu+\varepsilon} \int_R^{R+\delta} \left(r^2 \int_{|\mathbf{x}|=r} |f(\mathbf{x})|^2 \sin \theta \, d\theta d\varphi \right) dr \geq R^{\frac{\varepsilon}{2}} hc^2 \left(\frac{1}{1 + \frac{\delta}{R}} \right)^{2\mu+\frac{\varepsilon}{2}},$$

which proves eq. (2.12). Noting that $\varepsilon > 0$ was arbitrary concludes the proof of the theorem. \square

The following two corollaries are an important consequence from preceding discussion.

Corollary 2.7. *Let $f \in C^1(B(R_0, 0)^C \rightarrow \mathbb{C}^4)$ be a non-trivial solution to eq. (2.1) on the domain $B(R_0, 0)^C$ and let the \mathbf{A} -field fulfill Condition B. Let furthermore*

$$\int_{R_0}^{\infty} p_k(r) \, dr < \infty.$$

We then have

$$\liminf_{R \rightarrow \infty} R^2 \int_{|\mathbf{x}|=R} k^2 |f(\mathbf{x})|^2 + \left| \frac{\partial}{\partial r} f(\mathbf{x}) \right|^2 \sin \theta \, d\theta d\varphi > 0.$$

Proof. As before we have

$$r^2 \int_{|\mathbf{x}|=r} |f(\mathbf{x})|^2 \sin \theta \, d\theta d\varphi = r^2 \|f\|^2 = \|g\|^2.$$

Futhermore,

$$r^2 \int_{|\mathbf{x}|=r} \left| \frac{\partial}{\partial r} f(\mathbf{x}) \right|^2 \sin \theta \, d\theta d\varphi = r^2 \|f'\|^2 = \left\| g' - \frac{g}{r} \right\|^2.$$

Therefore, we get

$$\begin{aligned} r^2 \int_{|\mathbf{x}|=r} k^2 |f(\mathbf{x})|^2 + \left| \frac{\partial}{\partial r} f(\mathbf{x}) \right|^2 \sin \theta \, d\theta d\varphi &= k^2 \|g\|^2 + \left\| g' - \frac{g}{r} \right\|^2 = \\ &= k^2 \|g\|^2 + \|g'\|^2 + \frac{1}{r^2} \|g\|^2 - \frac{2}{r} \Re(g', g) \geq \\ &\geq k^2 \|g\|^2 + \|g'\|^2 + \frac{1}{r^2} \|g\|^2 - \frac{2}{r} \|g'\| \|g\| = \\ &= \left(k^2 - \frac{1}{r^2} \right) \|g\|^2 + \frac{1}{2} \|g'\|^2 + \frac{1}{2} \left(\|g'\| - \frac{2}{r} \|g\| \right)^2 \geq \\ &\geq \left(k^2 - \frac{1}{r^2} \right) \|g\|^2 + \frac{1}{2} \|g'\|^2. \end{aligned}$$

Observe that $k^2 - \frac{1}{r^2} > \frac{k^2}{2}$ for sufficiently large r . Application of Lemma 2.5 then proves the statement. \square

Corollary 2.8. *Let $f \in C^1(\mathbb{R}^3 \rightarrow \mathbb{C}^4)$ be a solution to eq. (2.1) and let the \mathbf{A} -field fulfill Condition B. We then have:*

1. *if $f \in o\left(\frac{1}{|\mathbf{x}|^{\mu+1}}\right)$ for large x then $f \equiv 0$ on all of \mathbb{R}^3 .*
2. *if $f \in L^2(\mathbb{R}^3 \rightarrow \mathbb{C}^4)$ and $\mu < \frac{1}{2}$ then $f \equiv 0$ on all of \mathbb{R}^3 .*
3. *the Dirac operator has no eigenvalues outside the gap (i.e. $|E_k| > 1$) if $p_k(r) = o\left(\frac{1}{r}\right)$.*

Proof. It suffices to show that $f \equiv 0$ only outside a ball of radius R_0 for then we can apply the unique continuation property of the Dirac operator (see e.g. [Jer86]) to obtain that f vanishes everywhere. Now, let $f \in o\left(\frac{1}{|\mathbf{x}|^{\mu+1}}\right)$, i.e. there exists an $h > 0$ such that $|f(\mathbf{x})| \leq \frac{C}{|\mathbf{x}|^{\mu+1+h}}$ for $|\mathbf{x}|$ large enough. We then have

$$r^2 \int_{|\mathbf{x}|=r} |f(\mathbf{x})|^2 \sin \theta \, d\theta d\varphi \leq \frac{4\pi C}{r^{2(\mu+h)}},$$

for sufficiently large r . Hence, we get

$$\begin{aligned} 4\pi C \lim_{R \rightarrow \infty} R^{2\mu+\varepsilon} \int_R^{R+\delta} \left(r^2 \int_{|\mathbf{x}|=r} |f(\mathbf{x})|^2 \sin \theta \, d\theta d\varphi \right) dr &\leq 4\pi C \lim_{R \rightarrow \infty} R^{2\mu+\varepsilon} \int_R^{R+\delta} \frac{1}{r^{2(\mu+h)}} dr \leq \\ &\leq 4\pi C \lim_{R \rightarrow \infty} \frac{R^{2\mu+\varepsilon}}{R^{2(\mu+h)}} \int_R^{R+\delta} dr = 4\pi C \delta \lim_{R \rightarrow \infty} \frac{1}{R^{2h-\varepsilon}} = 0, \end{aligned}$$

for $\varepsilon < 2h$. Thus, f can only be the trivial solution according to Theorem 2.6. To prove the second statement, assume that $\mu < \frac{1}{2}$ and $f \not\equiv 0$. Due to Theorem 2.6 we get with $\varepsilon = 1 - 2\mu > 0$ and sufficiently large R (see also [Kat59])

$$\int_R^{R+1} \left(r^2 \int_{|x|=r} |f(\mathbf{x})|^2 \sin \theta \, d\theta d\varphi \right) dr \geq \frac{c}{R}$$

with $c > 0$ and independent of R . Hence,

$$\int_{|x| \geq R_0} |f(\mathbf{x})|^2 \, d^3x = \int_{R_0}^{\infty} \int_{|x|=r} |f(\mathbf{x})|^2 r^2 \sin \theta \, d\theta d\varphi dr \geq c \sum_{n \geq R} \frac{1}{n} = \infty,$$

with $R > R_0$ large enough but fixed. The third statement is a direct consequence of the second statement, because if $p_k(r) \in o\left(\frac{1}{r}\right)$ we have $\mu = 0$. \square

3. Eigenfunction expansion

3.1. Introduction

We now turn to the theory of eigenfunction expansion for the Dirac operator with a vector potential. Eigenfunction expansion can be a useful instrument in quantum theory as it allows us to define unitary transformations which diagonalize operators of interest like the hamiltonian. Assume, $\{\phi_n\}_{n \in \mathbb{N}}$ is an orthonormal basis of eigenfunctions of some hamiltonian H . For any ψ we have

$$\psi = \sum_n \langle \phi_n, \psi \rangle \phi_n .$$

Thus, we can define the map $\mathcal{F} : \mathcal{H} \rightarrow \ell^2$ via

$$\mathcal{F}[\psi](n) = \langle \phi_n, \psi \rangle .$$

The inverse is then given by

$$\mathcal{F}^{-1}[\widehat{\psi}](\mathbf{x}) = \sum_n \phi_n(\mathbf{x}) \widehat{\psi}(n) .$$

A short computation shows that the transformed hamiltonian $\widehat{H} = \mathcal{F} H \mathcal{F}^{-1}$ is then diagonal on the sequence space ℓ^2 ,

$$\widehat{H} \widehat{\psi}(n) = \lambda_n \widehat{\psi}(n) ,$$

for any $\widehat{\psi}(n) \in \ell^2$ with λ_n being the eigenvalue associated with ϕ_n . Unfortunately, it is in general not possible to find an eigenbasis for an arbitrary hamiltonian. The reason is that the spectrum of a hamiltonian is usually not purely discrete but also contains a continuous part. Nevertheless, we can generalize the previous idea if we allow $\lambda_k \in \sigma(H)$ to take on any value in the spectrum and look for solutions of

$$H \phi_k = \lambda_k \phi_k ,$$

where H is now to be understood as a general differential operator. If ϕ_k exists and is not an element of the Hilbert space we call it *generalized eigenfunction*. Drawing further the analogy from the discrete case we expect the maps $\mathcal{F}, \mathcal{F}^{-1}$ formally to be

$$\mathcal{F}[\psi](k) = \langle \phi_k, \psi \rangle ,$$

and

$$\mathcal{F}^{-1}[\widehat{\psi}](\mathbf{x}) = \int \phi_k(\mathbf{x}) \widehat{\psi}(k) dk.$$

Of course, it is a priori not clear what $\langle \phi_k, \psi \rangle$ is supposed to mean as the inner product is only defined for functions in \mathcal{H} . Assume, e.g. the Hilbert space is the L^2 -function space. One thus would have to make sense of

$$\mathcal{F}[\psi](k) = \int \phi_k^\dagger(\mathbf{x}) \psi(\mathbf{x}) d^3x.$$

The content of the theory of generalized eigenfunction expansion is thus to establish the existence of generalized eigenfunctions, the map \mathcal{F} and their properties. For example, the free Schrödinger hamiltonian has the spectrum $\sigma(H_{Sch}) = [0, \infty)$ and e^{-ikx} fulfills

$$-\Delta e^{-ikx} = k^2 e^{-ikx}$$

for any $k^2 \in \sigma(H_{Sch})$. Thus, the map \mathcal{F} is simply the ordinary Fourier transformation. For the general Schrödinger hamiltonian including a potential term, the theory was mainly initiated by Ikebe [Ike60]. Since then, it developed to a satisfying degree and was also applied to the Dirac equation (see [Nen75] and [Eck74]). Nevertheless, it is still lacking certain regularity properties for the Dirac hamiltonian with a magnetic potential which we need in the subsequent chapters. Hence, we will thoroughly investigate the generalized eigenfunctions for this case in a similar manner as Ikebe has.

For the free Dirac hamiltonian the spectrum is given by $(-\infty, -1] \cup [1, \infty)$ and it is well known that

$$\begin{aligned} \phi_0^{+,1}(\mathbf{x}, \mathbf{k}) &= \frac{e^{ik \cdot \mathbf{x}}}{\sqrt{2E_k(E_k+1)}} \begin{pmatrix} E_k+1 \\ 0 \\ k_3 \\ k_1+ik_2 \end{pmatrix}, & \phi_0^{+,2}(\mathbf{x}, \mathbf{k}) &= \frac{e^{ik \cdot \mathbf{x}}}{\sqrt{2E_k(E_k+1)}} \begin{pmatrix} 0 \\ E_k+1 \\ k_1-ik_3 \\ -k_3 \end{pmatrix}, \\ \phi_0^{-,1}(\mathbf{x}, \mathbf{k}) &= \frac{e^{ik \cdot \mathbf{x}}}{\sqrt{2E_k(E_k+1)}} \begin{pmatrix} -k_3 \\ -k_1-ik_2 \\ E_k+1 \\ 0 \end{pmatrix}, & \phi_0^{-,2}(\mathbf{x}, \mathbf{k}) &= \frac{e^{ik \cdot \mathbf{x}}}{\sqrt{2E_k(E_k+1)}} \begin{pmatrix} -k_1+ik_2 \\ k_3 \\ 0 \\ E_k+1 \end{pmatrix}, \end{aligned}$$

fulfill the stationary Dirac equation

$$(-i\boldsymbol{\alpha}\nabla + \beta) \phi_0^{\pm,j}(\mathbf{x}, \mathbf{k}) = \pm E_k \phi_0^{\pm,j}(\mathbf{x}, \mathbf{k})$$

with $E_k = \sqrt{k^2 + 1}$ and $k \geq 0$. This can be written more compactly

$$(-i\boldsymbol{\alpha}\nabla + \beta) \underline{\phi}_0(\mathbf{x}, \mathbf{k}) = \underline{\phi}_0(\mathbf{x}, \mathbf{k}) \underline{E}_k$$

with the matrices $\underline{E}_k = \beta E_k$ and

$$\underline{\phi}_0(\mathbf{x}, \mathbf{k}) = (\phi_0^{+,1}, \phi_0^{+,2}, \phi_0^{-,1}, \phi_0^{-,2})(\mathbf{x}, \mathbf{k}) = \left(a_+(k) - a_-(k) \beta \frac{\boldsymbol{\alpha} \mathbf{k}}{k} \right) e^{i\mathbf{k}\mathbf{x}} = \underline{u}(\mathbf{k}) e^{i\mathbf{k}\mathbf{x}}$$

where

$$a_{\pm}(k) = \frac{1}{\sqrt{2E_k}} \sqrt{E_k \pm 1}.$$

With a vector potential the generalized eigenfunctions have to fulfill

$$(-i\boldsymbol{\alpha}\nabla + \beta - \boldsymbol{\alpha}A(\mathbf{x})) \underline{\phi}(\mathbf{x}, \mathbf{k}) = \underline{\phi}(\mathbf{x}, \mathbf{k}) \underline{E}_k. \quad (3.1)$$

The ansatz is to rewrite this equation into

$$(-i\boldsymbol{\alpha}\nabla + \beta \mp E_k) \phi^{\pm,j}(\mathbf{x}, \mathbf{k}) = \boldsymbol{\alpha}A(\mathbf{x}) \phi^{\pm,j}(\mathbf{x}, \mathbf{k})$$

and interpret the right-hand side as an inhomogeneity to the free Dirac equation. As we have seen in Chapter 1.2 the solution of the inhomogeneous Dirac equation is given by the convolution of the inhomogeneity with the fundamental solution. Hence, we formally get

$$\phi^{\pm,j}(\mathbf{x}, \mathbf{k}) = \phi_0^{\pm,j}(\mathbf{x}, \mathbf{k}) + \int_{\mathbb{R}^3} G_k^{\pm}(\mathbf{x} - \mathbf{y}) \boldsymbol{\alpha}A(\mathbf{y}) \phi^{\pm,j}(\mathbf{y}, \mathbf{k}) d^3y.$$

where $G_k^{\pm}(\mathbf{x})$ is the fundamental solution from eq. (1.3) with $z = \pm\sqrt{k^2 + 1}$. We write

$$\underline{\phi}(\mathbf{x}, \mathbf{k}) = \underline{\phi}_0(\mathbf{x}, \mathbf{k}) + \int_{\mathbb{R}^3} G_k(\mathbf{x} - \mathbf{y}) \boldsymbol{\alpha}A(\mathbf{y}) \underline{\phi}(\mathbf{y}, \mathbf{k}) d^3y.$$

in matrix notation where z from the fundamental solution is replaced by \underline{E}_k which is understood to act from the right side onto $\underline{\phi}(\mathbf{x}, \mathbf{k})$ like in eq. (3.1). This iterative equation is called Lippmann-Schwinger equation and will be our starting point in the analysis of generalized eigenfunctions.

3.2. Generalized eigenfunctions

In this section we prove that, under certain conditions on the external field, there exist unique solutions to the Lippmann-Schwinger equation and they solve the stationary Dirac equation. Furthermore, we will show the uniform boundedness of the eigenfunctions which becomes important for the second quantized Dirac theory. The following space is a useful tool to establishing the theory of eigenfunction expansion.

Definition and Lemma 3.1. *Let \mathcal{B} be the space of 4×4 matrices with their elements being continuous functions tending uniformly to zero as $|\mathbf{x}| \rightarrow \infty$, equipped with the following norm*

$$\|M\|_{\mathcal{B}} := \|M(\mathbf{x})\|_{\infty} = \sup_{\mathbf{x} \in \mathbb{R}^3} |M(\mathbf{x})|.$$

The space \mathcal{B} is a Banach space.

Proof. It is well known that the space of continuous functions tending uniformly to zero at infinity equipped with the infinity norm is a Banach space. The same arguments apply here. \square

We begin with an analysis of the integral operator defined by the convolution of the fundamental solution with the vector potential and the eigenfunctions in the Lippmann-Schwinger equation.

Lemma 3.2. *Let the vector potential $\mathbf{A}(\mathbf{x})$ be bounded and of order $|\mathbf{x}|^{-2-h}$ ($h > 0$) at infinity and let $f \in \mathcal{B}$. The family of operators T_k defined by*

$$T_k[f](\mathbf{x}) := \int_{\mathbb{R}^3} G_k(\mathbf{x} - \mathbf{y}) \boldsymbol{\alpha} \mathbf{A}(\mathbf{y}) f(\mathbf{y}) d^3 y$$

for $k \geq 0$ are compact linear operators on \mathcal{B} to \mathcal{B} and continuous in the parameter k . The function $T_k[f](\mathbf{x})$ is Hölder-continuous in \mathbf{x} with degree $\frac{1}{2}$.

Proof. The proof consists of four steps:

1. Vanishing at infinity

Let $f \in \mathcal{B}$. For $G_k(\mathbf{x})$ we write

$$G_k(\mathbf{x}) = \frac{e^{ik|\mathbf{x}|}}{4\pi|\mathbf{x}|} (S_k^1(\mathbf{x}) + S_k^2(\mathbf{x}))$$

with

$$S_k^1(\mathbf{x}) = \pm E_k + \beta + k \frac{\boldsymbol{\alpha} \mathbf{x}}{x} \quad \text{and} \quad S_k^2(\mathbf{x}) = i \frac{\boldsymbol{\alpha} \mathbf{x}}{x^2}.$$

We have $S_k^1(\mathbf{x} - \mathbf{y}) \boldsymbol{\alpha} \mathbf{A}(\mathbf{y}) f(\mathbf{y}) = \mathcal{O}(|\mathbf{y}|^{-2-h})$ ($h > 0$) for $|\mathbf{y}| \rightarrow \infty$, independently of \mathbf{x} , and all the matrix elements are obviously locally integrable for all $\mathbf{k}, \mathbf{x} \in \mathbb{R}^3$. Thus, we obtain from [Ike60, Lemma 3.1] that

$$\left| \int_{\mathbb{R}^3} \frac{e^{ik|\mathbf{x}-\mathbf{y}|}}{|\mathbf{x}-\mathbf{y}|} S_k^1(\mathbf{x}-\mathbf{y}) \boldsymbol{\alpha} \mathbf{A}(\mathbf{y}) f(\mathbf{y}) d^3 y \right| \rightarrow 0$$

as $|\mathbf{x}| \rightarrow \infty$. For the second term we have

$$\begin{aligned} & \left| \frac{1}{4\pi} \int_{\mathbb{R}^3} \frac{e^{ik|\mathbf{x}-\mathbf{y}|}}{|\mathbf{x}-\mathbf{y}|^2} \boldsymbol{\alpha} \frac{\mathbf{x}-\mathbf{y}}{|\mathbf{x}-\mathbf{y}|} \boldsymbol{\alpha} \mathbf{A}(\mathbf{y}) f(\mathbf{y}) d^3 y \right| \leq \\ & \leq \frac{1}{\pi} \int_{B(\mathbf{x},1)} \frac{|\mathbf{A}(\mathbf{y}) f(\mathbf{y})|}{|\mathbf{x}-\mathbf{y}|^2} d^3 y + \frac{1}{\pi} \int_{\mathbb{R}^3 \setminus B(\mathbf{x},1)} \frac{|\mathbf{A}(\mathbf{y}) f(\mathbf{y})|}{|\mathbf{x}-\mathbf{y}|^2} d^3 y = I_1 + I_2. \end{aligned}$$

Let R be such that $|A(\mathbf{x})f(\mathbf{x})| \leq C|\mathbf{x}|^{-1}$ for all $|\mathbf{x}| \geq R$. If we choose $|\mathbf{x}| \geq 1 + R$ we get for the first integral

$$\begin{aligned} I_1 &= \frac{1}{\pi} \int_{B(0,1)} \frac{|A(\mathbf{x}-\mathbf{y})f(\mathbf{x}-\mathbf{y})|}{|\mathbf{y}|^2} d^3y \leq C \frac{1}{\pi} \int_{B(0,1)} |\mathbf{y}|^{-2} |\mathbf{x}-\mathbf{y}|^{-1} d^3y = \\ &= C \frac{1}{|\mathbf{x}|} \int_0^1 \frac{1}{r} (|\mathbf{x}| + r - |\mathbf{x} - r|) dr = \frac{C}{|\mathbf{x}|}. \end{aligned}$$

We can estimate the second integral by

$$I_2 \leq \frac{1}{2\pi} \int_{\mathbb{R}^3} \frac{|A(\mathbf{y})f(\mathbf{y})|}{|\mathbf{x}-\mathbf{y}|} d^3y$$

because the integrand is positive and $1 \leq |\mathbf{x}-\mathbf{y}|$. Again, [Ike60, Lemma 3.1] tells us that the right hand side vanishes as $|\mathbf{x}| \rightarrow \infty$. Putting it all together we have

$$|T_k[f](\mathbf{x})| \rightarrow 0$$

as $|\mathbf{x}| \rightarrow \infty$ for every $k \geq 0$.

2. Hölder continuity

Next, we have to prove the Hölder-continuity of $T_k[f](\mathbf{x})$ in \mathbf{x} . We proceed in similar fashion as in [Ike60, Lemma 4.1] and take a look at the difference

$$\begin{aligned} T_k[f](\mathbf{x}) - T_k[f](\mathbf{x}') &= -\frac{1}{4\pi} \int_{\mathbb{R}^3} (e^{ik|\mathbf{x}-\mathbf{y}|} - e^{ik|\mathbf{x}'-\mathbf{y}|}) \frac{S_k(\mathbf{x}-\mathbf{y})}{|\mathbf{x}-\mathbf{y}|} \alpha A(\mathbf{y})f(\mathbf{y}) d^3y \\ &\quad - \frac{(E_k + \beta)}{4\pi} \int_{\mathbb{R}^3} e^{ik|\mathbf{x}'-\mathbf{y}|} \left(\frac{1}{|\mathbf{x}-\mathbf{y}|} - \frac{1}{|\mathbf{x}'-\mathbf{y}|} \right) \alpha A(\mathbf{y})f(\mathbf{y}) d^3y \\ &\quad - \frac{k}{4\pi} \int_{\mathbb{R}^3} e^{ik|\mathbf{x}'-\mathbf{y}|} \alpha \left(\frac{(\mathbf{x}-\mathbf{y})}{|\mathbf{x}-\mathbf{y}|^2} - \frac{(\mathbf{x}'-\mathbf{y})}{|\mathbf{x}'-\mathbf{y}|^2} \right) \alpha A(\mathbf{y})f(\mathbf{y}) d^3y \\ &\quad - \frac{i}{4\pi} \int_{\mathbb{R}^3} e^{ik|\mathbf{x}'-\mathbf{y}|} \alpha \left(\frac{(\mathbf{x}-\mathbf{y})}{|\mathbf{x}-\mathbf{y}|^3} - \frac{(\mathbf{x}'-\mathbf{y})}{|\mathbf{x}'-\mathbf{y}|^3} \right) \alpha A(\mathbf{y})f(\mathbf{y}) d^3y = \\ &= I_1 + I_2 + I_3 + I_4. \end{aligned}$$

Using following two inequalities

$$|e^{ik|\mathbf{x}-\mathbf{y}|} - e^{ik|\mathbf{x}'-\mathbf{y}|}| \leq k |\mathbf{x} - \mathbf{x}'|$$

and

$$\left| \frac{1}{|\mathbf{x}-\mathbf{y}|} - \frac{1}{|\mathbf{x}'-\mathbf{y}|} \right| \leq \frac{|\mathbf{x} - \mathbf{x}'|}{|\mathbf{x}-\mathbf{y}||\mathbf{x}'-\mathbf{y}|},$$

we get for the first two Integrals,

$$\begin{aligned} |I_1| &\leq |\mathbf{x} - \mathbf{x}'| \|f\|_{\mathcal{B}} \left(C \int_{\mathbb{R}^3} \frac{|A(\mathbf{y})|}{|\mathbf{x} - \mathbf{y}|} d^3 y + C \int_{\mathbb{R}^3} \frac{|A(\mathbf{y})|}{|\mathbf{x} - \mathbf{y}|^2} d^3 y \right) = |\mathbf{x} - \mathbf{x}'| \|f\|_{\mathcal{B}} (J_1 + J_2), \\ |I_2| &\leq |\mathbf{x} - \mathbf{x}'| \|f\|_{\mathcal{B}} \left(C \int_{\mathbb{R}^3} \frac{|A(\mathbf{y})|}{|\mathbf{x} - \mathbf{y}| |\mathbf{x}' - \mathbf{y}|} d^3 y \right) = |\mathbf{x} - \mathbf{x}'| \|f\|_{\mathcal{B}} J_3. \end{aligned}$$

Ikebe proved in [Ike60, Lemma 2.2] that $J_1 \leq C < \infty$ with C independent of \mathbf{x} . For J_2 we get

$$\begin{aligned} \int_{\mathbb{R}^3} \frac{|A(\mathbf{y})|}{|\mathbf{x} - \mathbf{y}|^2} d^3 y &= \int_{B(\mathbf{x},1)} \frac{|A(\mathbf{y})|}{|\mathbf{x} - \mathbf{y}|^2} d^3 y + \int_{\mathbb{R}^3 \setminus B(\mathbf{x},1)} \frac{|A(\mathbf{y})|}{|\mathbf{x} - \mathbf{y}|^2} d^3 y \leq \\ &\leq \sup_{\mathbf{x} \in \mathbb{R}^3} |A(\mathbf{x})| \int_{B(\mathbf{x},1)} \frac{1}{|\mathbf{x} - \mathbf{y}|^2} d^3 y + \int_{\mathbb{R}^3 \setminus B(\mathbf{x},1)} \frac{|A(\mathbf{y})|}{|\mathbf{x} - \mathbf{y}|} d^3 y \leq \\ &\leq \sup_{\mathbf{x} \in \mathbb{R}^3} |A(\mathbf{x})| + J_1 < \infty, \end{aligned}$$

as the A -field is bounded. Finally, J_3 can be bounded by multiples of J_2 . Thus, we are left to prove the Hölder-continuity of I_3 and I_4 . It is clear that they are bounded (by above computations). Thus, we can restrict ourselves to $\delta = |\boldsymbol{\delta}| < 1$ where $\boldsymbol{\delta} := \frac{1}{2}(\mathbf{x} - \mathbf{x}')$. With $j = 2, 3$ and $\mathbf{z} = \mathbf{x} - \boldsymbol{\delta} = \mathbf{x}' + \boldsymbol{\delta}$ we have

$$\begin{aligned} \int_{\mathbb{R}^3} \alpha \left(\frac{(\mathbf{x} - \mathbf{y})}{|\mathbf{x} - \mathbf{y}|^j} - \frac{(\mathbf{x}' - \mathbf{y})}{|\mathbf{x}' - \mathbf{y}|^j} \right) |A(\mathbf{y})| d^3 y &= \int_{B(\mathbf{z}, \sqrt{\delta})} \alpha \left(\frac{(\mathbf{x} - \mathbf{y})}{|\mathbf{x} - \mathbf{y}|^j} - \frac{(\mathbf{x}' - \mathbf{y})}{|\mathbf{x}' - \mathbf{y}|^j} \right) |A(\mathbf{y})| d^3 y \\ &+ \int_{\mathbb{R}^3 \setminus B(\mathbf{z}, \sqrt{\delta})} \alpha \left(\frac{(\mathbf{x} - \mathbf{y})}{|\mathbf{x} - \mathbf{y}|^j} - \frac{(\mathbf{x}' - \mathbf{y})}{|\mathbf{x}' - \mathbf{y}|^j} \right) |A(\mathbf{y})| d^3 y = \\ &= K_1 + K_2. \end{aligned}$$

For K_1 we get

$$\begin{aligned} |K_1| &\leq \sup_{\mathbf{x} \in \mathbb{R}^3} |A(\mathbf{x})| \left(\int_{B(\mathbf{z}, \sqrt{\delta})} \frac{1}{|\mathbf{x} - \mathbf{y}|^{j-1}} d^3 y + \int_{B(\mathbf{z}, \sqrt{\delta})} \frac{1}{|\mathbf{x}' - \mathbf{y}|^{j-1}} d^3 y \right) = \\ &= \sup_{\mathbf{x} \in \mathbb{R}^3} |A(\mathbf{x})| \left(\int_{B(\boldsymbol{\delta}, \sqrt{\delta})} \frac{1}{|\mathbf{y}|^{j-1}} d^3 y + \int_{B(-\boldsymbol{\delta}, \sqrt{\delta})} \frac{1}{|\mathbf{y}|^{j-1}} d^3 y \right) \leq \\ &\leq 2 \sup_{\mathbf{x} \in \mathbb{R}^3} |A(\mathbf{x})| \int_{B(0, \sqrt{\delta})} \frac{1}{|\mathbf{y}|^{j-1}} d^3 y = 8\pi \sup_{\mathbf{x} \in \mathbb{R}^3} |A(\mathbf{x})| \frac{1}{4-j} \delta^{\frac{4-j}{2}} \leq C\sqrt{\delta} \end{aligned}$$

as $\delta < 1$. In the third step we used that for a given radius the integral of $\frac{1}{|\mathbf{y}|^{j-1}}$ is maximal if the ball is centered at the singularity, $\mathbf{y} = 0$. For the constant we have $C < \infty$ and it is

independent of \mathbf{x} . Using the following inequality

$$\begin{aligned}
\left| \frac{(\mathbf{x} - \mathbf{y})}{|\mathbf{x} - \mathbf{y}|^j} - \frac{(\mathbf{x}' - \mathbf{y})}{|\mathbf{x}' - \mathbf{y}|^j} \right| &= \left| \frac{\mathbf{x} - \mathbf{x}'}{|\mathbf{x} - \mathbf{y}|^j} + \frac{(\mathbf{x}' - \mathbf{y})(|\mathbf{x}' - \mathbf{y}|^j - |\mathbf{x} - \mathbf{y}|^j)}{|\mathbf{x} - \mathbf{y}|^j |\mathbf{x}' - \mathbf{y}|^j} \right| \leq \\
&\leq \frac{|\mathbf{x} - \mathbf{x}'|}{|\mathbf{x} - \mathbf{y}|^j} + \frac{||\mathbf{x}' - \mathbf{y}|^j - |\mathbf{x} - \mathbf{y}|^j|}{|\mathbf{x} - \mathbf{y}|^j |\mathbf{x}' - \mathbf{y}|^{j-1}} = \\
&= \frac{|\mathbf{x} - \mathbf{x}'|}{|\mathbf{x} - \mathbf{y}|^j} + \frac{||\mathbf{x} - \mathbf{y}| - |\mathbf{x}' - \mathbf{y}|| \sum_{n=0}^{j-1} |\mathbf{x} - \mathbf{y}|^n |\mathbf{x}' - \mathbf{y}|^{j-1-n}}{|\mathbf{x} - \mathbf{y}|^j |\mathbf{x}' - \mathbf{y}|^{j-1}} \leq \\
&\leq \frac{|\mathbf{x} - \mathbf{x}'|}{|\mathbf{x} - \mathbf{y}|^j} + \sum_{n=0}^{j-1} \frac{|\mathbf{x} - \mathbf{x}'|}{|\mathbf{x} - \mathbf{y}|^{j-n} |\mathbf{x}' - \mathbf{y}|^n} \leq \\
&\leq \sum_{n=0}^j \frac{|\mathbf{x} - \mathbf{x}'|}{|\mathbf{x} - \mathbf{y}|^{j-n} |\mathbf{x}' - \mathbf{y}|^n},
\end{aligned}$$

we get for K_2

$$\begin{aligned}
|K_2| &\leq 2 \int_{\mathbb{R}^3 \setminus B(\mathbf{z}, \sqrt{\delta})} \left| \frac{(\mathbf{x} - \mathbf{y})}{|\mathbf{x} - \mathbf{y}|^j} - \frac{(\mathbf{x}' - \mathbf{y})}{|\mathbf{x}' - \mathbf{y}|^j} \right| |\mathbf{A}(\mathbf{y})| \, d^3 y \leq \\
&\leq C |\mathbf{x} - \mathbf{x}'| \int_{\mathbb{R}^3 \setminus B(\mathbf{z}, \sqrt{\delta})} \sum_{n=0}^j \frac{1}{|\mathbf{x} - \mathbf{y}|^{j-n} |\mathbf{x}' - \mathbf{y}|^n} |\mathbf{A}(\mathbf{y})| \, d^3 y \leq \\
&\leq (j+1)C |\mathbf{x} - \mathbf{x}'| \int_{\mathbb{R}^3 \setminus B(\mathbf{0}, \sqrt{\delta})} \frac{1}{|\mathbf{y}|^j} |\mathbf{A}(\mathbf{z} - \mathbf{y})| \, d^3 y \leq \\
&\leq C |\mathbf{x} - \mathbf{x}'| \sup_{\mathbf{x} \in \mathbb{R}} |\mathbf{A}(\mathbf{x})| \int_{\sqrt{\delta}}^1 \frac{1}{y} \, dy + C |\mathbf{x} - \mathbf{x}'| \int_{\mathbb{R}^3 \setminus B(\mathbf{0}, 1)} \frac{|\mathbf{A}(\mathbf{z} - \mathbf{y})|}{|\mathbf{y}|^j} \, d^3 y \leq \\
&\leq C\sqrt{\delta} + C\delta \int_{\mathbb{R}^3 \setminus B(\mathbf{0}, 1)} \frac{|\mathbf{A}(\mathbf{z} - \mathbf{y})|}{|\mathbf{y}|} \, d^3 y \\
&\leq C\sqrt{\delta} + C\delta \int_{\mathbb{R}^3} \frac{|\mathbf{A}(\mathbf{z} - \mathbf{y})|}{|\mathbf{y}|} \, d^3 y \leq C\sqrt{\delta} + C J_1 \delta.
\end{aligned}$$

In the third inequality we again observed that the center of the ball of integration is away from the singularities. In the fifth step we used that $|1 - \ln(\sqrt{\delta})| \leq \frac{1}{\sqrt{\delta}}$ and we have already shown that J_1 is uniformly bounded. Therefore we have for I_3 and I_4 ,

$$|I_{3/4}| \leq C |\mathbf{x} - \mathbf{x}'|^{\frac{1}{2}} \|f\|_{\mathcal{B}}.$$

Thus, $T_k[f](\mathbf{x})$ is continuous in \mathbf{x} and therefore T_k maps from \mathcal{B} onto \mathcal{B} . Moreover $T_k[f](\mathbf{x})$ is even Hölder continuous of degree $\frac{1}{2}$.

3. Continuity in k

We have to show that

$$\sup_{\mathbf{x} \in \mathbb{R}^3} \frac{|\mathbb{T}_k[f](\mathbf{x}) - \mathbb{T}_{k'}[f](\mathbf{x})|}{\|f\|_{\mathcal{B}}} \xrightarrow{k' \rightarrow k} 0,$$

which is easy with help of the computations carried out above.

$$\begin{aligned} |\mathbb{T}_k[f](\mathbf{x}) - \mathbb{T}_{k'}[f](\mathbf{x})| &\leq 2 \|f\|_{\mathcal{B}} \int \frac{|e^{ik|\mathbf{x}-\mathbf{y}} - e^{ik'|\mathbf{x}-\mathbf{y}}|}{|\mathbf{x}-\mathbf{y}|} |S_k(\mathbf{x}-\mathbf{y})| |A(\mathbf{y})| d^3y \\ &\quad + 2 \|f\|_{\mathcal{B}} \int \frac{|A(\mathbf{y})|}{|\mathbf{x}-\mathbf{y}|} \left| E_k - E_{k'} + \alpha \frac{\mathbf{x}-\mathbf{y}}{|\mathbf{x}-\mathbf{y}|} (k-k') \right| d^3y. \end{aligned}$$

In the proof of Hölder continuity we have shown that

$$\int \frac{|A(\mathbf{y})|}{|\mathbf{x}-\mathbf{y}|} d^3y$$

is uniformly bounded in \mathbf{x} . Thus, the last integral vanishes uniformly in \mathbf{x} for $k' \rightarrow k$. For the first integral remember that

$$\int \frac{|e^{ik|\mathbf{x}-\mathbf{y}} - e^{ik'|\mathbf{x}-\mathbf{y}}|}{|\mathbf{x}-\mathbf{y}|} |S_k(\mathbf{x}-\mathbf{y})| |A(\mathbf{y})| d^3y \xrightarrow{|\mathbf{x}| \rightarrow \infty} 0$$

uniformly in k' . Thus, there exists an $R > 0$ such that for all k'

$$\begin{aligned} \sup_{\mathbf{x} \in \mathbb{R}^3} \int \frac{|e^{ik|\mathbf{x}-\mathbf{y}} - e^{ik'|\mathbf{x}-\mathbf{y}}|}{|\mathbf{x}-\mathbf{y}|} |S_k(\mathbf{x}-\mathbf{y})| |A(\mathbf{y})| d^3y &= \\ = \sup_{\mathbf{x} \in B(R,0)} \int \frac{|e^{ik|\mathbf{x}-\mathbf{y}} - e^{ik'|\mathbf{x}-\mathbf{y}}|}{|\mathbf{x}-\mathbf{y}|} |S_k(\mathbf{x}-\mathbf{y})| |A(\mathbf{y})| d^3y. \end{aligned}$$

Now, let $R' > R$ and such that $|A(\mathbf{y})| < \frac{C}{|\mathbf{y}|^{2+h}}$ for $|\mathbf{y}| > R'$. Then, for $j = 1, 2$

$$\begin{aligned} \sup_{\mathbf{x} \in B(R,0)} \int_{\mathbb{R}^3 \setminus B(R',0)} \frac{1}{|\mathbf{x}-\mathbf{y}|^j} |A(\mathbf{y})| d^3y &\leq C \sup_{\mathbf{x} \in B(R,0)} \int_{\mathbb{R}^3 \setminus B(R',0)} \frac{1}{|\mathbf{x}-\mathbf{y}|^j} \frac{1}{|\mathbf{y}|^{2+h}} d^3y \leq \\ &\leq C \int_{R'}^{\infty} \frac{1}{(r-R)^j} \frac{1}{r^\varepsilon} dr \leq C \frac{1}{h} \frac{1}{\left(1 - \frac{R}{R'}\right)^2} \frac{1}{R'^h}. \end{aligned}$$

Finally, we have

$$\begin{aligned} \sup_{\mathbf{x} \in B(R,0)} \int_{B(R',0)} \frac{|e^{ik|\mathbf{x}-\mathbf{y}} - e^{ik'|\mathbf{x}-\mathbf{y}}|}{|\mathbf{x}-\mathbf{y}|} |S_k(\mathbf{x}-\mathbf{y})| |A(\mathbf{y})| d^3y &\leq \\ &\leq |k-k'| \sup_{\mathbf{x} \in B(R,0)} \int_{B(R',0)} |S_k(\mathbf{x}-\mathbf{y})| |A(\mathbf{y})| d^3y \leq |k-k'| \left(C \sup_{\mathbf{x} \in \mathbb{R}^3} |A(\mathbf{x})| R'^2 + J_1 \right) \end{aligned}$$

where we have used $|e^{ik|x-y|} - e^{ik'|x-y|}| \leq |k - k'| |\mathbf{x} - \mathbf{y}|$ and that J_1 is uniformly bounded in \mathbf{x} . Thus, we can always choose R , R' and k' such that

$$\sup_{\mathbf{x} \in \mathbb{R}^3} \frac{|T_k[f](\mathbf{x}) - T_{k'}[f](\mathbf{x})|}{\|f\|_{\mathcal{B}}}$$

becomes arbitrarily small.

4. Compactness

It is clear by the computations above that T_k is a bounded operator. To prove compactness we have to show that for every bounded sequence f_n in \mathcal{B} , there exists a norm-convergent subsequence in $(T_k[f_n])_{n \in \mathbb{N}}$. Once again we will closely follow Ikebe, [Ike60, Lemma 4.2]. Let $(f_n)_{n \in \mathbb{N}}$ be a family of functions in \mathcal{B} with $\|f_n\|_{\mathcal{B}} \leq M < \infty$ for all $n \in \mathbb{N}$. We denote the image of these functions with $g_n = T_k[f_n]$. By re-examining the proof of boundedness of T_k we see that $\|g_n\|_{\mathcal{B}} \leq M' < \infty$ independent of n . In particular the g_n are uniformly bounded (in n) on any compact domain of \mathbb{R}^3 . By the proof of the Hölder continuity above it is also clear that they are uniformly continuous in \mathbf{x} and n . Thus, they are uniformly equicontinuous. Therefore, by using Arzela-Ascolis theorem, on any compact domain $K \subset \mathbb{R}^3$ there exists a subsequence g_{n_k} which converges uniformly to some g on K . As, again by looking at the proof of the Hölder continuity, the $g_n(\mathbf{x}) \rightarrow 0$ uniformly in n for $|\mathbf{x}| \rightarrow \infty$ we also have $g(\mathbf{x}) \rightarrow 0$ for $|\mathbf{x}| \rightarrow \infty$ and thus for all compact $K \subset \mathbb{R}^3$

$$\begin{aligned} \|g - g_{n_k}\|_{\mathcal{B}} &= \sup_{\mathbf{x} \in K \cup (\mathbb{R}^3 \setminus K)} |g(\mathbf{x}) - g_{n_k}(\mathbf{x})| \leq \\ &\leq \sup_{\mathbf{x} \in K} |g(\mathbf{x}) - g_{n_k}(\mathbf{x})| + \sup_{\mathbb{R}^3 \setminus K} |g(\mathbf{x})| + \sup_{\mathbb{R}^3 \setminus K} |g_{n_k}(\mathbf{x})|. \end{aligned}$$

For any $\varepsilon > 0$ we can find a K around the origin big enough such that the last two terms are each smaller than $\frac{\varepsilon}{3}$ and for any given K there is an $N \in \mathbb{N}$ such that the first term is smaller than $\frac{\varepsilon}{3}$ for all $k > N$. \square

Remark. Note that the proof of Hölder continuity and $T_k[f]$ vanishing at infinity does not depend on f being in \mathcal{B} . It is only used that $f \in \mathcal{B}$ implies that f is bounded. Thus, for any bounded function f we have that the function $T_k[f](\mathbf{x})$ is Hölder continuous and vanishes at infinity and hence $T_k[f] \in \mathcal{B}$.

To establish the existence of solutions to the Lippmann-Schwinger equation we make use of the Fredholm alternative which can be formulated as follows (see e.g. [Rus86]). Let T be a compact operator on a Banach space \mathcal{B} and $g \in \mathcal{B}$. The operator $\text{id} - T$ is invertible if and only if

$$f' = T[f']$$

implies that $f' \equiv 0$. In this case the equation

$$f = g + T[f]$$

has a unique solution in \mathcal{B} which is given by

$$f = \frac{1}{1 - \mathbb{T}}[g].$$

We can now use this to prove the main theorem of this chapter.

Theorem 3.3. *Let the vector potential $A \in C^\infty(\mathbb{R}^3 \rightarrow \mathbb{R}^3)$ and be of order $|\mathbf{x}|^{-2-h}$ ($h > 0$) at infinity. Let furthermore its first partial derivatives be of order $|\mathbf{x}|^{-1-h}$ ($h > 0$) at infinity. Then there exist unique solutions $\underline{\phi}(\cdot, \mathbf{k}) \in C^\infty(\mathbb{R}^3 \rightarrow \mathbb{C}^{4 \times 4})$ of*

$$\underline{\phi}(\mathbf{x}, \mathbf{k}) = \underline{\phi}_0(\mathbf{x}, \mathbf{k}) + \int_{\mathbb{R}^3} G_k(\mathbf{x} - \mathbf{y}) \alpha A(\mathbf{y}) \underline{\phi}(\mathbf{y}, \mathbf{k}) d^3 y. \quad (3.2)$$

for all $\mathbf{k} \in \mathbb{R}^3 \setminus \{0\}$. They fulfill

$$[(-i\alpha\nabla - \alpha A(\mathbf{x})) + \beta] \underline{\phi}(\mathbf{x}, \mathbf{k}) = \underline{\phi}(\mathbf{x}, \mathbf{k}) \underline{E}_k, \quad (3.3)$$

with $\underline{E}_k = E_k \beta$ and $E_k = \sqrt{\mathbf{k}^2 + 1}$. These solutions are continuous in $\mathbf{k} \in \mathbb{R}^3 \setminus \{0\}$ and are uniformly bounded and uniformly continuous in $\mathbf{x} \in \mathbb{R}^3$.

Proof. To proof the existence of a solution we define

$$f_k(\mathbf{x}) := \underline{\phi}(\mathbf{x}, \mathbf{k}) - \underline{\phi}_0(\mathbf{x}, \mathbf{k}).$$

It fulfills

$$\begin{aligned} f_k(\mathbf{x}) &= g_k(\mathbf{x}) + \int_{\mathbb{R}^3} G_k(\mathbf{x} - \mathbf{y}) \alpha A(\mathbf{y}) f_k(\mathbf{x}) d^3 y = \\ &= g_k(\mathbf{x}) + \mathbb{T}_k[f_k](\mathbf{x}), \end{aligned} \quad (3.4)$$

with

$$g_k(\mathbf{x}) = \int_{\mathbb{R}^3} G_k(\mathbf{x} - \mathbf{y}) \alpha A(\mathbf{y}) \underline{\phi}_0(\mathbf{y}, \mathbf{k}) d^3 y.$$

It is sufficient to proof that eq. (3.4) has a unique solution. As $\underline{\phi}_0(\mathbf{x}, \mathbf{k})$ is a bounded function it is clear by the remark to the proof of Lemma 3.2 that $g_k \in \mathcal{B}$ and as \mathbb{T}_k is a compact operator on \mathcal{B} we can use the Fredholm alternative which leaves us to prove that

$$f(\mathbf{x}) = \int_{\mathbb{R}^3} G_k(\mathbf{x} - \mathbf{y}) \alpha A(\mathbf{y}) f(\mathbf{y}) d^3 y$$

for any $f \in \mathcal{B}$ implies $f(\mathbf{x}) \equiv 0$. If $f \in \mathcal{B}$ it follows that $\alpha A(\mathbf{x}) f(\mathbf{x})$ is locally integrable. Hence, we can use Lemma 1.1 which shows that f fulfills the Dirac equation. As f is continuous by assumption and the A -field is smooth it follows that f is also smooth (see [Rud91]). We furthermore

observe the following about the decay of f . Assume that $f \in \mathcal{O}(1)$ at infinity and by assumption we have $\mathbf{A} \in \mathcal{O}(|\mathbf{x}|^{-2-h})$. Hence, $f\boldsymbol{\alpha}\mathbf{A} \in \mathcal{O}(|\mathbf{x}|^{-2-h})$ and it follows by our proof of Lemma 3.2 and [Ike60, Lemma 3.1] that the decay of $T_k[f]$ at infinity is $\mathcal{O}(|\mathbf{x}|^{-1}) + \mathcal{O}(|\mathbf{x}|^{-h})$. As $f = T_k[f]$, we also have that $f \in \mathcal{O}(|\mathbf{x}|^{-1}) + \mathcal{O}(|\mathbf{x}|^{-h})$ and therefore $f\boldsymbol{\alpha}\mathbf{A} \in \mathcal{O}(|\mathbf{x}|^{-2-2h})$. This then implies that $T_k[f] \in \mathcal{O}(|\mathbf{x}|^{-1}) + \mathcal{O}(|\mathbf{x}|^{-2h})$ and again this is also true for f . Repeating this argument over and over we conclude that $f \in \mathcal{O}(|\mathbf{x}|^{-1})$ at infinity. Now, the Dirac kernel can be written as

$$G_k^\pm(\mathbf{x}) = (-i\boldsymbol{\alpha}\nabla + \beta \pm E_k) \frac{e^{ik|\mathbf{x}|}}{4\pi|\mathbf{x}|}.$$

Hence, as f fulfills the Dirac equation and \mathbf{A} is differentiable we find

$$\begin{aligned} f(\mathbf{x}) &= \int_{\mathbb{R}^3} G_k^\pm(\mathbf{x} - \mathbf{y})\boldsymbol{\alpha}\mathbf{A}(\mathbf{y})f(\mathbf{y}) \, d^3y = \\ &= (-i\boldsymbol{\alpha}\nabla_x + \beta \pm E_k) \int_{\mathbb{R}^3} \frac{e^{ik|\mathbf{x}-\mathbf{y}|}}{4\pi|\mathbf{x}-\mathbf{y}|} \boldsymbol{\alpha}\mathbf{A}(\mathbf{y})f(\mathbf{y}) \, d^3y = \\ &= (-i\boldsymbol{\alpha}\nabla_x + \beta \pm E_k) \int_{\mathbb{R}^3} \frac{e^{ik|\mathbf{y}|}}{4\pi|\mathbf{y}|} \boldsymbol{\alpha}\mathbf{A}(\mathbf{x} - \mathbf{y})f(\mathbf{x} - \mathbf{y}) \, d^3y = \\ &= \int_{\mathbb{R}^3} \frac{e^{ik|\mathbf{y}|}}{4\pi|\mathbf{y}|} (-i\boldsymbol{\alpha}\nabla_x + \beta \pm E_k) \boldsymbol{\alpha}\mathbf{A}(\mathbf{x} - \mathbf{y})f(\mathbf{x} - \mathbf{y}) \, d^3y = \\ &= - \int_{\mathbb{R}^3} \frac{e^{ik|\mathbf{x}-\mathbf{y}|}}{4\pi|\mathbf{x}-\mathbf{y}|} (-i\boldsymbol{\alpha}\nabla_y + \beta \pm E_k) \boldsymbol{\alpha}\mathbf{A}(\mathbf{y})f(\mathbf{y}) \, d^3y. \end{aligned}$$

As f fulfills the Dirac equation we see that $|\nabla f|$ can be bounded by $|f|$ for $|\mathbf{x}|$ sufficiently large and has therefore the same decay at infinity. Furthermore, both \mathbf{A} and $\partial_i\mathbf{A}$ decay with $|\mathbf{x}|^{-2-h}$. Thus, we have $(-i\boldsymbol{\alpha}\nabla_y + \beta \pm E_k) \boldsymbol{\alpha}\mathbf{A}(\mathbf{y})f(\mathbf{y}) \in \mathcal{O}(|\mathbf{x}|^{-3-h})$ and we can use [Ike60, Lemma 3.3] which shows that f fulfills the radiation condition

$$\lim_{|\mathbf{x}| \rightarrow \infty} |\mathbf{x}| \left| \frac{\partial}{\partial |\mathbf{x}|} f - ikf \right| = 0.$$

A similar derivation as in [Eck74, Lemma C3] shows that

$$\begin{aligned} R^2 \int_{S(R,0)} \left| \frac{\partial}{\partial |\mathbf{x}|} f - ikf \right|^2 \sin \theta \, d\theta \, d\varphi &= \\ &= R^2 \int_{S(R,0)} \left| \frac{\partial}{\partial |\mathbf{x}|} f(\mathbf{x}) \right|^2 + k^2 |f(\mathbf{x})|^2 \sin \theta \, d\theta \, d\varphi + \mathcal{O}(R^{-h}) \end{aligned}$$

where $S(R,0)$ is the sphere with radius R and the extra term comes from the non-compactness of the \mathbf{A} -field during integration by parts. Using the radiation condition we conclude that

$$\lim_{R \rightarrow \infty} R^2 \int_{S(R,0)} \left| \frac{\partial}{\partial |\mathbf{x}|} f(\mathbf{x}) \right|^2 + k^2 |f(\mathbf{x})|^2 \sin \theta \, d\theta \, d\varphi = 0.$$

Corollary 2.7 shows then that f has to be the trivial solution at least outside a sufficiently large ball. Similarly as in Corollary 2.8 this implies that f vanishes everywhere by unique continuation. Hence, the Fredholm alternative tells us that there is a unique solution to

$$f_k(\mathbf{x}) = T_k[\underline{\phi}_0(\cdot, \mathbf{k})](\mathbf{x}) + T_k[f_k](\mathbf{x})$$

which can be written as

$$f_k(\mathbf{x}) = (\text{id}_{\mathcal{B}} - T_k)^{-1} T_k[\underline{\phi}_0(\cdot, \mathbf{k})](\mathbf{x}).$$

By Lemma 3.2 we know that the operator T_k is continuous in k for all $k \geq 0$ and as $(\text{id}_{\mathcal{B}} - T_k)^{-1}$ exists for all $k > 0$ we find by the resolvent identity that also $(\text{id}_{\mathcal{B}} - T_k)^{-1}$ is continuous for all $k > 0$. The boundedness and uniform continuity for the generalized eigenfunctions in \mathbf{x} follow immediately from eq. (3.4), Lemma 3.2 and $f_k \in \mathcal{B}$.

To show that $\underline{\phi}(\mathbf{x}, \mathbf{k})$ fulfills the Dirac equation we first note that $\alpha A(\mathbf{x}) \underline{\phi}(\mathbf{x}, \mathbf{k})$ is locally integrable for every $\mathbf{k} \in \mathbb{R}^3 \setminus \{0\}$ as it is continuous in \mathbf{x} . Thus, Lemma 1.1 gives

$$\begin{aligned} [-i\alpha\nabla + \beta] \int_{\mathbb{R}^3} G_k(\mathbf{x} - \mathbf{y}) \alpha A(\mathbf{y}) \underline{\phi}(\mathbf{y}, \mathbf{k}) d^3 y &= \alpha A(\mathbf{x}) \underline{\phi}(\mathbf{x}, \mathbf{k}) \\ &+ \int_{\mathbb{R}^3} G_k(\mathbf{x} - \mathbf{y}) \alpha A(\mathbf{y}) \underline{\phi}(\mathbf{y}, \mathbf{k}) d^3 y \underline{E}_k. \end{aligned}$$

By the definition of $\underline{\phi}_0(\mathbf{x}, \mathbf{k})$ we have

$$[-i\alpha\nabla + \beta] \underline{\phi}_0(\mathbf{x}, \mathbf{k}) = \underline{\phi}_0(\mathbf{x}, \mathbf{k}) \underline{E}_k.$$

Hence, we get

$$\begin{aligned} [-i\alpha\nabla + \beta] \underline{\phi}(\mathbf{x}, \mathbf{k}) &= \\ &= \underline{\phi}_0(\mathbf{x}, \mathbf{k}) \underline{E}_k + \int_{\mathbb{R}^3} G_k(\mathbf{x} - \mathbf{y}) \alpha A(\mathbf{y}) \underline{\phi}(\mathbf{y}, \mathbf{k}) d^3 y \underline{E}_k + \alpha A(\mathbf{x}) \underline{\phi}(\mathbf{x}, \mathbf{k}) \\ &= \underline{\phi}(\mathbf{x}, \mathbf{k}) \underline{E}_k + \alpha A(\mathbf{x}) \underline{\phi}(\mathbf{x}, \mathbf{k}). \end{aligned}$$

As before, the smoothness follows again from the regularity theorem for elliptic partial differential equations. \square

With further restrictions on the external field we will be able to show that the generalized eigenfunctions are uniformly bounded in \mathbf{k} . We already know from Theorem 3.3 that the eigenfunctions are bounded and continuous for every compact subset of \mathbb{R}^3 not containing the origin. Thus, we have to investigate the behavior at infinity and at zero. We start with the former.

Lemma 3.4. *Let the vector potential fulfill the prerequisites of Theorem 3.3. Let it furthermore be such that all of its partial derivatives up to second order are integrable. Then*

$$\lim_{k \rightarrow \infty} \|f_k(\cdot)\|_{\mathcal{B}} = 0.$$

Proof. We start by showing that $T_k[\underline{\phi}_0(\cdot, \mathbf{k})](\mathbf{x})$ vanishes for $k \rightarrow \infty$. Let for the moment $\mathbf{A} \in C_0^\infty$ and note that the fundamental solution to the Dirac equation can be written as

$$G_k^\pm(\mathbf{x}) = (H_0 \pm E_k) G_k^{\text{Schr}}(\mathbf{x}) = (H_0 \pm E_k) \frac{e^{ik|\mathbf{x}|}}{4\pi|\mathbf{x}|}.$$

Therefore, we have

$$\begin{aligned} \int G_k^\pm(\mathbf{x} - \mathbf{y}) \boldsymbol{\alpha} \mathbf{A}(\mathbf{y}) \phi_0^\pm(\mathbf{k}, \mathbf{y}) d^3 y &= (H_0 \pm E_k) \int \frac{e^{ik|\mathbf{x}-\mathbf{y}|}}{4\pi|\mathbf{x}-\mathbf{y}|} \boldsymbol{\alpha} \mathbf{A}(\mathbf{y}) \phi_0^\pm(\mathbf{k}, \mathbf{y}) d^3 y = \\ &= (H_0 \pm E_k) \int \frac{e^{ik|\mathbf{y}|}}{4\pi|\mathbf{y}|} \boldsymbol{\alpha} \mathbf{A}(\mathbf{x} - \mathbf{y}) \phi_0^\pm(\mathbf{k}, \mathbf{x} - \mathbf{y}) d^3 y \\ &= (H_0 \pm E_k) \int \frac{e^{ik|\mathbf{y}|}}{4\pi|\mathbf{y}|} \boldsymbol{\alpha} \mathbf{A}(\mathbf{x} - \mathbf{y}) e^{-iy \cdot \mathbf{k}} d^3 y \phi_0^\pm(\mathbf{k}, \mathbf{x}) \end{aligned}$$

where we used $\phi_0^\pm(\mathbf{k}, \mathbf{x} - \mathbf{y}) = u^\pm(\mathbf{k}) e^{i(\mathbf{x}-\mathbf{y}) \cdot \mathbf{k}} = e^{-iy \cdot \mathbf{k}} \phi_0^\pm(\mathbf{k}, \mathbf{x})$ in the last step. Using the anti commutation relations we get

$$\begin{aligned} \int G_k^\pm(\mathbf{x} - \mathbf{y}) \boldsymbol{\alpha} \mathbf{A}(\mathbf{y}) \phi_0^\pm(\mathbf{k}, \mathbf{y}) d^3 y &= \int \frac{e^{ik|\mathbf{y}|}}{4\pi|\mathbf{y}|} (-i \boldsymbol{\alpha} \nabla \boldsymbol{\alpha} \mathbf{A}(\mathbf{x} - \mathbf{y})) e^{-iy \cdot \mathbf{k}} d^3 y \phi_0^\pm(\mathbf{k}, \mathbf{x}) \\ &\quad - 2i \int \frac{e^{ik|\mathbf{y}|}}{4\pi|\mathbf{y}|} A_i(\mathbf{x} - \mathbf{y}) e^{-iy \cdot \mathbf{k}} d^3 y \partial_i \phi_0^\pm(\mathbf{k}, \mathbf{x}) \\ &\quad + \int \frac{e^{ik|\mathbf{y}|}}{4\pi|\mathbf{y}|} \boldsymbol{\alpha} \mathbf{A}(\mathbf{x} - \mathbf{y}) e^{-iy \cdot \mathbf{k}} d^3 y (-H_0 \pm E_k) \phi_0^\pm(\mathbf{k}, \mathbf{x}) = \\ &= \int \frac{e^{ik|\mathbf{y}|}}{4\pi|\mathbf{y}|} (-i \boldsymbol{\alpha} \nabla \boldsymbol{\alpha} \mathbf{A}(\mathbf{x} - \mathbf{y})) e^{-iy \cdot \mathbf{k}} d^3 y \phi_0^\pm(\mathbf{k}, \mathbf{x}) \\ &\quad + 2 \int \frac{e^{ik|\mathbf{y}|}}{4\pi|\mathbf{y}|} \mathbf{k} \cdot \mathbf{A}(\mathbf{x} - \mathbf{y}) e^{-iy \cdot \mathbf{k}} d^3 y \phi_0^\pm(\mathbf{k}, \mathbf{x}), \end{aligned}$$

where we used $(H_0 \mp E_k) \phi_0^\pm(\mathbf{k}, \mathbf{x}) = 0$ and $\nabla \phi_0^\pm(\mathbf{k}, \mathbf{x}) = i \mathbf{k} \phi_0^\pm(\mathbf{k}, \mathbf{x})$. First, we will prove the desired k -dependency for second term as it is of leading order in \mathbf{k} . We choose the coordinate system of the integral such that \mathbf{k} is in the z -direction,

$$\int \frac{e^{ik|\mathbf{y}|}}{4\pi|\mathbf{y}|} \mathbf{k} \cdot \mathbf{A}(\mathbf{x} - \mathbf{y}) e^{-iy \cdot \mathbf{k}} d^3 y = \sum_{i=1}^3 k_i \int \frac{e^{ik(|y|-y_3)}}{4\pi|\mathbf{y}|} A_i(\mathbf{x} - \mathbf{y}) d^3 y.$$

Note that in polar coordinates we have

$$\frac{-i|\mathbf{y}|}{k} \frac{d}{d\rho} e^{ik(|y|-y_3)} = e^{ik(|y|-y_3)}$$

and

$$\frac{d}{d\rho} = \frac{\partial y_1}{\partial \rho} \frac{\partial}{\partial y_1} + \frac{\partial y_2}{\partial \rho} \frac{\partial}{\partial y_2} + \frac{\partial y_3}{\partial \rho} \frac{\partial}{\partial y_3} = \frac{y_1}{\rho} \frac{\partial}{\partial y_1} + \frac{y_2}{\rho} \frac{\partial}{\partial y_2}.$$

This gives

$$\begin{aligned} \sum_{i=1}^3 k_i \int \frac{e^{ik(|y|-y_3)}}{4\pi|y|} A_i(\mathbf{x}-\mathbf{y}) d^3y &= \frac{-i}{4\pi} \sum_{i=1}^3 \frac{k_i}{k} \int \frac{d}{d\rho} e^{ik(|y|-y_3)} \frac{A_i(\mathbf{x}-\mathbf{y})}{\rho} d^3y = \\ &= \frac{-i}{4\pi} \sum_{i=1}^3 \frac{k_i}{k} \int \left(\frac{\partial}{\partial y_1} e^{ik(|y|-y_3)} \right) \frac{y_1}{\rho^2} A_i(\mathbf{x}-\mathbf{y}) + \left(\frac{\partial}{\partial y_2} e^{ik(|y|-y_3)} \right) \frac{y_2}{\rho^2} A_i(\mathbf{x}-\mathbf{y}) d^3y. \end{aligned}$$

Integration by parts using the compact support of the A -field yields

$$\begin{aligned} \sum_{i=1}^3 \frac{k_i}{k} \int \frac{e^{ik(|y|-y_3)}}{4\pi|y|} A_i(\mathbf{x}-\mathbf{y}) d^3y &= \\ &= \frac{i}{4\pi} \sum_{i=1}^3 \frac{k_i}{k} \int e^{ik(|y|-y_3)} \frac{\partial}{\partial y_1} \frac{y_1}{\rho^2} A_i(\mathbf{x}-\mathbf{y}) + e^{ik(|y|-y_3)} \frac{\partial}{\partial y_2} \frac{y_2}{\rho^2} A_i(\mathbf{x}-\mathbf{y}) d^3y = \\ &= \frac{i}{4\pi} \sum_{i=1}^3 \frac{k_i}{k} \int e^{ik(|y|-y_3)} \frac{1}{\rho} \left(\frac{y_1}{\rho} \frac{\partial}{\partial y_1} + \frac{y_2}{\rho} \frac{\partial}{\partial y_2} \right) A_i(\mathbf{x}-\mathbf{y}) d^3y \\ &\quad + \frac{i}{4\pi} \sum_{i=1}^3 \frac{k_i}{k} \int e^{ik(|y|-y_3)} \left(\frac{2}{\rho^2} - 2 \frac{y_1^2 + y_2^2}{\rho^4} \right) A_i(\mathbf{x}-\mathbf{y}) d^3y = \\ &= \frac{i}{4\pi} \sum_{i=1}^3 \frac{k_i}{k} \int e^{ik(\sqrt{z^2+\rho^2}-z)} \frac{d}{d\rho} A_i(x_3-z, \phi_x, \phi, \rho_x, \rho) d\rho d\phi dz, \end{aligned}$$

where we switched to polar coordinates in the last step. Substituting ρ with $\rho|z|$ yields.

$$\begin{aligned} \sum_{i=1}^3 \frac{k_i}{k} \int \frac{e^{ik(|y|-y_3)}}{4\pi|y|} A_i(\mathbf{x}-\mathbf{y}) d^3y &= \\ &= \frac{i}{4\pi} \sum_{i=1}^3 \frac{k_i}{k} \int_{-\infty}^{\infty} \int_0^{\infty} \int_0^{2\pi} e^{ik(|z|\sqrt{1+\rho^2}-z)} \left(\frac{d}{d\rho} A_i(x_3-z, \phi_x, \phi, \rho_x, \bar{\rho}) \right) \Big|_{\bar{\rho}=\rho|z|} |z| d\rho d\phi dz. \end{aligned}$$

For $\rho \neq 0$ and z on the positive axis we can use the oscillatory behavior to show that the integral

vanishes for large k . Let $\alpha, \beta > 0$

$$\begin{aligned}
& \int_{k^{-\beta}}^{\infty} \int_{k^{-\alpha}}^{\infty} e^{ikz(\sqrt{1+\rho^2}-1)} \left(\frac{d}{d\rho} A_i(x_3 - z, \phi_x, \phi, \rho_x, \bar{\rho}) \right) \Big|_{\bar{\rho}=\rho z} z dz d\rho = \\
&= \frac{-i}{k} \int_{k^{-\beta}}^{\infty} \int_{k^{-\alpha}}^{\infty} \left(\frac{d}{dz} e^{ik(z\sqrt{1+\rho^2}-1)} \right) \frac{1}{\sqrt{1+\rho^2}-1} \left(z \frac{d}{d\rho} A_i(x_3 - z, \phi_x, \phi, \rho_x, \bar{\rho}) \right) \Big|_{\bar{\rho}=\rho z} dz d\rho = \\
&= \frac{i}{k} \int_{k^{-\beta}}^{\infty} \int_{k^{-\alpha}}^{\infty} e^{ik(z\sqrt{1+\rho^2}-1)} \frac{1}{\sqrt{1+\rho^2}-1} \frac{d}{dz} \left(z \frac{d}{d\rho} A_i(x_3 - z, \phi_x, \phi, \rho_x, \bar{\rho}) \right) \Big|_{\bar{\rho}=\rho z} dz d\rho = \\
&= \frac{i}{k} \int_{k^{-\beta}}^{\infty} \int_{zk^{-\alpha}}^{\infty} e^{ik(z\sqrt{1+\rho^2}-1)} \frac{1}{\sqrt{z^2+\rho^2}-z} \frac{d}{dz} z \frac{d}{d\rho} A_i(x_3 - z, \phi_x, \phi, \rho_x, \rho) dz d\rho = \\
&= \frac{i}{k} \int_{k^{-\beta}}^{\infty} \int_{zk^{-\alpha}}^{\infty} e^{ik(z\sqrt{1+\rho^2}-1)} \frac{1}{\sqrt{z^2+\rho^2}-z} \frac{d}{d\rho} A_i(x_3 - z, \phi_x, \phi, \rho_x, \rho) dz d\rho \\
&\quad + \frac{i}{k} \int_{k^{-\beta}}^{\infty} \int_{zk^{-\alpha}}^{\infty} e^{ik(z\sqrt{1+\rho^2}-1)} \frac{z}{\sqrt{z^2+\rho^2}-z} \frac{d}{dz} \frac{d}{d\rho} A_i(x_3 - z, \phi_x, \phi, \rho_x, \rho) dz d\rho
\end{aligned}$$

where we integrated by parts in the z variable and substituted back for ρ . We estimate the first term to be smaller than

$$\begin{aligned}
& \left| \frac{i}{k} \int_{k^{-\beta}}^{\infty} \int_{zk^{-\alpha}}^{\infty} e^{ik(z\sqrt{1+\rho^2}-1)} \frac{1}{\sqrt{z^2+\rho^2}-z} \frac{d}{d\rho} A_i(z_x - z, \phi_x, \phi, \rho_x, \rho) dz d\rho \right| \leq \\
& \leq \frac{1}{k^{1-\beta-\alpha}} \frac{1}{\sqrt{1+k^{-2\alpha}}-1} \int_0^{\infty} \int_0^{\infty} \left| \frac{d}{d\rho} A_i(z_x - z, \phi_x, \phi, \rho_x, \rho) \right| dz \rho d\rho.
\end{aligned}$$

For the second term we find

$$\begin{aligned}
& \left| \frac{i}{k} \int_{k^{-\beta}}^{\infty} \int_{zk^{-\alpha}}^{\infty} e^{ik(z\sqrt{1+\rho^2}-1)} \frac{z}{\sqrt{z^2+\rho^2}-z} \frac{d}{dz} \frac{d}{d\rho} A_i(x_3 - z, \phi_x, \phi, \rho_x, \rho) dz d\rho \right| \leq \\
& \leq \frac{1}{k^{1-\alpha}} \frac{1}{\sqrt{1+k^{-2\alpha}}-1} \int_{k^{-\beta}}^{\infty} \int_{zk^{-\alpha}}^{\infty} \left| \frac{d}{dz} \frac{d}{d\rho} A_i(x_3 - z, \phi_x, \phi, \rho_x, \rho) \right| dz \rho d\rho.
\end{aligned}$$

The integral close to $\rho = 0$ can be estimated by its volume

$$\begin{aligned}
& \left| \int_0^{\infty} \int_0^{k^{-\alpha}} e^{ikz(\sqrt{1+\rho^2}-1)} \left(\frac{d}{d\rho} A_i(z_x - z, \phi_x, \phi, \rho_x, \bar{\rho}) \right) \Big|_{\bar{\rho}=\rho z} z dz d\rho \right| \leq \\
& \leq k^{-\alpha} \int_0^{\infty} \max_{\rho} \left| z \frac{d}{d\rho} A_i(z_x - z, \phi_x, \phi, \rho_x, \rho) \right| dz
\end{aligned}$$

and similarly for z ,

$$\left| \int_0^{k^{-\beta}} \int_0^\infty e^{ikz(\sqrt{1+\rho^2}-1)} \left(\frac{d}{d\rho} A_i(z_x - z, \phi_x, \phi, \rho_x, \bar{\rho}) \right) \Big|_{\bar{\rho}=\rho z} z dz d\rho \right| \leq \\ \leq k^{-\beta} \int_0^\infty \max_z \left| z \frac{d}{d\rho} A_i(z_x - z, \phi_x, \phi, \rho_x, \rho) \right| d\rho.$$

For the negative z -axis there is no singularity in ρ . Hence, an integration by parts as performed above yields that this term is proportional to $\frac{1}{k}$. Choosing $\alpha = \beta = \frac{1}{5}$ we find

$$\left| \int \frac{e^{ik(|y|-y_3)}}{4\pi|y|} \mathbf{k} \cdot \mathbf{A}(\mathbf{x} - \mathbf{y}) d^3y \right| \leq \frac{C}{k^{\frac{1}{5}}},$$

and C can be bounded according to the derivation above with

$$\sum_{i=1,\dots,3} \left(\sum_{x,y} \| \mathbf{D}_{x,y}^2 A_i \|_{L^1} + \left\| \frac{1}{\rho} \sup_z |z \partial_\rho A_i| \right\|_{L^1(\rho, \phi)} + \left\| \sup_\rho |z \partial_\rho A_i| \right\|_{L^1(z, \phi)} \right).$$

Every function $f \in C^{2,1}(\mathbb{R}^3 \rightarrow \mathbb{R}^3)$ can be approximated by a C_0^∞ function and the Sobolev norm. Furthermore, every continuous function which goes to zero at infinity can also be approximated by C_0^∞ functions with the infinity norm. Combining this with continuity and decay we see that every potential which fulfills the prerequisites of Theorem 3.3 and is furthermore in $C^{2,1}$ can be approximated in the norm above by C_0^∞ functions. Hence, we have for all such potentials that $\|T_k[\underline{\phi}_0(\mathbf{k}, \cdot)]\|_{\mathcal{B}}$ vanishes for $k \rightarrow \infty$.

Now, similar as in [Teu99] we also have that $\|T_k^2\| \rightarrow 0$ for $k \rightarrow \infty$. Hence, the Neumann series of $(\text{id}_{\mathcal{B}} - T_k^2)^{-1}$ exists and is uniformly bounded for k large enough. Therefore, we conclude

$$\|f_k\|_{\mathcal{B}} = \left\| \frac{1}{\text{id}_{\mathcal{B}} - T_k} T_k[\underline{\phi}_0(\mathbf{k}, \cdot)] \right\|_{\mathcal{B}} = \left\| \frac{1}{\text{id}_{\mathcal{B}} - T_k^2} \left(T_k[\underline{\phi}_0(\mathbf{k}, \cdot)] + T_k^2[\underline{\phi}_0(\mathbf{k}, \cdot)] \right) \right\|_{\mathcal{B}} \leq \\ \leq \left\| \frac{1}{1 - T_k^2} \right\| \left(\|T_k[\underline{\phi}_0(\mathbf{k}, \cdot)]\|_{\mathcal{B}} + \|T_k^2\| \right) \rightarrow 0$$

for $k \rightarrow \infty$. □

It remains to show that the generalized eigenfunctions are bounded in vicinity of the origin. For this purpose it suffices to prove the existence of eigenfunctions for $\mathbf{k} = 0$. By the same argument as in the proof of Theorem 3.3 we then obtain that f_k is continuous for all \mathbf{k} . Hence, the generalized eigenfunctions are in particular bounded in \mathbf{k} for any compact subset D containing the origin. In the Schrödinger case, singular behavior at the origin occurs if a zero energy eigenstate or a zero resonance is present (see [Teu99], [JK79]). The zero resonances can be understood as eigenstates

to zero kinetic energy in a slightly enlarged space, namely the weighted space L^2_γ which is defined as

$$L^2_\gamma(\mathbb{R}^3 \rightarrow \mathbb{C}^4) = \left\{ f \mid (1 + |\mathbf{x}|^2)^{-\frac{\gamma}{2}} f(\mathbf{x}) \in L^2(\mathbb{R}^3 \rightarrow \mathbb{C}^4) \right\}$$

for some $\gamma > 0$. Hence, to avoid singular behavior at the spectral edge for the Dirac operator we exclude eigenstates on such a space.

Proposition 3.5. *Let the \mathbf{A} -field fulfill the prerequisites of Theorem 3.3 and Lemma 3.4 and let it be such that there are no eigenstates for zero kinetic energy of the extended Dirac operator to the space $L^2_{1/2+\varepsilon}(\mathbb{R}^3 \rightarrow \mathbb{C}^4)$ for some $\varepsilon > 0$. Then, the generalized eigenfunctions exist for all $(\mathbf{x}, \mathbf{k}) \in \mathbb{R}^3 \times \mathbb{R}^3$ and are uniformly bounded.*

Proof. Let $f \in \mathcal{B}$ be a solution to $f = T_0[f]$. Then f is also a solution to

$$f = (T_0)^n [f]$$

for any $n \in \mathbb{N}$. Hence, by repeated application of [Ike60, Lemma 3.1] we find that eventually $|f(\mathbf{x})| \leq \frac{C}{|\mathbf{x}|}$ for large $|\mathbf{x}| \rightarrow \infty$. Therefore, we have $f_j \in L^2_{1/2+\varepsilon}$ for any $\varepsilon > 0$ where f_j denotes the j -th column of the matrix valued function f . Similar to Theorem 3.3 and because of Lemma 1.1, we note that if f is a solution to $f = T_0[f]$ it is also a solution to the Dirac equation

$$H f_j(\mathbf{x}) = \pm f_j(\mathbf{x})$$

with the extended Dirac operator and $+$ for $j = 1, 2$ and $-$ for $j = 3, 4$. But by assumption there is an $\varepsilon > 0$ such that there are no eigenstates of the extended Dirac operator in $L^2_{1/2+\varepsilon}$ for zero kinetic energy. We conclude that $f = 0$. Hence, the Fredholm alternative shows that $\text{id} - T_0$ is invertible and there exists a unique solution $\underline{\phi}(\mathbf{x}, \mathbf{0}) \in \mathcal{B}$ to the Dirac equation. The continuity argument of Theorem 3.3 extends now also to $\mathbf{k} = 0$ and the uniform boundedness then follows from Lemma 3.4. \square

3.3. Generalized Fourier transform

Given the existence and boundedness of the generalized eigenfunctions we can return to our initial idea and expand wave functions into generalized eigenfunctions via the map \mathcal{F} , which we call *generalized Fourier transform*.

Definition and Theorem 3.6. *Let the \mathbf{A} -field fulfill the prerequisites of Theorem 3.3 and Proposition 3.5. We then have:*

i) *Let $\psi \in L^2(\mathbb{R}^3 \rightarrow \mathbb{C}^4)$. The generalized Fourier transform¹*

$$\mathcal{F}[\psi](\mathbf{k}) := \text{l.i.m.} \int_{\mathbb{R}^3} \underline{\phi}^\dagger(\mathbf{k}, \mathbf{x}) \psi(\mathbf{x}) d^3x$$

of ψ exists and is again in $L^2(\mathbb{R}^3 \rightarrow \mathbb{C}^4)$.

¹l.i.m. means $\lim_{R \rightarrow \infty} \int_{B(R,0)}$ in the L^2 -norm and stands for “limit in mean”. In the subsequent sections we will usually suppress it.

ii) Let $\widehat{\psi} \in L^2(\mathbb{R}^3 \rightarrow \mathbb{C}^4)$. The inverse generalized Fourier transform

$$\mathcal{F}^{-1}[\widehat{\psi}](\mathbf{x}) := \text{l.i.m.} \int_{\mathbb{R}^3} \underline{\phi}(\mathbf{x}, \mathbf{k}) \widehat{\psi}(\mathbf{k}) d^3k$$

of $\widehat{\psi}$ exists and we have $\mathcal{F}^{-1}[\widehat{\psi}] \in L^2(\mathbb{R}^3 \rightarrow \mathbb{C}^4)$.

iii) The generalized Fourier transform is unitary.

iv) For $\psi, \widehat{\psi} \in L^2(\mathbb{R}^3 \rightarrow \mathbb{C}^4)$ we have

$$\begin{aligned} \psi &= \mathcal{F}^{-1}[\mathcal{F}[\psi]] \\ \widehat{\psi} &= \mathcal{F}[\mathcal{F}^{-1}[\widehat{\psi}]]. \end{aligned}$$

v) Let $\psi \in \mathcal{D}(H)$, then

$$\mathcal{F}[H\psi](\mathbf{k}) = \underline{E}_k \mathcal{F}[\psi](\mathbf{k}).$$

vi) H has only an absolute continuous spectrum.

Remark. According to general conventions we call the usual Hilbert space “position space”, denoted by \mathcal{H} and the generalized Fourier transform thereof “momentum space”, denoted by \mathcal{FH} . If the external field is time-dependent so are the generalized eigenfunctions and the Fourier transform. We will denote this with a subscript t .

Proof. We start by showing that there are no eigenvalues in the mass gap under the conditions of Theorem 3.3 on the external field. Note to this end that on $C_0^\infty(\mathbb{R}^3 \rightarrow \mathbb{C}^4)$ we have

$$\begin{aligned} H_t^2 &= \alpha_k \alpha_l (-i\partial_k - A_k) (-i\partial_l - A_l) + \beta^2 + \{\alpha_k, \beta\} (-i\partial_k - A_k) \\ &= \alpha_k \alpha_l (-\partial_k \partial_l + A_k A_l + i(\partial_k A_l + A_k \partial_l)) + 1 \\ &= -\Delta + \mathbf{A}^2 + i\alpha_k \alpha_l (\partial_k A_l + A_k \partial_l) + 1 \\ &= -\Delta + \mathbf{A}^2 + i(\nabla \cdot \mathbf{A} + \mathbf{A} \cdot \nabla) - \gamma_5 \alpha_k ([\nabla \times \mathbf{A}]_k + [\mathbf{A} \times \nabla]_k) + 1 \end{aligned}$$

where we applied the identity $\alpha_k \alpha_l = (\delta_{kl} + i\gamma_5 \alpha_n \varepsilon_{kln})$ in the last step and with the definition of

$$\gamma_5 = -i\alpha_1 \alpha_2 \alpha_3 = \begin{pmatrix} 0 & \mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix}$$

in standard representation. Using the identity $\nabla \times (\mathbf{A}\psi) + \mathbf{A} \times (\nabla\psi) = (\text{curl } \mathbf{A})\psi$ from vector calculus we get

$$\begin{aligned} H_t^2 &= (-i\nabla - \mathbf{A}(\mathbf{x}, t))^2 - \gamma_5 \alpha_k (\text{curl } \mathbf{A}(\mathbf{x}, t))_k + 1 \\ &= (-i\nabla - \mathbf{A}(\mathbf{x}, t))^2 - \gamma_5 \boldsymbol{\alpha} \mathbf{B}(\mathbf{x}, t) + 1 \end{aligned}$$

with the magnetic field strength $\mathbf{B}(\mathbf{x}, t) = \text{curl } \mathbf{A}(\mathbf{x}, t)$. This is nothing else than the Pauli hamiltonian H_p plus one. The Pauli hamiltonian is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3 \rightarrow \mathbb{C}^4)$ under the conditions of Theorem 3.3 on the external field. This can be seen as follows. If the vector potential is continuously differentiable then the magnetic Schrödinger hamiltonian, $(-i\nabla - \mathbf{A}(\mathbf{x}, t))^2$, is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3 \rightarrow \mathbb{C}^4)$ (see [Hun79]). The condition on the derivative of the vector potential ensures that the symmetric operator of multiplication, $\gamma_5 \boldsymbol{\alpha} \mathbf{B}(\mathbf{x}, t)$, is a bounded operator. Hence, the Pauli hamiltonian is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3 \rightarrow \mathbb{C}^4)$ and the equality above extends for the whole domain

$$H_t^2 = H_p + 1.$$

Now, repeat the derivation above with the massless Dirac hamiltonian and use the same argument concerning self-adjointness again. This shows that the Pauli hamiltonian is also the same as the square of the massless Dirac operator in the case of a vanishing electrical field. Therefore, we find

$$H_t^2 = H_{m=0}^2 + 1.$$

By using the Borel functional calculus for unbounded functions (see [DS63, Thm XII.2.9]) we conclude that

$$\sigma(H_t)^2 = \sigma(H_{m=0})^2 + 1.$$

And as $\sigma(H_{m=0}) \in \mathbb{R}$ we have in particular $\sigma(H_t) \subset (-\infty, -1] \cup [1, \infty)$. We also note that due to Corollary 2.8 there are no embedded eigenvalues in the continuous spectrum and possible eigenvalues can only appear at the edge of the mass gap with $\lambda = \pm 1$. The prerequisites of Proposition 3.5 forbid such a case. Hence, the point spectrum is empty.

We can now essentially adopt the results from [Eck74] if we note the following. First, it is easily seen that the \mathbf{A} -field fulfills the prerequisites there, either directly because it is bounded and vanishes at infinity or by the computations carried out for the proof of Lemma 3.2. Under the conditions of Proposition 3.5 we know that the eigenfunctions exist for all $k \geq 0$ which means that the set Z in [Eck74, Theorem 1] is empty. Combining the nonexistence of the point spectrum with [Eck74, Theorem 1,b)] then yields $\sigma(H) \cap \sigma_{sing}(H) = \sigma_{ess}(H) \cap \sigma_{sing}(H) = \emptyset$. Hence, there is also no singular continuous spectrum and we have $\sigma(H) = \sigma_{a.c.}(H)$. This leads to the conclusion that $P_{a.c.}$, the projection onto the absolute continuous subspace, is the identity. This observation together with [Eck74, Theorem 1, d)] proves i) and shows that \mathcal{F} is an isometry. In [Eck74, Section 6] we find that \mathcal{F} is onto which then finishes iii). Our definition of the inverse generalized Fourier transform coincides with the adjoint of \mathcal{F} given in [Eck74, Section 6] if one reminds oneself that Z is empty. Thus, ii) is true and together with iii) we see \mathcal{F}^{-1} is indeed the inverse map of \mathcal{F} . Finally, part v) is a direct consequence of [Eck74, Theorem 1, d)] together with \mathcal{F} being unitary and $P_{a.c.} = \text{id}_{\mathcal{H}}$.

□

4. Negative energies and the Dirac sea

We already mentioned the existence of negative energy solutions to the Dirac equation in Chapter 1 and explained why they cannot be simply rejected as unphysical like in classical relativistic mechanics. Hence, we have to include them in the physical and mathematical discussion of the Dirac theory. We start off by identifying the parts of the Hilbert space which correspond to negative and positive energy states.

4.1. Spectral projections and subspaces

The definition of the spectral subspaces is very natural and straightforward in momentum space where the upper two components of any state $\widehat{\psi}$ correspond to positive energies and the lower ones to negative energies¹. Thus, to ensure the existence of an appropriate Fourier transform we assume the external field to fulfill the following condition.

Condition C. *Let the external field \mathbb{A}_t be such that there exists a generalized Fourier transform with the properties in Theorem 3.6.*

Now, observe the following properties of the bounded operators on momentum space given by $\widehat{P}^\pm = \frac{1}{2}(1 \pm \beta)$, with β from the Dirac matrices, which are easy to verify

$$\widehat{P}^\pm \widehat{P}^\pm = \widehat{P}^\pm, \quad \widehat{P}^\pm = (\widehat{P}^\pm)^\dagger.$$

They are thus orthogonal projections on the Hilbert space \mathcal{FH} (see e.g. [RS80, Chapter VI.2]). The corresponding projections on position space are then simply

$$P^\pm = \mathcal{F}^{-1} \widehat{P}^\pm \mathcal{F}.$$

It is then also trivial to verify that

$$P^\pm P^\mp = 0, \quad P^+ + P^- = \text{id}_{\mathcal{H}},$$

and therefore $P^+ \mathcal{H} \oplus P^- \mathcal{H}$ is a complete orthogonal decomposition of \mathcal{H} . Finally, due to Condition C we know that the hamiltonian is diagonal in \mathcal{FH} and due to the unitarity of the generalized Fourier transform, we get

$$\langle \psi, H \psi \rangle = \langle \mathcal{F} \psi, \mathcal{F} H \mathcal{F}^{-1} \mathcal{F} \psi \rangle = \langle \widehat{\psi}, \underline{E}_k \widehat{\psi} \rangle. \quad (4.1)$$

¹The upper two components are the amplitudes of the positive eigenfunction solutions in the eigenfunction expansion and similar for the lower components.

For $\psi \in \mathcal{H}^+ = P^+ \mathcal{H}$ we have $\widehat{\psi} \in \widehat{P}^+ \mathcal{F}\mathcal{H}$ and due to $\underline{E}_k \widehat{P}^\pm = E_k \beta \widehat{P}^\pm = \pm E_k \widehat{P}^\pm$ we find that eq. (4.1) is non-negative. Similarly, the negative counterpart holds for \mathcal{H}^- and thus, \mathcal{H}^\pm are the subspaces connected to the positive and negative part of the spectrum.

It is now easy to define the absolute value of the hamiltonian via the spectral subspaces, which is simply the hamiltonian on the positive subspace and the negative hamiltonian on the negative energy subspace,

$$|H| = H (P^+ - P^-) = H \operatorname{sgn} H . \quad (4.2)$$

For any $\psi \in \mathcal{H}$ we have

$$\begin{aligned} \mathcal{F}[|H| \psi](\mathbf{k}) &= \mathcal{F}[|H| (P^+ + P^-) \psi](\mathbf{k}) = \mathcal{F}[H (P^+ - P^-) \psi](\mathbf{k}) = \\ &= \underline{E}_k \mathcal{F}[(P^+ - P^-) \psi](\mathbf{k}) = \underline{E}_k (\widehat{P}^+ - \widehat{P}^-) \mathcal{F}[\psi](\mathbf{k}) = E_k \mathcal{F}[\psi](\mathbf{k}) . \end{aligned} \quad (4.3)$$

In momentum space it is now also clear that the spectrum of $|H|$ reduces to the positive part of the spectrum of the Dirac hamiltonian. Note finally, if the external field is time-dependent, so is the generalized Fourier transform and hence the spectral projections and the subspaces. We denote this by adding a subscript t to the entities when necessary.

4.2. Dirac sea

Dirac [Dir30] himself proposed a heuristic solution in 1930 to the dilemma of negative energies. He suggested that all the states belonging to the negative part of the spectrum are already occupied by electrons. Thus, a positive energy electron cannot fall down due to the Pauli exclusion principle and the vacuum as we perceive it is not empty but rather filled with infinitely many particles. This idea might seem absurd at first glance but has striking consequences. It obviously raises the question why we do not see this so called Dirac sea. While this is not completely true as we will explain in a second, there are two things one should be concerned about. This model results in an infinite energy density and infinite charge density and we have to see how to deal with them. Due to the Pauli principle and the electromagnetic repulsion the electrons in the sea are spread out in a very homogeneous way. Hence, a positive energy test particle feels a net force of zero and acts like a free particle². Regarding the infinite energy density we note that it is the energy differences that matter in physics, not the total energy. Hence, the total energy of the vacuum is irrelevant. Only deviations thereof matter³. Mathematically speaking, these quantities can be renormalized away. Though this might seem unsatisfactory at the beginning, the presence of the Dirac sea leads to a whole branch of new phenomena. Most striking is probably the prediction of pair creation which one can expect if a negative energy electron absorbs e.g. a photon with

²There is no rigorous proof of that for the Dirac equation. A first attempt with non-relativistic Fermions can be found in [JMPP17] which shows that this topic is actually more subtle than explained here.

³Note, that this only true in a non-gravitational context. Hence, the vacuum energy has to be taken into account if one wants incorporate gravitation. This is indeed one of the big puzzles in modern day physics.

energy $\geq 2mc^2$ and is lifted to the positive energy subspace. It should thus be visible now as a free electron. But not only the electron, also the missing charge in the sea should be detectable as a deviation from the filled sea which we assume to be the equilibrium - as a particle with the same mass as the electron, but of opposite charge. The positron was then discovered two years after the proposal of the Dirac sea.

One should pause here for a moment and think about this achievement. The sole search for a quantum mechanical wave equation which obeys special relativity together with the fundamental physical principal that any system strives towards its lowest state of energy has lead us directly to a many body theory, predicting the antiparticle of the electron. It provides us for the first time with a non trivial model for the vacuum and opens up a bag of completely new physical effects, most of which have been confirmed to an incredible precision up to this day. Surely, one of the great triumphs of physics.

The only drawback to this model is that there is no good interpretation of the Dirac equation as a one particle equation anymore. Even though it is believed to describe the behavior of an electron correctly in certain situations like the Hydrogen atom we need the Dirac sea to give a coherent physical interpretation. The modern view replaced the Dirac sea by QED which is based on the construction of a Fock space instead of the Dirac sea. This concept will be introduced in Chapter 7.2. The reasons why the idea of the Dirac sea seemed to be abandoned over the course of time are likely its heuristic character and lack of mathematical rigor as well as the inelegance of the infinitely many particle presumption in favor of a finitely many particle theory which QED is. Nevertheless, it should be mentioned that it is indeed possible to construct a mathematical rigorous model of the Dirac sea as was done by Deckert et al. [DDMS10]. Furthermore, QED contains not more physical insight⁴ than the Dirac sea picture. It is rather derived from it by a mathematical transformation. Hence, the same problems which come from the presence of infinitely many particles in the Dirac sea picture are still present in QED but swept under the rug. In the context of external fields the two models are mathematically equivalent, and as the Dirac sea provides one with a nice intuition we will refer to it frequently in the remainder of this work which is not unusual in the discussion of strong field QED, see e.g. [GMR85].

We finish this chapter with the mathematical connection between negative energy states and positive energy states with positive charge and introduce thereby the concept of *charge conjugation*. We have for all $\psi^+ \in P^+ \mathcal{D}(H)$ that

$$\langle \psi^+, H \psi^+ \rangle = \langle \widehat{\psi}^+, \underline{E}_k \widehat{\psi}^+ \rangle = \langle \widehat{\psi}^+, E_k \widehat{\psi}^+ \rangle \geq 1$$

and similarly for all $\psi^- \in P^- \mathcal{D}(H)$

$$\langle \psi^-, H \psi^- \rangle = \langle \widehat{\psi}^-, \underline{E}_k \widehat{\psi}^- \rangle = -\langle \widehat{\psi}^-, E_k \widehat{\psi}^- \rangle \leq -1.$$

Now, define

$$H^C = -CHC^{-1}$$

⁴At least the external field model of QED. While it is true that there is no rigorous mathematical Dirac sea model with interaction also QED with interaction can not be considered to be a rigorous mathematical theory.

with C being some anti-unitary operator. We then have

$$\langle C\psi^-, H^C C\psi^- \rangle = -\langle C\psi^-, C H \psi^- \rangle = -\langle H \psi^-, \psi^- \rangle \geq 1.$$

Hence, H^C is bounded from below on $C\mathcal{H}^-$. Furthermore, let $\psi(t)$ be a solution to the Dirac equation with external field. We then have

$$i \frac{\partial}{\partial t} C\psi(t) = -C i \frac{\partial}{\partial t} \psi(t) = -C H \psi(t) = H^C C\psi(t).$$

Therefore, by an anti-unitary transformation we can transform the space of negative energies into one of positive energies. For the anti-unitary transformation $C\psi = U_C \bar{\psi}$ where U_C is some unitary 4×4 matrix⁵ fulfilling $\beta U_C = -U_C \bar{\beta}$ and $\alpha_i U_C = U_C \bar{\alpha}_i$ we find a particular nice interpretation of H^C . Let $\psi \in C_0^\infty(\mathbb{R}^3 \rightarrow \mathbb{C}^4)$. We then have

$$\begin{aligned} H^C \psi &= -C H C^{-1} \psi = -\overline{U_C (-i\boldsymbol{\alpha}\nabla + \beta - \boldsymbol{\alpha}\mathbf{A}(\mathbf{x}) + \phi(\mathbf{x})) U_C^\dagger} \psi = \\ &= (-i\boldsymbol{\alpha}\nabla + \beta + \boldsymbol{\alpha}\mathbf{A}(\mathbf{x}) - \phi(\mathbf{x})) \psi = (H_0 - \mathcal{A}) \psi. \end{aligned}$$

This relation then also holds for all ψ in the domain of H . Looking back at Section 1.1 we remember that the sign in front of the external field corresponds to the charge. Hence, H^C describes a particle in an external field⁶ with an opposite charge to the electron but otherwise exactly the same behavior (governed by the Dirac equation). This particular choice for the operator C is therefore called *charge conjugation*.

⁵In the standard representation we use throughout this work, take $U_C = i\beta\alpha_2$.

⁶If there is no external field, then there is no way to distinguish particles with different charge as they have the same mass.

5. Commutator relations

After having covered the Dirac equation with external potential and related topics we will now discuss commutator relations of the following type which frequently appear in the proof of the adiabatic theorem,

$$[H_t, A] = B,$$

where H_t is the Dirac hamiltonian with time-dependent magnetic potential and A and B are bounded operators such that the commutator is well defined. We will see that most of the time only the off-diagonal parts, $P_t^\pm A P_t^\mp$, are of real interest. For these, the above equation turns into an anti-commutator relation

$$\{ |H_t|, P_t^\pm A P_t^\mp \} = \pm P_t^\pm B P_t^\mp.$$

We will see that it is important for us to be able to solve such operator equations for A given a specific B . As $|H_t|$ is invertible but does not commute with A , it is a priori not clear how to achieve this. Therefore, this section is devoted to develop a method to unravel such relations which is the main content of Theorem 5.2. The subsequent proofs are done in the momentum space, hence the external field has to be such that the generalized Fourier transform exists.

Condition D. *Let the external field A_t be such that there exists a generalized Fourier transform with the properties in Theorem 3.6.*

We already noted in the preceding chapter that the spectrum of the absolute value of the hamiltonian is non-negative. Hence, the resolvent, which we write as

$$\frac{1}{|H_t| - z},$$

is defined for all negative real numbers. In particular also for $z = -1$ which we need in the following lemma.

Lemma 5.1. *Let the external field fulfill Condition D. The operator*

$$R_t(n) = \frac{1}{(|H_t| + 1)} \left((|H_t| - 1) \frac{1}{(|H_t| + 1)} \right)^n$$

is bounded on \mathcal{H} for all $n \in \mathbb{N}$ with norm $\frac{1}{2^{n+1}} \left(\frac{n}{n+1} \right)^n$.

Remark. This formula holds also for the case $n = 0$ with the convention $0^0 = 1$.

Proof. First note, that the resolvent maps into the domain of the Hamiltonian, hence the operator is defined on all of \mathcal{H} and maps into the domain of the hamiltonian again. Furthermore, we have that $\frac{(E_k-1)^n}{(E_k+1)^{n+1}}$ has a maximum as it is a positive continuous function which tends to zero for $k \rightarrow \infty$ and is equal to zero at $k = 0$. To determine the maximum we differentiate which yields

$$\begin{aligned} \frac{d}{dk} \frac{(E_k-1)^n}{(E_k+1)^{n+1}} &= \frac{n(E_k-1)^{n-1} \frac{d}{dk} E_k}{(E_k+1)^{n+1}} - \frac{(n+1)(E_k-1)^n \frac{d}{dk} E_k}{(E_k+1)^{n+2}} = \\ &= \left(\frac{d}{dk} E_k \right) \frac{(E_k-1)^{n-1}}{(E_k+1)^{n+2}} (n(E_k+1) - (n+1)(E_k-1)) \stackrel{!}{=} 0. \end{aligned}$$

The solutions are given by $k = 0$ and $E_k = 2n + 1$ which implies $k \neq 0$. At $k = 0$ the function obviously has a minimum and it also turns to zero again for $k \rightarrow \infty$. Hence, we get

$$\sup_{k \in \mathbb{R}_0^+} \frac{(E_k-1)^n}{(E_k+1)^{n+1}} = \frac{(2n+1-1)^n}{(2n+1+1)^{n+1}} = \frac{1}{2(n+1)} \left(1 + \frac{1}{n}\right)^{-n} \quad \text{for } n \in \mathbb{N}. \quad (5.1)$$

Because the external field fulfills Condition D there exists a generalized Fourier transform. The operator norm is then easy to determine in momentum space as we have

$$\|R_t(n)\|_{\mathcal{H}} = \|\mathcal{F}R_t(n)\mathcal{F}^{-1}\|_{\mathcal{FH}} = \left\| \frac{(E_k-1)^n}{(E_k+1)^{n+1}} \right\|_{\mathcal{FH}} = \sup_{k \in \mathbb{R}_0^+} \frac{(E_k-1)^n}{(E_k+1)^{n+1}}.$$

The last equality holds because $\frac{(E_k-1)^n}{(E_k+1)^{n+1}}$ acts as an operator of multiplication and is a bounded function for all n . \square

The next lemma solves the anti-commutator relation problem.

Theorem 5.2. *Let $A : \mathcal{H} \rightarrow \mathcal{H}$ be a bounded operator and let the external field fulfill Condition D. We define the operator S_A to be*

$$S_A = 2 \sum_{n=0}^{\infty} R_t(n) A R_t(n). \quad (5.2)$$

It has the following properties:

1. S_A is a bounded operator on $\mathcal{H} \rightarrow \mathcal{H}$. Its norm can be estimated by

$$\|S_A\| \leq \frac{1}{2} \sum_{n=0}^{\infty} \frac{1}{(n+1)^2} \left(\frac{n}{n+1}\right)^{2n} \|A\|.$$

2. S_A is continuous in its operator argument.

3. We have the identity $A = \{ |H_t|, S_A \}$ on the domain of the hamiltonian, i.e. the operator S_B is a solution to the operator equation $\{ |H_t|, A \} = B$ for any bounded operator B and A unknown. This solution is unique in the Banach space of bounded operators.

Proof. 1. It is clear that

$$S_A^N := 2 \sum_{n=0}^N R(n) A R(n)$$

is a bounded operator for all $N \in \mathbb{N}$. The norm can be easily estimated with the help of Lemma 5.1 as we have

$$\|S_A^N\| \leq 2 \sum_{n=0}^N \|R_t(n) A R_t(n)\| \leq 2 \sum_{n=0}^N \|R_t(n)\|^2 \|A\| \leq \frac{1}{2} \sum_{n=0}^N \frac{1}{(n+1)^2} \left(\frac{n}{n+1} \right)^{2n} \|A\|.$$

As this last series obviously converges it is clear that $(S_A^N)_{N \in \mathbb{N}}$ forms a Cauchy-sequence in the Banach space of bounded operators,

$$\|S_A^N - S_A^M\| \leq \frac{1}{2} \sum_{n=M+1}^N \frac{1}{(n+1)^2} \left(\frac{n}{n+1} \right)^{2n} \|A\| \xrightarrow{N, M \rightarrow \infty} 0.$$

Hence, the sequence $(S_A^N)_{N \in \mathbb{N}}$ converges and eq. (5.2) defines a bounded operator on \mathcal{H} . For the norm estimate, use the continuity of the operator norm and perform the limit $N \rightarrow \infty$ in the inequality above.

2. Let $(A_N)_{N \in \mathbb{N}}$ be a sequence of bounded operators with $A_N \rightarrow A$ in operator norm. We have

$$\begin{aligned} \|S_{A_N} - S_A\| &\leq 2 \sum_{n=0}^{\infty} \|R_t(n) (A_N - A) R_t(n)\| \leq \\ &\leq \frac{1}{2} \sum_{n=0}^{\infty} \frac{1}{(n+1)^2} \left(\frac{n}{n+1} \right)^{2n} \|A_N - A\| \xrightarrow{N \rightarrow \infty} 0. \end{aligned}$$

3. The operator S_A maps into the domain of the hamiltonian due to the same property of $R(n)$. Hence, the anticommutator is well defined on the domain. Because the Hamiltonian fulfills Condition D there exists a generalized Fourier transform which diagonalizes H_t according to Theorem 3.6. For every $\psi \in \mathcal{D}(H_t)$ with $\widehat{\psi} = \mathcal{F}_t \psi$ we have

$$\begin{aligned} \mathcal{F}_t \{ |H_t|, S_A \} \mathcal{F}_t^{-1} [\widehat{\psi}] (\mathbf{k}) &= \\ &= E_k \mathcal{F}_t S_A \mathcal{F}_t^{-1} [\widehat{\psi}] (\mathbf{k}) + \mathcal{F}_t S_A \mathcal{F}_t^{-1} [E_{(\cdot)} \widehat{\psi}] (\mathbf{k}) = \\ &= 2 \sum_{n=0}^{\infty} \frac{(E_k - 1)^n}{(E_k + 1)^{n+1}} \left(E_k \widehat{A} \left[\frac{(E_{(\cdot)} - 1)^n}{(E_{(\cdot)} + 1)^{n+1}} \widehat{\psi}(\cdot) \right] (\mathbf{k}) + \widehat{A} \left[E_{(\cdot)} \frac{(E_{(\cdot)} - 1)^n}{(E_{(\cdot)} + 1)^{n+1}} \widehat{\psi}(\cdot) \right] (\mathbf{k}) \right) = \\ &= \lim_{N \rightarrow \infty} \widehat{A} \left[2 \sum_{n=0}^N (E_k + E_{(\cdot)}) \frac{(E_k - 1)^n}{(E_k + 1)^{n+1}} \frac{(E_{(\cdot)} - 1)^n}{(E_{(\cdot)} + 1)^{n+1}} \widehat{\psi}(\cdot) \right] (\mathbf{k}) \end{aligned}$$

where we pulled out the series in the first step as the Fourier transform is continuous and used the linearity of $\widehat{A} = \mathcal{F} A \mathcal{F}^{-1}$ in the last equation (k acts like a fixed parameter for the operator \widehat{A}). Note that by using the formula for the geometric sum we get for all $k \in \mathbb{R}_0^+$

$$\begin{aligned}
& 2 \sum_{n=0}^N (E_k + E_{k'}) \frac{(E_k - 1)^n}{(E_k + 1)^{n+1}} \frac{(E_{k'} - 1)^n}{(E_{k'} + 1)^{n+1}} \widehat{\psi}(\mathbf{k}') = \\
& = 2 \frac{E_k + E_{k'}}{(E_k + 1)(E_{k'} + 1)} \frac{1 - \left(\frac{E_k - 1}{E_k + 1} \frac{E_{k'} - 1}{E_{k'} + 1}\right)^N}{1 - \frac{(E_k - 1)(E_{k'} - 1)}{(E_k + 1)(E_{k'} + 1)}} \widehat{\psi}(\mathbf{k}') = \\
& = \frac{2E_k + 2E_{k'}}{(E_k + 1)(E_{k'} + 1) - (E_k - 1)(E_{k'} - 1)} \left(1 - \left(\frac{E_k - 1}{E_k + 1} \frac{E_{k'} - 1}{E_{k'} + 1}\right)^N\right) \widehat{\psi}(\mathbf{k}') = \\
& = 1 - \left(\frac{E_k - 1}{E_k + 1} \frac{E_{k'} - 1}{E_{k'} + 1}\right)^N \widehat{\psi}(\mathbf{k}').
\end{aligned}$$

This converges to $\widehat{\psi}$ in norm and uniformly in k as we have

$$\left\| \left(\frac{E_k - 1}{E_k + 1} \frac{E_{(\cdot)} - 1}{E_{(\cdot)} + 1} \right)^N \widehat{\psi}(\cdot) \right\|_{\mathcal{FH}} \leq \left\| \left(\frac{E_{(\cdot)} - 1}{E_{(\cdot)} + 1} \right)^N \widehat{\psi}(\cdot) \right\|_{\mathcal{FH}} \xrightarrow{N \rightarrow \infty} 0$$

for every $k \in \mathbb{R}_0^+$. The last step can be seen by the following argument. For every $\varphi \in \mathcal{C}_0^\infty$ we have

$$\left\| \left(\frac{E_{(\cdot)} - 1}{E_{(\cdot)} + 1} \right)^N \varphi(\cdot) \right\|_{\mathcal{FH}} \leq \max_{k \in \text{supp } \varphi} |\varphi(\mathbf{k})| \text{Vol}(\text{supp } \varphi) \max_{k \in \text{supp } \varphi} \left(\frac{E_k - 1}{E_k + 1} \right)^N \xrightarrow{N \rightarrow \infty} 0$$

and by a density argument the convergence also holds true for any $\widehat{\psi} \in L^2$. Therefore, we end up with

$$\mathcal{F}_t \{ |H_t\rangle, S_A \} \mathcal{F}_t^{-1}[\widehat{\psi}] = \mathcal{F}_t A \mathcal{F}_t^{-1}[\widehat{\psi}]$$

which proves the statement. Note furthermore that this also shows

$$A = \{ |H_t\rangle, S_A \} = S_{\{|H_t\rangle, A\}}$$

on the domain of the hamiltonian.

Let the A' be another bounded operator which fulfills $\{ |H_t\rangle, A' \} = B$. We have by using the identity property twice

$$A' = S_{\{|H_t\rangle, A'\}} = S_B = S_{\{|H_t\rangle, A\}} = A.$$

□

This method can now be used to show the existence and explicit form of operators which are defined via commutator relations. We start with the projection and its time derivative.

Proposition 5.3. *Let the external field and its time derivative define a bounded operator of multiplication. The limit of the following expression then exists with respect to the operator norm*

$$\dot{P}_t^\pm := \lim_{h \rightarrow 0} \frac{1}{h} (P_{t+h}^\pm - P_t^\pm)$$

and is given by

$$\dot{P}_t^\pm = \pm S_{\mathbb{A}}^{\text{odd}}$$

where $\dot{\mathbb{A}}_t^{\text{odd}} = P_t^+ \dot{\mathbb{A}}_t P_t^- + P_t^- \dot{\mathbb{A}}_t P_t^+$.

Remark. Note the following properties:

1. \dot{P}_t^\pm is a bounded operator
2. $\dot{P}_t^\pm = P_t^+ \dot{P}_t^\pm P_t^- + P_t^- \dot{P}_t^\pm P_t^+$ is an odd operator.

Proof. As P_t^+ is a projection we have

$$(P_{t+h}^+)^2 - (P_t^+)^2 = (P_{t+h}^+)^3 - (P_t^+)^3.$$

This can be expanded to

$$\begin{aligned} & (P_{t+h}^+ - P_t^+) P_{t+h}^+ + P_t^+ (P_{t+h}^+ - P_t^+) \\ &= (P_{t+h}^+ - P_t^+) (P_{t+h}^+)^2 + P_t^+ (P_{t+h}^+ - P_t^+) P_{t+h}^+ + (P_t^+)^2 (P_{t+h}^+ - P_t^+). \end{aligned}$$

Again, as $(P_t^+)^2 = P_t^+$, this implies

$$P_t^+ (P_{t+h}^+ - P_t^+) P_{t+h}^+ = 0.$$

We get the following trivial relation for the other diagonal element

$$P_t^- (P_{t+h}^+ - P_t^+) P_{t+h}^- = 0.$$

For the off-diagonal elements, we use $[H_t, P_t^+] = 0$ to derive

$$\begin{aligned} 0 &= H_{t+h} P_{t+h}^+ - H_t P_t^+ - (P_{t+h}^+ H_{t+h} - P_t^+ H_t) = \\ &= (H_{t+h} - H_t) P_{t+h}^+ + H_t (P_{t+h}^+ - P_t^+) - (P_{t+h}^+ - P_t^+) H_{t+h} - P_t^+ (H_{t+h} - H_t) \end{aligned}$$

Using the differentiability of the external field with respect to time and introducing the notion $P_t^h = \frac{1}{h} (P_{t+h}^+ - P_t^+)$ this is equivalent to

$$\begin{aligned} H_t P_t^h - P_t^h H_{t+h} &= P_t^+ \dot{A}_t - \dot{A}_t P_{t+h}^+ + \frac{1}{h} o(h) \\ \Rightarrow H_t P_t^h - P_t^h H_t &= P_t^+ \dot{A}_t - \dot{A}_t P_{t+h}^+ + h P_t^h \dot{A}_t + \frac{1}{h} o(h) = [P_{t+h}^+, \dot{A}_t] + \frac{1}{h} o(h) \\ \Rightarrow \pm (|H_t| P_t^\pm P_t^h P_t^\mp + P_t^\pm P_t^h P_t^\mp |H_t|) &= P_t^\pm [P_{t+h}^+, \dot{A}_t] P_t^\mp + \frac{1}{h} o(h) \\ \Rightarrow \{|H_t|, P_t^\pm P_t^h P_t^\mp\} &= \pm P_t^\pm [P_{t+h}^+, \dot{A}_t] P_t^\mp + \frac{1}{h} o(h). \end{aligned}$$

The right-hand side is bounded. Hence, we can use Theorem 5.2 and get

$$P_t^\pm P_t^h P_t^\mp = \pm S_{P_t^\pm [P_{t+h}^+, \dot{A}_t]} P_t^\mp + \frac{1}{h} o(h).$$

Adding it all together, we end up with

$$P_t^h = S_{P_t^+ [P_{t+h}^+, \dot{A}_t]} P_t^- - P_t^- [P_{t+h}^+, \dot{A}_t] P_t^+ + \frac{1}{h} o(h).$$

The operators P_t^\pm and \dot{A}_t are bounded, S is continuous in its operator argument and

$$\lim_{h \rightarrow 0} P_t^\pm [P_{t+h}^+, \dot{A}_t] P_t^\mp = \pm P_t^\pm \dot{A}_t P_t^\mp$$

in operator norm. We can therefore perform the limit $h \rightarrow 0$ and arrive at

$$\frac{d}{dt} P_t^+ = \lim_{h \rightarrow 0} P_t^h = S_{P_t^+ \dot{A}_t P_t^- + P_t^- \dot{A}_t P_t^+}.$$

It is clear that $\dot{P}_t^+ = -\dot{P}_t^-$ because we have $P_t^+ + P_t^- = \text{id}_{\mathcal{H}}$. □

Using this method we can determine the time-derivative of the operator S_A if A is an odd operator.

Proposition 5.4. *Let A be an odd and bounded time-dependent operator which is differentiable with respect to time such that its derivative also is a bounded operator. We then have*

$$\frac{d}{dt} S_A = [\dot{P}_t^+, \text{sgn } H_t S_A] + S_{[\text{sgn } H_t S_A, \dot{A}_t]}^{\text{odd}} + S_{(A)}^{\text{odd}}.$$

Proof. If A is odd then so is S_A . This means that the even part of the time derivative of S_A is given by $[\dot{P}_t^+, \text{sgn } H_t S_A]$. For the odd part we use the identity property of S which states that

$$A = \{|H_t|, S_A\} = [H_t, S_{\text{sgn } H_t A}]$$

where the last equality follows from S_A being odd. To show that this expression is differentiable one can use the same method as in the previous proof. We therefore skip this part and differentiate this expression which yields

$$\dot{A} - \left[\dot{A}_t, S_{\text{sgn } H_t A} \right] = \left[H_t, \left(\frac{d}{dt} S_{\text{sgn } H_t A} \right) \right].$$

By using $\text{sgn } H_t S_A = S_{\text{sgn } H_t A}$ throughout the following computations we find

$$(\dot{A})^{\text{odd}} - \left[\dot{A}_t, S_{\text{sgn } H_t A} \right]^{\text{odd}} = \left\{ |H_t|, \text{sgn } H_t \left(\frac{d}{dt} S_{\text{sgn } H_t A} \right)^{\text{odd}} \right\}$$

which we can solve by

$$\left(\frac{d}{dt} S_{\text{sgn } H_t A} \right)^{\text{odd}} = S_{\text{sgn } H_t} (\dot{A})^{\text{odd}} - S_{[\dot{A}_t, S_A]}^{\text{odd}}.$$

Now, note that

$$\left(\left(\frac{d}{dt} \text{sgn } H_t \right) S_A \right)^{\text{odd}} = (2\dot{P}_t^+ S_A)^{\text{odd}} = 0$$

as $\dot{P}_t^+ S_A$ is an even operator. Thus, we have

$$\left(\frac{d}{dt} S_A \right)^{\text{odd}} = S_{(\dot{A})}^{\text{odd}} - S_{[\dot{A}_t, \text{sgn } H_t S_A]}^{\text{odd}}.$$

□

Using the previous computations we can now easily determine the second derivative of the spectral projections.

Corollary 5.5. *Let the external field and its first and second time derivative define bounded operators of multiplication. Then the spectral projection is twice differentiable and given by*

$$\ddot{P}_t^+ = -2 \text{sgn } H_t (\dot{P}_t^+)^2 + S_{[\text{sgn } H_t \dot{P}_t^+, \dot{A}_t]}^{\text{odd}} + S_{(\ddot{A})}^{\text{odd}}.$$

Proof. The first derivative of the projection is

$$\dot{P}_t^+ = S_{\dot{A}_t}^{\text{odd}}.$$

As the external field is twice differentiable we can use Proposition 5.4 to derive the second derivative of the projection as

$$\begin{aligned} \ddot{P}_t^+ &= [\dot{P}_t^+, \text{sgn } H_t \dot{P}_t^+] + S_{[\text{sgn } H_t \dot{P}_t^+, \dot{A}_t]}^{\text{odd}} + S_{(\ddot{A})}^{\text{odd}} = \\ &= -2 \text{sgn } H_t (\dot{P}_t^+)^2 + S_{[\text{sgn } H_t \dot{P}_t^+, \dot{A}_t]}^{\text{odd}} + S_{(\ddot{A})}^{\text{odd}}. \end{aligned}$$

□

6. Adiabatic theorem

We now come to the main chapter of the first part of this thesis. Before we state the main result in Theorems 6.1 and 6.3 we start with a short introduction to time-adiabatic perturbation theory in general and then explain adiabatic behavior from a heuristic point of view.

6.1. Introduction

It is, in general, not possible to find exact solutions to a quantum mechanical system with a time-dependent potential. This is what time-dependent perturbation theories are for. Time adiabatic perturbation theory in particular applies to those cases where one has slowly varying external potentials. Roughly speaking one could say that if a physical system is given enough time to adapt to the external changes it will stay in an “equilibrium”. Now, what does this mean for a quantum system? For example, assume the initial state to be an eigenstate to some eigenvalue. We then expect such a state to stay approximately an eigenstate to the time-evolved hamiltonian and that, in particular, there appear no transitions to other subspaces. More generally speaking, an initial state in some spectral subspace will stay in the corresponding time-evolved spectral subspace if the external field varies slowly and the change of the subspaces is regular enough. This is the main content of (time-) adiabatic perturbation theory.

The question demanding an answer is obviously what does “slowly enough” mean? Let us assume the external field is an electromagnetic wave. The time scale on which this potential varies is given by the frequency or period T of the wave. In SI-units we therefore have

$$A = A \left(\frac{2\pi}{T} t \right).$$

On the contrary the time scale of a wave function fulfilling the Dirac equation is given by the natural time $\tau = \frac{\hbar}{mc^2}$ as we explained in Chapter 1.1. The external field on this time scale reads

$$A = A \left(\frac{2\pi\tau}{T} \frac{t}{\tau} \right) = A \left(\frac{2\pi\tau}{T} t' \right) = A(\varepsilon t'),$$

where t' is now the time measured in natural units and the dimensionless constant $\varepsilon = \frac{2\pi\tau}{T}$ is called *adiabatic parameter*. It is a measure for the separation of these two different time scales. We call an electromagnetic wave adiabatic if ε is close to zero, i.e. if the field is almost constant on the time scale of the wave function. The slow time scale is then also called macroscopic time whereas the short time scale is called microscopic. The Dirac equation on the microscopic time

is then

$$i \frac{\partial}{\partial t'} \psi = (-i \boldsymbol{\alpha} \nabla - \boldsymbol{\alpha} \mathbf{A}(\varepsilon t') + \beta) \psi.$$

Usually, experiments are performed on the time-scale of the external field. Hence, one is more likely interested in solutions on the macroscopic time. To this end we rescale the Dirac equation which yields

$$i \varepsilon \frac{\partial}{\partial t} \psi = (-i \boldsymbol{\alpha} \nabla - \boldsymbol{\alpha} \mathbf{A}(t) + \beta) \psi,$$

with

$$t = \varepsilon t'.$$

The goal of any time-adiabatic theorem is now to find approximate solutions to equations of such a form and state the error in dependency of the adiabatic parameter ε .

The history of adiabatic perturbation theory goes back to a paper by Born and Fock [BF28] in 1928 treating the Schrödinger operator with distinct eigenvalues. The theory has developed significantly since then (see [Teu03] for an in depth discussion) but it still seems necessary to prove a new version of the adiabatic theorem for the Dirac equation with an electromagnetic wave as external potential for several reasons. First of all, at the heart of time adiabatic theorems is the change of the spectral subspaces under time. Thus, one has to show certain regularity features of the spectral projections. This is mostly done via the Cauchy-Riesz integral formula (see e.g. [Nen80], [ASY87], [Joy07]) which provides an explicit formula for the spectral projections. To be able to use it one has to choose the path of integration such that it encircles the part of the spectrum one is interested in. But this is only possible if this part is separated by a gap from the rest of the spectrum. This is not the case for the Dirac operator when one would like to investigate the evolution of the whole negative energy subspace. All other results, to the best of our knowledge, assume the regularity of the projections or something similar to prove the adiabatic behavior (see e.g. [Nen81], [AE99], [Teu01]). But this is indeed the most difficult part as we will see in Chapter 6.3, for which we have to use the methods developed in Chapter 5.

Furthermore, it is difficult enough to give explicit upper bounds on the constants which appear in estimating the error of the adiabatic evolution. For electromagnetic waves the adiabatic parameter will scale with the frequency. But due to the dispersion if one varies the frequency this also affects the wave length. Hence, any external potential describing an electromagnetic wave will also scale in the position variable with ε . This in turn means that the hamiltonian for such a system, no matter what units we choose, always depends on the adiabatic parameter and thus also the constants in the error estimate! Hence, one has to show that this ε -dependence does not cancel the time adiabatic behavior. At last, if one likes to use adiabatic perturbation theory in the context of second quantization one is usually not interested in the operator norm estimate of the transitions to other subspaces anymore but in the Hilbert-Schmidt norm. It turns out that

our proof is easily extendable to this case yielding an Hilbert-Schmidt version of the adiabatic theorem with explicit bounds. This result has, to the best of our knowledge, not been available at all so far.

6.2. Heuristic explanation

We continue our discussion with a heuristic explanation of how the adiabatic theorem can be understood physically. We focus again on the Dirac equation but our argument is not bound to it. Afterwards, we will sketch how one can transform these ideas into a rigorous proof which is the content of the subsequent chapter. Please note that, as this is a heuristic discussion, we do not aim for mathematical rigorousness.

It is helpful to switch to the so called interaction picture which separates the time evolution into two parts. The first one which we call $U_r(t, s)$ is mainly the intrinsic quantum mechanical time evolution which every time-independent system also exhibits. The second one, written as $U_A(t, s)$, adds the time dependent behavior and is thus governed mainly by the external field. To see this, fix some r and define $U_r(t, s)$ through

$$i\varepsilon \frac{\partial}{\partial t} U_r(t, s) = H_r U_r(t, s)$$

where r now acts as a parameter. Hence, we have

$$U_r(t, s) = \exp\left[-\frac{i}{\varepsilon}(t-s) H_r\right]$$

for any $t, s \in \mathbb{R}$. We can evaluate $U_r(t, s)$ at $r = s$ and then define $U_A(t, s)$ through

$$U(t, s) = U_s(t, s) U_A(t, s)$$

where $U(t, s)$ is the full time evolution to the time dependent system. Applying the evolution equation we get

$$\begin{aligned} H_t U(t, s) &= i\varepsilon \frac{\partial}{\partial t} U(t, s) = \left(i\varepsilon \frac{\partial}{\partial t} U_s(t, s) \right) U_A(t, s) + U_s(t, s) i\varepsilon \frac{\partial}{\partial t} U_A(t, s) = \\ &= H_s U_s(t, s) U_A(t, s) + U_s(t, s) i\varepsilon \frac{\partial}{\partial t} U_A(t, s) \end{aligned}$$

and thus

$$\begin{aligned} i\varepsilon \frac{\partial}{\partial t} U_A(t, s) &= U_s(s, t) (H_t - H_s) U(t, s) = U_s(s, t) \boldsymbol{\alpha} [A(t, \mathbf{x}) - A(s, \mathbf{x})] U_s(t, s) U_A(t, s) = \\ &= \Delta_s(t) U_A(t, s). \end{aligned}$$

For small time intervals $|t - s| \ll 1$ we have that $\Delta_s(t) = \mathcal{O}(|t - s|)$. Hence, by using the Dyson series for $U_A(t, s)$,

$$U_A(t, s) = 1 - \frac{i}{\varepsilon} \int_s^t \Delta_s(r) U_A(r, s) dr$$

we see that $U_A(t, s) = 1 + \mathcal{O}(\frac{|t-s|^2}{\varepsilon})$. On the other hand we have for the same time interval $U_s(t, s) = 1 + \mathcal{O}(\frac{|t-s|}{\varepsilon})$. Thus, on the microscopic time scale and in the adiabatic setting i.e. where $|t - s| \propto \varepsilon$ and $\varepsilon \ll 1$ we see that $U_A(t, s) \approx 1$, i.e. the full time evolution is approximately the same as $U_s(t, s)$ on this scale. This is, of course, no surprise as adiabatic setting means precisely that the external field is almost constant on the microscopic scale and as such the time evolution should only yield a phase function due to the quantum mechanical evolution equation.

Assume now, that the time interval $[s, t]$ is on the macroscopic level and start with a wave function which is entirely in the negative subspace at time s . We are interested in parts of the wave function which tunnel through the spectral gap during the time interval $[s, t]$ and end up in the positive energy subspace. As we have

$$U(t, s) = U(t, r)U(r, s)$$

we can split up the time interval into N smaller intervals of length $\Delta s = \frac{t-s}{N}$ and look at the transitions there (Figure 6.1).

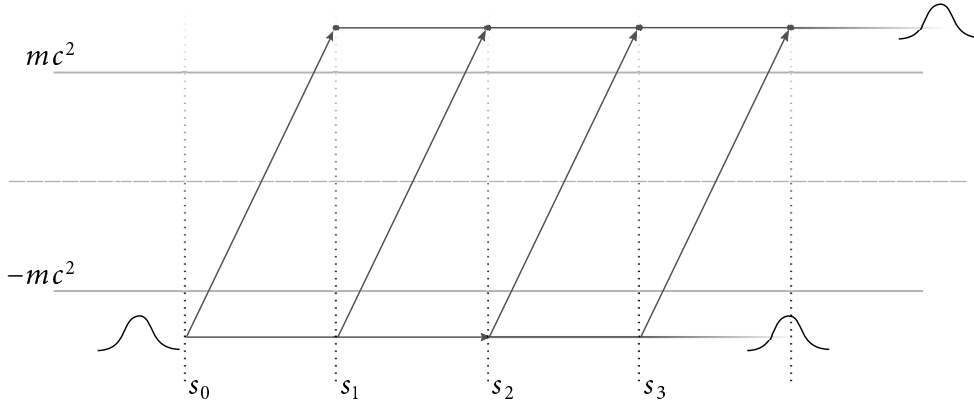


Figure 6.1.: Transitions of the wave function at different points in time.

It is not difficult to show (via a recursion relation) that the part of the wave function ending up in the positive subspace is given by

$$P_t^+ U(t, s) P_s^- = \sum_{n=1}^N \left(\prod_{m=0}^{N-n-1} P_{s_{N-m}}^+ U(s_{N-m}, s_{N-m-1}) \right) P_{s_n}^+ U(s_n, s_{n-1}) P_{s_{n-1}}^- U(s_{n-1}, s) P_s^- \quad (6.1)$$

with $s_n = s_{n-1} + \Delta s$ and $s_0 = s$. By a brute force norm estimate we immediately see that

$$P_t^+ U(t, s) P_s^- = \sum_{n=1}^N \mathcal{O}(P_{s_n+\Delta s}^+ U(s_n + \Delta s, s_n) P_{s_n}^-).$$

A Taylor expansion of $P_{s+\Delta s}^+ = P_s^+ + \mathcal{O}(\Delta s)$ yields

$$\begin{aligned} P_{s+\Delta s}^+ U(s + \Delta s, s) P_s^- &= P_s^+ U(s + \Delta s, s) P_s^- + \mathcal{O}(\Delta s) = \\ &= P_s^+ \exp\left[-\frac{i}{\varepsilon} \Delta s H_s\right] U_A(s + \Delta s, s) P_s^- + \mathcal{O}(\Delta s) = \\ &= \exp\left[-\frac{i}{\varepsilon} \Delta s |H_s|\right] P_s^+ U_A(s + \Delta s, s) P_s^- + \mathcal{O}(\Delta s) = \exp\left[-\frac{i}{\varepsilon} \Delta s |H_s|\right] \mathcal{O}\left(\frac{\Delta s^2}{\varepsilon}\right) + \mathcal{O}(\Delta s) \end{aligned}$$

where we used the Dyson series estimate for $U_A(s + \Delta s, s)$ in the last step. Thus, a naive estimate would yield

$$\begin{aligned} P_t^+ U(t, s) P_s^- &= \sum_{n=1}^N \mathcal{O}(P_{s_n+\Delta s}^+ U(s_n + \Delta s, s_n) P_{s_n}^-) = \mathcal{O}\left(N \frac{\Delta s^2}{\varepsilon}\right) + \mathcal{O}(N \Delta s) \\ &= \mathcal{O}\left(\frac{|t-s|^2}{N\varepsilon}\right) + \mathcal{O}(|t-s|) = \mathcal{O}(|t-s|) \end{aligned}$$

for $N \rightarrow \infty$. Hence, we have transitions through the spectral gap which should not surprise us as we have not taken adiabatic behavior into account. Transitions at each point in time simply stem from the fact that the spectral subspaces change over time due to the time-dependent external field. With $|t-s|$ being on the macroscopic scale the external field changes significantly and thus, we could indeed expect the wave function to tunnel through the gap. However, a more careful consideration shows that we missed an important effect. Let us take a look at pairs of transitions (Figure 6.2) being (up to now) arbitrarily far apart.

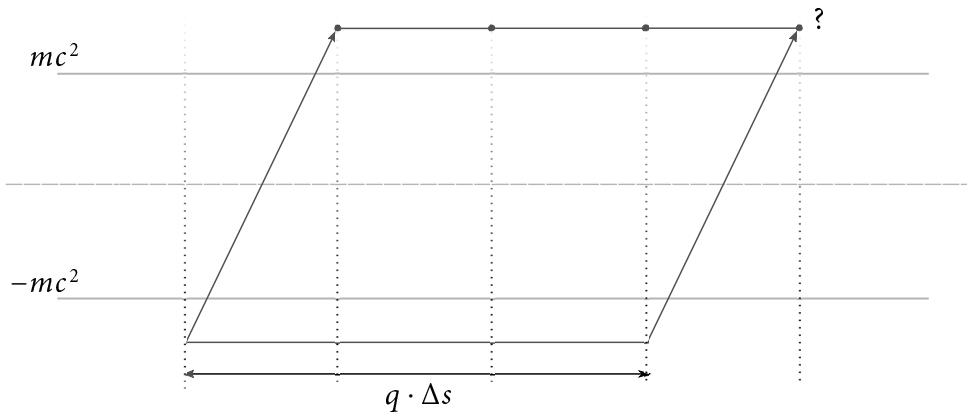


Figure 6.2.: A pair of transitions with (arbitrary) distance $q \cdot \Delta s$

The time evolution in the positive and negative subspace is given by

$$\begin{aligned} P_{n \cdot \Delta s + s}^\pm U(n \cdot \Delta s + s, s) P_s^\pm &= P_s^\pm U(n \cdot \Delta s + s, s) P_s^\pm + \mathcal{O}(n \cdot \Delta s) = \\ &= \exp \left[\mp \frac{i}{\varepsilon} n \cdot \Delta s |H_s| \right] P_s^\pm U_A(n \cdot \Delta s + s, s) P_s^\pm + \mathcal{O}(n \cdot \Delta s) = \\ &= \exp \left[\mp \frac{i}{\varepsilon} n \cdot \Delta s |H_s| \right] + \mathcal{O}(n \cdot \Delta s) \end{aligned}$$

where n is an arbitrary integer. We switch to momentum space as it is easier to handle the phase function there. We get for the first path in figure 6.2

$$\begin{aligned} \widehat{P}_{s_{n+1}}^+ \widehat{U}(s_{n+1}, s_1) \widehat{P}_{s_1}^+ \widehat{U}(s_1, s) \widehat{P}_s^- &= \\ &= \left(\exp \left[-\frac{i}{\varepsilon} n \cdot \Delta s E_k \right] + \mathcal{O}(n \cdot \Delta s) \right) \widehat{P}_{s_1}^+ \widehat{U}(s_1, s) \widehat{P}_s^- = \\ &= \exp \left[-\frac{i}{\varepsilon} n \cdot \Delta s E_k \right] \mathcal{O}(\Delta s) + \mathcal{O}(n \cdot \Delta s^2) \end{aligned}$$

and similarly for the second one

$$\begin{aligned} \widehat{P}_{s_{n+1}}^+ \widehat{U}(s_{n+1}, s_n) \widehat{P}_{s_n}^- \widehat{U}(s_n, s_0) \widehat{P}_{s_0}^- &= \\ &= \exp \left[+\frac{i}{\varepsilon} n \cdot \Delta s E_{k'} \right] \mathcal{O}(\Delta s) + \mathcal{O}(n \cdot \Delta s^2). \end{aligned}$$

The sum of the two then yields

$$\left(\exp \left[-\frac{i}{\varepsilon} n \cdot \Delta s E_k \right] + \exp \left[+\frac{i}{\varepsilon} n \cdot \Delta s E_{k'} \right] \right) \mathcal{O}(\Delta s) + \mathcal{O}(n \cdot \Delta s^2).$$

Note that the first term is proportional to

$$\begin{aligned} \cos \left((E_{k'} + E_k) \frac{n \cdot \Delta s}{\varepsilon} \right) \mathcal{O}(\Delta s) &= \left(n \cdot \Delta s - \frac{\pi}{2} \frac{\varepsilon}{E_k + E_{k'}} \right) \mathcal{O}(\Delta s) = \\ &= \left(\frac{n}{N} - \frac{\pi}{2} \frac{\varepsilon}{E_k + E_{k'}} \frac{1}{|t-s|} \right) \mathcal{O} \left(\frac{1}{N} \right), \end{aligned}$$

for

$$\frac{n}{N} \approx \frac{\pi}{2} \frac{\varepsilon}{E_{k'} + E_k} \frac{1}{|t-s|}$$

and it is well known that we can always find two integers such that this is true up to order $\frac{1}{N^2}$. Hence, taking into account these phase cancellations we can always find a pair of transitions that add up to

$$\begin{aligned} \left(\exp \left[-\frac{i}{\varepsilon} n \cdot \Delta s E_k \right] + \exp \left[+\frac{i}{\varepsilon} n \cdot \Delta s E_{k'} \right] \right) \mathcal{O}(\Delta s) + \mathcal{O}(n \cdot \Delta s^2) &= \\ &= \mathcal{O} \left(\frac{1}{N^3} \right) + \mathcal{O} \left(\frac{\varepsilon}{E_k + E_{k'}} \frac{|t-s|}{N} \right) \end{aligned}$$

and as we have $\frac{N}{2}$ of such pairs we get in total

$$\sum^{N/2} \mathcal{O}\left(\frac{1}{N^3}\right) + \mathcal{O}\left(\frac{\varepsilon}{E_k + E_{k'}} \frac{|t-s|}{N}\right) = \mathcal{O}\left(\frac{\varepsilon}{E_k + E_{k'}} |t-s|\right) + \mathcal{O}\left(\frac{1}{N^2}\right).$$

Finally, as N was completely arbitrary we must have for the full transition of a negative-energy mode $\psi_s^-(\mathbf{k})$ to a positive energy mode $\psi_t^+(\mathbf{k}')$

$$\widehat{P}_t^+ \widehat{U}(t, s) \widehat{P}_s^- = \mathcal{O}\left(\frac{\varepsilon}{E_k + E_{k'}} |t-s|\right).$$

Hence, the better the scales are separated, the more the tunneling is suppressed due to better phase cancelation. This is the main content of adiabatic perturbation theory. Note furthermore that transitions happen most likely from the edge of the spectral gap and are less likely from “deep out of the Dirac sea”. A fact which becomes important when one looks at the second quantized theory.

In the remaining part of this section we show how this previous argument can be made rigorous. From a mathematical point of view the sum in eq. (6.1) is not a very smart place to start as the computations get tedious very quickly. Also from a physical perspective, it seems counter-intuitive to use a discrete splitting of time as we expect to have transitions at every moment of time. Hence, after the heuristic detour above we should take the limit $N \rightarrow \infty$ to replace the sum with an integral. To be able to do so we have to find a way to take the limit of the product which appears in eq. (6.1). To figure out how to do this we look closer at what this product actually does. Its job is to keep track only of the fraction that stays in the positive subspace. If we replace the product by $P_t^+ U(t, s_n) P_{s_n}^+$, then this would also include paths which go back to the negative subspace and up again, see Figure 6.3.

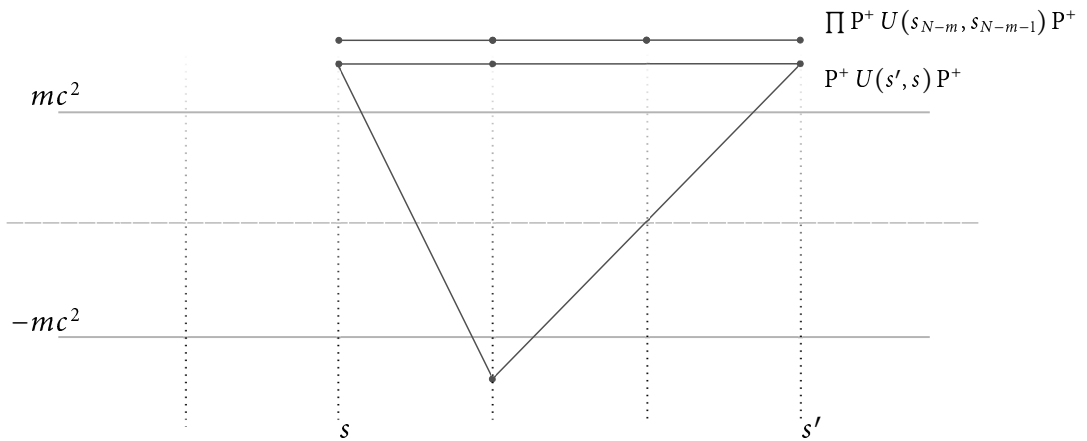


Figure 6.3.: The expression $P_{s'}^+ U(s', s) P_s^+$ contains the path which stays in the positive subspace and others which go back to the negative subspace and up again.

Hence, in order to do the replacement we need to subtract all the paths which go back to negative spectrum and up again. The correction terms are given by¹

$$\sum_{n=1}^N P_t^+ U(t, s_{n-1}) P_{s_n}^- U(s_n, s_{n-1}) P_{s_{n-1}}^+ U(s_{n-1}, s) P_s^- .$$

Replacing the product in eq. (6.1) by $P_t^+ U(t, s_n) P_{s_n}^+$ and subtracting the correction terms yields

$$P_t^+ U(t, s) P_s^- = \sum_{n=1}^N P_t^+ U(t, s_{n-1}) \left(P_{s_n}^+ U(s_n, s_{n-1}) P_{s_{n-1}}^- - P_{s_n}^- U(s_n, s_{n-1}) P_{s_{n-1}}^+ \right) U(s_{n-1}, s) P_s^- .$$

With this trick, it is easy to take the limit $N \rightarrow \infty$ if we note the following

$$\begin{aligned} & P_{s+\Delta s}^+ U(s + \Delta s, s) P_s^- - P_{s+\Delta s}^- U(s + \Delta s, s) P_s^+ = \\ & = P_s^+ U(s + \Delta s, s) P_s^- - P_s^- U(s + \Delta s, s) P_s^+ \\ & \quad + \Delta s \left(\left(\frac{d}{ds} P_s^+ \right) U(s + \Delta s, s) P_s^- - \left(\frac{d}{ds} P_s^- \right) U(s + \Delta s, s) P_s^+ \right) + o(\Delta s) = \\ & = P_s^+ \exp \left[-\frac{i}{\epsilon} \Delta s H_s \right] P_s^- - P_s^- \exp \left[-\frac{i}{\epsilon} \Delta s H_s \right] P_s^+ + \mathcal{O} \left(\frac{\Delta^2}{\epsilon} \right) \\ & \quad + \Delta s \left(\left(\frac{d}{ds} P_s^+ \right) U(s + \Delta s, s) P_s^- - \left(\frac{d}{ds} P_s^- \right) U(s + \Delta s, s) P_s^+ \right) + o(\Delta s) . \end{aligned}$$

Hence,

$$\lim_{\Delta s \rightarrow 0} \frac{1}{\Delta s} (P_{s+\Delta s}^+ U(s + \Delta s, s) P_s^- - P_{s+\Delta s}^- U(s + \Delta s, s) P_s^+) = \left(\frac{d}{ds} P_s^+ \right) P_s^- - \left(\frac{d}{ds} P_s^- \right) P_s^+ =: \dot{P}_s^+$$

which we denote for the time being with \dot{P}_s^+ . The integral is then

$$P_t^+ U(t, s) P_s^- = P_t^+ \int_s^t U(t, r) \dot{P}_r^+ U(r, s) dr P_s^- .$$

This equation is the starting point for the proof of the adiabatic theorem in Chapter 6.3, where we will derive it in a much simpler and mathematical rigorous way. To see how we can derive adiabatic behavior from this, we use the interaction picture again and switch to momentum space as before. The free part of the time evolution, $U_s(t, s)$, then yields a phase and the integral is therefore similar to an oscillatory integral

$$\int_s^t e^{-\frac{i}{\epsilon} (E_k + E_{k'}) r} \psi(r) dr .$$

¹We do not prove here that these are indeed the right terms because this chapter is thought of as a heuristic discussion. Instead, they are incorporated in the rigorous proof in the next chapter which is simple and elegant. However, if one sketches the extra paths one can convince oneself quickly that these are the right correction terms.

By writing

$$e^{-\frac{i}{\varepsilon}(E_k+E_{k'})r}\psi(r) = \frac{i\varepsilon}{E_k+E_{k'}} \frac{d}{dr} e^{-\frac{i}{\varepsilon}(E_k+E_{k'})r}\psi(r) - \frac{i\varepsilon}{E_k+E_{k'}} e^{-\frac{i}{\varepsilon}(E_k+E_{k'})r} \frac{d}{dr}\psi(r),$$

we get

$$\left| \int_s^t e^{-\frac{i}{\varepsilon}(E_k+E_{k'})r}\psi(r) dr \right| \leq \frac{\varepsilon}{E_k+E_{k'}} \left(|\psi(t) - \psi(s)| + |t-s| \sup_{r \in [s,t]} \left| \frac{d}{dr}\psi(r) \right| \right).$$

Hence, if $\frac{d}{dr}\psi(r)$ is bounded in ε , i.e. if we are in the adiabatic regime, the integral vanishes for small ε . Thus, to prove the adiabatic theorem we first have to show rigorously that the integrand can indeed be rewritten like we just did and, secondly, we need to prove the boundedness of the derivative. These two tasks are the content of following section.

6.3. The theorem

To begin with, we derive the expression for transitions through the gap which we have heuristically argued for in the preceding section. The transitions through the gap after the time interval $[s, t]$ has passed are given by $P_t^\pm U(t, s) P_s^\mp$. For the moment we restrict ourselves to the domain $\mathcal{D}(H_0)$ of the free hamiltonian and remember that $\mathcal{D}(H_0) = \mathcal{D}(H_t)$ for all t . Manipulating the off-diagonal terms by using the properties of projections yields

$$\begin{aligned} P_t^\pm U(t, s) P_s^\mp &= P_t^\pm U(t, s) P_s^\mp - P_t^\pm U(t, s) P_s^\pm P_s^\mp = \\ &= P_t^\pm (U(t, t) P_t^\pm U(t, s) - U(t, s) P_s^\pm U(s, s)) P_s^\mp = \\ &= P_t^\pm \int_s^t \frac{d}{dr} (U(t, r) P_r^\pm U(r, s)) dr P_s^\mp = \\ &= P_t^\pm \int_s^t \left(U(t, r) \dot{P}_r^\pm U(r, s) + U(t, r) \frac{i}{\varepsilon} [H_r, P_r^\pm] U(r, s) \right) dr P_s^\mp = \\ &= P_t^\pm \int_s^t U(t, r) \dot{P}_r^\pm U(r, s) dr P_s^\mp \end{aligned}$$

where the integral is understood as Bochner-integral on the Banach space of bounded linear operators. To evaluate this integral we assume that there exists a family of bounded operators $(X_t)_{t \in \mathbb{R}}$, differentiable with respect to t and such that the following relation holds on the domain of the hamiltonian,

$$\dot{P}_t^\pm = \pm [H_t, X_t].$$

Differentiating the expression $U(t, r) X_r U(r, s)$ yields

$$\frac{d}{dr} U(t, r) X_r U(r, s) = \frac{i}{\varepsilon} U(t, r) [H_r, X_r] U(r, s) + U(t, r) \left(\frac{d}{dr} X_r \right) U(r, s)$$

which is then equivalent to

$$U(t, r) \dot{P}_r^\pm U(r, s) = \pm i\varepsilon U(t, r) \left(\frac{d}{dr} X_r \right) U(r, s) \mp i\varepsilon \frac{d}{dr} U(t, r) X_r U(r, s).$$

We can now evaluate the above integral to be

$$\begin{aligned} P_t^\pm \int_s^t U(t, r) \dot{P}_r^\pm U(r, s) dr P_s^\mp &= \mp i\varepsilon P_t^\pm (X_t U(t, s) - U(t, s) X_s) P_s^\mp \\ &\pm i\varepsilon P_t^\pm \int_s^t U(t, r) \left(\frac{d}{dr} X_r \right) U(r, s) dr P_s^\mp. \end{aligned}$$

As every operator in the term above is bounded we can estimate the norm of the transitions by

$$\|P_t^\pm U(t, s) P_s^\mp\| \leq \varepsilon \left(\|X_t\| + \|X_s\| + \int_s^t \left\| \frac{d}{dr} X_r \right\| dr \right),$$

where we used the unitarity of the time evolution, $\|P_t^\pm\| = 1$ and the Minkowski inequality for the Bochner integral. Thus, the remaining task for the adiabatic theorem is to show that there exists such a family of operators $(X_t)_{t \in \mathbb{R}}$ and to determine the bound and the bound of its time-derivative.

Theorem 6.1 (Adiabatic theorem). *Let the vector potential $A(t, \mathbf{x})$ be such that there exists a generalized Fourier transform according to Theorem 3.6 and that $A(t, \mathbf{x})$ and its first two time derivatives define bounded operators of multiplication. The Dirac time evolution has then the following property*

$$\|P_t^\pm U(t, s) P_s^\mp\| \leq \varepsilon C^2 \left(\|\dot{A}_t\| + \|\dot{A}_s\| + \int_s^t 6C \|\dot{A}_r\|^2 + \|\ddot{A}_r\| dr \right)$$

where C is

$$C = \sum_{n=0}^{\infty} \frac{1}{(n+1)^2} \left(\frac{n}{n+1} \right)^{2n}.$$

Proof. The prerequisites on the external field guarantee the existence of the time evolution by Proposition 1.4 and the existence and boundedness of \dot{P}_t^\pm by Proposition 5.3. Thus, we can use the considerations above which leave to prove the existence and differentiability of X_t . As \dot{P}_t^\pm has only off-diagonal elements we can choose $P_t^\pm X_t P_t^\pm = 0$ as well. The defining commutator relation reduces then to the off-diagonal elements

$$P_t^\pm \dot{P}_t^\pm P_t^\mp = P_t^\pm [H_t, X_t] P_t^\mp = \pm \{ |H_t|, P_t^\pm X_t P_t^\mp \}.$$

The left-hand side is bounded, therefore we can use Theorem 5.2 and get

$$X_t = S_{\text{sgn } H_t} \dot{P}_t^\pm = S_{\text{sgn } H_t}^{(2)} \left(\dot{A}_t \right)^{\text{odd}}, \quad (6.2)$$

with $S_A^{(2)} = S_{S_A}$. For the norm we have according to Theorem 5.2,

$$\|X_t\| \leq \frac{1}{2} \sum_{n=0}^{\infty} \frac{1}{(n+1)^2} \left(\frac{n}{n+1}\right)^{2n} \|\dot{P}_t^+\| = C \|\dot{P}_t^+\| \leq C^2 \|\dot{A}_t\|. \quad (6.3)$$

The derivative of X_t is then derived with Proposition 5.4 and given by

$$\dot{X}_t = [\dot{P}_t^+, \text{sgn } H_t X_t] + S_{[\text{sgn } H_t X_t, \dot{A}_t]^{\text{odd}}} + S_{\text{sgn } H_t (\dot{P}^+)^{\text{odd}}}. \quad (6.4)$$

To estimate the norm of the derivative, we first note that

$$\|S_{(\dot{P}^+)^{\text{odd}}}\| \leq \|S_{[\text{sgn } H_t \dot{P}^+, \dot{A}_t]^{\text{odd}}}\| + \|S_{(\dot{A}_t)^{\text{odd}}}\| \leq 2C^3 \|\dot{A}_t\|^2 + C^2 \|\ddot{A}_t\| \quad (6.5)$$

due to Corollary 5.5. Therefore, we find

$$\begin{aligned} \|\dot{X}_t\| &\leq 2 \left(\|\dot{P}_t^+\| + C \|\dot{A}_t\| \right) \|X_t\| + \|S_{(\dot{P}^+)^{\text{odd}}}\| \leq \\ &\leq 4C^3 \|\dot{A}_t\|^2 + \|S_{(\dot{P}^+)^{\text{odd}}}\| \leq 6C^3 \|\dot{A}_t\|^2 + C^2 \|\ddot{A}_t\|. \end{aligned} \quad (6.6)$$

□

We can now extend the previous argument to higher orders in ε . To this end assume there exist two families of bounded operators $(X_n)_{n \in \mathbb{N}}$ and $(Y_n)_{n \in \mathbb{N}}$ which are time-dependent and differentiable with respect to time and such that

$$(\dot{X}_n)^{\text{odd}} + \{\dot{P}_t^+, \text{sgn } H_t Y_n\} = [H_t, X_{n+1}] \quad (6.7)$$

and

$$(\dot{Y}_n)^{\text{even}} + [\dot{P}_t^+, \text{sgn } H_t X_n] = [H_t, Y_{n+1}]. \quad (6.8)$$

First, note that if X_1 is odd and Y_1 is even then it follows by induction that X_n is odd and Y_n is even for all n . Secondly, we get that

$$\begin{aligned} \frac{d}{dr} U(t, r) (X_{n+1} + Y_{n+1}) U(r, s) &= \frac{i}{\varepsilon} U(t, r) ([H_r, X_{n+1}] + [H_r, Y_{n+1}]) U(r, s) \\ &\quad + U(t, r) (\dot{X}_{n+1} + \dot{Y}_{n+1}) U(r, s) = \\ &= \frac{i}{\varepsilon} U(t, r) \left((\dot{X}_n)^{\text{odd}} + \{\dot{P}_t^+, \text{sgn } H_t Y_n\} + (\dot{Y}_n)^{\text{even}} + [\dot{P}_t^+, \text{sgn } H_t X_n] \right) U(r, s) \\ &\quad + U(t, r) (\dot{X}_n + \dot{Y}_n) = \\ &= \frac{i}{\varepsilon} U(t, r) (\dot{X}_n + \dot{Y}_n) U(r, s) + U(t, r) (\dot{X}_{n+1} + \dot{Y}_{n+1}) U(r, s) \end{aligned}$$

and therefore

$$\begin{aligned} \int_s^t U(t, r) (\dot{X}_n + \dot{Y}_n) U(r, s) dr &= -i\varepsilon ((X_{n+1} + Y_{n+1}) U(t, s) - U(t, s) (X_{n+1} + Y_{n+1})) \\ &+ i\varepsilon \int_s^t U(t, r) (\dot{X}_{n+1} + \dot{Y}_{n+1}) U(r, s) dr. \end{aligned}$$

If we furthermore assume that there are some s and t such that $X_{n+1} = Y_{n+1} = 0$ at these times (this is the case, i.e. if the external field is being switched off at s and t) we have

$$\int_s^t U(t, r) (\dot{X}_n + \dot{Y}_n) U(r, s) dr = i\varepsilon \int_s^t U(t, r) (\dot{X}_{n+1} + \dot{Y}_{n+1}) U(r, s) dr.$$

By induction we can conclude that

$$\int_s^t U(t, r) (\dot{X}_1 + \dot{Y}_1) U(r, s) dr = (i\varepsilon)^n \int_s^t U(t, r) (\dot{X}_{n+1} + \dot{Y}_{n+1}) U(r, s) dr. \quad (6.9)$$

Looking back at the first order adiabatic theorem we see that X_1 is given by X_r and $Y_1 = 0$. We can now start to solve the commutator relations to any desired order in ε . For X_n , we can solve the corresponding commutator equation by using Theorem 5.2 as we did in the proof of the previous theorem. For example, for X_2 we get

$$X_2 = S_{\text{sgn } H_t(\dot{X}_1)^{\text{odd}}}. \quad (6.10)$$

For Y_2 , we note that

$$[\dot{P}_t^+, \text{sgn } H_t X_1] = [[H_t, X_1], \text{sgn } H_t X_1] = [H_t, -\text{sgn } H_t (X_1)^2]$$

and therefore, we have

$$Y_2 = -\text{sgn } H_t (X_1)^2. \quad (6.11)$$

Hence, the transition elements in second order adiabatic theory are,

$$\begin{aligned} P_t^\pm U(t, s) P_s^\mp &= \\ &= i\varepsilon P_t^\pm \int_s^t U(t, r) \dot{X}_1 U(r, s) dr P_s^\mp = \\ &= \varepsilon^2 P_t^\pm \int_s^t U(t, r) \frac{d}{dr} (X_2 + Y_2) U(r, s) dr P_s^\mp. \end{aligned} \quad (6.12)$$

The derivative of X_2 is due to Proposition 5.4 given by

$$\dot{X}_2 = [\dot{P}_r^+, \text{sgn } H_r X_2] + S_{[\text{sgn } H_t X_2, \dot{A}_r]^{\text{odd}}} + S_{\text{sgn } H_r (\ddot{X}_1)^{\text{odd}}}. \quad (6.13)$$

The first derivative of X_1 is given by eq. (6.4). Its second derivative is therefore

$$\begin{aligned}
(\ddot{X}_1)^{\text{odd}} &= [(\ddot{P}_r^+), \text{sgn } H_r X_1]^{\text{odd}} + 2[\dot{P}_r^+, \dot{P}_r^+ X_1]^{\text{odd}} + [\dot{P}_r^+, \text{sgn } H_t \dot{X}_1]^{\text{odd}} \\
&\quad + \left(\frac{d}{dr} S_{[\text{sgn } H_r X_1, \dot{A}_r]}^{\text{odd}} \right)^{\text{odd}} + \left(\frac{d}{dr} S_{\text{sgn } H_t (\dot{P}_r^+)^{\text{odd}}} \right)^{\text{odd}} = \\
&= [(\ddot{P}_r^+)^{\text{even}}, \text{sgn } H_r X_1] + [\dot{P}_r^+, [\dot{P}_r^+, X_1]] \\
&\quad + \left(\frac{d}{dr} S_{[\text{sgn } H_r X_1, \dot{A}_r]}^{\text{odd}} \right)^{\text{odd}} + \left(\frac{d}{dr} S_{\text{sgn } H_t (\dot{P}_r^+)^{\text{odd}}} \right)^{\text{odd}} = \\
&= -\{\dot{P}_r^+, \{\dot{P}_r^+, X_1\}\} + \left(\frac{d}{dr} S_{[\text{sgn } H_r X_1, \dot{A}_r]}^{\text{odd}} \right)^{\text{odd}} + \left(\frac{d}{dr} S_{\text{sgn } H_t (\dot{P}_r^+)^{\text{odd}}} \right)^{\text{odd}}
\end{aligned}$$

where we used $[\dot{P}_r^+, \text{sgn } H_t \dot{X}_1]^{\text{odd}} = [\dot{P}_r^+, \text{sgn } H_t (\dot{X}_1)^{\text{even}}]$ in the first step and $(\ddot{P}_r^+)^{\text{even}} = -2(\dot{P}_r^+)^2$ in the second step. To obtain the remaining derivatives we can again use Proposition 5.4 which yields

$$\begin{aligned}
(\ddot{X}_1)^{\text{odd}} &= -\{\dot{P}_r^+, \{\dot{P}_r^+, X_1\}\} + S_{[S_{[X_1, \dot{A}_r]}^{\text{odd}}, \dot{A}_r]}^{\text{odd}} + S_{[(\dot{X}_1)^{\text{odd}}, \dot{A}_r]}^{\text{odd}} + S_{[X_1, \ddot{A}_r]}^{\text{odd}} \\
&\quad + S_{[S_{(\dot{P}_r^+)^{\text{odd}}, \dot{A}_r]}^{\text{odd}} + S_{(\dot{P}_r^+)^{\text{odd}}}. \tag{6.14}
\end{aligned}$$

Note that we actually mean $(\ddot{P}_t^+)^{\text{odd}} = \left(\frac{d}{dt} (\dot{P}_t^+)^{\text{odd}} \right)^{\text{odd}}$. For \dot{Y}_2 we have

$$\dot{Y}_2 = -2\dot{P}_r^+ (X_1)^2 - \text{sgn } H_r \{X_1, \dot{X}_1\}. \tag{6.15}$$

All the terms which appear in the two derivatives are well known by the previous proofs except for $\frac{d^3}{dt^3} P_t^+$. It can again be computed by using Proposition 5.4 and we will do so in the next section. In principle we could continue with this procedure to any arbitrary power in ε . For example for the third and fourth order one finds

$$\begin{aligned}
X_3 &= \text{sgn } H_r \left(S_{(\dot{X}_2)^{\text{odd}}} - S_{\{\dot{P}_r^+, (X_1)^2\}} \right) \\
Y_3 &= -\text{sgn } H_t \{X_1, X_2\},
\end{aligned}$$

and

$$\begin{aligned}
X_4 &= \text{sgn } H_r \left(S_{(\dot{X}_3)^{\text{odd}}} - S_{\{\dot{P}_r^+, \{X_1, X_2\}\}} \right) \\
Y_4 &= -\text{sgn } H_r \left((X_1)^4 + (X_2)^2 + \{X_1, X_3\} \right).
\end{aligned}$$

However, to be able to compute time-derivatives of the operators we need some regularity of the external field. Otherwise, the time-derivatives will not exist. For N -th order in ε it certainly suffices if the first to the $(N + 1)$ -th derivative of the external field defines a bounded operator of multiplication. Then, all derivatives of operators in the expression above can be determined by consecutive use of Proposition 5.4.

6.4. A Hilbert-Schmidt version

In the context of second quantization we will see that quite often one does not only need the operator norm of the off-diagonal elements of the time evolution but rather the Hilbert-Schmidt norm. We will show in this section that our previous result can be strengthened to include also this case. To this end we will need the following lemma.

Lemma 6.2. *Let the vector potential be such that there exists a generalized Fourier transform according to Theorem 3.6 and such that the generalized eigenfunctions are uniformly bounded. Let T be a bounded operator on the Hilbert space and let $\mathbf{B}(\mathbf{x}) \in L^2(\mathbb{R}^3 \rightarrow \mathbb{R}^3)$ such that it defines a bounded multiplication operator. Denote the matrix-valued multiplication operator defined by $\alpha\mathbf{B}(\mathbf{x})$ with B . It follows that the operator $S_{TB}^{(2)} := S_{S_{TB}}$ is a Hilbert-Schmidt operator with*

$$\|S_{TB}^{(2)}\|_{HS} \leq \pi \sup_{\mathbf{x}, \mathbf{k} \in \mathbb{R}^3} |\underline{\phi}(\mathbf{x}, \mathbf{k})| \|\mathbf{B}\|_{L^2} \|T\|.$$

Proof. The generalized eigenfunctions are uniformly bounded. Hence, also $\alpha\mathbf{B}(\cdot)\underline{\phi}(\cdot, \mathbf{k}) \in L^2$ for all $\mathbf{k} \in \mathbb{R}^3$. Thus, we can define

$$h(\mathbf{k}, \mathbf{k}') = \frac{\mathcal{F}T[\alpha\mathbf{B}(\cdot)\underline{\phi}(\cdot, \mathbf{k}')](\mathbf{k})}{(E_k + E_{k'})^2}.$$

Using $(E_k + E_{k'})^4 \geq E_{k'}^4$ we get

$$\begin{aligned} \int |h(\mathbf{k}, \mathbf{k}')|^2 d^3k d^3k' &= \int \frac{|\mathcal{F}T[\alpha\mathbf{B}(\cdot)\underline{\phi}(\cdot, \mathbf{k}')](\mathbf{k})|^2}{(E_k + E_{k'})^4} d^3k d^3k' \leq \\ &\leq \int \frac{1}{E_{k'}^4} \left(\int |\mathcal{F}T[\alpha\mathbf{B}(\cdot)\underline{\phi}(\cdot, \mathbf{k}')](\mathbf{k})|^2 d^3k \right) d^3k' = \\ &= \int \frac{1}{E_{k'}^4} \|\mathcal{F}T[\alpha\mathbf{B}(\cdot)\underline{\phi}(\cdot, \mathbf{k}')]\|_{L^2}^2 d^3k' \leq \int \frac{1}{E_{k'}^4} \|\alpha\mathbf{B}(\cdot)\underline{\phi}(\cdot, \mathbf{k}')\|_{L^2}^2 d^3k' \|T\|^2 \leq \\ &\leq \int \frac{\sup_{\mathbf{x} \in \mathbb{R}^3} |\underline{\phi}(\mathbf{x}, \mathbf{k}')|^2}{E_{k'}^4} d^3k' \|\mathbf{B}\|_{L^2}^2 \|T\|^2 \leq \pi^2 \sup_{\mathbf{x}, \mathbf{k} \in \mathbb{R}^3} |\underline{\phi}(\mathbf{x}, \mathbf{k})|^2 \|\mathbf{B}\|_{L^2}^2 \|T\|^2 \end{aligned}$$

where we used the unitarity of the generalized Fourier transform in the fourth step. Hence, $h(\mathbf{k}, \mathbf{k}')$ defines a Hilbert-Schmidt integral operator $K : L^2 \rightarrow L^2$. By the definition of the generalized Fourier transform in Theorem 3.6 and $\alpha \mathbf{B}(\cdot) \underline{\phi}(\cdot, \mathbf{k}) \in L^2$ for all \mathbf{k} we get

$$\mathcal{F} S_{\text{TB}}^2 \mathcal{F}^{-1}[\widehat{\psi}] = K[\widehat{\psi}]$$

for all $\widehat{\psi} \in L^1 \cap L^2$ and thus, by the density of $L^1 \cap L^2$, this equality extends to all $\widehat{\psi} \in L^2$. By the unitarity of the generalized Fourier transform we get for the Hilbert-Schmidt norm of S_{TB}^2 ,

$$\begin{aligned} \|S_{\text{TB}}^2\|_{HS} &= \|\mathcal{F} S_{\text{TB}}^2 \mathcal{F}^{-1}\|_{HS} = \|K\|_{HS} = \left(\int |h(\mathbf{k}, \mathbf{k}')|^2 d^3k d^3k' \right)^{\frac{1}{2}} \leq \\ &\leq \pi \sup_{x, k \in \mathbb{R}^3} \left| \underline{\phi}(\mathbf{x}, \mathbf{k}) \right| \|\mathbf{B}\|_{L^2} \|\mathbf{T}\|. \end{aligned}$$

□

We can now prove the adiabatic theorem for the Hilbert-Schmidt norm.

Theorem 6.3 (Adiabatic theorem for Hilbert-Schmidt norm). *Let the vector potential be such that there exists a generalized Fourier transform according to Theorem 3.6 and such that the generalized eigenfunctions are uniformly bounded. Let it furthermore be such that $\mathbf{A}(t, \mathbf{x})$ and its first two time-derivatives define bounded operators of multiplication and let the first and second time derivative be square integrable. The Dirac time evolution has then the following property*

$$\begin{aligned} \|\mathbf{P}_t^\pm U(t, s) \mathbf{P}_s^\mp\|_{HS} &\leq \pi \varepsilon \left(\sup_{x, k \in \mathbb{R}^3} \left| \underline{\phi}_s(\mathbf{x}, \mathbf{k}) \right| \|\dot{\mathbf{A}}(t, \cdot)\|_{L^2} + \sup_{x, k \in \mathbb{R}^3} \left| \underline{\phi}_s(\mathbf{x}, \mathbf{k}) \right| \|\dot{\mathbf{A}}(s, \cdot)\|_{L^2} \right. \\ &\quad \left. + \int_s^t \sup_{x, k \in \mathbb{R}^3} \left| \underline{\phi}_r(\mathbf{x}, \mathbf{k}) \right| \left(6C \|\dot{\mathbf{A}}_r\| \|\dot{\mathbf{A}}(r, \cdot)\|_{L^2} + \|\ddot{\mathbf{A}}(r, \cdot)\|_{L^2} \right) dr \right) \end{aligned} \quad (6.16)$$

where C is

$$C = \sum_{n=0}^{\infty} \frac{1}{(n+1)^2} \left(\frac{n}{n+1} \right)^{2n}.$$

Proof. Recalling the proof of the adiabatic theorem we see that we only used the triangle inequality for the Bochner integral and unitarity of the time evolution to arrive at

$$\|\mathbf{P}_t^\pm U(t, s) \mathbf{P}_s^\mp\| \leq \varepsilon \left(\|X_t\| + \|X_s\| + \varepsilon \int_s^t \left\| \frac{d}{dr} X_r \right\| dr \right).$$

It is easy to see that the triangle inequality for the Bochner integral also holds for the Hilbert-Schmidt norm. Hence, we have

$$\|\mathbf{P}_t^\pm U(t, s) \mathbf{P}_s^\mp\|_{HS} \leq \varepsilon \left(\|X_t\|_{HS} + \|X_s\|_{HS} + \varepsilon \int_s^t \left\| \frac{d}{dr} X_r \right\|_{HS} dr \right)$$

and are thus left to prove the Hilbert-Schmidt property for X_t and \dot{X}_t . Remember that X_t is given by eq. (6.2)

$$X_t = S^2_{\text{sgn H}_t(\dot{A}_t)^{\text{odd}}}.$$

Therefore, we have by Lemma 6.2 that

$$\|X_t\|_{HS} = \left\| S^2_{\text{sgn H}_t(\dot{A}_t)^{\text{odd}}} \right\|_{HS} \leq \|S^2_{\dot{A}_t}\|_{HS} \leq \pi \sup_{x, k \in \mathbb{R}^3} |\phi(\mathbf{x}, \mathbf{k})| \|\dot{A}(t, \cdot)\|_{L^2}. \quad (6.17)$$

The operator \dot{X}_t from eq. (6.4) is given as

$$\dot{X}_t = [\dot{P}_t^+, \text{sgn H}_t X_t] + S_{[\text{sgn H}_t X_t, \dot{A}_t]^{\text{odd}}} + S_{\text{sgn H}_t(\dot{P}_t^+)^{\text{odd}}}.$$

To determine its norm we note first that

$$\begin{aligned} \left\| S_{(\dot{P}_t^+)^{\text{odd}}} \right\|_{HS} &\leq \left\| S_{\dot{A}_t^{+-} - \dot{A}_t^{-+}}^{(2)} \right\|_{HS} + \left\| S_{[\dot{P}_t^+, \dot{A}_t]^{+-} + [\dot{P}_t^+, \dot{A}_t]^{-+}}^{(2)} \right\|_{HS} \leq \\ &\leq \left\| S_{\dot{A}_t}^{(2)} \right\|_{HS} + \left\| S_{[\dot{P}_t^+, \dot{A}_t]}^{(2)} \right\|_{HS} \leq \\ &\leq \pi \sup_{x, k \in \mathbb{R}^3} |\phi(\mathbf{x}, \mathbf{k})| \left(\|\ddot{A}(t, \cdot)\|_{L^2} + 2C \|\dot{A}_t\| \|\dot{A}(t, \cdot)\|_{L^2} \right) \end{aligned} \quad (6.18)$$

where we used

$$\left\| S_{\dot{A}_t, \dot{P}_t^+}^{(2)} \right\|_{HS} = \left\| \left(S_{\dot{P}_t^+, \dot{A}_t}^{(2)} \right)^\dagger \right\|_{HS} = \left\| S_{\dot{P}_t^+, \dot{A}_t}^{(2)} \right\|_{HS}$$

and Lemma 6.2 in the last step. Thus, we find

$$\begin{aligned} \|\dot{X}_t\|_{HS} &\leq 2 \|\dot{P}_t^+\| \|X_t\|_{HS} + \left\| S_{[X_t, \dot{A}_t]^{\text{odd}}} \right\|_{HS} + \left\| S_{\text{sgn H}_t(\dot{P}_t^+)^{\text{odd}}} \right\|_{HS} \leq \\ &\leq 2 \left(\|\dot{P}_t^+\| + C \|\dot{A}_t\| \right) \|X_t\|_{HS} + \left\| S_{(\dot{P}_t^+)^{\text{odd}}} \right\|_{HS} \\ &\leq 4C \|\dot{A}_t\| \|X_t\|_{HS} + \left\| S_{(\dot{P}_t^+)^{\text{odd}}} \right\|_{HS} \\ &\leq \pi \sup_{x, k \in \mathbb{R}^3} |\phi(\mathbf{x}, \mathbf{k})| \left(\|\ddot{A}(t, \cdot)\|_{L^2} + 6C \|\dot{A}_t\| \|\dot{A}(t, \cdot)\|_{L^2} \right). \end{aligned} \quad (6.19)$$

□

Of course, this theorem can now also be extended to higher orders in ε . The starting point is again eq. (6.9). For example, to establish the second order we have to determine the Hilbert-Schmidt norm of $\dot{X}_2 + \dot{Y}_2$. For \dot{Y}_2 we get due to eq. (6.15)

$$\begin{aligned} \|\dot{Y}_2\|_{HS} &\leq 2 \left(\|\dot{P}_r^+\| \|X_1\| + \|\dot{X}_1\| \right) \|X_1\|_{HS} \leq \left(14C^3 \|\dot{A}_t\|^2 + 2C^2 \|\ddot{A}_t\| \right) \|X_1\|_{HS} \leq \\ &\leq \pi \left(14C^3 \|\dot{A}_t\|^2 + 2C^2 \|\ddot{A}_t\| \right) \sup_{x, k \in \mathbb{R}^3} \left| \phi(\mathbf{x}, \mathbf{k}) \right| \|\dot{A}(t, \cdot)\|_{L^2}, \end{aligned} \quad (6.20)$$

where we used eq. (6.3) and eq. (6.6) in the first step and eq. (6.17) in the last step. For \dot{X}_2 we have

$$\begin{aligned} \|\dot{X}_2\|_{HS} &\leq 2 \|\dot{P}_r^+\| \|X_2\|_{HS} + \left\| S_{[\text{sgn } H_t X_2, \dot{A}_r]}^{\text{odd}} \right\|_{HS} + \left\| S_{\text{sgn } H_r(\dot{X}_1)}^{\text{odd}} \right\|_{HS} \leq \\ &\leq 2 \left(\|\dot{P}_r^+\| + C \|\dot{A}_r\| \right) \|X_2\|_{HS} + \left\| S_{(\dot{X}_1)}^{\text{odd}} \right\|_{HS} \leq \\ &\leq 4C^2 \|\dot{A}_r\| \left\| (\dot{X}_1)^{\text{odd}} \right\|_{HS} + \left\| S_{(\dot{X}_1)}^{\text{odd}} \right\|_{HS}. \end{aligned}$$

For the last term we find with eq. (6.14) and Lemma 6.2 that

$$\begin{aligned} \left\| S_{(\dot{X}_1)}^{\text{odd}} \right\|_{HS} &\leq 4C \|\dot{P}_r^+\|^2 \|X_1\|_{HS} \\ &+ 2\pi \left(\left\| S_{[X_1, \dot{A}_r]} \right\| + \left\| (\dot{X}_1)^{\text{odd}} \right\| + \left\| S_{(\dot{P}_r^+)}^{\text{odd}} \right\| \right) \sup_{x, k \in \mathbb{R}^3} \left| \phi(\mathbf{x}, \mathbf{k}) \right| \|\dot{A}(t, \cdot)\|_{L^2} \\ &+ 2\pi \|X_1\| \sup_{x, k \in \mathbb{R}^3} \left| \phi(\mathbf{x}, \mathbf{k}) \right| \|\ddot{A}(t, \cdot)\|_{L^2} + \left\| S_{(\dot{P}_r^+)}^{(2)\text{odd}} \right\|_{HS} \leq \\ &\leq 2\pi \left(2C^3 \|\dot{A}_r\|^2 + 2C \|\dot{A}_r\| \|X_1\| + \left\| (\dot{X}_1)^{\text{odd}} \right\| + \left\| S_{(\dot{P}_r^+)}^{\text{odd}} \right\| \right) \sup_{x, k \in \mathbb{R}^3} \left| \phi(\mathbf{x}, \mathbf{k}) \right| \|\dot{A}(t, \cdot)\|_{L^2} \\ &+ 2\pi C^2 \|\dot{A}_r\| \sup_{x, k \in \mathbb{R}^3} \left| \phi(\mathbf{x}, \mathbf{k}) \right| \|\ddot{A}(t, \cdot)\|_{L^2} + \left\| S_{(\dot{P}_r^+)}^{(2)\text{odd}} \right\|_{HS} \leq \\ &\leq 2\pi \left(6C^3 \|\dot{A}_r\|^2 + 2 \left\| S_{(\dot{P}_r^+)}^{\text{odd}} \right\| \right) \sup_{x, k \in \mathbb{R}^3} \left| \phi(\mathbf{x}, \mathbf{k}) \right| \|\dot{A}(t, \cdot)\|_{L^2} \\ &+ 2\pi C^2 \|\dot{A}_r\| \sup_{x, k \in \mathbb{R}^3} \left| \phi(\mathbf{x}, \mathbf{k}) \right| \|\ddot{A}(t, \cdot)\|_{L^2} + \left\| S_{(\dot{P}_r^+)}^{(2)\text{odd}} \right\|_{HS} \leq \\ &\leq 2\pi \left(10C^3 \|\dot{A}_r\|^2 + 2C^2 \|\ddot{A}_r\| \right) \sup_{x, k \in \mathbb{R}^3} \left| \phi(\mathbf{x}, \mathbf{k}) \right| \|\dot{A}(t, \cdot)\|_{L^2} \\ &+ 2\pi C^2 \|\dot{A}_r\| \sup_{x, k \in \mathbb{R}^3} \left| \phi(\mathbf{x}, \mathbf{k}) \right| \|\ddot{A}(t, \cdot)\|_{L^2} + \left\| S_{(\dot{P}_r^+)}^{(2)\text{odd}} \right\|_{HS}. \end{aligned}$$

Finally, we have to estimate the last term from above. The third derivative of the projection is given by

$$\left(\frac{d}{dr} (\dot{P}_r^+)^{\text{odd}} \right)^{\text{odd}} = S_{[S_{[\dot{P}_r^+, \dot{A}_r]^{\text{odd}}} \dot{A}_r]^{\text{odd}}} + S_{[(\dot{P}_r^+)^{\text{odd}}, \dot{A}_r]^{\text{odd}}} + S_{[\dot{P}_r^+, \ddot{A}_r]^{\text{odd}}} + S_{\frac{d}{dr} \ddot{A}_r}^{\text{odd}}.$$

Hence, we have

$$\begin{aligned} \left\| S_{(\dot{P}_r^+)^{\text{odd}}}^{(2)} \right\|_{HS} &\leq \pi C \left(\left\| S_{[\dot{P}_r^+, \dot{A}_r]^{\text{odd}}} \right\| + \left\| (\dot{P}_r^+)^{\text{odd}} \right\| \right) \sup_{x, k \in \mathbb{R}^3} \left| \phi_{\underline{t}}(\mathbf{x}, \mathbf{k}) \right| \left\| \dot{A}(t, \cdot) \right\|_{L^2} \\ &\quad + \pi C \left\| \dot{P}_r^+ \right\| \sup_{x, k \in \mathbb{R}^3} \left| \phi_{\underline{t}}(\mathbf{x}, \mathbf{k}) \right| \left\| \dot{A}(t, \cdot) \right\|_{L^2} + \pi C \sup_{x, k \in \mathbb{R}^3} \left| \phi_{\underline{t}}(\mathbf{x}, \mathbf{k}) \right| \left\| \frac{d^3}{dt^3} A(t, \cdot) \right\|_{L^2} \\ &\leq \pi C \left(4C^2 \left\| \dot{A}_r \right\|^2 + C \left\| \ddot{A}_r \right\| \right) \sup_{x, k \in \mathbb{R}^3} \left| \phi_{\underline{t}}(\mathbf{x}, \mathbf{k}) \right| \left\| \dot{A}(t, \cdot) \right\|_{L^2} \\ &\quad + \pi C^2 \left\| \dot{A}_r \right\| \sup_{x, k \in \mathbb{R}^3} \left| \phi_{\underline{t}}(\mathbf{x}, \mathbf{k}) \right| \left\| \ddot{A}(t, \cdot) \right\|_{L^2} + \pi C \sup_{x, k \in \mathbb{R}^3} \left| \phi_{\underline{t}}(\mathbf{x}, \mathbf{k}) \right| \left\| \frac{d^3}{dt^3} A(t, \cdot) \right\|_{L^2}. \end{aligned}$$

Summing it all up, we find

$$\begin{aligned} \left\| \dot{X}_2 \right\|_{HS} &\leq 4\pi C^2 \left\| \dot{A}_r \right\| \sup_{x, k \in \mathbb{R}^3} \left| \phi_{\underline{t}}(\mathbf{x}, \mathbf{k}) \right| \left(\left\| \ddot{A}(t, \cdot) \right\|_{L^2} + 4C \left\| \dot{A}_r \right\| \left\| \dot{A}(t, \cdot) \right\|_{L^2} \right) \\ &\quad + 2\pi \left(10C^3 \left\| \dot{A}_r \right\|^2 + 2C^2 \left\| \ddot{A}_r \right\| \right) \sup_{x, k \in \mathbb{R}^3} \left| \phi_{\underline{t}}(\mathbf{x}, \mathbf{k}) \right| \left\| \dot{A}(t, \cdot) \right\|_{L^2} \\ &\quad + 2\pi C^2 \left\| \dot{A}_r \right\| \sup_{x, k \in \mathbb{R}^3} \left| \phi_{\underline{t}}(\mathbf{x}, \mathbf{k}) \right| \left\| \ddot{A}(t, \cdot) \right\|_{L^2} \\ &\quad + \pi C \left(4C^2 \left\| \dot{A}_r \right\|^2 + C \left\| \ddot{A}_r \right\| \right) \sup_{x, k \in \mathbb{R}^3} \left| \phi_{\underline{t}}(\mathbf{x}, \mathbf{k}) \right| \left\| \dot{A}(t, \cdot) \right\|_{L^2} \\ &\quad + \pi C^2 \left\| \dot{A}_r \right\| \sup_{x, k \in \mathbb{R}^3} \left| \phi_{\underline{t}}(\mathbf{x}, \mathbf{k}) \right| \left\| \ddot{A}(t, \cdot) \right\|_{L^2} + \pi C \sup_{x, k \in \mathbb{R}^3} \left| \phi_{\underline{t}}(\mathbf{x}, \mathbf{k}) \right| \left\| \frac{d^3}{dt^3} A(t, \cdot) \right\|_{L^2} = \\ &= \pi C \sup_{x, k \in \mathbb{R}^3} \left| \phi_{\underline{t}}(\mathbf{x}, \mathbf{k}) \right| \left(40C^2 \left\| \dot{A}_r \right\|^2 \left\| \dot{A}(t, \cdot) \right\|_{L^2} + 5C \left\| \ddot{A}_r \right\| \left\| \dot{A}(t, \cdot) \right\|_{L^2} \right. \\ &\quad \left. + 7C \left\| \dot{A}_r \right\| \left\| \ddot{A}(t, \cdot) \right\|_{L^2} + \left\| \frac{d^3}{dt^3} A(t, \cdot) \right\|_{L^2} \right). \end{aligned} \tag{6.21}$$

The next corollary is a trivial consequence of Theorem 6.3. However, it is important in the context of second quantization. Thus, we state it as a result of its own.

Corollary 6.4. *Let $A(t, \mathbf{x}) \in C^\infty(\mathbb{R} \times \mathbb{R}^3 \rightarrow \mathbb{R}^3)$ be of order $|\mathbf{x}|^{-2-h}$ at infinity and such that its first partial derivatives with respect to position are of order $|\mathbf{x}|^{-1-h}$. Furthermore, let its partial derivatives with respect to position and up to second order be integrable and let the first and second derivative*

with respect to time be square integrable. Finally, let the vector potential be such that there are no eigenstates for zero kinetic energy of the extended Dirac operator to the space $L^2_{1/2+\varepsilon}(\mathbb{R}^3 \rightarrow \mathbb{C}^4)$ for some $\varepsilon > 0$. The off-diagonal parts of the time evolution, $P_t^\pm U(t, s) P_s^\mp$, are then Hilbert-Schmidt operators.

Proof. The assumptions fulfill the prerequisites of Theorem 6.3 (see Chapter 3). The adiabatic parameter might not be small for an arbitrary external field but is always finite. Thus, the right-hand-side of eq. (6.16) is an upper bound on the Hilbert-Schmidt norm. \square

Part II.

External field QED

7. Second quantization

7.1. Introduction

Quantum electrodynamics is the theory which describes the interaction between electromagnetic fields and matter. In the following chapters we will discuss the so called *external field model of QED* which neglects the interaction between particles and assumes the presence of an electromagnetic field generated by some external source. The reasons we restrict ourselves to such a model are twofold. First, up to now it has not been possible to formulate a rigorous quantum mechanical theory of electrodynamics and even external field QED poses difficult problems. Thus, from a fundamental perspective it is highly interesting to understand the structure and mathematics of external field QED as groundwork towards the fully interacting QED. The second interesting aspect of external field QED is its application to strong field physics. There, the external fields reach strengths where the particle interaction can be neglected to a good degree of approximation. This drew our attention to external field QED initially as we would like to describe the process of pair creation in strong laser fields.

To set up the theory one usually starts by defining the necessary Hilbert space – called Fock space. A constructive approach can be found in [Tha92, Chapter 10]. This works generally well for static external fields. However, as soon as one tries to incorporate a time-dependent vector potential in the theory this approach breaks down. The time evolution operator ceases to exist which was shown by Ruijsenaars [Rui77] using the results of Shale and Stinespring [SS65]. This is commonly referred to as *time evolution problem of external field QED*. A solution to this was proposed by Deckert et al. [DDMS10]. There, the authors develop an extensive new mathematical framework to rigorously establish the idea of the Dirac sea and to solve the time evolution problem by introducing *infinite wedge spaces*. The key observation by Deckert et al. is that the change of the external field also changes what we perceive as ground state or vacuum. Thus, the Hilbert space of the theory – in their case the infinite wedge space – also has to be *time-dependent* instead of being fixed. We adopt this idea and will construct time-dependent Fock spaces in a similar constructive way as in [Tha92, Chapter 10]. We then go on to define the canonical time evolution on this family of Hilbert spaces and prove a generalized version of the Shale-Stinespring criterion. Together with the result from Corollary 6.4 this shows that the time evolution operator indeed exists for a wide range of vector potentials.

We would now like to sketch the whole idea of Fock spaces, second quantization and its connection to the Dirac sea. In Chapter 1 we encountered the negative energy solutions of the Dirac equation and explained Dirac's idea of a "sea" filled with infinitely many electrons of negative energy. This sea ought to be very homogeneous due to electromagnetic repulsion and the Pauli exclusion principle. Thus, a free positive energy particle would not be able to feel the Dirac sea as

the forces cancel out. Furthermore, it cannot fall down to a lower energy state by the emission of radiation as all lower states are already occupied by other electrons. A test particle would therefore “fly” through all the sea electrons without detecting them¹. This filled sea is called the vacuum state. Physically relevant objects (in the sense of being detectable) are thus not all the electrons in the sea but rather deviations from it. Such deviations can either be electrons with positive energy or missing electrons of negative energy. We saw in Chapter 1 that the latter behave like positive energy particles with positive charge by the mechanism of charge conjugation. Concentrating only on the net deviations solves the problem of constructing a theory for infinitely many particles. But this theory has now to be capable of dealing with a varying amount of particles as transitions from the negative to the positive part and vice versa can happen, which correspond to the creation and annihilation of electrons and positrons. Therefore, we need a Hilbert space which can handle states with different numbers of particles and superpositions thereof. This space is called the Fock space and is constructed out of the spectral subspaces for positive and negative energy. We will do so in detail in the upcoming section. Furthermore, to jump between states of different particle numbers we need to be able to create and annihilate particles. We call the operators for this task creation and annihilation operators for electrons and positrons respectively. They are denoted by a^\dagger , a and b^\dagger , b . From the antisymmetry of fermionic states we conclude that the order matters in which we create or annihilate particles. Assume that we add two electrons which are in the states $\varphi, \psi \in \mathcal{H}^+$ to an existing Fock space state Ψ . We get by the antisymmetry consideration

$$a^\dagger[\varphi]a^\dagger[\psi]\Psi = -a^\dagger[\psi]a^\dagger[\varphi]\Psi.$$

Thus, we have to impose an anticommutator condition on these operators

$$\{a^\dagger[\varphi], a^\dagger[\psi]\} = 0 \quad \{a[\varphi], a[\psi]\} = 0$$

and similarly for the antiparticle operators. Note that the creation and annihilation operators for the electron are only valid for states $\varphi \in \mathcal{H}^+$ and the ones for the positron only for $\varphi \in \mathcal{H}^-$. Especially in a time-dependent setting where the spectral subspaces change over time this leads to mathematical troubles. Hence, from a mathematical point of view it would be desirable to have an operator which fulfills the anticommutation rules and is defined on the whole Hilbert space \mathcal{H} . The most direct way is to take the sum of the particle and antiparticle operators. We will see by the Propositions 7.2 and 7.3 in Section 7.3 that one should take a and b^\dagger to form the Fock space operator

$$\Gamma[\varphi] = a[\mathbb{P}^+ \varphi] + b^\dagger[\mathbb{P}^- \varphi]$$

for all states $\varphi \in \mathcal{H}$. It can then be shown (Proposition 7.7) that this operator and its adjoint indeed have similar properties as the creation and annihilation operators. But also from a physical point of view this definition is very intuitive (at least in the Dirac sea picture). It annihilates a

¹Although the mechanisms are different modern physics suggests similar behavior for neutrinos. As they interact only weakly with matter, every second large numbers of neutrinos flow right through us without being notified.

positive energy electron and creates a negative energy hole, i.e. also annihilates a negative energy electron. Thus, it can be interpreted as the Fock space representation of the annihilation and creation operators for electrons in the Dirac sea picture where we only have this one type of particles. The operator $\Gamma[\varphi]$ is usually called the *field operator* and the mapping $\varphi \mapsto \Gamma[\varphi]$, i.e. the assignment of a Hilbert space state to an operator fulfilling the anticommutation rules, is called second quantization. Although this term is often accompanied with some mystery it is in its fundamentals not much more than a neat procedure to get rid of the infinitely many particles in the Dirac sea. Taking into account only the net deviations from the Dirac sea turns it into a theory with a varying amount of finitely many particles. Nevertheless, one should keep in mind that many mathematical problems which stem from the infinite amount of particles are still present in the second quantized theory and are sometimes even harder to solve there as their origin is blurred.

We now show this procedure explicitly using the example of the second quantized Dirac hamiltonian. Please note that this is a non-rigorous derivation which simply serves to demonstrate the considerations above. We will see that one needs a simple form of renormalization to make sense of the resulting expression. In many presentations this seems to be introduced arbitrarily and might be hard to understand but it is indeed consequent if second quantization is understood in the context we just described. Our idea is the following. As the electrons do not interact in the free field case (and also in the external field model) each electron should evolve independently in time due to the one-particle time evolution. We will thus take one electron out of the sea, evolve it in time and put it back. If the electron has a negative energy this is similar to creating a hole, evolve it in time and annihilate it afterwards. Let us start with N positive energy electrons and N holes, described by the state $\Psi(t)$ at time t . We can write $\Psi(t)$ as a deviation from the vacuum state Ω where all electrons have negative energy in the following way

$$\Psi(t) = \sum_{\substack{i_1 < i_2 < \dots < i_n \\ j_1 < j_2 < \dots < j_m}}^N \alpha_{i_1, \dots, i_n, j_1, \dots, j_m}^* a^\dagger[\phi_{i_1}^+] \dots a^\dagger[\phi_{i_n}^+] b^\dagger[\phi_{j_1}^-] \dots b^\dagger[\phi_{j_m}^-] \Omega$$

with $\{\phi_n^\pm\}$ being an orthonormal basis of \mathcal{H}^\pm . According to the considerations above this state evolves to

$$\begin{aligned} \Psi(t + \Delta t) &= \widehat{U}(t + \Delta t, t) \Psi(t) = \\ &= \sum_{\substack{i_1 < i_2 < \dots < i_n \\ j_1 < j_2 < \dots < j_m}}^N \prod_{i \in \{i_1, \dots, i_n\}} a^\dagger[U(t + \Delta t, t) \phi_i^+] a[\phi_i^+] \prod_{j \notin \{j_1, \dots, j_m\}} b[U(t + \Delta t, t) \phi_j^-] b^\dagger[\phi_j^-] \\ &\quad \cdot \alpha_{i_1, \dots, i_n, j_1, \dots, j_m}^* a^\dagger[\phi_{i_1}^+] \dots a^\dagger[\phi_{i_n}^+] b^\dagger[\phi_{j_1}^-] \dots b^\dagger[\phi_{j_m}^-] \Omega = \\ &= \sum_{\substack{i_1 < i_2 < \dots < i_n \\ j_1 < j_2 < \dots < j_m}}^N \prod_{i \in \{i_1, \dots, i_n\}} a^\dagger[(1 - i\Delta t D) \phi_i^+] a[\phi_i^+] \prod_{j \notin \{j_1, \dots, j_m\}} b[(1 - i\Delta t D) \phi_j^-] b^\dagger[\phi_j^-] \\ &\quad \cdot \alpha_{i_1, \dots, i_n, j_1, \dots, j_m}^* a^\dagger[\phi_{i_1}^+] \dots a^\dagger[\phi_{i_n}^+] b^\dagger[\phi_{j_1}^-] \dots b^\dagger[\phi_{j_m}^-] \Omega + \mathcal{O}(\Delta t^2) \end{aligned}$$

where $U(t + \Delta t, t) = 1 - i\Delta t D + \mathcal{O}(\Delta t^2)$ is the one-particle time evolution. Note that we have in general

$$[a^\dagger[\phi_j^+] a[\phi_j^+], a^\dagger[\phi_i^+] a[\phi_i^+]] = [b[\phi_j^-] b^\dagger[\phi_j^-], b[\phi_i^-] b^\dagger[\phi_i^-]] = 0.$$

Furthermore, let $k, i \in \{i_1, \dots, i_n\}$ with $k \neq i$. We then have

$$[a^\dagger[D\phi_k^+] a[\phi_k^+], a^\dagger[\phi_i^+] a[\phi_i^+]] = -\langle \phi_i^+, D\phi_k^+ \rangle a[\phi_k^+] a^\dagger[\phi_i^+]$$

and thus

$$[a^\dagger[D\phi_k^+] a[\phi_k^+], a^\dagger[\phi_i^+] b[\phi_i^-]] a^\dagger[\phi_{i_1}^+] \dots a^\dagger[\phi_{i_n}^+] \Omega = 0.$$

Similarly, if $l, j \notin \{j_1, \dots, j_m\}$ with $l \neq j$ we find

$$[b[D\phi_l^-] b^\dagger[\phi_l^-], b[\phi_j^-] b^\dagger[\phi_j^-]] = -\langle \phi_j^-, D\phi_l^- \rangle b^\dagger[\phi_l^-] b[\phi_j^-]$$

and therefore

$$[b[D\phi_l^-] b^\dagger[\phi_l^-], b[\phi_j^-] b^\dagger[\phi_j^-]] b^\dagger[\phi_{j_1}^-] \dots b^\dagger[\phi_{j_m}^-] \Omega = 0$$

Hence, the order in the products above does not matter and we get by linearity of the creation and annihilation operators

$$\begin{aligned} \Psi_{t+\Delta t} &= \sum_{\substack{i_1 < i_2 < \dots < i_n \\ j_1 < j_2 < \dots < j_m}}^N \alpha_{i_1, \dots, i_n, j_1, \dots, j_m}^* \prod_{i \in \{i_1, \dots, i_n\}} a^\dagger[\phi_i^+] a[\phi_i^+] \prod_{j \notin \{j_1, \dots, j_m\}} b[\phi_j^-] b^\dagger[\phi_j^-] \\ &\quad \cdot a^\dagger[\phi_{i_1}^+] \dots a^\dagger[\phi_{i_n}^+] b^\dagger[\phi_{j_1}^-] \dots b^\dagger[\phi_{j_m}^-] \Omega \\ &\quad - i\Delta t \sum_{\substack{i_1 < i_2 < \dots < i_n \\ j_1 < j_2 < \dots < j_m}}^N \alpha_{i_1, \dots, i_n, j_1, \dots, j_m}^* \sum_{k \in \{i_1, \dots, i_n\}} \left(a^\dagger[D\phi_k^+] a[\phi_k^+] \prod_{\substack{i \in \{i_1, \dots, i_n\} \\ i \neq k}} a^\dagger[\phi_i^+] a[\phi_i^+] \right) \\ &\quad \cdot \prod_{j \notin \{j_1, \dots, j_m\}} b[\phi_j^-] b^\dagger[\phi_j^-] a^\dagger[\phi_{i_1}^+] \dots a^\dagger[\phi_{i_n}^+] b^\dagger[\phi_{j_1}^-] \dots b^\dagger[\phi_{j_m}^-] \Omega \\ &\quad - i\Delta t \sum_{\substack{i_1 < i_2 < \dots < i_n \\ j_1 < j_2 < \dots < j_m}}^N \alpha_{i_1, \dots, i_n, j_1, \dots, j_m}^* \sum_{l \notin \{j_1, \dots, j_m\}} \left(b[D\phi_l^-] b^\dagger[\phi_l^-] \prod_{\substack{j \in \{j_1, \dots, j_m\} \\ j \neq l}} b[\phi_j^-] b^\dagger[\phi_j^-] \right) \\ &\quad \cdot \prod_{i \in \{i_1, \dots, i_n\}} a^\dagger[\phi_i^+] a[\phi_i^+] a^\dagger[\phi_{i_1}^+] \dots a^\dagger[\phi_{i_n}^+] b^\dagger[\phi_{j_1}^-] \dots b^\dagger[\phi_{j_m}^-] \Omega + \mathcal{O}(\Delta t^2). \end{aligned}$$

Adding a particle and subtracting it again if it was not present or subtracting a particle and adding it again if it was present does not change the state. Thus, $\prod_{i \in \{i_1, \dots, i_n\}} a^\dagger[\phi_i^+] a[\phi_i^+]$ acts as a mere

identity and the same holds for the hole analogon. Hence, the first term is just $\Psi(t)$ again and the second and third term simplify a lot. The time derivative of the state is therefore

$$\begin{aligned} i \frac{d}{dt} \Psi(t) &= \lim_{\Delta t \rightarrow 0} \frac{\Psi(t + \Delta t) - \Psi(t)}{\Delta t} = \\ &= \sum_{\substack{i_1 < i_2 < \dots < i_n \\ j_1 < j_2 < \dots < j_m}}^N \sum_l \left(\sum_{k \in \{i_1, \dots, i_n\}} \langle \phi_l^+, D\phi_k^+ \rangle a^\dagger[\phi_l^+] a[\phi_k^+] + \sum_{k \notin \{j_1, \dots, j_m\}} \langle \phi_l^-, D\phi_k^- \rangle b[\phi_l^-] b^\dagger[\phi_k^-] \right) \\ &\quad \cdot \alpha_{i_1, \dots, i_n, j_1, \dots, j_m}^* a^\dagger[\phi_{i_1}^+] \dots a^\dagger[\phi_{i_n}^+] b^\dagger[\phi_{j_1}^-] \dots b^\dagger[\phi_{j_m}^-] \Omega \end{aligned}$$

where we expanded $D\phi_k^\pm$ in terms of basis vectors. We can extend both inner sums to all basis vectors ϕ_n^\pm as the extra factors are equal to zero when acting on $a^\dagger[\phi_{i_1}^+] \dots a^\dagger[\phi_{i_n}^+] b^\dagger[\phi_{j_1}^-] \dots b^\dagger[\phi_{j_m}^-] \Omega$. This yields

$$\begin{aligned} i \frac{d}{dt} \Psi_t &= \sum_{l,k} \langle \phi_l^+, D\phi_k^+ \rangle a^\dagger[\phi_l^+] a[\phi_k^+] + \langle \phi_l^-, D\phi_k^- \rangle b[\phi_l^-] b^\dagger[\phi_k^-] \\ &\quad \cdot \sum_{\substack{i_1 < i_2 < \dots < i_n \\ j_1 < j_2 < \dots < j_m}}^N \alpha_{i_1, \dots, i_n, j_1, \dots, j_m}^* a^\dagger[\phi_{i_1}^+] \dots a^\dagger[\phi_{i_n}^+] b^\dagger[\phi_{j_1}^-] \dots b^\dagger[\phi_{j_m}^-] \Omega = \\ &= \left(\sum_{l,k} \langle \phi_l^+, D\phi_k^+ \rangle a^\dagger[\phi_l^+] a[\phi_k^+] + \langle \phi_l^-, D\phi_k^- \rangle b[\phi_l^-] b^\dagger[\phi_k^-] \right) \Psi_t = \\ &= \widehat{H}' \Psi_t. \end{aligned}$$

We arrive at a partial differential equation for the time evolution of a state $\Psi(t)$, which has the form of a Schrödinger equation. Let us compute the expectation value of the operator \widehat{H}' and a state Ψ . For the vacuum we get

$$\begin{aligned} \langle \Omega, \widehat{H}' \Omega \rangle &= \sum_{l,k} \langle \Omega, (\langle \phi_l^+, D\phi_k^+ \rangle a^\dagger[\phi_l^+] a[\phi_k^+] + \langle \phi_l^-, D\phi_k^- \rangle b[\phi_l^-] b^\dagger[\phi_k^-]) \Omega \rangle = \\ &= \sum_l \langle \phi_l^-, D\phi_l^- \rangle = -\infty \end{aligned}$$

and as any state Ψ can be built out of the vacuum by adding the corresponding amount of finitely many particles the same holds true for any $\langle \Psi, \widehat{H}' \Psi \rangle$. This is of course bad news, so what went wrong? Up to this point we have computed the dynamics of all electrons present. As there are infinitely many particles in the sea it is of no surprise that the energy operator \widehat{H}' will always yield an expectation value of $-\infty$. In particular, the expectation value of the vacuum $E_{vac} = \langle \Omega, \widehat{H}' \Omega \rangle$ is precisely the sum of the expectation values of all electron states in the Dirac sea. As we said before we would like the theory to be only about the deviations from the sea as this is what we

can observe. Note that due to the anticommutation rules we have

$$\begin{aligned} i \frac{d}{dt} \Psi_t &= \left(\sum_{l,k} \langle \phi_l^+, D \phi_k^+ \rangle a^\dagger [\phi_l^+] a [\phi_k^+] + \langle \phi_l^-, D \phi_k^- \rangle b [\phi_l^-] b^\dagger [\phi_k^-] \right) \Psi_t = \\ &= \left(\sum_{l,k} \langle \phi_l^+, D \phi_k^+ \rangle a^\dagger [\phi_l^+] a [\phi_k^+] - \langle \phi_l^-, D \phi_k^- \rangle b^\dagger [\phi_k^-] b [\phi_l^-] \right) \Psi_t + E_{vac} \Psi_t = \\ &= \widehat{H} \Psi_t + E_{vac} \Psi_t. \end{aligned}$$

The operator \widehat{H} is now clearly positive as all of its summands are positive and for the vacuum we get

$$\langle \Omega, \widehat{H} \Omega \rangle = 0,$$

and therefore

$$0 \leq \langle \Psi, \widehat{H} \Psi \rangle < \infty.$$

This operator is called the second quantized Dirac operator which is nothing else than the hamiltonian for only the positive energy electrons and the holes. It is indeed simply derived by taking the Hamiltonian for the infinitely many particle system and subtracting the filled Dirac sea.

In the next chapter we will construct the Hilbert space for our theory of net deviations from the Dirac sea – the Fock space – in a mathematically rigorous manner. The resulting Hamiltonian in the free field case, given as the generator of the time evolution, would then have automatically the right form, and there is no need for the somewhat vague vacuum energy renormalization we performed above. However, given a time-dependent field there is no straightforward way to construct a Hamiltonian as it is not possible to formulate the theory in one fixed Fock space. We rather have to take a family of Fock spaces to be able to construct a time evolution. Therefore, it is not a priori clear how to formulate a partial differential equation on such a construction as we are missing the necessary algebraic structure. Thus, we will focus on the construction of the time evolution rather than the hamiltonian in the following.

7.2. Fock space

We now start with the general construction of Fock spaces. The results from this and the subsequent section will then be applied in the next chapter to define the time-dependent Fock spaces. The way we construct our Fock spaces is a generalization of the procedure in [Tha92]. We therefore follow a similar route to Fock spaces as described there. Let \mathcal{H} be the Hilbert space of the one-particle Dirac equation and let $V \subset \mathcal{H}$ be a closed subspace. We can then decompose the Hilbert space into

$$\mathcal{H} = V \oplus V^\perp$$

where V^\perp is the orthogonal complement to V . These subspaces equipped with the usual scalar product are again Hilbert spaces. We call V a *polarization*. The standard choice of these subspaces to construct a Fock space would be \mathcal{H}^+ and \mathcal{H}^- , but for now we will keep this freedom of the splitting. Let C be the charge conjugation operator defined in Chapter 4.2. We define the particle and antiparticle sector to be

$$\mathcal{F}_p^{(1)} := V \quad \text{and} \quad \mathcal{F}_a^{(1)} := CV^\perp.$$

The n -particle Hilbert space is then the n -fold anti-symmetrized Hilbert space tensor product of $\mathcal{F}_p^{(1)}$, i.e.

$$\mathcal{F}_p^{(n)} = \bigwedge^n V$$

which is constructed as follows. Let $\varphi_1, \dots, \varphi_n \in V$ and define the following map

$$\begin{aligned} \varphi_1 \wedge \dots \wedge \varphi_n &: V \times \dots \times V \rightarrow \mathbb{C}, \\ (\varphi_1 \wedge \dots \wedge \varphi_n) [\psi_1, \dots, \psi_n] &= \frac{1}{\sqrt{n!}} \sum_{\sigma \in \mathcal{S}_n} \text{sgn}(\sigma) \langle \varphi_1, \psi_{\sigma(1)} \rangle_{\mathcal{H}} \dots \langle \varphi_n, \psi_{\sigma(n)} \rangle_{\mathcal{H}}. \end{aligned}$$

It is by construction antisymmetric under permutation of any two φ_i and φ_j and antilinear in each φ_i . The addition and scalar multiplication of two such maps is given by pointwise addition and scalar multiplication. Let $\{\phi_j\}_{j \in \mathbb{N}}$ be an orthonormal basis of V and define $\mathcal{B}_p^{(n)}$ to be the ordered set of all such maps with elements from this orthonormal basis, i.e.

$$\mathcal{B}_p^{(n)} = \{ \phi_{j_1} \wedge \dots \wedge \phi_{j_n} \mid j_1 < \dots < j_n \}.$$

The canonical inner product on the space of all finite linear combinations, $\text{span } \mathcal{B}^{(n)}$, is then simply a sesquilinear form $\langle \cdot, \cdot \rangle : \text{span } \mathcal{B}_p^{(n)} \times \text{span } \mathcal{B}_p^{(n)} \rightarrow \mathbb{C}$ defined by

$$\langle \phi_{j_1} \wedge \dots \wedge \phi_{j_n}, \phi_{i_1} \wedge \dots \wedge \phi_{i_n} \rangle = \delta_{j_1 i_1} \dots \delta_{j_n i_n}$$

with $j_1 < \dots < j_n$ and $i_1 < \dots < i_n$.

Proposition 7.1. $\langle \cdot, \cdot \rangle$ is an inner product and $\mathcal{B}_p^{(n)}$ is an orthonormal basis of $\text{span } \mathcal{B}_p^{(n)}$.

Proof. Let $\psi \in \text{span } \mathcal{B}_p^{(n)}$ be the null vector. As ψ is a finite linear combination of elements of $\mathcal{B}_p^{(n)}$ we have for every $\varphi = (\varphi_1, \dots, \varphi_n) \in V \times \dots \times V$

$$\begin{aligned} 0 = \psi[\varphi] &= \sum_{j_1 < \dots < j_n}^N \psi_{j_1, \dots, j_n} (\phi_{j_1} \wedge \dots \wedge \phi_{j_n}) [\varphi_1, \dots, \varphi_n] = \\ &= \frac{1}{\sqrt{n!}} \sum_{\sigma \in \mathcal{S}_n} \text{sgn}(\sigma) \sum_{j_1 < \dots < j_n}^N \psi_{j_1, \dots, j_n} \langle \phi_{\sigma(j_1)}, \varphi_1 \rangle_{\mathcal{H}} \dots \langle \phi_{j_n}, \varphi_n \rangle_{\mathcal{H}}. \end{aligned}$$

Now, set $\varphi_1 = \phi_{i_1}, \dots, \varphi_n = \phi_{i_n}$ for a sequence $i_1 < \dots < i_n$. All terms vanish except where $\sigma(j_k) = i_k$ for all $1 \leq k \leq n$. This can only be fulfilled for $j_k = i_k$ and the identity permutation as the i_k and j_k are ordered. Thus, the only term surviving is ψ_{i_1, \dots, i_n} which is then identical to zero. By choosing such sequences repetitively we end up with $\psi_{i_1, \dots, i_n} = 0$ for every choice of $i_1 < \dots < i_n$. Hence, the $\phi_{i_1} \wedge \dots \wedge \phi_{i_n}$ are linearly independent and $\mathcal{B}_p^{(n)}$ is therefore a basis of $\text{span } \mathcal{B}_p^{(n)}$. The sesquilinearity and definition of $\langle \cdot, \cdot \rangle$ give

$$\langle \psi, \varphi \rangle = \sum_{j_1 < \dots < j_n} \bar{\psi}_{j_1, \dots, j_n} \varphi_{j_1, \dots, j_n}.$$

which shows positive definiteness. It is then obvious from the definition of $\langle \cdot, \cdot \rangle$ that $\mathcal{B}_p^{(n)}$ is in particular an orthonormal basis. \square

The n -fold anti-symmetrized Hilbert space product of V is now given as the usual Hilbert space completion (see e.g. [RS80]) of $\text{span } \mathcal{B}_p^{(n)}$ with respect to this inner product. Note that the resulting Hilbert space (and thus the inner product) does not depend on the choice of the orthonormal basis used in the construction of $\mathcal{B}_p^{(n)}$. Thus, any $\mathcal{B}_p^{(n)}$ constructed in the way above is an orthonormal basis of the wedge product space². The n -antiparticle sector is constructed in the same way starting with the space CV^\perp

$$\mathcal{F}_a^{(n)} = \bigwedge^n CV^\perp.$$

The space where no particle or antiparticle is present is called the vacuum state. There should only be one physical state associated with the vacuum and the rules of quantum mechanics teach us that every physical state is represented by a ray of vectors in a Hilbert space. Thus the Hilbert space for the vacuum is simply the complex numbers with the usual inner product

$$\mathcal{F}^{(0,0)} = \mathbb{C}.$$

The vacuum state, denoted by Ω , is then represented by a complex number with absolute value one. A state with n -particles and m -antiparticles is an element of the Hilbert space tensor product of $\mathcal{F}_p^{(n)}$ and $\mathcal{F}_a^{(m)}$

$$\mathcal{F}^{(n,m)} := \mathcal{F}_p^{(n)} \otimes \mathcal{F}_a^{(m)}.$$

The canonical inner product of these spaces is

$$\langle \varphi_p \otimes \eta_a, \psi_p \otimes \phi_a \rangle_{(n,m)} = \langle \varphi_p, \psi_p \rangle_n \langle \eta_a, \phi_a \rangle_m.$$

The basis of this tensor product is simply (see e.g. [RS80])

$$\mathcal{B}^{(n,m)} = \left\{ \phi_i^p \otimes \phi_j^a \mid \phi_i^p \in \mathcal{B}_p^{(n)}, \phi_j^a \in \mathcal{B}_a^{(m)}, i, j \in \mathbb{N} \right\}.$$

²It is actually not $\mathcal{B}_p^{(n)}$ itself but $\mathcal{B}_p^{(n)}$ under an isometric embedding which serves as basis.

To be able to handle states with a varying number of particles and antiparticles we define the *Fock space* with respect to the polarization V to be

$$\mathcal{F}_V = \bigoplus_{n,m=0}^{\infty} \mathcal{F}^{(n,m)},$$

where \bigoplus is the usual direct sum of countably many Hilbert spaces. Thus, elements of \mathcal{F}_V are sequences $(\varphi_{n,m})_{n,m}$ with $\varphi_{n,m} \in \mathcal{F}^{(n,m)}$ which are square summable

$$\sum_{n,m=0}^{\infty} \|\varphi_{n,m}\|_{(n,m)}^2 < \infty.$$

We name these elements with capital greek letters and write

$$\Psi = \Psi^{(0,0)} + \Psi^{(1,0)} + \Psi^{(0,1)} + \dots \equiv (\Psi^{(0,0)}, \Psi^{(1,0)}, \Psi^{(0,1)}, \dots).$$

For example, the vacuum state corresponds to the sequence $\Omega = (e^{i\alpha}, 0, 0, \dots)$ for any $\alpha \in \mathbb{R}$. The canonical inner product is given by

$$\langle \Psi, \Phi \rangle = \sum_{n,m=0}^{\infty} \langle \Psi^{(n,m)}, \Phi^{(n,m)} \rangle_{n,m}.$$

Such a space is then again a Hilbert space (see e.g. [RS80]) and the union of the basissets $\mathcal{B}^{(n,m)}$

$$\mathcal{B} = \bigcup_{n,m \in \mathbb{N}} \mathcal{B}^{(n,m)},$$

is then an orthonormal basis of this Fock space³.

Remark. We began the construction of our Fock space in the dual space $V^* \times \dots \times V^*$ rather than in the space $V \times \dots \times V$ of L^2 -functions. However, the connection is clear. We associate to every $\phi_{j_1} \wedge \dots \wedge \phi_{j_n}$ the function $\frac{1}{\sqrt{n!}} \sum_{\sigma \in \mathcal{S}_n} \text{sgn}(\sigma) \phi_{\sigma(j_1)}(x_1) \dots \phi_{j_n}(x_n)$. This is the unique association according to the Riesz representation theorem and connects our abstract Fock space and its inner product to the one used in [Tha92].

7.3. Creation and annihilation operators

To be able to jump between different particle sectors in the Fock space, we need operators which add and remove particles and antiparticles to a given state. To this end we will now define the creation and annihilation operators. We remind ourselves that states in V are to be interpreted as particles. Hence, a particle creation operator shall be able to add a state from V to an existing

³Again, we actually mean the union over the *canonical embeddings* of the basissets $\mathcal{B}^{(n,m)}$ into the Fock space \mathcal{F}_V .

(n, m) -particle state and turn it into an $(n + 1, m)$ -particle state. Let $\varphi \in V$ and let $\{\phi_n\}_{n \in \mathbb{N}}$ be an orthonormal basis of V . The *particle creation operator* is then a linear operator

$$a_V[\varphi] : \mathcal{F}_V \rightarrow \mathcal{F}_V .$$

defined via its action on the basis vectors of the particle sector

$$a_V^\dagger[\varphi] (\phi_{j_1} \wedge \cdots \wedge \phi_{j_n}) = \sum_{k=1}^{\infty} \langle \phi_k, \varphi \rangle \phi_k \wedge \phi_{j_1} \wedge \cdots \wedge \phi_{j_n}$$

and the *particle annihilation operator* is given by

$$a_V[\varphi] (\phi_{j_1} \wedge \cdots \wedge \phi_{j_n}) = \sum_{k=1}^n (-1)^{k-1} \overline{\langle \phi_{j_k}, \varphi \rangle} \phi_{j_1} \wedge \cdots \wedge \phi_{j_{k-1}} \wedge \phi_{j_{k+1}} \wedge \cdots \wedge \phi_{j_n}$$

and

$$a_V[\varphi] \Omega = 0 .$$

On the antiparticle sector they are defined to act as mere identity. It is also easy to see that the definition above is independent of the choice of basis vectors. Similarly, we define the *antiparticle creation* and *annihilation operators* to be linear operators on the Fock space by their action on the basis vectors of the antiparticle sector. Let $\{\phi_n^\dagger\}_{n \in \mathbb{N}}$ be an orthonormal basis of CV^\perp and $\varphi \in V^\perp$. We define

$$b_V^\dagger[\varphi] (\phi_{j_1}^\dagger \wedge \cdots \wedge \phi_{j_n}^\dagger) = (-1)^n \sum_{k=1}^{\infty} \langle \phi_k^\dagger, C\varphi \rangle \phi_k^\dagger \wedge \phi_{j_1}^\dagger \wedge \cdots \wedge \phi_{j_n}^\dagger$$

$$b_V[\varphi] (\phi_{j_1}^\dagger \wedge \cdots \wedge \phi_{j_n}^\dagger) = (-1)^n \sum_{k=1}^n (-1)^{k-1} \overline{\langle \phi_{j_k}^\dagger, C\varphi \rangle} \phi_{j_1}^\dagger \wedge \cdots \wedge \phi_{j_{k-1}}^\dagger \wedge \phi_{j_{k+1}}^\dagger \wedge \cdots \wedge \phi_{j_n}^\dagger$$

and

$$b_V[\varphi] \Omega = 0 .$$

Again, they shall act as the identity on the particle sector. The next two propositions summarize the important properties of these operators.

Proposition 7.2. *Let $\varphi, \varphi_1, \varphi_2 \in V$. The operators a_V^\dagger and a_V have the following properties:*

1. $\{a_V[\varphi_1], a_V[\varphi_2]\} = \{a_V^\dagger[\varphi_1], a_V^\dagger[\varphi_2]\} = 0 ,$
2. $\{a_V[\varphi_1], a_V^\dagger[\varphi_2]\} = \langle \varphi_1, \varphi_2 \rangle_{\mathcal{H}} ,$
3. $a_V^\dagger[\varphi] = (a_V[\varphi])^\dagger ,$

4. $\|a_V^\dagger[\varphi]\Psi\|^2 + \|a_V[\varphi]\Psi\|^2 = \|\varphi\|_{\mathcal{H}}^2 \|\Psi\|^2$ for any $\Psi \in \mathcal{F}_V$,
5. the mapping $\varphi \mapsto a_V[\varphi]$ is antilinear whereas the mapping $\varphi \mapsto a_V^\dagger[\varphi]$ is linear,
6. $a_V[\varphi]\Omega = 0$ and $a_V^\dagger[\varphi]\Omega = (0, \varphi, 0, 0, \dots)$,
7. $(a_V[\varphi])^2 \Psi = (a_V^\dagger[\varphi])^2 \Psi = 0$ for any $\Psi \in \mathcal{F}_V$.

Remark. The first two points are called the *canonical anticommutation relation* or CAR and the last point is the rigorous version of the *Pauli exclusion principle*.

Proof. 1. This follows directly from the anti-symmetry of the wedge product under exchange of any two functions.

2. This follows from the completeness of the orthonormal basis used in the definition of a_V^\dagger and a sign difference due to the alternating factor $(-1)^{k-1}$ in the definition of a_V .
3. We have

$$\begin{aligned} & \langle a_V[\varphi](\phi_{i_1} \wedge \dots \wedge \phi_{i_{n+1}}), \phi_{j_1} \wedge \dots \wedge \phi_{j_n} \rangle = \\ & = \sum_{k=1}^n (-1)^{k-1} \langle \phi_{i_k}, \varphi \rangle \delta_{i_1 j_1} \dots \delta_{i_{k-1} j_{k-1}} \delta_{i_{k+1} j_k} \dots \delta_{i_{n+1} j_n} = \\ & = \langle \phi_{i_1} \wedge \dots \wedge \phi_{i_{n+1}}, a_V^\dagger[\varphi](\phi_{j_1} \wedge \dots \wedge \phi_{j_n}) \rangle. \end{aligned}$$

4. Use 2) with $\varphi_1 = \varphi_2$ and 3).
5. See definition.
6. $a_V^\dagger[\varphi]\Omega = \sum_{k=1}^{\infty} \langle \phi_k, \varphi \rangle \phi_k = \varphi$ as $\{\phi_k\}_k$ is an orthonormal basis of V .
7. Use 1) with $\varphi_1 = \varphi_2$.

□

Proposition 7.3. Let $\varphi, \varphi_1, \varphi_2 \in V^\perp$. The operators b_V^\dagger and b_V have the following properties:

1. $\{b_V[\varphi_1], b_V[\varphi_2]\} = \{b_V^\dagger[\varphi_1], b_V^\dagger[\varphi_2]\} = 0$,
2. $\{b_V[\varphi_1], b_V^\dagger[\varphi_2]\} = \overline{\langle \varphi_1, \varphi_2 \rangle_{\mathcal{H}}}$,
3. $b_V^\dagger[\varphi] = (b_V[\varphi])^\dagger$,
4. $\|b_V^\dagger[\varphi]\Psi\|^2 + \|b_V[\varphi]\Psi\|^2 = \|\varphi\|_{\mathcal{H}}^2 \|\Psi\|^2$ for any $\Psi \in \mathcal{F}(V)$,
5. the mapping $\varphi \mapsto b_V[\varphi]$ is linear whereas the mapping $\varphi \mapsto b_V^\dagger[\varphi]$ is antilinear,

$$6. b_V[\varphi]\Omega = 0 \text{ and } b_V^\dagger[\varphi]\Omega = (0, 0, C\varphi, 0, \dots),$$

$$7. (b_V[\varphi])^2\Psi = (b_V^\dagger[\varphi])^2\Psi = 0 \text{ for any } \Psi \in \mathcal{F}_V.$$

Proof. Analogous to the previous one. \square

Proposition 7.4. *Let $\varphi_1 \in V$ and $\varphi_2 \in V^\perp$. We then have*

$$\{a_V[\varphi_1], b_V^\dagger[\varphi_2]\} = \{a_V^\dagger[\varphi_1], b_V[\varphi_2]\} = 0.$$

Proof. Interchanging the particle and antiparticle operators yields a minus sign due to the particle sector dependent minus sign in the definition of b_V and b_V^\dagger . \square

Now, as we are able to jump back and forth between states of different particle numbers one might think that we should be able to create every thinkable state out of the vacuum by adding the appropriate particle states and form superpositions thereof. This is the content of the next proposition.

Proposition 7.5. *Let $\{\phi_n\}$ and $\{\phi_n^\perp\}$ be the orthonormal bases of V and V^\perp which were used in the construction of \mathcal{B} . We then have*

$$\mathcal{B} = \left\{ a_V^\dagger[\phi_{i_1}] \dots a_V^\dagger[\phi_{i_n}] b_V^\dagger[\phi_{j_1}^\perp] \dots b_V^\dagger[\phi_{j_m}^\perp] \Omega \mid n, m \in \mathbb{N}_0 \right. \\ \left. \text{and } i_1 < i_2 < \dots < i_n, j_1 < j_2 < \dots < j_m \right\}.$$

Proof. Note that for $\{\phi_n^\perp\}$ being an orthonormal basis of V^\perp , $\{C\phi_n^\perp\}$ is an orthonormal basis of CV^\perp . Let $j_1 < \dots < j_n$ be an ordered sequence. It follows that

$$b_V^\dagger[\phi_{j_1}^\perp] (C\phi_{j_2}^\perp \wedge \dots \wedge C\phi_{j_n}^\perp) = C\phi_{j_1}^\perp \wedge C\phi_{j_2}^\perp \wedge \dots \wedge C\phi_{j_n}^\perp,$$

is a basis vector of \mathcal{B} and as $b_V^\dagger[\phi_{j_n}^\perp]\Omega = C\phi_{j_n}^\perp$ we can represent any basis vector of \mathcal{B} in the form of the statement. The same holds true for a_V^\dagger . \square

As we have explained in the introductory section it is useful from a mathematical and physical point of view to introduce the field operators.

Definition 7.6. *Let $\varphi \in \mathcal{H}$. The field operators on Fock space with polarizations V , called Γ_V and Γ_V^\dagger are defined as*

$$\Gamma_V^\dagger[\varphi] = a_V^\dagger[P_V \varphi] + b_V[P_V^\perp \varphi], \\ \Gamma_V[\varphi] = a_V[P_V \varphi] + b_V^\dagger[P_V^\perp \varphi].$$

Their properties are easily derived from those of a_V and b_V .

Proposition 7.7. *Let $\varphi, \varphi_1, \varphi_2 \in \mathcal{H}$. The field operators have the following properties:*

1. $\{\Gamma_V[\varphi_1], \Gamma_V[\varphi_2]\} = \{\Gamma_V^\dagger[\varphi_1], \Gamma_V^\dagger[\varphi_2]\} = 0$,
2. $\{\Gamma_V[\varphi_1], \Gamma_V^\dagger[\varphi_2]\} = \langle \varphi_1, \varphi_2 \rangle_{\mathcal{H}}$,
3. $\Gamma_V^\dagger[\varphi] = (\Gamma_V[\varphi])^\dagger$,
4. $\|\Gamma_V^\dagger[\varphi]\Psi\|^2 + \|\Gamma_V[\varphi]\Psi\|^2 = \|\varphi\|_{\mathcal{H}}^2 \|\Psi\|^2$ for any $\Psi \in \mathcal{F}_V$,
5. The mapping $\varphi \mapsto \Gamma_V[\varphi]$ is antilinear whereas the mapping $\varphi \mapsto \Gamma_V^\dagger[\varphi]$ is linear,
6. $\|\Gamma_V^\dagger[\varphi]\| = \|\Gamma_V[\varphi]\| = \|\varphi\|_{\mathcal{H}}$.

Proof. Use Propositions 7.2, 7.3 and 7.4 in a straightforward way. For the last point we use 4) to conclude that $\|\Gamma_V[\varphi]\| \leq \|\varphi\|$. Furthermore, if $P_V^+ \varphi \neq 0$ choose $\Psi = a_V^\dagger[P^+ \varphi]\Omega$ otherwise choose $\Psi = \Omega$. With 4) we get $\|\Gamma_V[\varphi]\Psi\| = \|\varphi\|_{\mathcal{H}} \|\Psi\|$ and therefore $\|\Gamma_V[\varphi]\| \geq \|\varphi\|_{\mathcal{H}}$. The proof for Γ_V^\dagger is the same. \square

Finally, we would like to define creation and annihilation operators of multiparticle states. These operators are crucial to derive the scattering amplitudes for pair creation in a second quantized setting. Following Proposition 7.5, it is possible to write any state with n -particles and m -antiparticles $\Psi^{(n,m)} \in \mathcal{F}_V$ as

$$\begin{aligned} \Psi^{(n,m)} &= \sum_{\substack{i_1 < i_2 < \dots < i_n \\ j_1 < j_2 < \dots < j_m}} \bar{\alpha}_{i_1, \dots, i_n, j_1, \dots, j_m} a_V^\dagger[\phi_{i_1}] \dots a_V^\dagger[\phi_{i_n}] b_V^\dagger[\phi_{j_1}^\perp] \dots b_V^\dagger[\phi_{j_m}^\perp] \Omega = \\ &= \sum \bar{\alpha}_{i_1, \dots, i_n, j_1, \dots, j_m} \Gamma_V^\dagger[\phi_{i_1}] \dots \Gamma_V^\dagger[\phi_{i_n}] \Gamma_V[\phi_{j_1}^\perp] \dots \Gamma_V[\phi_{j_m}^\perp] \Omega \end{aligned}$$

with $\|\Psi^{(n,m)}\|_{\mathcal{F}} = \left(\sum |\alpha_{i_1, \dots, i_n, j_1, \dots, j_m}|^2 \right)^{1/2}$. This justifies the following definition of the corresponding annihilation and creation operator for an (n, m) -particle state.

Definition 7.8. Let $\Psi^{(n,m)} \in \mathcal{F}_V$ be an (n, m) -particle state. We can decompose this state according to Proposition 7.5. The corresponding annihilation and creation operators on the Fock space for this state are defined as

$$\begin{aligned} \widehat{\Psi}^{(n,m)} &= \sum_{\substack{i_1 < i_2 < \dots < i_n \\ j_1 < j_2 < \dots < j_m}} \alpha_{i_1, \dots, i_n, j_1, \dots, j_m} \Gamma_V^\dagger[\phi_{j_m}^\perp] \dots \Gamma_V^\dagger[\phi_{j_1}^\perp] \Gamma_V[\phi_{i_n}] \dots \Gamma_V[\phi_{i_1}] \\ \widehat{\Psi}^{(n,m)\dagger} &= \sum_{\substack{i_1 < i_2 < \dots < i_n \\ j_1 < j_2 < \dots < j_m}} \bar{\alpha}_{i_1, \dots, i_n, j_1, \dots, j_m} \Gamma_V^\dagger[\phi_{i_1}] \dots \Gamma_V^\dagger[\phi_{i_n}] \Gamma_V[\phi_{j_1}^\perp] \dots \Gamma_V[\phi_{j_m}^\perp]. \end{aligned}$$

We chose to give the definition with the field operators instead of the particle creation and annihilation operators. In time-independent field theory there is no preferred choice but as we remarked before this is different in time-dependent QED where the spectral subspaces are not invariant anymore. Hence, one should use the field operators to stay out of trouble. We finish this section with expectable properties of the operator above.

Proposition 7.9. *Let $\Psi^{(n,m)} \in \mathcal{F}_V$ be an (n, m) -particle state. We have*

1. $\Psi^{(n,m)} = \widehat{\Psi}^{(n,m)\dagger} \Omega$,
2. $\widehat{\Psi}^{(n,m)} \Psi^{(n,m)} = \|\Psi^{(n,m)}\|_{\mathcal{F}}^2 \Omega$,
3. $\|\widehat{\Psi}^{(n,m)}\| = \|\Psi^{(n,m)}\|_{\mathcal{F}}$.

Proof. 1. This is obvious by definition.

2. Plugging in the definitions yields

$$\begin{aligned} \widehat{\Psi}^{(n,m)} \Psi^{(n,m)} &= \sum_{\substack{k_1 < k_2 < \dots < k_n \\ l_1 < l_2 < \dots < l_m}} \sum_{\substack{i_1 < i_2 < \dots < i_n \\ j_1 < j_2 < \dots < j_m}} \alpha_{k_1, \dots, k_n, l_1, \dots, l_m} \bar{\alpha}_{i_1, \dots, i_n, j_1, \dots, j_m} \\ &\cdot \Gamma_V^\dagger[\phi_{l_m}^\perp] \dots \Gamma_V^\dagger[\phi_{l_1}^\perp] \Gamma_V[\phi_{k_n}] \dots \Gamma_V[\phi_{k_1}] \\ &\cdot \Gamma_V^\dagger[\phi_{i_1}] \dots \Gamma_V^\dagger[\phi_{i_n}] \Gamma_V[\phi_{j_1}^\perp] \dots \Gamma_V[\phi_{j_m}^\perp] \Omega. \end{aligned}$$

Let us look at each of the terms in the sum above where $\{k_1, \dots, k_n\} \neq \{i_1, \dots, i_n\}$ or $\{l_1, \dots, l_m\} \neq \{j_1, \dots, j_m\}$. Assume the former is the case. Then we can find at least one k_r such that $k_r \neq i_q$ for all $i_q \in \{i_1, \dots, i_n\}$. Therefore, $\Gamma_V[\phi_{k_r}]$ anti-commutes with all the other Γ_V^\dagger to its right. Furthermore, we have $\Gamma_V[\phi_{k_r}] \Omega = b_V[\phi_{k_r}] \Omega = 0$ and thus all terms in the sum where $\{k_1, \dots, k_n\} \neq \{i_1, \dots, i_n\}$ vanish. As we also have $k_1 < k_2 < \dots < k_n$ and $i_1 < i_2 < \dots < i_n$ it follows $k_1 = i_1, \dots, k_n = i_n$. The same argument holds for the case where $\{l_1, \dots, l_m\} \neq \{j_1, \dots, j_m\}$. Hence, we get

$$\begin{aligned} \widehat{\Psi}^{(n,m)} \Psi^{(n,m)} &= \sum_{\substack{i_1 < i_2 < \dots < i_n \\ j_1 < j_2 < \dots < j_m}} |\alpha_{i_1, \dots, i_n, j_1, \dots, j_m}|^2 \Gamma_V^\dagger[\phi_{j_m}^\perp] \dots \Gamma_V^\dagger[\phi_{j_1}^\perp] \Gamma_V[\phi_{i_n}] \dots \Gamma_V[\phi_{i_1}] \\ &\cdot \Gamma_V^\dagger[\phi_{i_1}] \dots \Gamma_V^\dagger[\phi_{i_n}] \Gamma_V[\phi_{j_1}^\perp] \dots \Gamma_V[\phi_{j_m}^\perp] \Omega. \end{aligned}$$

Now, we interchange $\Gamma_V[\phi_{i_1}] \Gamma_V^\dagger[\phi_{i_1}] = \text{id}_{\mathcal{F}} - \Gamma_V^\dagger[\phi_{i_1, t}] \Gamma_V[\phi_{i_1}^\perp]$. As $i_1 < i_2, \dots, i_n$, we obtain that $\Gamma_V[\phi_{i_1}]$ commutes with all the Γ_V^\dagger 's to its right and again as $\Gamma_V[\phi_{i_1}] \Omega = 0$, this term gives no contribution. Hence, we end up with

$$\begin{aligned} &\dots \Gamma_V[\phi_{i_2}] \Gamma_V[\phi_{i_1}] \Gamma_V^\dagger[\phi_{i_1}] \Gamma_V^\dagger[\phi_{i_2}] \dots \Omega = \\ &= \dots \Gamma[\phi_{i_3}] \Gamma_V[\phi_{i_2}] \Gamma_V^\dagger[\phi_{i_2}] \Gamma_V^\dagger[\phi_{i_3}] \dots \Omega = \\ &= \dots = \Omega, \end{aligned}$$

and thus

$$\widehat{\Psi}^{(n,m)} \Psi^{(n,m)} = \sum_{\substack{i_1 < i_2 < \dots < i_n \\ j_1 < j_2 < \dots < j_m}} |\alpha_{i_1, \dots, i_n, j_1, \dots, j_m}|^2 \Omega = \|\Psi^{(n,m)}\|_{\mathcal{F}}^2 \Omega.$$

3. Let $\Phi^{(q,r)} \in \mathcal{F}^{(q,r)}$. We immediately see that $\widehat{\Psi}^{(n,m)} \Phi^{(q,r)} = 0$ if $q < n$ or $r < m$. Otherwise we get with the same argument as above that the first n and m indices of the coefficient of $\Phi^{(q,r)}$ have to be the same as the indices of the coefficient of $\Psi^{(n,m)}$. Furthermore, by using the anticommutation rules* in the same fashion as before we see that only the field operators belonging to the indices i_{n+1}, \dots, i_q and j_{m+1}, \dots, j_r are left over,

$$\begin{aligned} \|\widehat{\Psi}^{(n,m)} \Phi^{(q,r)}\|_{\mathcal{F}} &= \left\| \sum_{\substack{i_1 < i_2 < \dots < i_n \\ j_1 < j_2 < \dots < j_n}} \alpha_{i_1, \dots, i_n, j_1, \dots, j_m} \left(\sum_{\substack{i_{n+1} < i_{n+2} < \dots < i_q \\ j_{m+1} < j_{m+2} < \dots < j_r}} \bar{\beta}_{i_1, \dots, i_q, j_1, \dots, j_r} \right. \right. \\ &\quad \left. \cdot \Gamma_V^\dagger[\phi_{i_{n+1}}] \dots \Gamma_V^\dagger[\phi_{i_q}] \Gamma_V[\phi_{j_{m+1}}^\dagger] \dots \Gamma_V[\phi_{j_r}^\dagger] \Omega \right\|_{\mathcal{F}} \leq \\ &\leq \sum_{\substack{i_1 < i_2 < \dots < i_n \\ j_1 < j_2 < \dots < j_n}} |\alpha_{i_1, \dots, i_n, j_1, \dots, j_m}| \left\| \sum_{\substack{i_{n+1} < i_{n+2} < \dots < i_q \\ j_{m+1} < j_{m+2} < \dots < j_r}} \bar{\beta}_{i_1, \dots, i_q, j_1, \dots, j_r} \right. \\ &\quad \left. \cdot a_V^\dagger[\phi_{i_{n+1}}] \dots a_V^\dagger[\phi_{i_q}] b_V^\dagger[\phi_{j_{m+1}}^\dagger] \dots b_V^\dagger[\phi_{j_r}^\dagger] \Omega \right\|_{\mathcal{F}}. \end{aligned}$$

As we use an orthogonal basis of \mathcal{H} the states $a_V^\dagger[\phi_{i_{n+1}}] \dots a_V^\dagger[\phi_{i_q}] b_V^\dagger[\phi_{j_{m+1}}^\dagger] \dots b_V^\dagger[\phi_{j_r}^\dagger] \Omega$ are also all orthogonal according to proposition 7.5 and have the norm one. Hence, the second sum is just $\left(\sum |\beta_{i_1, \dots, i_q, j_1, \dots, j_r}|^2 \right)^{\frac{1}{2}}$ and therefore

$$\begin{aligned} \|\widehat{\Psi}^{(n,m)} \Phi^{(q,r)}\|_{\mathcal{F}} &\leq \sum_{\substack{i_1 < i_2 < \dots < i_n \\ j_1 < j_2 < \dots < j_n}} \left(|\alpha_{i_1, \dots, i_n, j_1, \dots, j_m}| \left(\sum_{\substack{i_{n+1} < i_{n+2} < \dots < i_q \\ j_{m+1} < j_{m+2} < \dots < j_r}} |\beta_{i_1, \dots, i_q, j_1, \dots, j_r}|^2 \right)^{\frac{1}{2}} \right) \leq \\ &\leq \left(\sum_{\substack{i_1 < i_2 < \dots < i_n \\ j_1 < j_2 < \dots < j_n}} |\alpha_{i_1, \dots, i_n, j_1, \dots, j_m}|^2 \right)^{\frac{1}{2}} \left(\sum_{\substack{i_1 < i_2 < \dots < i_q \\ j_1 < j_2 < \dots < j_r}} |\beta_{i_1, \dots, i_q, j_1, \dots, j_r}|^2 \right)^{\frac{1}{2}} = \|\Psi^{(n,m)}\|_{\mathcal{F}} \|\Phi^{(q,r)}\|_{\mathcal{F}}. \end{aligned}$$

For any $\Phi \in \mathcal{F}_V$ we thus get

$$\begin{aligned} \|\widehat{\Psi}^{(n,m)} \Phi\|_{\mathcal{F}} &= \left(\sum_{k,l=0}^{\infty} \|\widehat{\Psi}^{(n,m)} \Phi^{(k,l)}\|^2 \right)^{\frac{1}{2}} \leq \|\Psi^{(n,m)}\|_{\mathcal{F}} \left(\sum_{k,l=0}^{\infty} \|\Phi^{(k,l)}\|^2 \right)^{\frac{1}{2}} = \\ &= \|\Psi^{(n,m)}\|_{\mathcal{F}} \|\Phi\|_{\mathcal{F}}. \end{aligned}$$

Together with part two this proves statement three. □

8. Time evolution

8.1. Motivation and definition

At the beginning of this chapter a motivation of time evolution in QED will be given. Again, the most intuitive way to approach this topic is via the Dirac sea picture. Assume we have a many-body system consisting of n particles of one (fermionic) species. The wave function is then in general a superposition of the n -fold wedge products defined in Chapter 7.2,

$$\Psi^{(n)} = \sum \alpha_{i_1, \dots, i_n} \phi_{i_1} \wedge \dots \wedge \phi_{i_n},$$

in some suitable Hilbert space. The time evolution of the many body Schrödinger or Dirac equation with an external field and no particle interaction is simply the one-particle time evolution applied to every ϕ_i ,

$$\widehat{U} \Psi^{(n)} = \sum \alpha_{i_1, \dots, i_n} (U \phi_{i_1}) \wedge \dots \wedge (U \phi_{i_n}).$$

This pattern stays the same for any n . QED is seen as an “infinitely-many particle system” in the Dirac sea interpretation. Thus, we have to take the limit $n \rightarrow \infty$ for $\Psi^{(n)}$ in some sense. Of course, it is a priori not clear what this is supposed to mean. It is possible to proceed in such a way and give a precise meaning to the so called *infinite wedge product* as was done by Deckert et al. [DDMS10]. In this setting, the second quantized time evolution is indeed the generalization of the many-body time evolution sketched above. Some serious mathematical work is required to set up the whole framework in which this theory can be formulated. It seems to be a little contrary to the idea of only considering the net deviations from the Dirac sea. Thus, it is not the standard way of defining the time evolution in external field QED but it can be shown that both paths are equivalent.

We would like to define the time evolution in a way which is independent of the size of the sea so that we can perform the limit $n \rightarrow \infty$. Assume we have a “bare” vacuum with no particles present at all – an empty sea so to say – and an operator A^\dagger which adds a particle to an existing state with n electrons. It is then possible to create every n -particle state out of the bare vacuum by subsequent application of A^\dagger to the vacuum. Now, let $\Psi^{(n)}$ be a product state. We then get according to the Chapters 7.2 and 7.3

$$A^\dagger[\varphi] \Psi^{(n)} = \sum_{k=1}^{\infty} \langle \phi_k, \varphi \rangle \phi_k \wedge \phi_{i_1} \wedge \dots \wedge \phi_{i_n}.$$

The time evolution of such an $(n + 1)$ -particle state is

$$\widehat{U} A^\dagger[\varphi] \Psi^{(n)} = \sum_{k=1}^{\infty} \langle \phi_k, \varphi \rangle (U \phi_k) \wedge (U \phi_{i_1}) \wedge \dots \wedge (U \phi_{i_n})$$

due to the considerations above. We can repeat this procedure with the state $\widehat{U} \Psi^{(n)}$ and add an arbitrary particle φ'

$$\begin{aligned} A^\dagger[\varphi'] \widehat{U} \Psi^{(n)} &= \sum_{k=1}^{\infty} \langle \phi_k, \varphi' \rangle (\phi_k) \wedge (\phi_{i_1}) \wedge \cdots \wedge (\phi_{i_n}) = \\ &= \sum_{k=1}^{\infty} \langle U \phi_k, \varphi' \rangle (U \phi_k) \wedge (U \phi_{i_1}) \wedge \cdots \wedge (U \phi_{i_n}) . \end{aligned}$$

We used the fact that the definition of a creation operator is independent of the choice of orthonormal basis and that $\{U \phi_k\}_{k \in \mathbb{N}}$ is an orthonormal basis if $\{\phi_k\}_{k \in \mathbb{N}}$ is one. Setting $\varphi' = U \varphi$, we get

$$A^\dagger[U \varphi] \widehat{U} \Psi^{(n)} = \sum_{k=1}^{\infty} \langle U \phi_k, U \varphi \rangle (U \phi_k) \wedge (U \phi_{i_1}) \wedge \cdots \wedge (U \phi_{i_n}) = \widehat{U} A^\dagger[\varphi] \Psi^{(n)} .$$

We conclude that for any n -particle system with one fermionic particle species, the time evolution defined via the usual many-body Schrödinger or Dirac equation is equivalent¹ to a unitary operator \widehat{U} fulfilling

$$A^\dagger[U \varphi] = \widehat{U} A^\dagger[\varphi] \widehat{U}^\dagger \quad \text{for all } \varphi \in \mathcal{H} .$$

This expression does not explicitly depend on the particle number anymore and could thus serve well as the definition of the time evolution on the infinitely-many particle system (if we can make sense of A^\dagger on such a space). As we said before, the field operator Γ^\dagger can be physically understood as creation operator for a Dirac electron. Thus, we will use it in the definition of the time evolution taking the place of A^\dagger from the heuristic argument above.

Now, before we state the precise definition of a time evolution we introduce the *time-dependent* Fock spaces. The reason we are forced to do so is the time evolution problem in usual external field QED which we discuss briefly in the next section. In usual QED the Fock space is built with respect to the polarization $V = \mathcal{H}^+$. An external field however changes these subspaces according to Chapter 4.1. Hence, we will define the family of time-dependent polarizations $(V_t)_{t \in \mathbb{R}}$ to be the positive spectral subspace at time t , $V_t = \mathcal{H}_t^+$. The *time-dependent Fock space* is then given as the family of Fock spaces corresponding to this polarization $\mathcal{F}_t = \mathcal{F}_{V_t}$. Note that the physical implications of this might be uncomfortable. What we call particles and antiparticles now depends on the external field and is not of universal objective nature anymore. Again, from the Dirac sea perspective this surprising result has a rather simple explanation. What we can detect as a particle and antiparticle depends on which electrons of the sea are visible or not to our detectors. And the presence of an electromagnetic force might indeed be able to change this.

The time evolution on these families of Fock spaces is now given by the following definition.

¹We swept some subtleties under the rug here. First, we have to be able to embed $\Psi^{(n)}$ into a space where states with lower particle numbers are also possible to be able to define A^\dagger . This is always possible in the external field setting via Fock spaces. Second, the time evolution operator \widehat{U} is defined on this bigger space and thus the n -particle Schrödinger time evolution is not strictly equivalent to but rather the restriction of \widehat{U} to the n -particle subspace.

Definition 8.1. Let $U(t, s)$ be a one-particle time evolution on a Hilbert space \mathcal{H} . Let Γ_t be the field operator corresponding to the splitting \mathcal{H}_t^+ . The time evolution on the time-dependent Fock space is a family of unitary operators $\widehat{U}(t, s) : \mathcal{F}_s \rightarrow \mathcal{F}_t$ which fulfill

1. $\Gamma_t[U(t, s)\varphi] = \widehat{U}(t, s) \Gamma_s[\varphi] (\widehat{U}(t, s))^\dagger$ for all $\varphi \in \mathcal{H}$,
2. $\widehat{U}(t, t) = \text{id}_{\mathcal{F}_t}$,
3. $\widehat{U}(t, s) = \widehat{U}(t, r)\widehat{U}(r, s)$.

We need to add some remarks to this definition. The first point in the definition is the standard way of lifting *any* unitary operator from the one-particle Hilbert space to Fock space. The only difference in the time-dependent setting is that now the field operators are also time-dependent. Properties 2) and 3) are well known in usual quantum mechanics. However, there one usually starts with a wave equation and Stone's theorem guarantees these properties. Hence, there they are a mathematical consequence. In time-dependent Fock space setting, as we mentioned earlier, there is usually no generator of a time evolution and Stone's theorem is not valid. However, from a physical point of view, those two properties seem to be immanent to the whole concept of a time evolution. Thus, they should be included in the definition.

Proposition 8.2. Let $\widehat{U}(t, s)$ be a unitary time evolution as stated in Definition 8.1. It has the following properties:

1. $(\widehat{U}(t, s))^\dagger = \widehat{U}(s, t)$,
2. $\widehat{U}(t, s)$ is unique up to a phase $e^{i\varphi(t, s)}$,
3. the phase function fulfills $\varphi(t, s) = \varphi(t, r) + \varphi(r, s)$ for any r and $\varphi(t, t) = 0$ modulo 2π .

Proof. 1. This follows directly from 2) and 3) in the Definition 8.1.

2. Let $\widehat{U}(t, s)$ and $\widehat{U}'(t, s)$ be two unitary time evolutions according to the definition above. We immediately get that $[\Gamma_s[\varphi], \widehat{U}(s, t)\widehat{U}'(t, s)] = 0$ for all $\varphi \in \mathcal{H}$ and likewise for $\Gamma_s^\dagger[\varphi]$. This yields

$$a_s[\varphi]\widehat{U}(s, t)\widehat{U}'(t, s)\Omega = 0 \quad \text{for all } \varphi \in \mathcal{H}_s^+,$$

which implies that $\widehat{U}(s, t)\widehat{U}'(t, s)\Omega$ is the vacuum state which is unique up to a phase. Thus,

$$\widehat{U}(s, t)\widehat{U}'(t, s)\Omega = e^{i\varphi(t, s)}\Omega.$$

Therefore, using Definition 7.8 of the multi-particle creation operator we have for every state $\Psi_s \in \mathcal{F}_s$

$$\begin{aligned} \widehat{U}(t, s) \widehat{U}'(t, s) \Psi_s &= \sum_{n, m} \alpha_{n, m} \widehat{\Psi}^{(n, m)} \widehat{U}(t, s) \widehat{U}'(t, s) \Omega = \\ &= \sum_{n, m} \alpha_{n, m} \widehat{\Psi}^{(n, m)} e^{i\varphi(t, s)} \Omega_s = e^{i\varphi(t, s)} \Psi_s. \end{aligned}$$

Hence,

$$\widehat{U}'(t, s) = e^{i\varphi(t, s)} \widehat{U}(t, s).$$

3. This also follows directly from 2) and 3) in the Definition 8.1. □

Hence, the time evolution given by Definition 8.1 is not unique. One phase function which fulfills the conditions in 3) is e.g. a time integral over the external field. This ambiguity in the time evolution does not matter in the determination of event probabilities as only the absolute values of the scattering matrix enter such quantities. And a phase function does not alter the absolute value. However, the variation of the scattering amplitudes with respect to the external field is linked to the QED current (see [Sch14]). The essence of this connection and possible further conditions for the definition of the time evolution are content of ongoing research. Deckert and Merkl have announced results to shed more light onto this.

8.2. Time evolution problem

The Definition 8.1 of the time evolution raises the question whether such unitary operators exist at all. In the usual formulation of external field QED, i.e. with a fixed Fock space constructed from the negative and positive energy subspaces of the free Hamiltonian, this question has been answered by Shale and Stinespring [SS65] and Ruijsenaars [Rui77]. Shale and Stinespring showed that a unitary one-particle operator can be lifted to Fock space in the sense of Definition 8.1 if and only if its off diagonal components, $P^+ U(t, s) P^-$ and $P^- U(t, s) P^+$ are Hilbert-Schmidt operators (see also [Tha92, Thm 10.6, Thm 10.7]). The spectral projections refer to the free Dirac hamiltonian. Ruijsenaars showed in 1977 that the off-diagonal components of the time evolution are Hilbert-Schmidt if and only if the magnetic vector potential A is equal to zero. This result is shattering as it is unclear what the non-existence of a time evolution is supposed to mean. Besides, there exist external fields where the vector potential can be gauged away. Hence, the existence of the time evolution could be explicitly gauge dependent in such a theory.

There are basically two conclusions which can be drawn here. Either the concept of a time evolution itself is not a proper one in the framework of QED anymore. Or the way it has been defined is incorrect in the presence of time-dependent fields. The former one seems to be more widespread and indeed most of QED is dealing with scattering situations where any external field

is not active anymore. If one adopts this point of view on the fundamental level though, it has to be made clear in a precise way what this means and especially how the explicit time-dependence in classical physics and quantum mechanics can arise from such a theory. To the best of our knowledge no such work is available and most textbooks seem to take a rather pragmatic view. Experiments are close to ideal scattering situations and as we are able to deal with them there is not much to worry about. This is rather unsatisfactory on a fundamental level though. Thus, there have been several approaches to fix this issue, one of them being time-dependent infinite wedge spaces of Deckert et al. (see e.g. [Laz11] for an overview of other approaches).

We will show in the next section that a time evolution does exist on the time-dependent Fock space as we constructed it.

8.3. Generalized Shale-Stinespring criterion

The next lemma gives us a nice characterization when and under which circumstances the canonical lift of a time evolution on the Hilbert space \mathcal{H} to the time-dependent Fock spaces is possible.

Lemma 8.3. *Let $s, t \in \mathbb{R}$ and let $U(t, s) : \mathcal{H} \rightarrow \mathcal{H}$ be a time evolution on the one-particle Hilbert space \mathcal{H} . Let $\Omega \in \mathcal{F}_s$ be the vacuum state, i.e.*

$$\Gamma_s[\varphi]\Omega = \Gamma_s^\dagger[\phi]\Omega = 0 \quad \text{for all } \varphi \in \mathcal{H}_s^+ \text{ and all } \phi \in \mathcal{H}_s^- .$$

There is a state $\Psi \in \mathcal{F}_t$ other than the null vector such that

$$\Gamma_t[U(t, s)\varphi]\Psi = \Gamma_t^\dagger[U(t, s)\phi]\Psi = 0 \quad \text{for all } \varphi \in \mathcal{H}_s^+ \text{ and all } \phi \in \mathcal{H}_s^- \quad (8.1)$$

if and only if there is a unitary operator $\widehat{U}(t, s) : \mathcal{F}_s \rightarrow \mathcal{F}_t$ such that

$$\Gamma_t[U(t, s)\psi] = \widehat{U}(t, s) \Gamma_s[\psi] (\widehat{U}(t, s))^\dagger \quad \text{for all } \psi \in \mathcal{H} . \quad (8.2)$$

Proof. If there exists a unitary operator fulfilling eq. (8.2) then it is easy to see that $\Psi = \widehat{U}(t, s)\Omega$ is the required state.

On the other hand, if there exists a state Ψ such that eq. (8.1) holds then we can construct an operator acting on the linear hull of basis vectors in \mathcal{F}_s

$$\begin{aligned} \widetilde{U}(t, s) : \text{span}(\mathcal{B}_s) &\rightarrow \mathcal{F}_t, \\ \Gamma_s^\dagger[\phi_{i_1}^+] \dots \Gamma_s^\dagger[\phi_{i_n}^+] \Gamma_s[\phi_{j_1}^-] \dots \Gamma_s[\phi_{j_m}^-] \Omega &\mapsto \\ \Gamma_t^\dagger[U(t, s)\phi_{i_1}^+] \dots \Gamma_t^\dagger[U(t, s)\phi_{i_n}^+] \Gamma_t[U(t, s)\phi_{j_1}^-] \dots \Gamma_t[U(t, s)\phi_{j_m}^-] \Psi \end{aligned}$$

where $\{\phi_n^+\}_{n \in \mathbb{N}}$ and $\{\phi_n^-\}_{n \in \mathbb{N}}$ are ONB of \mathcal{H}_s^+ and \mathcal{H}_s^- . Using the CAR and eq. (8.1) we can easily infer that eq. (8.2) holds for $\widetilde{U}(t, s)$ and the orthonormal bases $\{\phi_n^+\}_{n \in \mathbb{N}}$ and $\{\phi_n^-\}_{n \in \mathbb{N}}$. Due to

property 6) of Proposition 7.7, eq. (8.2) then also holds for any $\psi \in \mathcal{H}$. Thus, it is also true for the unique linear extension

$$\widehat{U}(t, s) : \mathcal{F}_s \rightarrow \mathcal{F}_t, \quad \widehat{U}(t, s)|_{\text{span}(\mathcal{B}_s)} = \widetilde{U}(t, s).$$

To prove unitarity we note that eq. (8.1), the CAR and the orthogonality of the Hilbert space basis vectors can be used to show that $\widetilde{U}(t, s)$ leaves the norm of all basis vectors in \mathcal{B}_s invariant and is thus norm preserving on $\text{span}(\mathcal{B}_s)$. The same is then also true for the linear extension. The action of $\widehat{U}(t, s)$ on

$$\mathcal{M} := \left\{ \Gamma_s^+ [U(s, t) \phi_{i_n}] \Gamma_s [U(s, t) \phi_{j_1}^+] \dots \Gamma_s [U(s, t) \phi_{j_m}^+] \Omega_s \mid \text{for all } i_1 < \dots, i_n, j_1 < \dots < j_m \right\}$$

is $\widehat{U}(t, s)\mathcal{M} = \mathcal{B}_t$. Thus, $\text{span } \mathcal{B}_t = \text{span } \widehat{U}(t, s)\mathcal{M} = \widehat{U}(t, s) \text{span } \mathcal{M}$ by linearity and therefore, $\text{span } \mathcal{B}_t \subseteq \text{ran } \widehat{U}(t, s) \subseteq \mathcal{F}_t$. The range of $\widehat{U}(t, s)$ is therefore dense and the operator is unitary. \square

Remark. The state Ψ is in general *not* the vacuum state of \mathcal{F}_t . This is the crucial difference between the time-independent Fock space setting and the family of time-dependent Fock spaces and allows e.g. for the process of pair creation.

Definition 8.4. *If the state Ψ from Lemma 8.3 exists, we call the one-particle operator $U(t, s)$ unitarily implementable.*

Before we go on to prove the two main results of this section, we need some relations between the spectral subspaces under the time evolution. Note that for the sake of notation we abbreviate $P_t^+ U(t, s) P_s^- = U_{t,s}^{+-}$ and similarly.

Lemma 8.5. 1. *We have $U_{t,s}^{+-} \ker U_{t,s}^{--} = P_t^+ \ker U_{s,t}^{++}$ and $U_{t,s}^{-+} \ker U_{t,s}^{++} = P_t^- \ker U_{s,t}^{--}$.*

2. *We have $U_{t,s}^{-+} (\ker U_{t,s}^{++})^\perp \perp \ker U_{s,t}^{--}$ and $U_{t,s}^{+-} (\ker U_{t,s}^{--})^\perp \perp \ker U_{s,t}^{++}$.*

3. *We have $U_{t,s}^{++} (\ker U_{t,s}^{++})^\perp \perp \ker U_{s,t}^{++}$ and $U_{t,s}^{--} (\ker U_{t,s}^{--})^\perp \perp \ker U_{s,t}^{--}$.*

4. *If $U_{t,s}^{+-} + U_{t,s}^{-+}$ is compact then $\ker U_{t,s}^{++}$ and $\ker U_{t,s}^{--}$ are finite dimensional subspaces.*

Proof. The proof of 1) and 4) can be found in [Tha92], Chapter 10.3.2, by noting that $U^{\text{even}} = U_{t,s}^{++} + U_{t,s}^{--}$ and $U^{\text{odd}} = U_{t,s}^{+-} + U_{t,s}^{-+}$ and $\ker U^{\text{even}}(t, s) = P_s^+ \ker U_{t,s}^{++} \oplus P_s^- \ker U_{t,s}^{--}$.

To prove 2) we start with $(\ker U_{t,s}^{++})^\perp \perp P_t^+ \ker U_{t,s}^{++}$ which is by 1) equivalent to $(\ker U_{t,s}^{++})^\perp \perp U_{s,t}^{+-} \ker U_{s,t}^{--}$ and thus $(U_{s,t}^{+-})^\dagger (\ker U_{t,s}^{++})^\perp \perp \ker U_{s,t}^{--}$ and similarly for the second part.

The third statement is easy to see as we have trivially $(\ker U_{t,s}^{++})^\perp \perp 0$ which can be written as $(\ker U_{t,s}^{++})^\perp \perp U_{s,t}^{++} \ker U_{s,t}^{++}$ and thus $(U_{s,t}^{++})^\dagger (\ker U_{t,s}^{++})^\perp \perp \ker U_{s,t}^{++}$. The second part is analogous.

For the last statement we note that the unitarity of the time evolution yields

$$(U_{s,t}^{++} + U_{s,t}^{--})(U_{t,s}^{++} + U_{t,s}^{--}) = \text{id}_{\mathcal{H}} - (U_{s,t}^{+-} + U_{s,t}^{-+})(U_{t,s}^{-+} + U_{t,s}^{+-}).$$

Therefore, we have

$$\begin{aligned} \ker(U_{t,s}^{++} + U_{t,s}^{--}) &\subset \ker(U_{s,t}^{++} + U_{s,t}^{--})(U_{t,s}^{++} + U_{t,s}^{--}) = \\ &= \ker(\text{id}_{\mathcal{H}} - (U_{s,t}^{+-} + U_{s,t}^{-+})(U_{t,s}^{-+} + U_{t,s}^{+-})). \end{aligned}$$

If $U_{t,s}^{-+} + U_{t,s}^{+-}$ is compact then the eigenvalues of $(U_{s,t}^{+-} + U_{s,t}^{-+})(U_{t,s}^{-+} + U_{t,s}^{+-})$ are isolated and of finite multiplicity, in particular if one is an eigenvalue then

$$\dim \ker(\text{id}_{\mathcal{H}} - (U_{s,t}^{+-} + U_{s,t}^{-+})(U_{t,s}^{-+} + U_{t,s}^{+-})) < \infty.$$

□

To prove the first part of the Shale-Stinespring criterion we need to construct a state according to Lemma 8.3. To do so, we define the rather abstract operator $\exp[A a_t^\dagger b_t^\dagger]$ for some operator A , where $A^{+-} : \mathcal{H}_t^- \mapsto \mathcal{H}_t^+$ is Hilbert-Schmidt, in the following way. For $n \in \mathbb{N}$ we define

$$(A a_t^\dagger b_t^\dagger)^n = \sum_{\substack{i_1, \dots, i_n \\ j_1, \dots, j_n}} \langle \phi_{i_1}^+, A \phi_{j_1}^- \rangle \dots \langle \phi_{i_n}^+, A \phi_{j_n}^- \rangle a_t^\dagger[\phi_{i_1}^+] \dots a_t^\dagger[\phi_{i_n}^+] b_t^\dagger[\phi_{j_1}^-] \dots b_t^\dagger[\phi_{j_n}^-] \quad (8.3)$$

with $\{\phi_n^+\}_n$ and $\{\phi_n^-\}_n$ being the orthonormal bases of \mathcal{H}_t^\pm . A straightforward computation using the CAR shows that

$$\|(A a_t^\dagger b_t^\dagger)^n \Omega\| = \|A^{+-}\|_{\text{HS}}^n.$$

Therefore, as $(A a_t^\dagger b_t^\dagger)^n$ commutes with every creation operator, the action of it on every $\Psi \in \text{span } \mathcal{B}$, where \mathcal{B} is the Fock space basis from Proposition 7.5, is well defined. The exponential is then given by

$$\exp[A a_t^\dagger b_t^\dagger] = \sum_n \frac{(A a_t^\dagger b_t^\dagger)^n}{n!}.$$

With the previous considerations at hand we find that

$$\|\exp[A a_t^\dagger b_t^\dagger] \Omega\| \leq \exp[\|A^{+-}\|_{\text{HS}}],$$

and by the same reasoning as before it is clear that $\exp[A a_t^\dagger b_t^\dagger]$ is well defined on $\text{span } \mathcal{B}$. Using the CAR it is now easy to see that for $\varphi_1 \in \mathcal{H}_t^+$

$$[\exp[A a_t^\dagger b_t^\dagger], a_t[\varphi_1]] = -b_t^\dagger[P_t^- A^\dagger \varphi_1] \exp[A a_t^\dagger b_t^\dagger] \quad (8.4)$$

and for $\varphi_2 \in \mathcal{H}_t^-$

$$[\exp[A a_t^\dagger b_t^\dagger], b_t[\varphi_2]] = a_t^\dagger[P_t^+ A \varphi_2] \exp[A a_t^\dagger b_t^\dagger]. \quad (8.5)$$

The next two theorems state that $P_t^\pm U(t, s) P_s^\mp$ being a Hilbert-Schmidt operator is necessary and sufficient for $U(t, s)$ being unitarily implementable. Again, the proofs follow closely the ones of [Tha92, Thm 10.6, Thm10.7], generalizing and elaborating where necessary.

Theorem 8.6. *Let $s, t \in \mathbb{R}$ and let $U(t, s)$ be a unitary operator on \mathcal{H} . If $P_t^\pm U(t, s) P_s^\mp$ are Hilbert-Schmidt operators then there exists a unitary operator $\widehat{U}(t, s) : \mathcal{F}_s \rightarrow \mathcal{F}_t$ which fulfills eq. (8.2) and we have*

$$\Psi = \widehat{U}(t, s)\Omega = k \prod_{i=1}^N a_t^\dagger[\phi_i^+] \prod_{j=1}^M b_t^\dagger[\phi_j^-] \exp \left[U_{t,s}^{+-} (U_{t,s}^{--})^{-1} a_t^\dagger b_t^\dagger \right] \Omega \quad (8.6)$$

where $\{\phi_i^+\}_{i=1,\dots,N}$ and $\{\phi_j^-\}_{j=1,\dots,M}$ are orthonormal bases of the finite dimensional subspaces $\ker U_{s,t}^{++}$ and $\ker U_{s,t}^{--}$ and where k is normalization constant.

Proof. By Lemma 8.3 we have to show that the state defined in eq. (8.6) fulfills eq. (8.1). We first prove that

$$\Gamma_t[U(t, s)\varphi]\Psi = 0 \quad \text{for all } \varphi \in \ker U_{t,s}^{++} \cap \mathcal{H}_s^+.$$

For such a state φ we have $\Gamma_t[U(t, s)\varphi] = b_t^\dagger[P_t^- U(t, s) P_s^+ \varphi] = \sum_{j=1}^M \alpha_j b_t^\dagger[\phi_j^-]$. The expansion is possible because $U_{t,s}^{+-} \ker U_{t,s}^{++} \subset \ker U_{s,t}^{--}$ which is finite dimensional due to Lemma 8.5. For every part in the expansion there is a matching counter part in the state Ψ such that we get $b_t^\dagger[\phi_j^-]\Psi = 0$ for all j .

Now, let $\varphi \in (\ker U_{t,s}^{++})^\perp \cap \mathcal{H}_s^+$. Lemma 8.5 shows that $U_{t,s}^{++}\varphi \perp \ker U_{s,t}^{++}$ and $U_{t,s}^{--}\varphi \perp \ker U_{s,t}^{--}$ and hence

$$\Gamma_t[U(t, s)\varphi] = a_t[P_t^+ U(t, s) P_s^+ \varphi] + b_t^\dagger[P_t^- U(t, s) P_s^+ \varphi]$$

can be pulled through the product in the state Ψ . Thus, we have

$$\begin{aligned} & (a_t[U_{t,s}^{++}\varphi] + b_t^\dagger[U_{t,s}^{--}\varphi]) \exp \left[U_{t,s}^{+-} (U_{t,s}^{--})^{-1} a_t^\dagger b_t^\dagger \right] \Omega = \\ & = \left(b_t^\dagger[P_t^- (U_{s,t}^{--})^{-1} U_{s,t}^{--} U_{t,s}^{++}\varphi] + b_t^\dagger[U_{t,s}^{--}\varphi] \right) \exp \left[U_{t,s}^{+-} (U_{t,s}^{--})^{-1} a_t^\dagger b_t^\dagger \right] \Omega \end{aligned}$$

where we used eq. (8.4). By the same reasoning as in [Tha92, Thm 10.6] we find that

$$P_t^- (U_{s,t}^{--})^{-1} U_{s,t}^{--} U_{t,s}^{++}\varphi = -U_{t,s}^{--}\varphi$$

which completes the proof. The proof for $\Gamma_t^\dagger[U(t, s)\varphi]$ is completely analogous. \square

Theorem 8.7. *Let $s, t \in \mathbb{R}$ and let $U(t, s)$ be a unitary operator on \mathcal{H} . The operators $P_t^\pm U(t, s) P_s^\mp$ are Hilbert-Schmidt if $U(t, s)$ is unitarily implementable.*

Proof. Note that if $P_t^+ \ker U_{s,t}^{++}$ is finite dimensional so is $U_{t,s}^{+-} \ker U_{t,s}^{--}$ due to Lemma 8.5. Thus, $U_{t,s}^{+-}$ would be a finite rank operator and as such also Hilbert-Schmidt on $\ker U_{t,s}^{--}$. Hence, we will first show that $P_t^+ \ker U_{s,t}^{++}$ is finite dimensional and then go on to prove the Hilbert-Schmidt property on $(\ker U_{t,s}^{--})^\perp$.

We observe that for $\Psi = \widehat{U}(t, s)\Omega$ being the evolved vacuum state according to Lemma 8.3 and for any $\varphi \in P_t^+ \ker U_{s,t}^{++}$ we have

$$\begin{aligned} a_t^\dagger[\varphi]\Psi &= \Gamma_t^\dagger[\varphi]\Psi = \widehat{U}(t, s)\Gamma_s^\dagger[U(s, t)\varphi] \left(\widehat{U}(t, s)\right)^\dagger \Psi = \widehat{U}(t, s)\Gamma_s^\dagger[U(s, t)\varphi]\Omega = \\ &= \widehat{U}(t, s)a_s^\dagger[P_s^+ U(s, t)\varphi]\Omega = \widehat{U}(t, s)a_s^\dagger[0]\Omega = 0 \end{aligned}$$

and in a similar way we get $b_t^\dagger[\varphi]\Psi = 0$ for any $\varphi \in P_t^- \ker U_{s,t}^{--}$. Now, let $\{\phi_n^+\}_{n \in \mathbb{N}}$ and $\{\phi_n^-\}_{n \in \mathbb{N}}$ be orthonormal bases of \mathcal{H}_t^\pm which contain orthonormal bases of $P_t^+ \ker U_{s,t}^{++}$ and $P_t^- \ker U_{s,t}^{--}$, respectively. Using these bases in the construction of the Fock space we can expand the state Ψ into

$$\Psi = \sum_{n,m} \Psi^{(n,m)}$$

where

$$\Psi^{(n,m)} = \sum_{\substack{i_1 < \dots < i_n \\ j_1 < \dots < j_m}} \bar{\alpha}_{i_1 \dots i_n, j_1 \dots j_m} a_t^\dagger[\phi_{i_1}^+] \dots a_t^\dagger[\phi_{i_n}^+] b_t^\dagger[\phi_{j_1}^-] \dots b_t^\dagger[\phi_{j_m}^-] \Omega \quad (8.7)$$

and the coefficients are given by

$$\bar{\alpha}_{i_1 \dots i_n, j_1 \dots j_m} = \langle a_t^\dagger[\phi_{i_1}^+] \dots a_t^\dagger[\phi_{i_n}^+] b_t^\dagger[\phi_{j_1}^-] \dots b_t^\dagger[\phi_{j_m}^-] \Omega, \Psi \rangle.$$

Let ϕ_l^+ be a basis vector which is in $P_t^+ \ker U_{s,t}^{++}$. If $l \notin \{i_1 \dots i_n\}$ for a particular coefficient we have

$$\begin{aligned} \bar{\alpha}_{i_1 \dots i_n, j_1 \dots j_m} &= \langle a_t^\dagger[\phi_{i_1}^+] \dots a_t^\dagger[\phi_{i_n}^+] b_t^\dagger[\phi_{j_1}^-] \dots b_t^\dagger[\phi_{j_m}^-] \Omega, \Psi \rangle = \\ &= \langle a_t^\dagger[\phi_{i_1}^+] \dots a_t^\dagger[\phi_{i_n}^+] b_t^\dagger[\phi_{j_1}^-] \dots b_t^\dagger[\phi_{j_m}^-] \Omega, \{a_t[\phi_l^+], a_t^\dagger[\phi_l^+]\} \Psi \rangle = 0 \end{aligned}$$

due to $a_t^\dagger[\phi_l^+]\Psi = 0$ and $a_t[\phi_l^+]\Omega = 0$. We can always find such a basis vector for $n < \dim P_t^+ \ker U_{s,t}^{++}$. The same argument applies for $m < \dim P_t^- \ker U_{s,t}^{--}$ and in this case we find

$$\Psi^{(n,m)} = 0.$$

We conclude that $P_t^+ \ker U_{s,t}^{++}$ and $P_t^- \ker U_{s,t}^{--}$ have to be finite dimensional. Otherwise we would have

$$0 = \left\| \sum_{n,m} \Psi^{(n,m)} \right\| = \|\Psi\| = \|\widehat{U}(t, s)\Omega\| = \|\Omega\| = 1.$$

This proves the Hilbert-Schmidt property on $\ker U_{t,s}^{--}$.

For the remaining part we reorder the basis vectors such that the first N and M elements of $\{\phi_n^+\}_{n \in \mathbb{N}}$ and $\{\phi_n^-\}_{n \in \mathbb{N}}$ are the basis vectors of $P_t^+ \ker U_{s,t}^{++}$ and $P_t^- \ker U_{s,t}^{--}$. Using the argument of

the vanishing coefficients from above we find that all the first N and M basis vectors must be present in the expansion of eq. (8.7). As the indices are ordered we have

$$\Psi^{(n,m)} = \sum_{\substack{N < i_{N+1} < \dots < i_n \\ M < j_{M+1} < \dots < j_m}} \bar{\alpha}_{1,\dots,N,i_{N+1},\dots,i_n,1,\dots,M,j_{M+1},\dots,j_m} a_t^\dagger[\phi_1] \dots a_t^\dagger[\phi_N] a_t^\dagger[\phi_{i_{N+1}}] \dots a_t^\dagger[\phi_{i_n}] \\ b_t^\dagger[\phi_1^-] \dots b_t^\dagger[\phi_M^-] b_t^\dagger[\phi_{j_{M+1}}^-] \dots b_t^\dagger[\phi_{j_m}^-] \Omega$$

for $n \geq N$ and $m \geq M$. Otherwise, $\Psi^{(n,m)}$ is identical to zero. The state $\Psi^{(N,M)}$ is thus a product state

$$\Psi^{(N,M)} = \alpha \prod_{n=1}^N a_t^\dagger[\phi_n^+] \prod_{m=1}^M b_t^\dagger[\phi_m^-] \Omega$$

with $\alpha = \bar{\alpha}_{1,\dots,N,1,\dots,M}$. To see that α cannot be zero we note that from $(\Gamma_t [U(t,s)\varphi] \Psi)^{(N+i,M+j)} = 0$ it follows

$$a_t [U_{t,s}^{++} \varphi] \Psi^{(N+i+1,M+j)} = -b_t^\dagger [U_{t,s}^{--} \varphi] \Psi^{(N+i,M+j-1)}$$

for all $\varphi \in \mathcal{H}_s^+$. As the dimension of $P_t^+ \ker U_{s,t}^{++}$ is equal to N there must be at least one state of $P_t^+ (\ker U_{s,t}^{++})^\perp$ present in $\Psi^{(N+i+1,M+j)}$ for $i \geq 0$. This, in turn, means that if $a_t [U_{t,s}^{++} \varphi] \Psi^{(N+i+1,M+j)} = 0$ for all $\varphi \in P_t^+ (\ker U_{s,t}^{++})^\perp$ we have $\Psi^{(N+i+1,M+j)} = 0$ (remember that $U_{t,s}^{++}$ is invertible on $(\ker U_{s,t}^{++})^\perp$). Hence, we can conclude that if $\Psi^{(N+i,M+j-1)} = 0$ then also $\Psi^{(N+i+1,M+j)} = 0$ for all $i, j \geq 0$. In particular if $\Psi^{(N,M)} = 0$ it follows that $\Psi^{(N+l,M+k)} = 0$ for all $l = k$. For $k \neq l$ we use that $\Psi^{(N+l,M-1)} = 0$ for every $l \geq 0$ which we have shown above. From there we get with our relations that

$$\Psi^{(N+k+l,M+l)} = 0$$

for all $k > 0$ and $l \geq 0$. The same conclusion can be drawn for

$$\Psi^{(N+l,M+k+l)} = 0$$

if we start with $(\Gamma_t^\dagger [U(t,s)\varphi] \Psi)^{(N+i,M+j)} = 0$. Both together yield $\Psi^{(N+l,M+k)} = 0$ if $k \neq l$. Thus, if $\alpha = 0$ it follows that $\Psi^{(N,M)} = 0$. This results in $\Psi = 0$ which is a contradiction.

Using the CAR we can now build every other non-zero (n,m) -sector out of $\Psi^{(N,M)}$. For example for $N+1$ and $M+1$ we get

$$\Psi^{(N+1,M+1)} = \sum_{\substack{i=N+1 \\ j=M+1}} \bar{\alpha}_{i,j} a_t^\dagger[\phi_i] b_t^\dagger[\phi_j^+] \Psi^{(N,M)} \quad (8.8)$$

with $\bar{\alpha}_{i,j} = (-1)^M \frac{\bar{\alpha}_{1,\dots,N,i,1,\dots,M,j}}{\alpha}$ and

$$\sum_{i,j} |\alpha_{i,j}|^2 \leq 1$$

as the norm of Ψ is one. Because of this we can we can define the following Hilbert-Schmidt operator

$$A[\varphi] = \sum_{\substack{i=N+1 \\ j=M+1}} \alpha_{i,j} \langle \phi_j^-, \varphi \rangle \phi_i^+$$

and using the definition from eq. (8.3) we can write

$$\Psi^{(N+1, M+1)} = A a_t^\dagger b_t^\dagger \Psi^{(N, M)}.$$

Now, as $\Gamma_t^\dagger [U(t, s)\varphi] \Psi = 0$ for all $\varphi \in \mathcal{H}_s^-$ we have in particular

$$\begin{aligned} 0 &= (\Gamma_t^\dagger [U(t, s)\varphi] \Psi)^{(N+1, M)} = (a_t^\dagger [P_t^+ U(t, s)\varphi] + b_t [P_t^- U(t, s)\varphi] \Psi)^{(N+1, M)} = \\ &= a_t^\dagger [P_t^+ U(t, s)\varphi] \Psi^{(N, M)} + b_t [P_t^- U(t, s)\varphi] \Psi^{(N+1, M+1)} = \\ &= a_t^\dagger [P_t^+ U(t, s)\varphi] \Psi^{(N, M)} + b_t [P_t^- U(t, s)\varphi] A a_t^\dagger b_t^\dagger \Psi^{(N, M)}. \end{aligned}$$

Using the definition of $A a_t^\dagger b_t^\dagger$ we compute

$$\begin{aligned} b_t [P_t^- U(t, s)\varphi] A a_t^\dagger b_t^\dagger &= \sum_{i,j} \langle \phi_i^+, A \phi_j^- \rangle b_t [P_t^- U(t, s)\varphi] a_t^\dagger [\phi_i^+] b_t^\dagger [\phi_j^-] = \\ &= \sum_{i,j} \langle A^\dagger \phi_i^+, \phi_j^- \rangle a_t^\dagger [\phi_i^+] (b_t^\dagger [\phi_j^-] b_t [P_t^- U(t, s)\varphi] - \langle \phi_j^-, P_t^- U(t, s)\varphi \rangle) = \\ &= \sum_{i,j} \langle A^\dagger \phi_i^+, \phi_j^- \rangle a_t^\dagger [\phi_i^+] b_t^\dagger [\phi_j^-] b_t [P_t^- U(t, s)\varphi] - a_t^\dagger [P_t^+ A P_t^- U(t, s)\varphi] \end{aligned}$$

and as $b_t [P_t^- U(t, s)\varphi] \Psi^{(N, M)} = \Gamma_t^\dagger [P_t^- U(t, s)\varphi] \Psi^{(N, M)} = 0$ we conclude that

$$a_t^\dagger [P_t^+ U(t, s)\varphi] \Psi^{(N, M)} = a_t^\dagger [P_t^+ A P_t^- U(t, s)\varphi] \Psi^{(N, M)}$$

for all $\varphi \in \mathcal{H}_s^-$. For $\varphi \in P_s^- (\ker U_{t,s}^{--})^\perp$ in particular we have $U_{t,s}^{+-} \varphi \perp P_t^+ \ker U_{s,t}^{++}$ by Lemma 8.5 and $P_t^+ A U_{t,s}^{--} \varphi \perp P_t^+ \ker U_{s,t}^{++}$ by the definition of A . Hence, plugging in the product formula for $\Psi^{(N, M)}$ we can pull $a_t^\dagger [P_t^+ U(t, s)\varphi]$ and $a_t^\dagger [P_t^+ A P_t^- U(t, s)\varphi]$ all the way through to the vacuum state and as the creation operators in the product are all invertible we conclude

$$a_t^\dagger [P_t^+ U(t, s)\varphi] \Omega = a_t^\dagger [P_t^+ A P_t^- U(t, s)\varphi] \Omega.$$

Therefore, we have

$$P_t^+ U(t, s) P_s^- \varphi = P_t^+ A P_t^- U(t, s)\varphi,$$

for all $\varphi \in P_s^- (\ker U_{t,s}^{--})^\perp$. The proof for $P_t^- U(t, s) P_s^+$ being Hilbert-Schmidt is analogous. \square

9. Vacuum transition amplitudes for finite times

After we have set up the whole framework of external field QED we can now use it to derive upper and lower bounds on the transition amplitudes from the vacuum into some (n, m) -particle state. We will see that these bounds depend solely on the transition properties of the one-particle Dirac equation. This can then be used to establish some sort of “second quantized adiabatic theorem” which we will do in Chapter 12. We put this into quotation marks as the question to answer will not be whether a state tunnels to another spectral subspace but rather to give an estimate on the transition amplitudes from one specific particle subspace to another if the external field is changing adiabatically. However, the results below are not only valid for adiabatic perturbation theory but can be applied whenever the transition amplitudes of the one-particle theory can be controlled.

We derive two formulas for an upper as well as for a lower bound. If the one-particle transition probability is high we can use the lower bound to conclude that the same is true in the second quantized context. Vice versa, if the one-particle amplitude is low we make use of the upper bound to show that the vacuum state will evolve into the vacuum again. However, there is an important distinction between the two results. For the lower bound it suffices to control only the usual operator norm of the one-particle transitions whereas for the upper bound the Hilbert-Schmidt norm is needed. From the Dirac sea interpretation this result is absolutely meaningful as transitions to other particle sectors in Fock space correspond to transitions from the Dirac sea to the positive energies. And as there are infinitely many particles in the sea we have to sum over all transition amplitudes which is precisely the Hilbert-Schmidt norm. Nevertheless, we stress that the results below are achieved completely in the framework of time-dependent external field QED and no reference to the Dirac sea is necessary for the proof. Our first theorem in this chapter is given by the following.

Theorem 9.1. *Let the external potential be such that there exists a unitarily implementable one-particle time evolution according to Definition 8.1 and let $s < t$. We then have for the transition amplitude from the vacuum to the (n, m) -particle sector*

$$|\beta_{n,m}| \leq \sum_{k=0}^{\min\{n,m\}} \frac{\sqrt{n!}\sqrt{m!}}{k!(n-k)!(m-k)!} \|P_t^- U(t,s) P_s^- U(s,t) P_t^+\|_{\text{HS}}^k \cdot \|P_s^+ U(s,t) P_t^-\|_{\text{HS}}^{m-k} \|P_s^- U(s,t) P_t^+\|_{\text{HS}}^{n-k} .$$

for $n + m \geq 1$.

Before we can give the proof of the theorem we need two technical lemmata involving products of creation and annihilation operators. To this end let V be a polarization as in the Chapters before. The first lemma is the binomial theorem for the creation and annihilation operators.

Lemma 9.2 (Binomial theorem). *Let $\varphi_i \in \mathcal{H}$ for $i = 1, \dots, n$. We then have*

$$\begin{aligned} & \prod_{i=1}^n (a_V [P_V \varphi_i] + b_V^\dagger [P_V^\perp \varphi_i]) = \\ & = \sum_{k=0}^n \sum_{\sigma \in S_n} \frac{\text{sgn } \sigma}{k!(n-k)!} a_V [P_V \varphi_{\sigma(1)}] \cdots a_V [P_V \varphi_{\sigma(n-k)}] b_V^\dagger [P_V^\perp \varphi_{\sigma(n-k+1)}] \cdots b_V^\dagger [P_V^\perp \varphi_{\sigma(n)}]. \end{aligned}$$

and similarly for the adjoint.

Proof. The proof is by induction and similar to the usual binomial theorem. We have

$$\begin{aligned} & \prod_{i=1}^{n+1} (a_V [P_V \varphi_i] + b_V^\dagger [P_V^\perp \varphi_i]) = \\ & = \prod_{i=1}^n (a_V [P_V \varphi_i] + b_V^\dagger [P_V^\perp \varphi_i]) \cdot (a_V [P_V \varphi_{n+1}] + b_V^\dagger [P_V^\perp \varphi_{n+1}]) = \\ & = \sum_{k=0}^n \sum_{\sigma \in S_n} \frac{\text{sgn } \sigma}{k!(n-k)!} a_V [P_V \varphi_{\sigma(1)}] \cdots a_V [P_V \varphi_{\sigma(n-k)}] \\ & \quad \cdot b_V^\dagger [P_V^\perp \varphi_{\sigma(n-k+1)}] \cdots b_V^\dagger [P_V^\perp \varphi_{\sigma(n)}] (a_V [P_V \varphi_{n+1}] + b_V^\dagger [P_V^\perp \varphi_{n+1}]) = \\ & = \sum_{k=0}^n \sum_{\substack{\sigma \in S_{n+1} \\ \sigma(n+1)=n+1}} \frac{\text{sgn } \sigma}{k!(n-k)!} a_V [P_V \varphi_{\sigma(1)}] \cdots a_V [P_V \varphi_{\sigma(n-k)}] \\ & \quad \cdot b_V^\dagger [P_V^\perp \varphi_{\sigma(n-k+1)}] \cdots b_V^\dagger [P_V^\perp \varphi_{\sigma(n)}] (a_V [P_V \varphi_{\sigma(n+1)}] + b_V^\dagger [P_V^\perp \varphi_{\sigma(n+1)}]). \end{aligned}$$

For the first term we find

$$\begin{aligned}
& \sum_{k=0}^n \sum_{\substack{\sigma \in \mathcal{S}_{n+1} \\ \sigma(n+1)=n+1}} \frac{\operatorname{sgn} \sigma}{k!(n-k)!} a_V [\mathbf{P}_V \varphi_{\sigma(1)}] \cdots a_V [\mathbf{P}_V \varphi_{\sigma(n-k)}] \\
& \quad \cdot b_V^\dagger [\mathbf{P}_V^\perp \varphi_{\sigma(n-k+1)}] \cdots b_V^\dagger [\mathbf{P}_V^\perp \varphi_{\sigma(n)}] a_V [\mathbf{P}_V \varphi_{\sigma(n+1)}] = \\
& = \sum_{k=0}^n (-1)^k \sum_{\substack{\sigma \in \mathcal{S}_{n+1} \\ \sigma(n+1)=n+1}} \frac{\operatorname{sgn} \sigma}{k!(n-k)!} a_V [\mathbf{P}_V \varphi_{\sigma(1)}] \cdots a_V [\mathbf{P}_V \varphi_{\sigma(n-k)}] a_V [\mathbf{P}_V \varphi_{\sigma(n+1)}] \\
& \quad \cdot b_V^\dagger [\mathbf{P}_V^\perp \varphi_{\sigma(n-k+1)}] \cdots b_V^\dagger [\mathbf{P}_V^\perp \varphi_{\sigma(n)}] = \\
& = \sum_{k=0}^n \sum_{\substack{\sigma \in \mathcal{S}_{n+1} \\ \sigma(n-k+1)=n+1}} \frac{\operatorname{sgn} \sigma}{k!(n-k)!} a_V [\mathbf{P}_V \varphi_{\sigma(1)}] \cdots a_V [\mathbf{P}_V \varphi_{\sigma(n-k)}] a_V [\mathbf{P}_V \varphi_{\sigma(n-k+1)}] \\
& \quad \cdot b_V^\dagger [\mathbf{P}_V^\perp \varphi_{\sigma(n-k+2)}] \cdots b_V^\dagger [\mathbf{P}_V^\perp \varphi_{\sigma(n+1)}] = \\
& = \sum_{\sigma \in \mathcal{S}_{n+1}} \operatorname{sgn} \sigma a_V [\mathbf{P}_V \varphi_{\sigma(1)}] \cdots a_V [\mathbf{P}_V \varphi_{\sigma(n+1)}] \\
& \quad + \sum_{k=0}^{n-1} \sum_{\substack{\sigma \in \mathcal{S}_{n+1} \\ \sigma(n-k)=n+1}} \frac{\operatorname{sgn} \sigma}{(k+1)!(n-k-1)!} a_V [\mathbf{P}_V \varphi_{\sigma(1)}] \cdots a_V [\mathbf{P}_V \varphi_{\sigma(n-k)}] \\
& \quad \cdot b_V^\dagger [\mathbf{P}_V^\perp \varphi_{\sigma(n-k+1)}] \cdots b_V^\dagger [\mathbf{P}_V^\perp \varphi_{\sigma(n+1)}]
\end{aligned}$$

and similarly for the second one

$$\begin{aligned}
& \sum_{k=0}^n \sum_{\substack{\sigma \in \mathcal{S}_{n+1} \\ \sigma(n+1)=n+1}} \frac{\operatorname{sgn} \sigma}{k!(n-k)!} a_V [\mathbf{P}_V \varphi_{\sigma(1)}] \cdots a_V [\mathbf{P}_V \varphi_{\sigma(n-k)}] \\
& \quad \cdot b_V^\dagger [\mathbf{P}_V^\perp \varphi_{\sigma(n-k+1)}] \cdots b_V^\dagger [\mathbf{P}_V^\perp \varphi_{\sigma(n)}] b_V^\dagger [\mathbf{P}_V^\perp \varphi_{\sigma(n+1)}] = \\
& = \sum_{k=0}^{n-1} \sum_{\substack{\sigma \in \mathcal{S}_{n+1} \\ \sigma(n+1)=n+1}} \frac{\operatorname{sgn} \sigma}{k!(n-k)!} a_V [\mathbf{P}_V \varphi_{\sigma(1)}] \cdots a_V [\mathbf{P}_V \varphi_{\sigma(n-k)}] \\
& \quad \cdot b_V^\dagger [\mathbf{P}_V^\perp \varphi_{\sigma(n-k+1)}] \cdots b_V^\dagger [\mathbf{P}_V^\perp \varphi_{\sigma(n+1)}] \\
& \quad + \sum_{\sigma \in \mathcal{S}_{n+1}} \operatorname{sgn} \sigma b_V^\dagger [\mathbf{P}_V^\perp \varphi_{\sigma(1)}] \cdots b_V^\dagger [\mathbf{P}_V^\perp \varphi_{\sigma(n+1)}].
\end{aligned}$$

Finally, we observe that

$$\begin{aligned}
& \sum_{\substack{\sigma \in \mathcal{S}_{n+1} \\ \sigma(n-k)=n+1}} \frac{\text{sgn } \sigma}{(k+1)!(n-k-1)!} a_V [\mathbf{P}_V \varphi_{\sigma(1)}] \cdots a_V [\mathbf{P}_V \varphi_{\sigma(n-k)}] \\
& \quad \cdot b_V^\dagger [\mathbf{P}_V^\perp \varphi_{\sigma(n-k+1)}] \cdots b_V^\dagger [\mathbf{P}_V^\perp \varphi_{\sigma(n+1)}] \\
& + \sum_{\substack{\sigma \in \mathcal{S}_{n+1} \\ \sigma(n+1)=n+1}} \frac{\text{sgn } \sigma}{k!(n-k)!} a_V [\mathbf{P}_V \varphi_{\sigma(1)}] \cdots a_V [\mathbf{P}_V \varphi_{\sigma(n-k)}] \\
& \quad \cdot b_V^\dagger [\mathbf{P}_V^\perp \varphi_{\sigma(n-k+1)}] \cdots b_V^\dagger [\mathbf{P}_V^\perp \varphi_{\sigma(n+1)}] = \\
& = \frac{1}{(k+1)!(n-k)!} \left(\sum_{\substack{\sigma \in \mathcal{S}_{n+1} \\ \sigma(n-k)=n+1}} (n-k) \text{sgn } \sigma a_V [\mathbf{P}_V \varphi_{\sigma(1)}] \cdots a_V [\mathbf{P}_V \varphi_{\sigma(n-k)}] \right. \\
& \quad \cdot b_V^\dagger [\mathbf{P}_V^\perp \varphi_{\sigma(n-k+1)}] \cdots b_V^\dagger [\mathbf{P}_V^\perp \varphi_{\sigma(n+1)}] \\
& \quad + \sum_{\substack{\sigma \in \mathcal{S}_{n+1} \\ \sigma(n+1)=n+1}} (k+1) \text{sgn } \sigma a_V [\mathbf{P}_V \varphi_{\sigma(1)}] \cdots a_V [\mathbf{P}_V \varphi_{\sigma(n-k)}] \\
& \quad \left. \cdot b_V^\dagger [\mathbf{P}_V^\perp \varphi_{\sigma(n-k+1)}] \cdots b_V^\dagger [\mathbf{P}_V^\perp \varphi_{\sigma(n+1)}] \right) = \\
& = \sum_{\sigma \in \mathcal{S}_{n+1}} \frac{\text{sgn } \sigma}{(k+1)!(n-k)!} a_V [\mathbf{P}_V \varphi_{\sigma(1)}] \cdots a_V [\mathbf{P}_V \varphi_{\sigma(n-k)}] \\
& \quad \cdot b_V^\dagger [\mathbf{P}_V^\perp \varphi_{\sigma(n-k+1)}] \cdots b_V^\dagger [\mathbf{P}_V^\perp \varphi_{\sigma(n+1)}].
\end{aligned}$$

Putting it all together we end up with

$$\begin{aligned}
& \prod_{i=1}^{n+1} (a_V [\mathbf{P}_V \varphi_i] + b_V^\dagger [\mathbf{P}_V^\perp \varphi_i]) = \\
& = \sum_{\sigma \in \mathcal{S}_{n+1}} \text{sgn } \sigma a_V [\mathbf{P}_V \varphi_{\sigma(1)}] \cdots a_V [\mathbf{P}_V \varphi_{\sigma(n+1)}] \\
& \quad + \sum_{k=0}^{n-1} \sum_{\sigma \in \mathcal{S}_{n+1}} \frac{\text{sgn } \sigma}{(k+1)!(n-k)!} a_V [\mathbf{P}_V \varphi_{\sigma(1)}] \cdots a_V [\mathbf{P}_V \varphi_{\sigma(n-k)}] \\
& \quad \cdot b_V^\dagger [\mathbf{P}_V^\perp \varphi_{\sigma(n-k+1)}] \cdots b_V^\dagger [\mathbf{P}_V^\perp \varphi_{\sigma(n+1)}] + \sum_{\sigma \in \mathcal{S}_{n+1}} \text{sgn } \sigma b_V^\dagger [\mathbf{P}_V^\perp \varphi_{\sigma(1)}] \cdots b_V^\dagger [\mathbf{P}_V^\perp \varphi_{\sigma(n+1)}] = \\
& = \sum_{k=0}^{n+1} \sum_{\sigma \in \mathcal{S}_{n+1}} \frac{\text{sgn } \sigma}{k!(n+1-k)!} a_V [\mathbf{P}_V \varphi_{\sigma(1)}] \cdots a_V [\mathbf{P}_V \varphi_{\sigma(n+1-k)}] \\
& \quad \cdot b_V^\dagger [\mathbf{P}_V^\perp \varphi_{\sigma(n+1-k+1)}] \cdots b_V^\dagger [\mathbf{P}_V^\perp \varphi_{\sigma(n+1)}].
\end{aligned}$$

□

The next lemma is a statement about the product of arbitrary many creation and annihilation operators acting on the vacuum.

Lemma 9.3. *Let $\varphi_i \in V$ for $i = 1, \dots, n$ and $\psi_j \in V$ for $j = 1, \dots, m$. We then have*

$$\begin{aligned} & a_V [\varphi_n] \dots a_V [\varphi_1] a_V^\dagger [\psi_1] \dots a_V^\dagger [\psi_m] \Omega = \\ & = \frac{1}{(m-n)!} \sum_{\sigma \in S_m} \operatorname{sgn} \sigma \langle \varphi_1, \psi_{\sigma(1)} \rangle \dots \langle \varphi_n, \psi_{\sigma(n)} \rangle a_V^\dagger [\psi_{\sigma(n+1)}] \dots a_V^\dagger [\psi_{\sigma(m)}] \Omega, \end{aligned}$$

if $m \geq n$, and similar for b_V and b_V^\dagger . Otherwise it is zero.

Proof. Let $n = 1$. We then have for $m = 1$

$$a_V [\varphi_1] a_V^\dagger [\psi_1] \Omega = -a_V^\dagger [\psi_1] a_V [\varphi_1] \Omega + \langle \varphi_1, \psi_1 \rangle \Omega = \frac{1}{0!} \sum_{\sigma \in S_1} \langle \varphi_1, \psi_{\sigma(1)} \rangle \Omega,$$

and thus by induction for all $m \geq n$

$$\begin{aligned} & a_V [\varphi_1] a_V^\dagger [\psi_1] \dots a_V^\dagger [\psi_{m+1}] \Omega = \\ & = (-1)^m a_V [\varphi_1] a_V^\dagger [\psi_{m+1}] a_V^\dagger [\psi_1] \dots a_V^\dagger [\psi_m] \Omega = \\ & = (-1)^m \left(-a_V^\dagger [\psi_{m+1}] a_V [\varphi_1] + \langle \varphi_1, \psi_{m+1} \rangle \right) a_V^\dagger [\psi_1] \dots a_V^\dagger [\psi_m] \Omega = \\ & = \frac{1}{(m-1)!} \sum_{\sigma \in S_m} \operatorname{sgn} \sigma \langle \varphi_1, \psi_{\sigma(1)} \rangle a_V^\dagger [\psi_{\sigma(2)}] \dots a_V^\dagger [\psi_{\sigma(m)}] a_V^\dagger [\psi_{m+1}] \Omega \\ & \quad + (-1)^m \langle \varphi_1, \psi_{m+1} \rangle a_V^\dagger [\psi_1] \dots a_V^\dagger [\psi_m] \Omega. \end{aligned}$$

The first term is equivalent to

$$\begin{aligned} & \frac{1}{(m-1)!} \sum_{\sigma \in S_m} \operatorname{sgn} \sigma \langle \varphi_1, \psi_{\sigma(1)} \rangle a_V^\dagger [\psi_{\sigma(2)}] \dots a_V^\dagger [\psi_{\sigma(m)}] a_V^\dagger [\psi_{m+1}] \Omega = \\ & = \frac{1}{(m-1)!} \sum_{\substack{\sigma \in S_{m+1} \\ \sigma(m+1)=m+1}} \operatorname{sgn} \sigma \langle \varphi_1, \psi_{\sigma(1)} \rangle a_V^\dagger [\psi_{\sigma(2)}] \dots a_V^\dagger [\psi_{\sigma(m)}] a_V^\dagger [\psi_{\sigma(m+1)}] \Omega = \\ & = \frac{1}{m(m-1)!} \sum_{\substack{\sigma \in S_{m+1} \\ \sigma(1) \neq m+1}} \operatorname{sgn} \sigma \langle \varphi_1, \psi_{\sigma(1)} \rangle a_V^\dagger [\psi_{\sigma(2)}] \dots a_V^\dagger [\psi_{\sigma(m)}] a_V^\dagger [\psi_{\sigma(m+1)}] \Omega. \end{aligned}$$

The second term above can be written as

$$\begin{aligned}
& (-1)^m \langle \varphi_1, P^+ \psi_{m+1} \rangle a^\dagger [P^+ \psi_1] \dots a^\dagger [P^+ \psi_m] \Omega = \\
& = \frac{(-1)^m}{m!} \sum_{\sigma \in S_m} \operatorname{sgn} \sigma \langle \varphi_1, P^+ \psi_{m+1} \rangle a^\dagger [P^+ \psi_{\sigma(1)}] \dots a^\dagger [P^+ \psi_{\sigma(m)}] \Omega = \\
& = \frac{-1}{m!} \sum_{\sigma \in S_m} \operatorname{sgn} \sigma \langle \varphi_1, P^+ \psi_{m+1} \rangle a^\dagger [P^+ \psi_{\sigma(2)}] \dots a^\dagger [P^+ \psi_{\sigma(m)}] a^\dagger [P^+ \psi_{\sigma(1)}] \Omega = \\
& = \frac{-1}{m!} \sum_{\substack{\sigma \in S_{m+1} \\ \sigma(m+1)=m+1}} \operatorname{sgn} \sigma \langle \varphi_1, P^+ \psi_{\sigma(m+1)} \rangle a^\dagger [P^+ \psi_{\sigma(2)}] \dots a^\dagger [P^+ \psi_{\sigma(1)}] \Omega = \\
& = \frac{1}{m!} \sum_{\substack{\sigma \in S_{m+1} \\ \sigma(1)=m+1}} \operatorname{sgn} \sigma \langle \varphi_1, P^+ \psi_{\sigma(1)} \rangle a^\dagger [P^+ \psi_{\sigma(2)}] \dots a^\dagger [P^+ \psi_{\sigma(m+1)}] \Omega
\end{aligned}$$

which proves the statement for $n = 1$ and any m . If $n > m$ we have more annihilation- than creation operators and this yields simply zero. For any $n < m$ we get by induction

$$\begin{aligned}
& a_V [\varphi_{n+1}] \dots a_V [\varphi_1] a_V^\dagger [\psi_1] \dots a_V^\dagger [\psi_m] \Omega = \\
& = \frac{1}{(m-n)!} \sum_{\sigma \in S_m} \operatorname{sgn} \sigma \langle \varphi_1, \psi_{\sigma(1)} \rangle \dots \langle \varphi_n, \psi_{\sigma(n)} \rangle a_V [\varphi_{n+1}] a_V^\dagger [\psi_{\sigma(n+1)}] \dots a_V^\dagger [\psi_{\sigma(m)}] \Omega = \\
& = \sum_{k=n+1}^m (-1)^{k-n-1} \frac{1}{(m-n)!} \sum_{\sigma \in S_m} \operatorname{sgn} \sigma \langle \varphi_1, \psi_{\sigma(1)} \rangle \dots \langle \varphi_n, \psi_{\sigma(n)} \rangle \langle \varphi_{n+1}, \Psi_{\sigma(k)} \rangle \\
& \quad \cdot a_V^\dagger [\psi_{\sigma(n+1)}] \dots a_V^\dagger [\psi_{\sigma(k-1)}] a_V^\dagger [\psi_{\sigma(k+1)}] \dots a_V^\dagger [\psi_{\sigma(m)}] \Omega = \\
& = \sum_{k=n+1}^m \frac{-1}{(m-n)!} \sum_{\sigma \in S_m} \operatorname{sgn} \sigma \langle \varphi_1, \psi_{\sigma(1)} \rangle \dots \langle \varphi_n, \psi_{\sigma(k)} \rangle \langle \varphi_{n+1}, \Psi_{\sigma(n+1)} \rangle \\
& \quad \cdot a_V^\dagger [\psi_{\sigma(n+2)}] \dots a_V^\dagger [\psi_{\sigma(k-1)}] a_V^\dagger [\psi_{\sigma(n+1)}] a_V^\dagger [\psi_{\sigma(k+1)}] \dots a_V^\dagger [\psi_{\sigma(m)}] \Omega = \\
& = \sum_{k=n+1}^m \frac{1}{(m-n)!} \sum_{\sigma \in S_m} \operatorname{sgn} \sigma \langle \varphi_1, \psi_{\sigma(1)} \rangle \dots \langle \varphi_n, \psi_{\sigma(n)} \rangle \langle \varphi_{n+1}, \Psi_{\sigma(n+1)} \rangle \\
& \quad \cdot a_V^\dagger [\psi_{\sigma(n+2)}] \dots a_V^\dagger [\psi_{\sigma(m)}] \Omega = \\
& = \frac{1}{(m-n-1)!} \sum_{\sigma \in S_m} \operatorname{sgn} \sigma \langle \varphi_1, \psi_{\sigma(1)} \rangle \dots \langle \varphi_{n+1}, \Psi_{\sigma(n+1)} \rangle a_V^\dagger [\psi_{\sigma(n+2)}] \dots a_V^\dagger [\psi_{\sigma(m)}] \Omega.
\end{aligned}$$

□

These results now enable us to give the proof of the theorem.

Proof of Theorem 9.1. We start by splitting the time-evolved state into the vacuum state and the orthogonal rest

$$\widehat{U}(t, s) \Omega = \alpha \Omega + \beta \Omega_t^\perp.$$

We can furthermore decompose Ω_t^\perp into the particle and antiparticle sectors which gives

$$\beta\Omega_t^\perp = \sum_{n+m \geq 1} \beta_{n,m} \Psi_t^{(n,m)},$$

with $\Psi_t^{(n,m)}$ normalized to one and $|\beta|^2 = \sum_{n+m \geq 1} |\beta_{n,m}|^2$. By comparing these two equations we see that for $n + m \geq 1$

$$\beta_{n,m} \Psi_t^{(n,m)} = (\widehat{U}(t,s)\Omega)^{(n,m)}.$$

Using Proposition 7.9 and $\|\Psi_t^{(n,m)}\|^2 = 1$ we find

$$\beta_{n,m} = \langle \Omega, \widehat{\Psi}_t^{(n,m)} (\widehat{U}(t,s)\Omega)^{(n,m)} \rangle_{\mathcal{F}_t} = \langle \Omega, \widehat{\Psi}_t^{(n,m)} \widehat{U}(t,s)\Omega \rangle_{\mathcal{F}_t}$$

where $\widehat{\Psi}_t^{(n,m)}$ is the multi-particle annihilation operator according to Definition 7.8 and the last equality is due to the orthogonality of different particle sectors from where it follows that

$$\langle \Omega, \widehat{\Psi}_t^{(n,m)} (\widehat{U}(t,s)\Omega)^{(k,l)} \rangle = 0$$

if $n \neq k$ or $m \neq l$. Using the unitarity of the time evolution this is equivalent to

$$\begin{aligned} \langle \Omega, \widehat{\Psi}_t^{(n,m)} \widehat{U}(t,s)\Omega \rangle_{\mathcal{F}_t} &= \langle \widehat{U}(s,t)\Omega, \widehat{U}(s,t)\widehat{\Psi}_t^{(n,m)}\widehat{U}(t,s)\Omega \rangle_{\mathcal{F}_s} = \\ &= \sum_{\substack{i_1 < \dots < i_n \\ j_1 < \dots < j_m}} \alpha_{i_1, \dots, i_n, j_1, \dots, j_m} \\ &\quad \cdot \langle \widehat{U}(s,t)\Omega, \widehat{U}(s,t)\Gamma_t^\dagger[\phi_{j_m}^-] \dots \Gamma_t^\dagger[\phi_{j_1}^-] \Gamma_t[\phi_{i_n}^+] \dots \Gamma_t[\phi_{i_1}^+] \widehat{U}(t,s)\Omega \rangle_{\mathcal{F}_s} = \\ &= \sum_{\substack{i_1 < \dots < i_n \\ j_1 < \dots < j_m}} \alpha_{i_1, \dots, i_n, j_1, \dots, j_m} \\ &\quad \cdot \langle \widehat{U}(s,t)\Omega, \Gamma_s^\dagger[U(s,t)\phi_{j_m}^-] \dots \Gamma_s^\dagger[U(s,t)\phi_{j_1}^-] \Gamma_s[U(s,t)\phi_{i_n}^+] \dots \Gamma_s[U(s,t)\phi_{i_1}^+] \Omega \rangle_{\mathcal{F}_s}. \end{aligned}$$

The second equality is simply the expansion of the multi-particle annihilation operator and for the third equality we used $\text{id}_{\mathcal{F}} = \widehat{U}(t,s)\widehat{U}(s,t)$ which we plugged in repeatedly and then used the defining property of the second quantized time evolution stated in Definition 8.1. Using that $\Gamma_s[\varphi]\Omega = (a_s[P^+\varphi] + b_s^\dagger[P^-\varphi])\Omega = b_s^\dagger[P^-\varphi]\Omega$ for any $\varphi \in \mathcal{H}$ as well as the CAR for the particle and antiparticle operators we get

$$\begin{aligned} \langle \Omega, \widehat{\Psi}_t^{(n,m)} \widehat{U}(t,s)\Omega \rangle_{\mathcal{F}_t} &= \sum_{\substack{i_1 < \dots < i_n \\ j_1 < \dots < j_m}} \alpha_{i_1, \dots, i_n, j_1, \dots, j_m} \langle \widehat{U}(s,t)\Omega, \Gamma_s^\dagger[U(s,t)\phi_{j_m}^-] \dots \Gamma_s^\dagger[U(s,t)\phi_{j_1}^-] \\ &\quad \cdot b_s^\dagger[P_s^- U(s,t)\phi_{i_n}^+] \dots b_s^\dagger[P_s^- U(s,t)\phi_{i_1}^+] \Omega \rangle_{\mathcal{F}_s}. \end{aligned}$$

We rewrite the remaining product of Γ 's with the help of the Lemma 9.2 and obtain

$$\begin{aligned} \langle \Omega, \widehat{\Psi}_t^{(n,m)} \widehat{U}(t,s) \Omega \rangle_{\mathcal{F}_t} &= \sum_{\substack{i_1 < \dots < i_n \\ j_1 < \dots < j_m}} \alpha_{i_1, \dots, i_n, j_1, \dots, j_m} \sum_{k=0}^m \frac{(-1)^{\frac{m(m-1)}{2}}}{k!(m-k)!} \sum_{\sigma \in \mathcal{S}_m} \text{sgn } \sigma \\ &\cdot \langle \widehat{U}(s,t) \Omega, a_s^\dagger [P_s^+ U(s,t) \phi_{j_{\sigma(1)}}^-] \dots a_s^\dagger [P_s^+ U(s,t) \phi_{j_{\sigma(m-k)}}^-] \\ &\cdot b_s [P_s^- U(s,t) \phi_{j_{\sigma(m-k+1)}}^-] \dots b_s [P_s^- U(s,t) \phi_{j_{\sigma(m)}}^-] \\ &\cdot b_s^\dagger [P_s^- U(s,t) \phi_{i_n}^+] \dots b_s^\dagger [P_s^- U(s,t) \phi_{i_1}^+] \Omega \rangle_{\mathcal{F}_s}. \end{aligned}$$

With the help of Lemma 9.3 we can pull all the remaining annihilation operators to the right, annihilating the vacuum. This results in the following expression, containing only creation operators

$$\begin{aligned} \langle \Omega, \widehat{\Psi}_t^{(n,m)} \widehat{U}(t,s) \Omega \rangle_{\mathcal{F}_t} &= \sum_{\substack{i_1 < \dots < i_n \\ j_1 < \dots < j_m}} \alpha_{i_1, \dots, i_n, j_1, \dots, j_m} \sum_{k=0}^{\min\{n,m\}} \frac{1}{k!(n-k)!(m-k)!} \\ &\cdot \sum_{\substack{\sigma \in \mathcal{S}_m \\ \tau \in \mathcal{S}_n}} \text{sgn } \sigma \text{sgn } \tau \langle U_{s,t}^{--} \phi_{j_{\sigma(m)}}^-, U_{s,t}^{-+} \phi_{i_{\tau(n)}}^+ \rangle \dots \langle U_{s,t}^{--} \phi_{j_{\sigma(m-k+1)}}^-, U_{s,t}^{-+} \phi_{i_{\tau(n-k+1)}}^+ \rangle \\ &\cdot \langle \widehat{U}(s,t) \Omega, a_s^\dagger [P_s^+ U(s,t) \phi_{j_{\sigma(1)}}^-] \dots a_s^\dagger [P_s^+ U(s,t) \phi_{j_{\sigma(m-k)}}^-] \\ &\cdot b_s^\dagger [P_s^- U(s,t) \phi_{i_{\tau(n-k)}}^+] \dots b_s^\dagger [P_s^- U(s,t) \phi_{i_{\tau(1)}}^+] \Omega \rangle_{\mathcal{F}_s}. \end{aligned}$$

Using Cauchy-Schwarz, the unitarity of the time evolution and the operator norm of the creation operators we find that

$$\begin{aligned} \left| \langle \Omega, \widehat{\Psi}_t^{(n,m)} \widehat{U}(t,s) \Omega \rangle_{\mathcal{F}_t} \right|^2 &= \left(\sum_{\substack{i_1 < \dots < i_n \\ j_1 < \dots < j_m}} |\alpha_{i_1, \dots, i_n, j_1, \dots, j_m}| \sum_{k=0}^{\min\{n,m\}} \frac{1}{k!(n-k)!(m-k)!} \right. \\ &\cdot \sum_{\substack{\sigma \in \mathcal{S}_m \\ \tau \in \mathcal{S}_n}} \left| \langle U_{s,t}^{--} \phi_{j_{\sigma(m)}}^-, U_{s,t}^{-+} \phi_{i_{\tau(n)}}^+ \rangle \dots \langle U_{s,t}^{--} \phi_{j_{\sigma(m-k+1)}}^-, U_{s,t}^{-+} \phi_{i_{\tau(n-k+1)}}^+ \rangle \right| \\ &\cdot \left\| P_s^+ U(s,t) \phi_{j_{\sigma(1)}}^- \right\|_{\mathcal{H}} \dots \left\| P_s^+ U(s,t) \phi_{j_{\sigma(m-k)}}^- \right\|_{\mathcal{H}} \\ &\cdot \left. \left\| P_s^- U(s,t) \phi_{i_{\tau(n-k)}}^+ \right\|_{\mathcal{H}} \dots \left\| P_s^- U(s,t) \phi_{i_{\tau(1)}}^+ \right\|_{\mathcal{H}} \right)^2. \end{aligned}$$

Pulling the two finite sums in front of all (which is possible as all the summands are positive) and

then using Cauchy-Schwarz in sequence space we obtain

$$\begin{aligned}
& \left| \langle \Omega, \widehat{\Psi}_t^{(n,m)} \widehat{U}(t,s) \Omega \rangle_{\mathcal{F}_i} \right| \leq \\
& \leq \sum_{\substack{\sigma \in S_m \\ \tau \in S_n}} \sum_{k=0}^{\min\{n,m\}} \frac{1}{k!(n-k)!(m-k)!} \left(\sum_{\substack{i_1 < \dots < i_n \\ j_1 < \dots < j_m}} |\alpha_{i_1, \dots, i_n, j_1, \dots, j_m}|^2 \right. \\
& \quad \cdot \sum_{\substack{i_1 < \dots < i_n \\ j_1 < \dots < j_m}} \left| \langle U_{s,t}^{--} \phi_{j_{\sigma(m)}}^-, U_{s,t}^{-+} \phi_{i_{\tau(n)}}^+ \rangle \right|^2 \cdots \left| \langle U_{s,t}^{--} \phi_{j_{\sigma(m-k+1)}}^-, U_{s,t}^{-+} \phi_{i_{\tau(n-k+1)}}^+ \rangle \right|^2 \\
& \quad \cdot \left\| P_s^+ U(s,t) \phi_{j_{\sigma(1)}}^- \right\|_{\mathcal{H}}^2 \cdots \left\| P_s^+ U(s,t) \phi_{j_{\sigma(m-k)}}^- \right\|_{\mathcal{H}}^2 \\
& \quad \cdot \left. \left\| P_s^- U(s,t) \phi_{i_{\tau(n-k)}}^+ \right\|_{\mathcal{H}}^2 \cdots \left\| P_s^- U(s,t) \phi_{i_{\tau(1)}}^+ \right\|_{\mathcal{H}}^2 \right)^{\frac{1}{2}}.
\end{aligned}$$

The series containing the α 's is equal to one due to the normalization of $\Psi_t^{(n,m)}$. For the other sum we note that in general, if we choose a set of n integers which are pair-wise different, then there are $n!$ possibilities to arrange these numbers but only one if we require an order, i.e. where $i_1 < \dots < i_n$. Hence, we can extend the sum over the ordered indices to all indices and correct it by the faculty of n and m ,

$$\begin{aligned}
& \left| \langle \Omega, \widehat{\Psi}_t^{(n,m)} \widehat{U}(t,s) \Omega \rangle_{\mathcal{F}_i} \right| \leq \\
& \leq \sum_{\substack{\sigma \in S_m \\ \tau \in S_n}} \sum_{k=0}^{\min\{n,m\}} \frac{1}{k!(n-k)!(m-k)! \sqrt{n!} \sqrt{m!}} \\
& \quad \cdot \left(\sum_{\substack{i_1, \dots, i_n \\ j_1, \dots, j_m}} \left| \langle U_{s,t}^{--} \phi_{j_{\sigma(m)}}^-, U_{s,t}^{-+} \phi_{i_{\tau(n)}}^+ \rangle \right|^2 \cdots \left| \langle U_{s,t}^{--} \phi_{j_{\sigma(m-k+1)}}^-, U_{s,t}^{-+} \phi_{i_{\tau(n-k+1)}}^+ \rangle \right|^2 \right. \\
& \quad \cdot \left\| P_s^+ U(s,t) \phi_{j_{\sigma(1)}}^- \right\|_{\mathcal{H}}^2 \cdots \left\| P_s^+ U(s,t) \phi_{j_{\sigma(m-k)}}^- \right\|_{\mathcal{H}}^2 \\
& \quad \cdot \left. \left\| P_s^- U(s,t) \phi_{i_{\tau(n-k)}}^+ \right\|_{\mathcal{H}}^2 \cdots \left\| P_s^- U(s,t) \phi_{i_{\tau(1)}}^+ \right\|_{\mathcal{H}}^2 \right)^{\frac{1}{2}}.
\end{aligned}$$

Because we sum over all indices, every permutation yields the same term and therefore

$$\begin{aligned}
& \left| \langle \Omega, \widehat{\Psi}_t^{(n,m)} \widehat{U}(t,s) \Omega \rangle_{\mathcal{F}_i} \right| \leq \\
& \leq \sum_{k=0}^{\min\{n,m\}} \frac{\sqrt{n!} \sqrt{m!}}{k!(n-k)!(m-k)!} \\
& \quad \cdot \left(\sum_{\substack{i_1, \dots, i_n \\ j_1, \dots, j_m}} |\langle U_{s,t}^{--} \phi_{j_m}^-, U_{s,t}^{++} \phi_{i_n}^+ \rangle|^2 \cdots |\langle U_{s,t}^{--} \phi_{j_{m-k+1}}^-, U_{s,t}^{++} \phi_{i_{n-k+1}}^+ \rangle|^2 \right. \\
& \quad \cdot \|P_s^+ U(s,t) \phi_{j_i}^-\|_{\mathcal{H}}^2 \cdots \|P_s^+ U(s,t) \phi_{j_{m-k}}^-\|_{\mathcal{H}}^2 \\
& \quad \left. \cdot \|P_s^- U(s,t) \phi_{i_{n-k}}^+\|_{\mathcal{H}}^2 \cdots \|P_s^- U(s,t) \phi_{i_1}^+\|_{\mathcal{H}}^2 \right)^{\frac{1}{2}} = \\
& = \sum_{k=0}^{\min\{n,m\}} \frac{\sqrt{n!} \sqrt{m!}}{k!(n-k)!(m-k)!} \left(\sum_{i=1, j=1} |\langle U_{s,t}^{--} \phi_j^-, U_{s,t}^{++} \phi_i^+ \rangle|^2 \right)^{\frac{k}{2}} \\
& \quad \cdot \left(\sum_{i=1} \|P_s^+ U(s,t) \phi_i^-\|_{\mathcal{H}}^2 \right)^{\frac{m-k}{2}} \left(\sum_{i=1} \|P_s^- U(s,t) \phi_i^+\|_{\mathcal{H}}^2 \right)^{\frac{n-k}{2}} = \\
& = \sum_{k=0}^{\min\{n,m\}} \frac{\sqrt{n!} \sqrt{m!}}{k!(n-k)!(m-k)!} \|P_t^- U(t,s) P_s^- U(s,t) P_t^+\|_{\text{HS}}^k \\
& \quad \cdot \|P_s^+ U(s,t) P_t^-\|_{\text{HS}}^{m-k} \|P_s^- U(s,t) P_t^+\|_{\text{HS}}^{n-k}.
\end{aligned}$$

□

The second theorem of this chapter is the counterpart of the one above. It gives a characterization of when transitions from the vacuum state to higher particle sectors in Fock space happen due to the one-particle time evolution. Note that in this case it is sufficient to control the behavior of a single one-particle state only. Again, in the view of the Dirac sea this is clear because if we can find a state which performs a transition from the negative energy part of the Hilbert space to the positive energy one we have created a pair and have thus left the vacuum. Also, in this case the proof is given solely on the framework of external field QED and no reference to the Dirac sea besides the interpretation is necessary. The theorem was inspired by a result in [PD08] where it was shown that if there exists a $\varphi \in \mathcal{H}$ such that $\lim_{t \rightarrow \infty} \lim_{s \rightarrow -\infty} \|P_t^- U(t,s) P_s^- \varphi\|_{\mathcal{H}}^2 = 0$ then we have

$$\lim_{t \rightarrow \infty} \lim_{s \rightarrow -\infty} \left| \langle \Omega, \widehat{U}(t,s) \Omega \rangle \right| = 0,$$

with Ω being the usual free-field vacuum. We generalize the statement to finite times using our time-dependent Fock space formalism and realistic settings where $\|P_t^- U(t,s) P_s^- \varphi\|_{\mathcal{H}}^2$ is close but not equal to zero.

Theorem 9.4. *Let the external potential be such that there exists a unitarily implementable one-particle time evolution and let $s < t$. We then have*

$$|\langle \Omega, \widehat{U}(t, s)\Omega \rangle| \leq \inf_{\substack{\varphi \in \mathcal{H}_s^- \\ \|\varphi\|=1}} \frac{2 \|\mathbb{P}_t^- U(t, s) \mathbb{P}_s^- \varphi\|_{\mathcal{H}}}{1 + \|\mathbb{P}_t^- U(t, s) \mathbb{P}_s^- \varphi\|_{\mathcal{H}}^2}.$$

Proof. Let $\varphi \in \mathcal{H}_s^-$ be normalized to one. We then have

$$\|\Gamma_s[\varphi]\Omega_s\|_{\mathcal{F}_s} = \|b_s^\dagger[\mathbb{P}_s^- \varphi]\Omega\|_{\mathcal{F}_s} = \|\mathbb{P}_s^- \varphi\|_{\mathcal{H}} = 1. \quad (9.1)$$

We decompose the time-evolved state into the vacuum fraction at time t and the orthogonal part to it

$$\widehat{U}(t, s)\Omega = \alpha\Omega + \beta\Omega_t^\perp.$$

The time evolution is unitary and Ω normalized to one. Hence, we can always choose Ω_t^\perp to be normalized to one together with $|\alpha|^2 + |\beta|^2 = 1$. Furthermore, we have

$$\|\Gamma_s[\varphi]\Omega\|_{\mathcal{F}_s} = \|\widehat{U}(t, s)\Gamma_s[\varphi]\Omega\|_{\mathcal{F}_t}.$$

Using the definition of the time evolution (Definition 8.1) yields

$$\begin{aligned} \|\Gamma_s[\varphi]\Omega\|_{\mathcal{F}_s} &= \|\widehat{U}(t, s)\Gamma_s[\varphi]\Omega\|_{\mathcal{F}_t} = \|\widehat{U}(t, s)\Gamma_s[\varphi]\widehat{U}(s, t)\widehat{U}(t, s)\Omega\|_{\mathcal{F}_t} = \\ &= \|\Gamma_t[U(t, s)\varphi]\widehat{U}(t, s)\Omega\|_{\mathcal{F}_t} = \|\Gamma_t[U(t, s)\varphi](\alpha\Omega + \beta\Omega_t^\perp)\|_{\mathcal{F}_t} = \\ &= \|\alpha(a_t[\mathbb{P}_t^+ U(t, s)\varphi] + b_t^\dagger[\mathbb{P}_t^- U(t, s)\varphi])\Omega + \beta\Gamma_t[U(t, s)\varphi]\Omega_t^\perp\|_{\mathcal{F}_t} = \\ &= \|\alpha b_t^\dagger[\mathbb{P}_t^- U(t, s)\varphi]\Omega + \beta\Gamma_t[U(t, s)\varphi]\Omega_t^\perp\|_{\mathcal{F}_t} \leq \\ &\leq |\alpha| \|b_t^\dagger[\mathbb{P}_t^- U(t, s)\varphi]\Omega\|_{\mathcal{F}_t} + |\beta| \|\Gamma_t[U(t, s)\varphi]\Omega_t^\perp\|_{\mathcal{F}_t} \leq \\ &\leq |\alpha| \|\mathbb{P}_t^- U(t, s)\varphi\|_{\mathcal{H}} + |\beta| \|U(t, s)\varphi\|_{\mathcal{H}} = |\alpha| \|\mathbb{P}_t^- U(t, s) \mathbb{P}_s^- \varphi\|_{\mathcal{H}} + |\beta| \end{aligned}$$

where we used part 4) of Proposition 7.3 and 7.7 in the first step of the last line. Together with eq. (9.1) and the normalization condition we get

$$1 - |\alpha| \|\mathbb{P}_t^- U(t, s) \mathbb{P}_s^- \varphi\|_{\mathcal{H}} \leq \sqrt{1 - |\alpha|^2}.$$

As both sides are positive we can take the square and obtain

$$1 - 2|\alpha| \|\mathbb{P}_t^- U(t, s) \mathbb{P}_s^- \varphi\|_{\mathcal{H}} + |\alpha|^2 \|\mathbb{P}_t^- U(t, s) \mathbb{P}_s^- \varphi\|_{\mathcal{H}}^2 \leq 1 - |\alpha|^2$$

which is equivalent to

$$|\alpha| \leq \frac{2 \|\mathbb{P}_t^- U(t, s) \mathbb{P}_s^- \varphi\|_{\mathcal{H}}}{1 + \|\mathbb{P}_t^- U(t, s) \mathbb{P}_s^- \varphi\|_{\mathcal{H}}^2}.$$

This expression holds for all $\varphi \in \mathcal{H}_s^-$ with $\|\varphi\|_{\mathcal{H}} = 1$ which proves the theorem. \square

Part III.

Pair creation by strong laser fields

10. Overview

The discovery of the Dirac equation soon led physicists to one of the most intriguing features of quantum electrodynamics – pair creation. In Dirac’s famous paper [Dir30] where he introduced the hole picture he already explained the possibility of pair creation and annihilation by the absorption and emission of radiation. For a single photon to be able to do so, its energy needs to be above the threshold of $2mc^2$. This is nowadays experimentally very well confirmed and daily routine to any high energy physicist. Nevertheless, there is another extreme region of QED where we should expect pair creation to happen – strong electromagnetic fields.

This part of QED has not been verified very well because of the necessary high field strengths. Thus, this area might be fruitful in future for experimental physicists with further technological development. But also from a theoretical point of view this is a highly interesting field of QED as one cannot simply apply the usual perturbative methods anymore due to the strong fields and new approaches have to be developed.

The first hint that pair creation might take place in strong potentials is due to a computation by Klein [Kle29]. Briefly summarized, it states that for a constant step-potential in the one-particle Dirac equation the transmission coefficient for an incoming wave is not zero as in non-relativistic quantum mechanics but stays high even if the potential is increased without limit. This unexpected behavior is called Klein’s paradox. Sauter [Sau31] showed that the sharp jump in the potential is not necessary for this effect and can indeed be smoothed if the full potential height of at least more than two electron masses is reached within the Compton wave length. From this one can infer that the field strength responsible for the potential has to be at least of order $10^{18} \frac{V}{m}$. Other important contributions to this side of QED were made by Heisenberg and Euler [HE36] and Schwinger [Sch51]. We will discuss these results more in depth in the subsequent chapters but the predicted threshold of the critical field strength always stays the same as the one computed by Sauter.

The use of high intensity lasers has been one proposal to create strong electrical fields to test the aforementioned effects. The theoretical work (see e.g. [MP77], [AHR⁺01], [Pop01], [Rin01], [NBMP04], [BPR⁺06], [BET⁺10]) done on this field is mainly based on Schwinger’s computation or on a slight generalization thereof by Brezin and Itzykson [BI70]. Schwinger computes the pair creation rate for a plane wave and a static electrical field, both extended infinitely. He finds that the pair creation rate for a plane wave is identical to zero. For the static external field pair creation should take place if the electrical field exceeds the same critical field strength which Sauter found. As a laser beam is close to a plane wave no one expects pair creation to take place in such a situation. The proposed experiments should rather superpose two laser beams to form a standing wave. The argument is then as follows. At the antinodes the electromagnetic field is almost spatially homogeneous on the scale of the Compton wave length. Therefore, it seems

legitimate to use Schwinger's result on a static, homogeneous electrical field to compute the mean number of created electron-positron pairs.

However, the same argument also applies to a single plane wave but we already know that the pair-creation rate of such a field is identical to zero. Furthermore, we note that all spatially homogeneous, i.e. infinitely extended fields ought to be limits of very wide but finitely extended fields in reality. Now, assume we have a static field which yields an asymptotic complete scattering system, i.e. which can be handled by scattering theory. Then, the one-particle scattering matrix S is defined and unitary (see [Tha92, Thm. 8.3]). Furthermore, the scattering matrix commutes with the free Dirac hamiltonian. Therefore, $P^+ S P^- = P^- S P^+ = 0$. The one-particle scattering matrix is therefore unitarily implementable due to Theorem 8.6 and we have $\widehat{S}\Omega = \Omega$. But this implies we do not have any pair creation¹. This is certainly puzzling as physicists usually assume that the fields behave nicely at infinity such that these mathematical technicalities are always fulfilled. Of course, we do not have a mathematical contradiction as a field or potential which is infinitely extended does not yield an asymptotic complete scattering system. However, we cannot expect that any mathematical tricks will lead the way out of this seemingly paradoxical situation. For example, take a nice bounded, smooth barrier-potential which increases to its full strength at the length of the Compton wave length. Such a static potential can not produce any pairs. However, if we take the limit such that it becomes a smoothed step-potential we suddenly have a constant flux of pairs which was shown by Klein, Sauter and finally Hansen and Ravndal [HR81].

We therefore believe that a careful analysis of the physics and mathematics is necessary to treat the process of pair creation in strong laser fields. This is the goal of the next two chapters.

¹See also [Tha92, Thm. 10.10] and the surrounding chapter for a more detailed discussion.

11. Pair creation in constant fields and potentials

11.1. Klein's paradox

The so called Klein paradox is tightly knotted to the possibility of creating electron-positron pairs out of the vacuum. Hence, we will give a quick summary of what it is about and then go on to explain its connection to pair creation.

It was soon after Dirac published his famous equation that Klein [Kle29] applied the Dirac equation to a common problem of non-relativistic quantum mechanics – the scattering of an incoming particle on a potential step,

$$V(x) = V \quad \text{for } x \geq 0$$

and

$$V(x) = 0 \quad \text{for } x < 0.$$

As in non-relativistic quantum mechanics, Klein was interested in the reflection and transmission coefficient for an incoming plane wave from the left side. He found for the reflection and transmission coefficient that

$$R = \frac{2Vm}{\frac{V}{c^2} - (p + p')^2} = \left(\frac{1 - r}{1 + r} \right)^2, \quad T = 1 - R = \frac{4r}{(1 + r)^2}.$$

The parameter r is given by

$$r = \frac{p'}{p} \frac{E + mc^2}{E - V + mc^2},$$

where p and p' are the momentum of the incoming wave and the penetrating one. In some papers and textbooks (see e.g. [BD64]) it is said that for $V > E + mc^2$ the parameter r becomes negative and the reflection coefficient is therefore greater than one, i.e. there are more reflected particles than incoming ones. However, this was not Klein's intention as he noted¹ that for an incoming wave from the left side the group velocity always has to be positive otherwise we also would have an incoming wave from the right side.

¹According to Klein it was actually Pauli who noted the necessary condition.

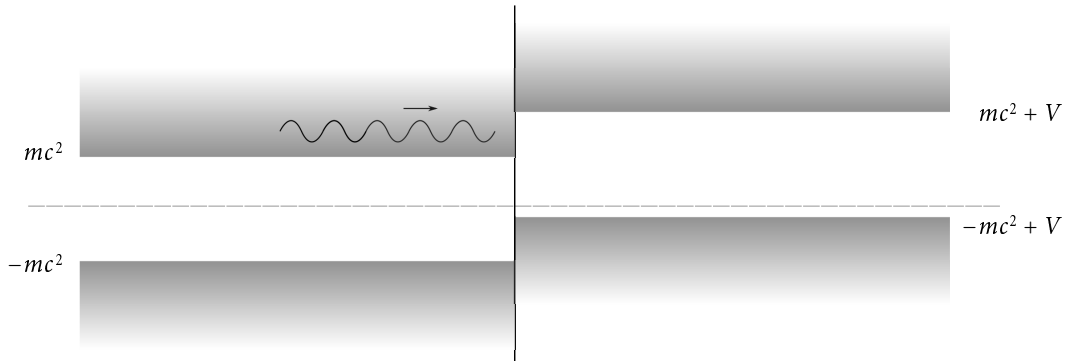


Figure 11.1.: A plane wave coming from the left side to the Klein step.

The group velocity for a wave inside the potential is given by the general formula

$$v = \frac{c^2}{E - V} p'.$$

In the interesting region $V > E + mc^2$ we see that the momentum p' is opposite to the velocity. Hence, p' becomes negative if the velocity is positive. Therefore, r is always positive and $R < 1$. The original paradoxical notion is rather that for an incoming wave in the energy band $mc^2 < E < V - mc^2$ the reflection coefficient is not equal to one as we would expect. There is a substantial percentage of particles for which this step is transparent and this behavior persists for any potential strength. In the limit $V \rightarrow \infty$ we have

$$\lim_{V \rightarrow \infty} R = \frac{E/c - p}{E/c + p}.$$

Klein also noted that a steep but finite increase of the potential would suffice to produce this effect. Sauter [Sau31] then showed that this behavior indeed persists if the potential increases linearly to its full strength at least within the Compton wave length of the electron. The necessary field strengths for this effect can thus be estimated with $2mc^2 < V$ and $\frac{V}{\lambda_c}$ to be at least approximately $10^{18} \frac{V}{m}$.

So how can one interpret this result? Hansen and Ravndal [HR81] were the first to show that for the Klein step there is a connection between the transmission coefficient T of the one-particle Dirac equation and the average rate of produced positron-electron pairs in QED. Following Caloggeracos and Dombey [CD99] the vacuum expectation value of the electric current is given by the following formula

$$\langle \Omega, j \Omega \rangle = -\frac{1}{2\pi} \int T(E) dE,$$

where the energy integral is over the Klein-zone $mc^2 < E < V - mc^2$. The resolution of the Klein paradox is the following (see e.g. [HR81], [GMR85]). The potential produces electron-positron pairs at the step. This is due to the fact that the potential lifts the negative energy continuum. For $V > 2mc^2$ the positive energy continuum to the left side of the step overlaps with the lower energy continuum inside the potential.

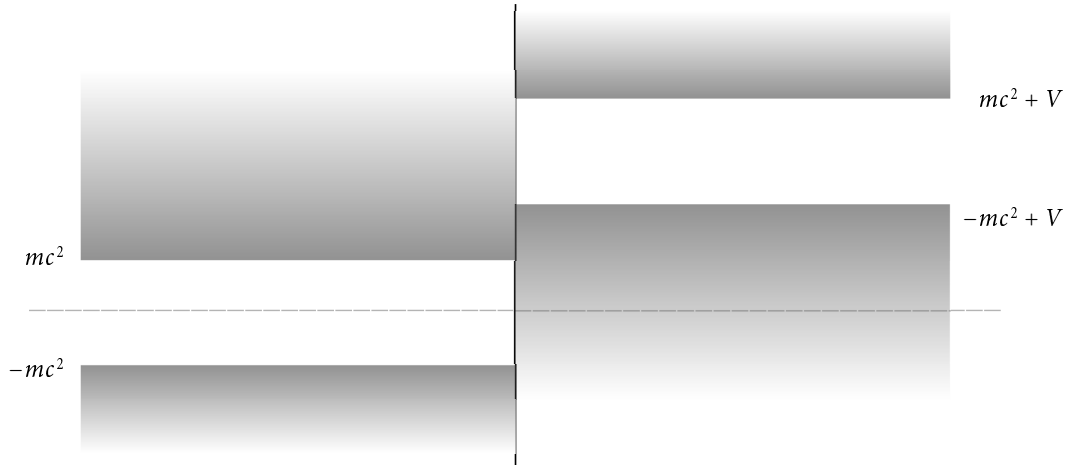


Figure 11.2.: The upper continuum to the left side overlaps with the lower continuum to the right side if the potential is stronger than $2mc^2$.

Assuming a filled Dirac sea this results in electrons from the right side of the step scattering to the left side, leaving a positive energy electron moving to the left and a hole, i.e. a positron moving to the right. If we have an additional electron coming from the left side it cannot scatter back into energies occupied by created electrons due to the Pauli principle. Therefore, such a plane wave has to be transmitted through the barrier (where the corresponding energy is now unoccupied!) resulting in a reflection coefficient smaller than one for an incoming electron from the left.

Hence, Klein's paradox was actually the first hint that electron-pair production out of the vacuum should be possible in strong external fields. However, there are no infinitely extended potentials in reality. Thus, to switch to a more realistic setting we assume the potential to be very wide but still finite,

$$V(x) = V \quad \text{for} \quad |x| \leq a,$$

and

$$V(x) = 0 \quad \text{for} \quad |x| > a.$$

But in this case we already know that there is no pair creation as we have explained in the previous chapter.

So how can this contradiction be reconciled? This is possible by the following careful observation. There are no real time-independent potentials, hence also the finite barrier has to be

switched on sometime. Furthermore, it contains bound states. When such a potential is gradually tuned up these bound states – which subsequently appear at the lower continuum edge – wander through the mass gap until they reach the upper continuum (see [DC99]). It is well known that such a behavior causes pair creation which was shown by Pickl [PD08]. The argument is that an electron from the sea occupies the bound state while it is at the lower continuum leaving a hole and this electron scatters into a free electron once the bound state reaches the upper continuum. The wider the potential is the more bound states there are in the potential and their energy spectrum is closer together. It takes time for the electrons to leave the barrier due to their finite velocity. This results in a current of electrons flowing from inside the potential. Of course, this flow is finite as there is only a finite amount of bound states inside the potential. But if one now takes the limit $a \rightarrow \infty$ we have more and more electrons in the potential and the time-dependent current becomes a steady time-independent current. One can now show that the vacuum expectation value of this current is connected to the transmission amplitude in the same way as for the Klein step (see [DC99]).

11.2. Schwinger mechanism

Schwinger [Sch51] computed the probability of positron-electron pair creation for a plane wave and a homogeneous, static electric field within the fully developed QED framework. Whereas the probability to create pairs with a plane wave is identical to zero for all field strengths the pair creation rate per unit volume and unit time is for a constant electric field of the order

$$w = \exp\left[-\frac{m^2 c^3}{e \hbar E}\right] = \exp\left[-\frac{E_{cr}}{E}\right],$$

where E is the electric field strength and $E_{cr} \approx 10^{18} \frac{\text{V}}{\text{m}}$ is the critical field strength. Of course, an infinitely extended electric field is not realistic. Wang and Wong [WW88] computed what they called the finite-size Schwinger mechanism, which corresponds to a constant electric field inside a plate capacitor and a vanishing field outside. They used numerical evaluations to analyze their derivations and found that pair creation is again lead by a term proportional to w if the plates are not too close together.

This result is not very surprising as such a field corresponds precisely to the potential considered by Sauter which we discussed in the previous chapter. In fact, the potential for the Schwinger field can be written as

$$\phi(x) = -E \cdot x = \sum_{n=-\infty}^{\infty} \phi_n(x),$$

with

$$\phi_n(x) = \begin{cases} 0 & x < d \cdot n \\ E \cdot (x - n \cdot d) & d \cdot n < x < d \cdot (n + 1) \\ \frac{2mc^2}{e} & d \cdot (n + 1) < x \end{cases},$$

with the electrical field strength E and the width $d = \frac{2mc^2}{eE}$. If E exceeds critical field strength E_{cr} we find that d becomes smaller than the Compton wave length. Therefore, each ϕ_n now acts as a Sauter potential being capable of creating pairs. The Schwinger mechanism can thus be understood as repeated versions of the Klein-Sauter effect with the same physical origin.

Our conclusion is that the pair-production mechanism in reality is *always* a result of the time-dependency of a particular external field. To investigate the possibility of pair-creation one therefore has to analyze if an external field is capable of lifting electrons through the mass gap.

12. Pair creation by strong laser fields

We explained how pair creation by strong fields always originates from the time-dependency of a particular field. If the external field is capable of creating bound states which cross the spectral gap we know that these bound states scatter once they dive into the positive energy continuum. This results in an electron-positron pair as was first proved by Pickl [Pic05].

How is the situation for intense laser? As we have already mentioned almost all work on that topic relies on the computation by Schwinger and its generalization by Brezin and Itzykson [BI70]. Although Brezin and Itzykson already had the application to intense lasers in mind their work should not be interpreted as a conjecture for pair creation by lasers. On the contrary, it was rather meant to discourage the hope for an early verification at that time. We find in their paper:

Instead of estimating the effect for an arbitrary electromagnetic field varying in space and time, we will content ourselves with a pure electric field oscillating with a frequency ω . In spite of the slightly unrealistic character of this assumption, we expect that it retains the main features of a more general situation. It is, of course, well known that specific anomalies can occur; for instance, there is no pair creation in a plane-wave field. Therefore, if the rate predicted by the theory were more favorable, one should pay more attention to the particular geometrical characterization.

Unfortunately, it seems that this precaution got lost in the course of time. As we explained in the previous chapter, the Schwinger mechanism is rooted in the capability of lifting bound states to the positive energy continuum. And such a behavior is certainly not a local effect but requires a “particular geometrical characterization” of a potential. While it is true that a standing wave can locally be approximated by a constant field it is nevertheless not able to lift bound states through the gap. This can be seen as follows. In Coulomb gauge the electromagnetic wave in the vacuum is described by a pure vector potential. And from Theorem 3.6 we know that the spectrum of such a potential is absolutely continuous. In particular, there are no bound states in the gap at any time and no lifting can occur. We conclude that any treatment of pair creation by strong lasers which only focuses on a locally achievable peak field strength is misleading and highly questionable in general.

To analyze the situation for lasers we have to combine the results and methods which we have developed in the first two parts into a statement about pair creation probability of certain external fields. To be able to use all previous results we have to impose the following regularity condition on the vector potential. However, this is more of technical nature and can most likely be further relaxed.

Condition E (Regularity condition). Let $\mathbf{A}(t, \mathbf{x}) \in C^\infty(\mathbb{R} \times \mathbb{R}^3 \rightarrow \mathbb{R}^3)$ such that it fulfills the following:

- let $\frac{d^j}{dt^j} \mathbf{A}(t, \mathbf{x}) \in L^\infty \cap L^2$ for $j = 1, 2, 3$
- let $\frac{\partial^j}{\partial t^j} \mathbf{A}(t, \mathbf{x}) \in L^1$ for $j = 1, 2$
- let $|\mathbf{A}(t, \mathbf{x})| \leq C |\mathbf{x}|^{-2-h}$ and $|\partial_{x_i} \mathbf{A}(t, \mathbf{x})| \leq C |\mathbf{x}|^{-1-h}$ for sufficiently large $|\mathbf{x}|$.
- let the vector potential be such that there are $s, t \in \mathbb{R}$ such that $\mathbf{A}(r, \mathbf{x}) = 0$ for all $r \notin (s, t)$.

We denote with $\mathbf{E} = -\frac{\partial}{\partial t} \mathbf{A}$ the electric field and with $E_0 = \sup_{(t, \mathbf{x}) \in \mathbb{R} \times \mathbb{R}^3} |\mathbf{E}(t, \mathbf{x})|$ the maximal field strength. With \dot{E}_0 and \ddot{E}_0 we mean the maximal amplitude of the time-derivatives of the electric field. Under these conditions we can formulate the following theorem¹.

Theorem 12.1. Let $A^\mu = (\phi, -\mathbf{A})$ be a four-vector potential with $\phi = 0$ and $\mathbf{A}(t, \mathbf{x}) \in C^3(\mathbb{R} \times \mathbb{R}^3 \rightarrow \mathbb{R}^3)$ such that it fulfills the regularity condition. Furthermore, let it be such that there are no eigenvalues for $\lambda \in \{-1, 1\}$ of the extended Dirac operator in the weighted space $L^2_\gamma(\mathbb{R}^3 \rightarrow \mathbb{C}^4)$ for some $\gamma > \frac{1}{2}$. We then have for the pair creation probability $p_{e^-e^+}$ and the mean value $\mu_{e^-e^+}$ during the time interval $[s, t]$ that

$$p_{e^-e^+} \leq \|P^+ U(t, s) P^-\|_{\text{HS}}^2 \frac{(1 + \|P^- U(t, s) P^+\|_{\text{HS}})}{1 - \|P^+ U(t, s) P^-\|_{\text{HS}} (1 + \|P^- U(t, s) P^+\|_{\text{HS}})}$$

and

$$\mu_{e^-e^+} \leq \|P^+ U(t, s) P^-\|_{\text{HS}}^2 \frac{1}{(1 - \|P^+ U(t, s) P^-\|_{\text{HS}} (1 + \|P^- U(t, s) P^+\|_{\text{HS}}))^2}$$

with

$$\|P^\pm U(t, s) P^\mp\|_{\text{HS}} \leq C \pi \varepsilon^2 |t - s| \sup_{\substack{\mathbf{x}, \mathbf{k} \in \mathbb{R}^3 \\ t \in \mathbb{R}}} |\phi_{\pm t}(\mathbf{x}, \mathbf{k})| \\ \cdot \sup_{t \in \mathbb{R}} \left(54 C^2 E_0^3 \left\| \frac{\mathbf{E}(t, \cdot)}{E_0} \right\|_{L^2} + 7 C E_0 \dot{E}_0 \left(\left\| \frac{\mathbf{E}(t, \cdot)}{E_0} \right\|_{L^2} + \left\| \frac{\dot{\mathbf{E}}(t, \cdot)}{\dot{E}_0} \right\|_{L^2} \right) + \ddot{E}_0 \left\| \frac{\ddot{\mathbf{E}}(r, \cdot)}{\ddot{E}_0} \right\|_{L^2} \right)$$

and

$$C = \sum_{n=0}^{\infty} \frac{1}{(n+1)^2} \left(\frac{n}{n+1} \right)^{2n}.$$

¹Remember that, in our system of units, position is measured in terms of the Compton wave length of the electron and time is measured in terms of *macroscopic time*, i.e. $\frac{t}{\varepsilon}$ with the natural time τ .

Proof. The probability of creating exactly n -pairs from the vacuum during the time-interval $[s, t]$ is given by the square of the amplitude in Theorem 9.1 with $n = m$

$$p_{e^-e^+}^{(n)} = |\beta_{n,n}|^2 .$$

Using the result of Theorem 9.1 we get

$$p_{e^-e^+}^{(n)} \leq \left(\sum_{k=0}^n \frac{n!}{k!(n-k)!(n-k)!} \|P_t^- U(t,s) P_s^- U(s,t) P_t^+\|_{\text{HS}}^k \cdot \|P_s^+ U(s,t) P_t^-\|_{\text{HS}}^{n-k} \|P_s^- U(s,t) P_t^+\|_{\text{HS}}^{n-k} \right)^2 .$$

The total probability that some pairs are created by the action of the external field is then simply the sum

$$p_{e^-e^+} = \sum_{n=1}^{\infty} p_{e^-e^+}^{(n)} \leq \sum_{n=1}^{\infty} \left(\sum_{k=0}^n \frac{n!}{k!(n-k)!(n-k)!} \|P_t^- U(t,s) P_s^- U(s,t) P_t^+\|_{\text{HS}}^k \cdot \|P_s^+ U(s,t) P_t^-\|_{\text{HS}}^{n-k} \|P_s^- U(s,t) P_t^+\|_{\text{HS}}^{n-k} \right)^2 .$$

Furthermore, the expected value of pairs in an experiment is given by

$$\mu_{e^-e^+} = \sum_{n=1}^{\infty} n \cdot p_{e^-e^+}^{(n)} = \sum_{n=1}^{\infty} n \left(\sum_{k=0}^n \frac{n!}{k!(n-k)!(n-k)!} \|P_t^- U(t,s) P_s^- U(s,t) P_t^+\|_{\text{HS}}^k \cdot \|P_s^+ U(s,t) P_t^-\|_{\text{HS}}^{n-k} \|P_s^- U(s,t) P_t^+\|_{\text{HS}}^{n-k} \right)^2 .$$

To evaluate these expressions we abbreviate

$$A := \|P_t^- U(t,s) P_s^- U(s,t) P_t^+\|_{\text{HS}} ,$$

and

$$B := \|P_s^+ U(s,t) P_t^-\|_{\text{HS}} \|P_s^- U(s,t) P_t^+\|_{\text{HS}} .$$

We then have for $p_{e^-e^+}^{(n)}$

$$p_{e^-e^+}^{(n)} \leq \left(\sum_{k=0}^n \frac{n!}{k!(n-k)!(n-k)!} A^k B^{n-k} \right)^2 \leq \left(\sum_{k=0}^n \frac{n!}{k!(n-k)!} A^k B^{n-k} \right)^2 = (A + B)^{2n} .$$

For $A + B < 1$ we can employ the geometric series to give a bound on the total probability

$$p_{e^-e^+} \leq \sum_{n=1}^{\infty} (A + B)^{2n} = \frac{(A + B)^2}{1 - (A + B)^2}$$

and similarly for the mean value

$$\mu_{e^-e^+} \leq \sum_{n=1}^{\infty} n (A + B)^{2n} = \frac{(A + B)^2}{(1 - (A + B)^2)^2}.$$

Using $P_s^- = (P_s^-)^2$ we can determine a bound on $A + B$ by

$$\begin{aligned} A + B &= \|P_t^- U(t, s) P_s^- U(s, t) P_t^+\|_{\text{HS}} + \|P_s^+ U(s, t) P_t^-\|_{\text{HS}} \|P_s^- U(s, t) P_t^+\|_{\text{HS}} \leq \\ &\leq \|P_t^- U(t, s) P_s^-\| \|P_s^- U(s, t) P_t^+\|_{\text{HS}} + \|P_s^+ U(s, t) P_t^-\|_{\text{HS}} \|P_s^- U(s, t) P_t^+\|_{\text{HS}} \leq \\ &\leq \|P_s^- U(s, t) P_t^+\|_{\text{HS}} (\|P_t^- U(t, s) P_s^-\| + \|P_s^+ U(s, t) P_t^-\|_{\text{HS}}) \leq \\ &\leq \|P_s^- U(s, t) P_t^+\|_{\text{HS}} (1 + \|P_s^+ U(s, t) P_t^-\|_{\text{HS}}). \end{aligned}$$

If $\|P_s^\pm U(s, t) P_t^\mp\|_{\text{HS}} < \frac{1}{2}$ we have that $A + B < 1$ and therefore

$$\begin{aligned} p_{e^-e^+} &\leq \|P_s^- U(s, t) P_t^+\|_{\text{HS}}^2 \frac{(1 + \|P_s^+ U(s, t) P_t^-\|_{\text{HS}})^2}{1 - \|P_s^- U(s, t) P_t^+\|_{\text{HS}}^2 (1 + \|P_s^+ U(s, t) P_t^-\|_{\text{HS}})^2} \leq \\ &\leq \|P_s^- U(s, t) P_t^+\|_{\text{HS}}^2 \frac{(1 + \|P_s^+ U(s, t) P_t^-\|_{\text{HS}})}{1 - \|P_s^- U(s, t) P_t^+\|_{\text{HS}} (1 + \|P_s^+ U(s, t) P_t^-\|_{\text{HS}})}, \end{aligned}$$

where we used the third binomial identity. Similarly, we obtain for the mean value

$$\mu_{e^-e^+} \leq \|P_s^- U(s, t) P_t^+\|_{\text{HS}}^2 \frac{1}{(1 - \|P_s^- U(s, t) P_t^+\|_{\text{HS}} (1 + \|P_s^+ U(s, t) P_t^-\|_{\text{HS}}))^2}.$$

Taking the adjoint of the operators yields the formula used in the statement of the theorem.

To estimate the Hilbert-Schmidt norm above we now use Theorem 6.3 and the remarks afterwards together with eq. (6.20) and eq. (6.21). Note, that the boundary terms vanish as the vector potential is assumed to be zero at the boundary of the interval. Also, the projections at s and t are then the spectral projections corresponding to the free Dirac operator. The electric field is given as the time-derivative of the vector potential (as we only have a vector potential) and the operator norm is just the infinity norm of the electric field and its time-derivatives. We denote the maximal field strength in the time interval $[s, t]$ with E_0 . Thus, we have the following estimate on the Hilbert-Schmidt norm

$$\begin{aligned} \|P^\pm U(t, s) P^\mp\|_{\text{HS}} &\leq C\pi\varepsilon^2 |t - s| \sup_{\substack{x, k \in \mathbb{R}^3 \\ t \in \mathbb{R}}} |\phi(x, k)| \\ &\cdot \sup_{t \in \mathbb{R}} \left(54C^2 E_0^3 \left\| \frac{\mathbf{E}(t, \cdot)}{E_0} \right\|_{L^2} + 7C E_0 \dot{E}_0 \left(\left\| \frac{\mathbf{E}(t, \cdot)}{E_0} \right\|_{L^2} + \left\| \frac{\dot{\mathbf{E}}(t, \cdot)}{\dot{E}_0} \right\|_{L^2} \right) + \ddot{E}_0 \left\| \frac{\ddot{\mathbf{E}}(r, \cdot)}{\ddot{E}_0} \right\|_{L^2} \right) \end{aligned}$$

under the conditions we have imposed here. \square

We now use these considerations to look further into the possibility of creating electron-positron pairs with ultra intense lasers. Plane waves do not produce any pairs as we have explained earlier. Hence, we assume to have two focused laser beams which are opposite to each other such that they form a standing wave. The interesting region where the maximal field strength is obtained is the focused spot with a radius roughly the size of the wave length. These are the two common assumption in the literature (see e.g. [AHR⁺01], [Pop01], [Rin01], [BPR⁺06], [BET⁺10]). The electromagnetic field outside of the focused spot is of no big relevance to pair production. Hence, we can require the necessary decay of the field far away from the spot region. Furthermore, we assume the vector potential to be infinitely often differentiable which is certainly the case for a standing wave. Therefore, we see by Theorem 3.6 that the spectral gap is free of any bound states and no lifting can occur.

However, to finally apply Theorem 12.1 we also have to show that there are no eigenvalues at the gap. This condition is more subtle and it enters the previous discussion in two ways. The first one is explicit through the prerequisite in Proposition 3.5. Generalized eigenfunctions will usually become singular at the spectral edge if there are eigenstates or resonances (see [Teu99], [Pic07]). And as the bound of the Hilbert-Schmidt operator in Lemma 6.2 depends on the absolute value of the generalized eigenfunctions we have to exclude such a behavior. However, the generalized eigenfunctions appear in the context of generalized Fourier transform and it could very well be that this bound can be improved with a better incorporation of certain properties of the Fourier transform.

But this is where we demanded the absence of eigenstates at the edge implicitly a second time. The spectral projections as we defined them are strictly speaking the spectral projections onto the absolutely continuous part of the positive and negative subspaces. We have shown in the proof of Theorem 3.6 that the spectrum is only absolutely continuous if there are no eigenvalues and resonances at the gap and therefore the absolutely continuous subspace is identical to the whole space. If there are eigenvalues at the edge then our proof of the adiabatic theorem is only valid for the absolutely continuous subspace and we have to distinguish two cases. In the first one, the eigenspace is finite dimensional. The transition operator onto this subspace is then a finite rank operator and hence Hilbert-Schmidt. The same also holds for transitions from this subspace by using the adjoint. Hence, we expect that our proof of the adiabatic theorem can be easily generalized to include also this case. However, the eigenspace can very well be infinite dimensional. In this case the Hilbert-Schmidt property is not obvious. One important property to establish finiteness of the Hilbert-Schmidt norm was that transitions are suppressed by the square of the inverse energy of a specific mode. This does not work for eigenstates at the gap edge anymore. Hence, there is no good heuristic argument why the Hilbert-Schmidt adiabatic theorem should also hold in the case of infinitely degenerated eigenvalues at the gap. Investigating this case is a near term future research goal. Furthermore, it should be clarified if this is connected to the possible singularity of the Hilbert-Schmidt norm in Lemma 6.2.

So how is the situation with lasers? Unfortunately, the question regarding eigenvalues at the gap is difficult. There are no general results concerned with the geometry of potentials which

would exclude such a behavior. However, we observe that eigenstates which have been explicitly constructed seem to be rather special (see [AMN99], [AMN00]). Furthermore, we also find in the paper of Saito and Umeda ([SU11]) that vector potentials which create eigenvalues at the gap edge are rather sparse. The precise statement is the following. If the vector potential is L^3 (which is true for our assumptions on the vector potential), then the set of vector potentials which do not have eigenvalues at the edge is dense in L^3 and a possible non-empty eigenspace is always finite dimensional.

Hence, we are lead to believe that a generic laser field does not possess this special and rather sparse ability to create electron-positron pairs by edge eigenvalues. Therefore, we strongly conjecture that the assumption of Theorem 12.1 regarding this point are fulfilled by a laser field. However, the rigorous analysis of this is certainly an interesting task for future research.

Generally, a laser puls or the focused spot of a laser beam is at least of order of the wave length. Thus, the volume of the interesting region, where possible pair creation can take place, scales inversely with the frequency. One has to take this behavior into account, otherwise the results of the adiabatic limit, where the frequency vanishes, would be physically misleading. The normalized L^2 -norm in the theorem precisely serves the purpose to measure the volume where pair-creation could happen and to take it into account. For a standing wave in the spot region we have

$$|\mathbf{E}(t, \mathbf{x})| \propto E_0 \sin\left(\frac{2\pi}{\lambda} \mathbf{x}\right) = E_0 \sin(\varepsilon \mathbf{x})$$

for \mathbf{x} in natural units. For the L^2 -norm to be ε independent we can rescale and substitute $\mathbf{x}' = \varepsilon \mathbf{x}$. This yields

$$\left\| \frac{\mathbf{E}(t, \cdot)}{E_0} \right\|_{L^2} = \left(\int \left| \frac{\mathbf{E}(t, \varepsilon \mathbf{x})}{E_0} \right|^2 d^3 x' \right)^{\frac{1}{2}} = \frac{1}{\varepsilon^{\frac{3}{2}}} \left(\int \left| \frac{\mathbf{E}(t, \mathbf{x}')}{E_0} \right|^2 d^3 x' \right)^{\frac{1}{2}}$$

where the latter integral is now a frequency independent constant. This is the reason why we used second order adiabatic perturbation theory in Theorem 12.1. Remember that we are on the time scale of the external field. Hence, the time derivative of the electromagnetic wave has also the amplitude E_0 . The Hilbert-Schmidt norm simplifies to

$$\|P^\pm U(t, s) P^\mp\|_{HS} \leq \varepsilon^{\frac{1}{2}} |t - s| \sup_{\substack{\mathbf{x}, \mathbf{k} \in \mathbb{R}^3 \\ t \in \mathbb{R}}} \left| \phi(\mathbf{x}, \mathbf{k}) \right| (C_3 E_0^3 + C_2 E_0 E_0^2 + C_1 E_0)$$

where we absorbed all ε -independent quantities into the constants. The eigenfunctions depend on the adiabatic parameter. Therefore, the absolute value could also scale inversely to ε like the support of the external field. However, in the Lippmann-Schwinger equation we also have a phase which oscillates proportional to ε^{-1} if we rescale the integral like we did with the L^2 -norm. Furthermore, we see that the generalized eigenfunctions enter the inequality above through the estimate carried out in Theorem 6.3. First, we note that the estimate there is a rough one and most likely not sharp. Secondly, possible singular behavior up to any arbitrary power in ε^{-1} could easily

be canceled by using higher order adiabatic perturbation theory as the generalized eigenfunctions will always be of linear order in the estimate of the Hilbert-Schmidt norm. In this case, we can take the adiabatic limit and see that for $\varepsilon \rightarrow 0$ no pair creation occurs no matter how strong the external field is. The resulting electric field, corresponding to the adiabatic limit, is infinitely extended, homogeneous and constant in time. In other words, it is precisely the Schwinger field. The completely different results come from different limiting procedures. Schwingers field can be thought of as Klein-Sauter potentials added up ad infinitum whereas we started with an electromagnetic wave. However, it exemplifies that the “geometric characterisation” of the field under investigation must be taken into account as Brezin and Itzykson already presumed. Furthermore, our limit seems to be better suited in the context of ultra intense lasers which in turn means that results for laser fields derived by use of Schwingers computations are highly questionable.

Furthermore, there is nothing which prevents us from going to ever higher orders in ε if the external field is infinitely often differentiable. It is just a matter of handling the corresponding estimates as we did in Chapter 6.3. From the way X_n and Y_n are defined in eq. (6.7) and eq. (6.8) we can already infer that $\dot{X}_{n+2} + \dot{Y}_{n+2}$ scale in leading order with

$$\|\dot{X}_{n+2}\| + \|\dot{Y}_{n+2}\| \propto E_0^{n+3} \left\| \frac{\mathbf{E}(t, \cdot)}{E_0} \right\|_{L^2}.$$

In particular the L^2 -norm enters always linearly. Thus, the Hilbert-Schmidt norm is in leading order of the peak field strength proportional to

$$\|P_s^- U(s, t) P_t^+\|_{HS} \propto \varepsilon^{\frac{1}{2}} E_0^3 C_n (\varepsilon E_0)^n$$

where $n = 0$ corresponds to the second order adiabatic perturbation which we have performed above. We note that in our choice of units we have

$$E = \frac{e\hbar}{m^2 c^3} E_{SI} = \frac{E_{SI}}{E_{cr}}$$

with $E = |\mathbf{E}|$, E_{SI} being the field strength in SI units and E_{cr} being the critical field strength. Hence, to have the estimate in a form independent of the unit system we have to write

$$p_{e^-e^+} \propto \|P_s^- U(s, t) P_t^+\|_{HS}^2 \lesssim \varepsilon \left(\frac{E_0}{E_{cr}} \right)^6 C_n \left(\varepsilon \frac{E_0}{E_{cr}} \right)^{2n}$$

in leading order of the peak field strength. This result is contrary to what can be found in the literature so far (e.g. see [MP77], [AHR⁺01], [Pop01], [Rin01], [NBMP04], [BPR⁺06], [BET⁺10]). There, the probability of creating electron-positron pairs is believed to be suppressed for

$$p_{e^-e^+} \propto \frac{E_0}{E_{cr}} \ll 1,$$

which is obtained by using the Schwinger computation. However, we have already argued against the validity of using Schwingers result in the context of electromagnetic waves. Our result now

suggests that the adiabatic parameter has been missing in the computations so far and possible transitions are suppressed if

$$\varepsilon \frac{E_0}{E_{cr}} \ll 1.$$

To demonstrate the drastic consequences we assume that

$$\frac{E_0}{E_{cr}} \approx 1.$$

This is the region where up to now it has been believed that pair creation should become observable. For common lasers with $\lambda_1 = 1 \mu\text{m}$ or $\lambda_2 = 1 \text{nm}$ we have

$$\varepsilon_1 = \frac{\lambda_C}{\lambda_1} \approx 2 \cdot 10^{-6} \quad \text{and} \quad \varepsilon_2 = \frac{\lambda_C}{\lambda_2} \approx 2 \cdot 10^{-3},$$

where λ_C is the Compton wave length of the electron. Hence, the mean value and probability to observe pair creation with intense lasers is at least a thousand to a million times lower than what has been assumed.

Finally, we also feel the need to stress that the computations above establish only an *upper* bound on the pair creation probability. All the estimates carried out in our derivations are most likely not the best ones. Hence, it could well be that the actual probability to observe pair creation with laser is well below our estimate. For example, note that if one could obtain a good grab on the constants C_n , i.e. if it could be shown that $\sqrt[n]{C_n}$ is bounded by some constant C uniformly for all n then we have

$$\left(\varepsilon \sqrt[n]{C_n} E_0 \right)^n < (\varepsilon C E_0)^n \quad \text{for all } n.$$

This in turn would show that pair creation probability and mean number of created pairs are identical to zero if $\varepsilon < (C E_0)^{-1}$ as the right hand side vanishes for $n \rightarrow \infty$.

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Eidesstattliche Versicherung

(Gemäß Promotionsordnung vom 12.07.11, §8, Abs. 2 Pkt. 5)

Hiermit erkläre ich an Eidesstatt, dass die Dissertation von mir selbstständig, ohne unerlaubte Beihilfe angefertigt ist.

Johannes Mattis Nissen-Meyer

München, den 18. April 2018