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The non-relativistic limit of Dirac operators with electrostatic and Lorentz scalar δ-shell interactions in $\mathbb{R}^3$

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Affidavit

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Abstract

In this master thesis the non-relativistic limit of Dirac operators with electrostatic and Lorentz scalar δ-shell interactions in $\mathbb{R}^3$ is investigated. These interactions appear, for instance, as idealizations in the description of a relativistic quantum particle with spin $1/2$ in the presence of strongly localized external fields. In order to describe δ-shell interactions, we consider the formal differential expression

$$\mathcal{A}_{\eta,\tau} = A_0 + (\eta I_4 + \tau\beta)\, \langle \delta_\Sigma, \cdot \rangle \delta_\Sigma$$

as a singular pertubation of the free Dirac operator A_0. Here, Σ is a compact, closed and C^2-smooth surface in $\mathbb{R}^3$, $\eta, \tau \in \mathbb{R}$ represent the strengths of interaction and $I_4, \beta \in \mathbb{C}^{4\times 4}$ are two matrices. Applying the theory of quasi boundary triples, self-adjoint operators $A_{\eta,\tau}$ can be constructed by encoding the effect of the δ-interactions in form of suitable jump conditions on the interface Σ. These operators are interpreted as realizations of the formal differential expression above.

Subsequently, for $\lambda \in \mathbb{C} \setminus \mathbb{R}$ the non-relativistic limit

$$\big(A_{\eta,\tau} - \big(\lambda + mc^2\big)\big)^{-1} \to \begin{pmatrix} (T_{\eta,\tau} - \lambda)^{-1} & 0 \\ 0 & 0 \end{pmatrix} \quad \text{for } c \to \infty$$

is determined for the resolvent, where $T_{\eta,\tau}$ is a self-adjoint operator. The corresponding convergence analysis and the characterization of the limit operator $T_{\eta,\tau}$ is done separately for the two cases $\eta + \tau \neq 0$ and $\eta + \tau = 0$, as in these the limit operators behave quite differently.

For the parameter combination $\eta + \tau \neq 0$, the limit operator $T_{\eta,\tau}$ turns out to be a Schrödinger operator with a δ-interaction of strength $\eta + \tau$. This indicates that the Dirac operators $A_{\eta,\tau}$ can indeed be regarded as relativistic counterparts of the well studied Schrödinger operators with δ-interactions.

Finally, it is shown that in the case of $\eta + \tau = 0$, the limit operator $T_{\eta,\tau}$ is a Schrödinger operator as well. However, the characterization of the domain of definition yields that, in contrast to the case $\eta + \tau \neq 0$, there are no jump conditions describing δ-interactions but oblique jump conditions.

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Contents

1 Introduction

In non-relativistic quantum mechanics, a free particle with mass m is described by the free Schrödinger equation

$$i\hbar \frac{\partial}{\partial t}\Psi = -\frac{\hbar^2}{2m}\Delta\Psi \tag{1.1}$$

with Planck's constant $\hbar$ and wave function Ψ. This equation neglects small details such as the spin of particles, which is necessary to explain the magnetic moment of particles as it was observed in the Stern-Gerlach experiment. A reason for this can be seen in the fact that the spin observable does not have a classical analogue and is therefore not taken into account when deriving the Schrödinger equation by applying substitution rules. In order to include the description of the spin of a particle, it has to be added retrospectively to non-relativistic quantum mechanics by means of a magnetic moment operator as it is done in the monograph [54, Chaper 5.2]. Furthermore, due to the asymmetry of temporal and spatial coordinates, it is obvious that the Schrödinger equation (1.1) is not invariant under Lorentz transformations. Dirac's aim was to generalize equation (1.1) to a relativistic equation, which besides the explanation of many other phenomena, provides a natural description of the particle spin. In the following we motivate the Dirac equation, based on Dirac's approach, as it is done in [54, Chapter 5.3] or [78, Chapter 1.1]. Firstly, observe that by formally replacing the numbers E and p_k in the classical, non-relativistic energy-momentum relationship of a free particle

$$E = \frac{p^2}{2m} = \frac{1}{2m}\sum_{k=1}^{3} p_k^2 \tag{1.2}$$

by the differential expressions $i\hbar\frac{\partial}{\partial t}$ and $-i\hbar\frac{\partial}{\partial x_k}$, the free Schrödinger equation (1.1) is obtained. Following the presentation in [54, Chaper 5.3] we introduce the relativisitic 4-momentum

$$(p^\mu) = \left(\frac{E}{c}, \gamma m v\right)$$

with the rest mass m, the speed of light c, the velocity of the particle v in the current inertial reference system and the γ-factor $\gamma = \left(1 - \frac{v^2}{c^2}\right)^{-\frac{1}{2}}$. Using the metric tensor of special relativity $(\eta_{\mu\nu})$, one obtains the Lorentz invariant energy-momentum relationship of a free particle

$$p_\mu p^\mu = \eta_{\mu\nu} p^\nu p^\mu = m^2 c^2$$

or equivalently

$$E^2 = c^2p^2 + m^2c^4 \tag{1.3}$$

with the relativistic 3-momentum $p = \gamma mv$. The first attempt in generalizing the Schrödinger equation (1.1) is to apply substitution rules, as we did above in deriving it from the energy-momentum relationship (1.2). In particular, we define the 4-gradient as

$$(\partial^\mu) = \left(\frac{1}{c}\frac{\partial}{\partial t}, -\nabla\right)$$

and replace the relativistic 4-momentum (p^μ) in the energy-momentum relationship (1.3) by the differential expression $(i\hbar\partial^\mu)$. This leads to the so-called Klein-Gordon equation

$$\left(\Delta - \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{m^2c^2}{\hbar^2}\right)\Psi = 0,$$

which is a Lorentz invariant partial differential equation of second order in temporal and spatial coordinates. Therefore more information about the system has to be known, since in addition to $\Psi(t_0,\cdot)$ also the initial condition $\frac{\partial}{\partial t}\Psi(t_0,\cdot)$ at a given time $t_0 \in \mathbb{R}$ has to be specified to solve this wave equation uniquely. Furthermore, the quantity resulting from the wave function Ψ, which is supposed to describe the location of the particle, can no longer be interpreted as a probability density, since it is not positive. Dirac did not believe that taking relativistic effects into account would lead to such drastic changes in the underlying description of the system. So instead of replacing the 4-momentum by a differential expression he proposed a linearization of the relativistic energy equation (1.3) in the following sense.

$$\left(E - c\sum_{k=1}^{3}\alpha_k p_k - mc^2\beta\right)\left(E + c\sum_{k=1}^{3}\alpha_k p_k + mc^2\beta\right) = 0 \tag{1.4}$$

A comparison of (1.3) and (1.4) shows that the unknown quantities α_k and β must be chosen so that they satisfy the anti-commutation relations

- $\alpha_k\alpha_j + \alpha_j\alpha_k = 2\delta_{kj}I_4$
- $\alpha_k\beta + \beta\alpha_k = 0$
- $\beta^2 = I$

for all $k, j \in \{1, 2, 3\}$. Let

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad , \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad , \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

be the Pauli spin matrices, then we define the Dirac matrices as

$$\alpha_k = \begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{pmatrix} \quad \text{and} \quad \beta = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}$$

and a direct calculation shows that these matrices fulfill the upper anti-commutation relations. For a more detailed discussion of the usage of 4×4 matrices we refer to the lecture notes [48]. Furthermore, it should be noted that we are using here the standard representation of the Dirac matrices, which was introduced by Dirac. For other equivalent representations of these matrices we refer to [78, Appendix 1.A]. Since E and p_k are numbers we have that every solution of

$$E \pm c \sum_{k=1}^{3} \alpha_k p_k \pm mc^2 \beta = 0 \tag{1.5}$$

is also a solution of (1.4) and therefore we will restrict ourselves to the case of the lower sign. This is not a loss of generality, since it can be shown that the resulting Dirac equation leads to the same physical predictions as if we had chosen the other sign. Using the usual substitutions E by $i\hbar\frac{\partial}{\partial t}$ and p by $-i\hbar\nabla$ for equation (1.5) one obtains the free Dirac equation

$$\left(i\hbar \frac{\partial}{\partial t} + ic\hbar \sum_{k=1}^{3} \alpha_k \frac{\partial}{\partial x_k} - mc^2 \beta \right) \Psi = 0$$

whose vector-valued solutions $\Psi : \mathbb{R}^3 \to \mathbb{C}^4$ are called Dirac spinors. As shown in [54, Chaper 5.3.2], the Dirac spinors describe particles with spin $1/2$ as, for example, electrons. By applying the notation $\alpha \cdot x = \sum_{k=1}^{3} \alpha_k x_k$ for a given $x \in \mathbb{R}^3$, the following more compact representation of the free Dirac equation is obtained.

$$i\hbar \frac{\partial}{\partial t} \Psi = \left(-ic\hbar(\alpha \cdot \nabla) + mc^2 \beta \right) \Psi \tag{1.6}$$

Next, we define the free Dirac operator as the formal differential expression

$$A_0 = -ic\hbar(\alpha \cdot \nabla) + mc^2 \beta$$

and thus obtain for the free Dirac equation (1.6) the representation

$$i\hbar \frac{\partial}{\partial t} \Psi = A_0 \Psi \tag{1.7}$$

for suitable Dirac spinors Ψ.

To define A_0 in a mathematically rigorous way it is necessary to choose a Hilbert space and a suitable subspace on which A_0 acts. This choice has a great influence on the properties of the operator. As it will be shown in Theorem 3.1, A_0 is a self-adjoint operator in the Hilbert space $L^2(\mathbb{R}^3; \mathbb{C}^4)$ defined on the standard Sobolev space $H^1(\mathbb{R}^3; \mathbb{C}^4) \subseteq L^2(\mathbb{R}^3; \mathbb{C}^4)$ and the spectrum is given by

$$\sigma(A_0) = (-\infty, -mc^2] \cup [mc^2, \infty).$$

This is interesting for two reasons. First, it shows that Planck's constant $\hbar$ can be set to 1 without loss of generality, since it does not affect the spectrum, and secondly that the free Dirac operator is not semi-bounded.

From a mathematical point of view the absence of semi-boundedness leads to serious difficulties, since many analytic tools, such as sesquilinear forms, cannot be applied to construct self-adjoint extensions of restrictions of A_0 and to study their properties. This is one of the main reasons why many results already shown for Schrödinger operators are still open problems when Dirac operators are considered.

From a physical point of view there are possible energy states of the system that are negative and these energies are not bounded from below. Therefore there must be some mechanism that prevents a particle with positive energy from dropping into lower and lower negative energy states and releasing an infinite amount of energy in the process. Dirac's solution to this problem was to postulate non-measurable particles that occupy almost all negative energy states. Due to Pauli's exclusion principle, this prevents particles with positive energies from dropping into these negative energy states. If a sufficiently large amount of energy is added to particles with negative energy, they can be excited to states of positive energy. The states that are now unoccupied in the negative energy range behave like particles themselves and are called holes. Using a anti-unitary transformation, called charge conjugation, for a fixed particle charge as in [78, Chapter 1.4], these holes can be interpreted as particles with opposite charge and positive energy. This led to the discovery of anti-particles, such as in the case of the electron, the positron.

Next, the influence of an external potential V on a relativistic quantum particle, will be investigated. In particular, we consider perturbations of the free Dirac operator of the form

$$\mathcal{A} = A_0 + V \tag{1.8}$$

with external potential V, which is described by a 4×4 hermitian matrix-valued function. This function acts like a multiplication operator on Dirac spinors. Since we are studying relativistic effects, these potentials must be invariant under Lorentz transformations. For a given scalar potential Φ the quantity $V = \Phi\beta$ is Lorentz invariant as shown in [78, Chapter 4.2]. Similarly, an electromagnetic field described by a scalar potential Φ and a vector potential F can be represented by the Lorentz-invariant quantity $V = \Phi I_4 - \alpha \cdot F$. This motivates the following formal ansatz for the Dirac operator of a relativistic quantum particle with spin $1/2$ moving in an external field consisting of a electrostatic potential Φ_{el} and a scalar potential Φ_s

$$\mathcal{A} = A_0 + (\Phi_{el} I_4 + \Phi_s \beta)\,. \tag{1.9}$$

In [78, Chapter 4.3] the self-adjointness and the essential spectrum of the operators A, defined as realizations of the expression (1.8), are investigated, but since these results are not applied in this thesis we skip their presentation and refer to the mentioned literature.

Of particular interest are strongly localized fields which only have an effect in a small neighbourhood of a set $\Sigma \subseteq \mathbb{R}^3$ with measure 0. An example for a field of this kind is the quark confinement inside a nucleon in form of the MIT bag model as it is discussed in [66, 75]. To describe these strongly localized fields it is often a useful simplification to replace them by so-called δ-potentials which are supported on Σ. Although this is only an idealized model, it reflects the physical behavior of such a system to a reasonable extend and is solvable. In this context "solvable" generally means that it is possible to provide a detailed description of the spectral properties of the underlying operators. In the following we consider a constant electrostatic potential and a constant Lorentz scalar potential which are both strongly localized in a neighbourhood of the surface $\Sigma \subseteq \mathbb{R}^3$ and approximated by δ-potentials supported on Σ. Applying the above formal ansatz (1.9) for the Dirac operator of a relativistic quantum particle with spin $1/2$ moving in these external potential fields, yields the formal expression

$$\mathcal{A}_{\eta,\tau} = A_0 + (\eta I_4 + \tau\beta)\,\langle\delta_\Sigma, \cdot\rangle\delta_\Sigma \tag{1.10}$$

with constant interaction strengths $\eta, \tau \in \mathbb{R}$. This formal differential expression is the starting point of this thesis and will be the main object of considerations.

The first task of this thesis is to give rigorous meaning to the formal expression (1.10). This is done as in [12, 14, 40] by using extension theoretical tools like quasi boundary triples and encoding the effect of the δ-potentials in form of jump conditions on the boundary $\Sigma \subseteq \mathbb{R}^3$ of a C^2-domain. In this way we are able to construct operators $A_{\eta,\tau}$, which are interpreted as realizations of the formal expression (1.10). As it will be shown in Section 3.2, $A_{\eta,\tau}$ are self-adjoint operators in the Hilbert space $L^2(\mathbb{R}^3;\mathbb{C}^4)$ for non-critical interaction strengths $\eta^2 - \tau^2 \neq 4c^2$. This property is necessary to interpret $A_{\eta,\tau}$ as a quantum mechanical observable, namely the total energy of the particle. Furthermore, the operators $A_{\eta,\tau}$ are explicitly given by

$$\begin{aligned}
\operatorname{dom}(A_{\eta,\tau}) = \Big\{ f = f_+ \oplus f_- \in H^1(\Omega_+;\mathbb{C}^4) \oplus H^1(\Omega_-;\mathbb{C}^4) \;\Big|& \\
ic\alpha\cdot\nu\,(\tau_+ f_+ - \tau_- f_-) + \frac{1}{2}(\eta I_4 + \tau\beta)(\tau_+ f_+ + \tau_- f_-) = 0 &\Big\} \\
A_{\eta,\tau} f = \big(-ic(\alpha\cdot\nabla) + mc^2\beta\big) f_+ \oplus \big(-ic(\alpha\cdot\nabla) + mc^2\beta\big) f_- &
\end{aligned}$$

where $\Omega_+ \subseteq \mathbb{R}^3$ is a bounded C^2-domain with boundary $\partial\Omega_+ = \Sigma$ and open complement $\Omega_- = \mathbb{R}^3 \setminus \overline{\Omega_+}$, ν is the outer unit normal vector on Σ and $\tau_\pm$ are the trace operators of the Sobolev spaces $H^1(\Omega_\pm;\mathbb{C}^4)$. This will lead to a variant of Krein's formula, which relates the resolvent of $A_{\eta,\tau}$ to the resolvent of the free Dirac operator A_0 and a pertubation term. This perturbation term can be represented by integral operators in $L^2(\mathbb{R}^3;\mathbb{C}^4)$ and $L^2(\Sigma;\mathbb{C}^4)$ and contains all information about the spectral properties of the operator $A_{\eta,\tau}$.

The treatment of critical interaction strengths $\eta, \tau \in \mathbb{R}$ with $\eta^2 - \tau^2 = 4c^2$ is much more complicated and will not be discussed in this thesis. However, this is not a restriction, since critical interaction strengths only occur in a single point $c > 0$ and are therefore insignificant for the non-relativistic limit $c \to \infty$. For a detailed discussion of critical interaction strengths, we refer to [14] and [40, Chapter 4.3] for the three-dimensional case and to [15] for the two-dimensional case.

The second task of this thesis is to determine the non-relativisitc limit of $A_{\eta,\tau}$ for $c \to \infty$. This establishes a connection between the relativistic and the non-relativistic description and thereby allows an interpretation of the operators $A_{\eta,\tau}$ by means of the well studied non-relativistic counterparts. Intuitively, one would expect that if the limiting velocity c for particles is removed the description of a relativistic quantum particle by means of the Dirac equation would turn into a description of a non-relativistic quantum particle by means of the Schrödinger equation. Roughly speaking, we are able to recover non-relativistic quantum mechanics if we perform the limit $c \to \infty$. In Sections 4.1 and 4.2 it is shown that this indeed is the case. In particular, if we consider the kinetic energy term $A_{\eta,\tau} - mc^2$ and an arbitrary number $\lambda \in \mathbb{C} \setminus \mathbb{R}$, the norm resolvent convergence

$$\lim_{c \to \infty} \left(A_{\eta,\tau} - \left(\lambda + mc^2 \right) \right)^{-1} = \begin{pmatrix} (T_{\eta,\tau} - \lambda)^{-1} & 0 \\ 0 & 0 \end{pmatrix}$$

follows with a self-adjoint Schrödinger operator $T_{\eta,\tau}$ in $L^2(\mathbb{R}^3; \mathbb{C}^2)$. This self-adjoint operator $T_{\eta,\tau}$ can be characterized by certain jump conditions on the surface $\Sigma \subseteq \mathbb{R}^3$ which depend on the interaction strengths η and τ. It will be shown that the behavior of $T_{\eta,\tau}$ depends strongly on whether $\eta + \tau = 0$ or $\eta + \tau \neq 0$ occurs.

- If η and τ are chosen such that $\eta + \tau \neq 0$ is valid, then for all $f \in \operatorname{dom}(T_{\eta,\tau})$ the jump conditions
$$\tau_+ f_+ = \tau_- f_-$$
for f and
$$(\eta + \tau) (\tau_+ f_+ + \tau_- f_-) = \frac{1}{2m} (\partial_\nu f_+ - \partial_\nu f_-)$$
for $\partial_\nu f$ follow on Σ. Here $\partial_\nu f_\pm$ denotes the normal derivative of the functions $f_\pm = f \upharpoonright \Omega_\pm : \Omega_\pm \to \mathbb{C}^2$ on Σ with respect to the outer unit normal vector ν. These interface conditions describe a Schrödinger operator with a δ-interaction of strength $\eta + \tau$ as discussed for instance in [18]. Therefore, in this case the non-relativistic limit yields the expected transition of the description by means of a Dirac operator to a description by means of a Schrödinger operator. Retrospectively we thereby get the justification that the imposed jump conditions for Dirac operators with δ-shell interactions were indeed chosen correctly.

- If η and τ are chosen such that $\eta + \tau = 0$ and initially $\eta - \tau = \varepsilon c^2$ for some $\varepsilon \in \mathbb{R}$ are valid, then for all $f \in \operatorname{dom}(T_{\eta,\tau})$ the jump conditions

  $$\tau_+ \left((\sigma \cdot \nabla) f_+ \right) = \tau_- \left((\sigma \cdot \nabla) f_- \right)$$

  for $(\sigma \cdot \nabla) f$ and

  $$i(\sigma \cdot \nu) \left(\tau_+ f_+ - \tau_- f_- \right) = \frac{\varepsilon}{2} \left(\tau_+ \left(\frac{i}{2m} (\sigma \cdot \nabla) f_+ \right) + \tau_- \left(\frac{i}{2m} (\sigma \cdot \nabla) f_- \right) \right)$$

  for f follow on Σ. Once again we have applied the notation $\sigma \cdot x = \sum_{k=1}^{3} \sigma_k x_k$ for a given $x \in \mathbb{R}^3$ and the Pauli spin matrices σ_k. These so-called oblique jump conditions seem to occur frequently in the analysis of Dirac operators and it is therefore assumed that there is a close relationship between Dirac operators and Schrödinger operators with oblique jump conditions. See, for instance, [5, Remark 5] where oblique jump conditions appear in the context of boundary value problems of Dirac operators in two dimensions.

As surprising as this very different behavior of the non-relativistic limit $T_{\eta,\tau}$ may seem, it reflects the following known result for Dirac operators with electrostatic and Lorentz scalar point interactions in one dimension. If $\eta + \tau \neq 0$ is valid, then the jump condition of a function $f \in \operatorname{dom}(T_{\eta,\tau})$ in $\Sigma = \{0\}$ corresponds to a Schrödinger operator with δ-interaction, whereas in the case $\eta + \tau = 0$ the jump condition corresponds to a Schrödinger operator with δ'-interaction. This can be shown using ordinary boundary triples or with a similar strategy as in [2, Appendix J]. The interesting aspect in three dimensions is that for $\eta + \tau = 0$ a different behaviour is observed and, in contrast to the one-dimensional case, there are no jump conditions which describe δ-interactions or δ'-interactions but oblique jump conditions.

While the non-relativistic limit of pure electrostatic or pure Lorentz scalar δ-shell interactions in $\mathbb{R}^3$ has been investigated in [10, 12, 40], the general case with arbitrary constant interaction strengths $\eta, \tau \in \mathbb{R}$ has not been considered so far, to the best knowledge of the author. Thus, the aim of this thesis is to make a small contribution in this field.

To conclude this introduction, we briefly outline the previous research on Dirac operators with δ-interactions. In 1987, Gestezy and Šeba first discussed Dirac operators with δ-interactions in one dimension in [32] and constructed self-adjoint realizations of the formal expressions by imposing suitable jump conditions. In addition to an explicit representation of the resolvent and a characterization of the spectrum, it could be shown that in the non-relativistic limit there is a convergence in the norm resolvent sense to a Schrödinger operator with δ-point interaction. An alternative approach to point interactions was presented in [72, 80] and it was shown that these interactions can be approximated by a sequence of so-called squeezed potentials with shrinking support and that this convergence is in the norm resolvent sense. For more recent publications on one-dimensional Dirac operators with point interactions, we refer for instance to [19, 20, 57].

Dirac operators with δ-shell interactions in three dimensions were first studied by Dittrich, Exner and Šeba in [23]. The authors considered electrostatic and Lorentz scalar δ-interactions supported on the surface of a sphere. By using spherical harmonics the problem was reduced to a one-dimensional problem and the self-adjointness of the operators $A_{\eta,\tau}$, as well as spectral properties and a representation of the resolvent could be shown. A first treatment of a more general class of surfaces $\Sigma \subseteq \mathbb{R}^3$ is found in [6, 7, 8]. For non-critical interaction strengths $\eta, \tau \in \mathbb{R}$ with $\eta^2 - \tau^2 \neq 4c^2$, the self-adjointness of the operators $A_{\eta,\tau}$ could be shown as well as spectral properties, in particular of the discrete spectrum, were discussed for the case $\tau = 0$. Furthermore, it was shown in [51, 52] that δ-shell interactions with $\eta = 0$ or $\tau = 0$ can be approximated by squeezed potentials as in the one-dimensional case. However, in general this convergence is taking place only in the strong resolvent sense. On the basis of the results in [7], it was shown in [10, 12] that the operators $A_{\eta,\tau}$ can alternatively be defined by means of quasi boundary triples and, in addition to an explicit resolvent formula, an extensive investigation of the spectral properties of the operators $A_{\eta,\tau}$ was carried out. Furthermore, the non-relativistic limit for purely electrostatic and purely Lorentz scalar δ-shell interactions was discussed and a Schrödinger operator with δ-interaction characterized as the limit operator. The case of critical interaction strengths $\eta, \tau \in \mathbb{R}$ with $\eta^2 - \tau^2 = 4c^2$ was considered in [14, 40] and it was shown that the properties of the operators $A_{\eta,\tau}$ differ significantly from those with non-critical interaction strengths. In particular, there is a reduction of the regularity of the functions in the domain of definition of $A_{\eta,\tau}$ as well as possible points from the essential spectrum located in the spectral gap $(-mc^2, mc^2)$.

2 Definitions and preliminary results

In this chapter we introduce all necessary definitions, tools and results to define and study Dirac operators with electrostatic and Lorentz scalar δ-shell interactions in a mathematical rigorous way.

In Section 2.1 we introduce linear operators and discuss their properties. Next, Section 2.2 is devoted to the abstract extension theoretic tool of quasi boundary triples. This will allow us to characterize Dirac operators with electrostatic and Lorentz scalar δ-shell interactions $A_{\eta,\tau}$ as self-adjoint extensions of restrictions of the free Dirac operator A_0 in the Hilbert space $L^2(\mathbb{R}^3;\mathbb{C}^4)$. Subsequently, an auxiliary result is presented in Section 2.3, which will allow us to show the self-adjointness of the Schrödinger operator $T_{\eta,\tau}$ in the non-relativistic limit $\eta+\tau=0$ and to characterize its domain of definition. In order to define the underlying Hilbert space and the domain of definition of the free Dirac operator and Dirac operators with electrostatic and Lorentz scalar δ-shell interactions, we will introduce L^2-spaces and Sobolev spaces on a domain $\Omega \subseteq \mathbb{R}^3$ in Section 2.4. Furthermore, L^2-spaces and Sobolev spaces on the boundary $\partial\Omega$ of a Lipschitz domain $\Omega \subseteq \mathbb{R}^3$ are introduced in Section 2.5. This allows us to characterize boundary values and regularity of functions which are defined on the boundary of the Lipschitz domain. Finally, in Section 2.6 certain integral operators in L^2-spaces are discussed, which appear in the representation formula of the resolvent of the operators $A_{\eta,\tau}$.

2.1 Linear operators

In this section we introduce unbounded linear operators, their adjoint operators and spectral properties. All the material is well known and can be found for instance in the books [45, 69, 81, 83] or in the lecture notes [65]. If a result comes from another source text, it is referred to at the respective passage. Although it is not the most general stetting, we assume throughout this entire section that $\mathcal{H}$ and $\mathcal{G}$ are Hilbert spaces over $\mathbb{C}$ unless stated otherwise.

Let $\mathrm{dom}(T) \subseteq \mathcal{H}$ be a subspace of $\mathcal{H}$, then a linear mapping $T : \mathrm{dom}(T) \to \mathcal{G}$ is called a linear operator from $\mathcal{H}$ to $\mathcal{G}$. The set $\mathrm{dom}(T)$ is called domain of definition of T or just domain of T if no confusion is possible. Next, we define the kernel of a linear operator T as

$$\ker(T) = \Big\{ x \in \operatorname{dom}(T) \,\Big|\, Tx = 0 \Big\} \subseteq \mathcal{H}$$

and the range of T as

$$\operatorname{ran}(T) = \Big\{ y \in \mathcal{G} \,\Big|\, \exists x \in \operatorname{dom}(T) \text{ such that } Tx = y \Big\} \subseteq \mathcal{G}.$$

It is obvious that these two sets are subspaces of $\mathcal{H}$ and $\mathcal{G}$, respectively. In the following we will always assume that T is a linear operator from $\mathcal{H}$ to $\mathcal{G}$, unless stated otherwise.

If two linear operators $T : \operatorname{dom}(T) \to \mathcal{G}$ and $S : \operatorname{dom}(S) \to \mathcal{G}$ are given, we write $S \subseteq T$ if $\operatorname{dom}(S) \subseteq \operatorname{dom}(T)$ and $Sx = Tx$ holds true for all $x \in \operatorname{dom}(S)$. In this case S is called a restriction of T and T is called an extension of S and we write $S = T \restriction \operatorname{dom}(S)$.

Definition 2.1. A linear operator $T : \operatorname{dom}(T) \to \mathcal{G}$ is called bounded, if there exists a constant $C > 0$ such that

$$\|Tx\|_{\mathcal{G}} \leq C \|x\|_{\mathcal{H}}$$

holds true for all $x \in \operatorname{dom}(T)$.

The norm of a linear and bounded operator is defined as the minimal C of Definition 2.1 and it can be shown that

$$\|T\| = \sup \left\{ \frac{\|Tx\|_{\mathcal{G}}}{\|x\|_{\mathcal{H}}} \,\middle|\, x \in \operatorname{dom}(T) \setminus \{0\} \right\}$$

holds true. We define $\mathcal{L}(\mathcal{H}, \mathcal{G})$ as the set of all linear and bounded operators T from $\mathcal{H}$ to $\mathcal{G}$ with $\operatorname{dom}(T) = \mathcal{H}$ and it is well known that $\mathcal{L}(\mathcal{H}, \mathcal{G})$ equipped with the above operator norm is a Banach space. In the special case of $\mathcal{H} = \mathcal{G}$ we simply write $\mathcal{L}(\mathcal{H}) = \mathcal{L}(\mathcal{H}, \mathcal{H})$ and observe that this space is even a unital Banach algebra. Furthermore, we define the dual space of $\mathcal{H}$ as $\mathcal{H}^* = \mathcal{L}(\mathcal{H}, \mathbb{C})$ and call its elements linear and bounded functionals.

Definition 2.2. A linear operator $T : \mathcal{H} \to \mathcal{G}$ is called compact if the image of every bounded set in $\mathcal{H}$ is relatively compact in $\mathcal{G}$. In other words, for every bounded set $B \subseteq \mathcal{H}$, the closure of $T(B) \subseteq \mathcal{G}$ is compact in $\mathcal{G}$.

As in the case of bounded operators we define $\mathcal{K}(\mathcal{H}, \mathcal{G})$ as the set of all linear and compact operators T from $\mathcal{H}$ to $\mathcal{G}$. It can be shown that every compact operator is bounded and therefore $\mathcal{K}(\mathcal{H}, \mathcal{G})$ is a subset of $\mathcal{L}(\mathcal{H}, \mathcal{G})$. In the special case of $\mathcal{H} = \mathcal{G}$, we simply write $\mathcal{K}(\mathcal{H}) = \mathcal{K}(\mathcal{H}, \mathcal{H})$ and it can be shown that $\mathcal{K}(\mathcal{H})$ is a closed, two-sided ideal in $\mathcal{L}(\mathcal{H})$.

The next result, also known as Fredholm's alternative, is formulated here in such a way that it is best suited for the considerations in the following chapters. In particular, we will use Theorem 2.3 to investigate certain types of integral operators that appear in the resolvent representation of Dirac operators with electrostatic and Lorentz scalar δ-shell interactions.

Theorem 2.3. Let $\mathcal{H}$ be a Hilbert space, $T \in \mathcal{K}(\mathcal{H})$ be a compact operator and $\lambda \in \mathbb{C} \setminus \{0\}$ an arbitrary number, then exactly one of the following statements is true.

i) The homogeneous problem $Tx - \lambda x = 0$ has only the trivial solution $x = 0$. In this case there exists for all $y \in \mathcal{H}$ a unique solution $x \in \mathcal{H}$ of the inhomogeneous problem $Tx - \lambda x = y$.

ii) There are $1 \leq n = \dim(\ker(T - \lambda)) < \infty$ linearly independent solutions of the homogeneous problem $Tx - \lambda x = 0$.

Since many important linear operators such as differential operators are not bounded, we have to consider a more general class of linear operators called closed operators. Although these operators are not bounded, they have properties similar to those of bounded operators but are still broad enough to cover most linear operators found in practice. Let $T : \operatorname{dom}(T) \to \mathcal{G}$ be a linear operator from $\mathcal{H}$ to $\mathcal{G}$, then we define the graph of T as the set

$$G(T) = \Big\{ (x, Tx) \;\Big|\; x \in \operatorname{dom}(T) \Big\} \subseteq \mathcal{H} \times \mathcal{G}.$$

Due to the linearity of the underlying operator, the graph is a linear subspace of $\mathcal{H} \times \mathcal{G}$ and it contains all the information about the operator.

Definition 2.4. A linear operator $T : \operatorname{dom}(T) \to \mathcal{G}$ is called closed, if the graph $G(T)$ of T is a closed subspace of $\mathcal{H} \times \mathcal{G}$ with respect to the product norm $\|\cdot\|_{\mathcal{H}\times\mathcal{G}}$ defined by $\|(x,y)\|_{\mathcal{H}\times\mathcal{G}} = \sqrt{\|x\|_{\mathcal{H}}^2 + \|y\|_{\mathcal{G}}^2}$ for all $(x,y) \in \mathcal{H} \times \mathcal{G}$.

At this point, it should be noted that for given norms on $\mathcal{H}$ and $\mathcal{G}$, other norms may be defined on the product space. However, since we are working with Hilbert spaces whose norms are induced by inner products, this choice is advantageous. The next result characterizes closed operators in a way which is usually more convenient to work with.

Theorem 2.5. Let $T : \operatorname{dom}(T) \to \mathcal{G}$ be a linear operator, then the following statements are equivalent.

i) T is closed

ii) For every sequence $(x_n)_{n \in \mathbb{N}} \subseteq \operatorname{dom}(T)$ with $x_n \to x$ in $\mathcal{H}$ and $Tx_n \to y$ in $\mathcal{G}$, it follows that $x \in \operatorname{dom}(T)$ and $Tx = y$ holds true.

iii) The space $(\operatorname{dom}(T), \|\cdot\|_T)$ equipped with the graph norm $\|x\|_T = \sqrt{\|x\|_{\mathcal{H}}^2 + \|Tx\|_{\mathcal{G}}^2}$ for every $x \in \operatorname{dom}(T)$ is complete and therefore a Hilbert space.

Using Theorem 2.5, it follows immediately that every linear and bounded operator $T \in \mathcal{L}(\mathcal{H}, \mathcal{G})$ is closed, but as shown in [83, Page 347 - Bsp a)], not every closed operator is bounded on its domain of definition. The next result, which contains the so-called closed graph theorem, shows the connection of bounded and closed linear operators.

Theorem 2.6. Let $T : \mathrm{dom}(T) \to \mathcal{G}$ be a linear operator, then two of the following properties imply the third.

i) T is closed.

ii) $\mathrm{dom}(T)$ is closed in $\mathcal{H}$.

iii) T is bounded on $\mathrm{dom}(T)$.

This result allows us to deduce the boundedness of the inverse operator as follows. Let $T : \mathrm{dom}(T) \to \mathcal{G}$ be a linear, closed and bijective operator, then it is easy to see that the inverse operator $T^{-1} : \mathcal{G} \to \mathrm{dom}(T)$ is closed as well. Since $\mathrm{dom}(T^{-1}) = \mathcal{G}$ is a Banach space, the boundedness of T^{-1} follows from Theorem 2.6. This will be used in Theorem 2.8 and in the considerations regarding the spectral properties of closed operators.

If a not necessarily closed operator is given, then it is in many cases important to know if closed extensions exist. This leads us to the concept of closable operators.

Definition 2.7. A linear operator $T : \mathrm{dom}(T) \to \mathcal{G}$ is called closable if the closure of $G(T)$ in $\mathcal{H} \times \mathcal{G}$ with respect to the product norm $\|\cdot\|_{\mathcal{H}\times\mathcal{G}}$ is the graph of a linear operator. This unique operator is the smallest closed extension of T with respect to the inclusion of linear operators and is denoted $\overline{T}$.

If T a closable opterator then it follows immediately from Definition 2.7 that the closure $\overline{T}$ is explicitly given by

$$\begin{aligned} \mathrm{dom}(\overline{T}) &= \left\{ x \in \mathcal{H} \;\middle|\; \exists (x_n)_{n\in\mathbb{N}} \subseteq \mathrm{dom}(T), y \in \mathcal{G} \text{ such that } x_n \to x \text{ and } Tx_n \to y \right\} \\ \overline{T}x &= y. \end{aligned}$$

In particular, every bounded operator is closable and $\mathrm{dom}\left(\overline{T}\right) = \overline{\mathrm{dom}(T)}$ is valid.

To conclude the considerations of closed operators we formulate a result which shows that the invertibility of a linear, closed and bijective operator is stable under small perturbations. The proof can be found for instance in [46, Thm. 1.16]. Theorem 2.8 will be of particular importance in the next chapter, since in the process of studying the non-relativisitc limit of Dirac operators with electrostatic and Lorentz scalar δ-shell interactions we will have to deduce the existence of the inverse of a sum of two linear operators. Before formulating the result recall the consideration above which showed that the inverse operator of a linear, closed and bijective operator is always bounded.

Theorem 2.8. Let $T : \operatorname{dom}(T) \to \mathcal{G}$ be a linear, closed and bijective operator with inverse $T^{-1} \in \mathcal{L}(\mathcal{G}, \mathcal{H})$ and let $A : \operatorname{dom}(A) \to \mathcal{G}$ be a given linear operator such that $\operatorname{dom}(T) \subseteq \operatorname{dom}(A)$ holds true. Furthermore, assume that there exist constants $a, b \geq 0$ such that $\|Ax\|_{\mathcal{G}} \leq a\|x\|_{\mathcal{H}} + b\|Tx\|_{\mathcal{G}}$ is valid for all $x \in \operatorname{dom}(T)$ and that a and b satisfy the inequality $a\|T^{-1}\| + b < 1$. Then $S = A + T$ is a linear and invertible operator with $S^{-1} \in \mathcal{L}(\mathcal{G}, \mathcal{H})$ and the estimate

$$\left\|S^{-1} - T^{-1}\right\| \leq \frac{\|T^{-1}\| \, (a\|T^{-1}\| + b)}{1 - a\|T^{-1}\| - b}.$$

holds true. If A is a bounded operator with $\|A\|\|T^{-1}\| < 1$ one can choose $a = \|A\|$ and $b = 0$.

Next, we consider adjoint operators which can be regarded as a generalization of the concept of the conjugate transpose of a complex matrix.

Definition 2.9. Let $T : \operatorname{dom}(T) \to \mathcal{G}$ be a linear and densely defined operator from $\mathcal{H}$ to $\mathcal{G}$. Then the uniquely defined linear operator

$$\begin{aligned} \operatorname{dom}(T^*) &= \left\{ y \in \mathcal{G} \,\middle|\, \exists y^* \in \mathcal{H} \text{ such that } (y^*, x)_{\mathcal{H}} = (y, Tx)_{\mathcal{G}} \ \forall x \in \operatorname{dom}(T) \right\} \subseteq \mathcal{G} \\ T^* y &= y^* \end{aligned}$$

is called the adjoint operator of T or just the adjoint of T if no confusion is possible.

Note that the density of $\operatorname{dom}(T) \subseteq \mathcal{H}$ in $\mathcal{H}$ is necessary to obtain a unique element $y^* \in \mathcal{H}$ and consequently a well-defined and unique operator T^*. The next theorem is a collection of well known results concerning the adjoint operator which will be useful in the following chapters when dealing with Dirac operators.

Theorem 2.10. Let $T : \operatorname{dom}(T) \to \mathcal{G}$ be a linear and densely defined operator and $\mathcal{F}$ be a given Hilbert space, then the following statements are true.

i) $T^* : \operatorname{dom}(T^*) \to \mathcal{H}$ is a closed operator.

ii) T is bounded on $\operatorname{dom}(T)$ if and only if $T^* \in \mathcal{L}(\mathcal{G}, \mathcal{H})$ and in this case $\|T\| = \|T^*\|$ holds true.

iii) $\operatorname{dom}(T^*)$ is dense in $\mathcal{G}$ if and only if T is closeable and in this case $\overline{T} = T^{**}$ holds true. Furthermore, if T is bounded, then T^{**} is the unique bounded extension of T to $\mathcal{H}$.

iv) If T is a closable operator, then $\overline{T}^* = T^*$ holds true.

v) Let $S : \operatorname{dom}(S) \to \mathcal{G}$ be a linear and densely defined operator from $\mathcal{H}$ to $\mathcal{G}$, then it follows from $S \subseteq T$ that $T^* \subseteq S^*$ holds true.

vi) Let $S \in \mathcal{L}(\mathcal{G}, \mathcal{F})$ be a given linear and bounded operator, then $(ST)^* = T^* S^*$ holds true.

vii) Let $S \in \mathcal{L}(\mathcal{H}, \mathcal{G})$ be a given linear and bounded operator, then $(S + T)^* = S^* + T^*$ holds true.

With the definition of the adjoint operator we are now able to define the important concepts of symmetric and self-adjoint operators. For the latter, a rich spectral theory can be developed and they are central quantities in the mathematical formulation of quantum mechanics.

Definition 2.11. A linear and densely defined operator $T : \operatorname{dom}(T) \to \mathcal{H}$ in $\mathcal{H}$ is called symmetric if $T \subseteq T^*$ holds true. A symmetric operator is called self-adjoint if even $T = T^*$ applies. Furthermore, a symmetric operator is called essentially self-adjoint if the closure $\overline{T}$ is self-adjoint.

To obtain a self-adjoint operator by modifying the domain of definition of a symmetric operator, the crucial step is to choose the "correct" domain of definition. This choice will be of great importance in the next chapter, as we want to define Dirac operators with electrostatic and Lorentz scalar δ-shell interactions as self-adjoint extensions of certain symmetric operators. The next theorem allows us to characterize self-adjoint operators in a very convenient way.

Theorem 2.12. Let $T : \operatorname{dom}(T) \to \mathcal{H}$ be a linear, densely defined and symmetric operator and $\lambda \in \mathbb{C} \setminus \mathbb{R}$ be a given complex number, then the following statements are equivalent.

i) T is self-adjoint.

ii) T is closed and $\ker(T^* + \lambda) = \ker(T^* + \overline{\lambda}) = \{0\}$.

iii) $\operatorname{ran}(T - \lambda) = \mathcal{H} = \operatorname{ran}(T - \overline{\lambda})$.

It shall be noted that a careful inspection of Theorem 2.12 shows that T is self-adjoint if and only if ii) or iii) is valid for one $\lambda_0 \in \mathbb{C} \setminus \mathbb{R}$ and hence for all $\lambda \in \mathbb{C} \setminus \mathbb{R}$.

Finally, we discuss the spectral theory of closed operators in Hilbert spaces. At this point it is noteworthy to remark, that without loss of generality we can restrict ourselves to closed operators, since the resolvent set of an non-closed operator is always empty as shown in [81, Bemerkung 5.1]. First, we introduce the resolvent set and the spectrum of a linear and closed operator.

Definition 2.13. Let $T : \operatorname{dom}(T) \to \mathcal{H}$ be a linear, densely defined and closed operator.

i) The resolvent set of T is defined as the set of all $\lambda \in \mathbb{C}$ such that the operator $T - \lambda$ is bijective

$$\rho(T) = \Big\{ \lambda \in \mathbb{C} \,\Big|\, T - \lambda : \operatorname{dom}(T) \to \mathcal{H} \text{ is bijective} \Big\}.$$

ii) The spectrum of T is defined as $\sigma(T) = \mathbb{C} \setminus \rho(T)$.

An application of the consideration following Theorem 2.6 shows that the resolvent $R(\lambda) = (T - \lambda)^{-1}$ is a linear and bounded operator in $\mathcal{H}$ for all $\lambda \in \rho(T)$. Sometimes a more detailed investigation of the spectrum may be necessary and therefore we decompose it further into several parts. To avoid technical details that would require a distinction between algebraic and geometric multiplicity of an eigenvalue, we formulate items ii) and iii) only for self-adjoint operators. For a detailed presentation in the case of not necessarily self-adjoint operators, we refer to [38, Chapter 6].

Definition 2.14. Let $T : \mathrm{dom}(T) \to X$ be a linear, densely defined and closed operator.

i) The point spectrum of T is defined as the set of all eigenvalues

$$\sigma_p(T) = \left\{ \lambda \in \mathbb{C} \;\middle|\; \ker(T - \lambda) \neq \{0\} \right\}.$$

The elements of the eigenspace $\ker(T - \lambda)$ are called eigenvectors of T to the eigenvalue λ.

ii) The discrete spectrum of a self-adjoint operator T is defined as the set of all isolated eigenvalues for which the eigenspace is finite dimensional

$$\sigma_{\mathrm{disc}}(T) = \left\{ \lambda \in \sigma_p(T) \;\middle|\; \lambda \text{ is isolated in } \sigma(T) \text{ and } \dim(\ker(T - \lambda)) < \infty \right\}.$$

iii) The essential spectrum of a self-adjoint operator T is defined as the set $\sigma_{\mathrm{ess}}(T) = \sigma(T) \setminus \sigma_{\mathrm{disc}}(T)$.

The last theorem of this section is a collection of well known results concerning the resolvent set and the spectrum of a linear and closed operator which will be useful in the following chapters when dealing with Dirac operators.

Theorem 2.15. Let $T : \mathrm{dom}(T) \to \mathcal{H}$ be a linear, closed and densely defined operator, then the following statements are true.

i) If T is a symmetric operator, then $\sigma_p(T) \subseteq \mathbb{R}$ holds true.

ii) If T is a self-adjoint operator, then $\sigma(T) \subseteq \mathbb{R}$ and $\mathbb{C} \setminus \mathbb{R} \subseteq \rho(T)$ hold true.

2.2 Quasi boundary triples

In this section we introduce the concept of quasi boundary triples, which is a powerful tool in the extension and spectral theory of symmetric operators. The following results for quasi boundary triples can be found in [16, 17, 18, 40]. If a result comes from another source text, it is referred to at the respective passage.

As in our case it is in general relatively easy to construct a symmetric operator from a formal differential expression by specifying a suitable domain of definition. If this operator is not self-adjoint, the question arises whether self-adjoint extensions exist and how they can be characterized.

To formulate our considerations in a more precise way we will always assume in the following that $\mathcal{H}$ is a Hilbert space and $S : \mathrm{dom}(S) \subseteq \mathcal{H} \to \mathcal{H}$ is a linear, densely defined, closed and symmetric operator in $\mathcal{H}$. From Theorem 2.10 it follows that a linear operator A is a self-adjoint extension of S if and only if A is a self-adjoint restriction of S^*. In particular, A is completely characterized by its domain of definition $\mathrm{dom}(A) \subseteq \mathrm{dom}(S^*)$ and the relation $A = S^* \upharpoonright \mathrm{dom}(A)$. Thus, the problem of finding self-adjoint extensions of S is equivalent to specifying their domains of definition. For this purpose quasi boundary triples can be used.

Definition 2.16. Let $T : \mathrm{dom}(T) \subseteq \mathcal{H} \to \mathcal{H}$ be a linear operator in $\mathcal{H}$ with $\overline{T} = S^*$. A triple $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ is called quasi boundary triple for the adjoint operator S^*, if $\mathcal{G}$ is a Hilbert space and the linear operators $\Gamma_0, \Gamma_1 : \mathrm{dom}(T) \subseteq \mathcal{H} \to \mathcal{G}$ satisfy the following conditions.

i) The abstract Green's identity

$$(Tf, g)_{\mathcal{H}} - (f, Tg)_{\mathcal{H}} = (\Gamma_1 f, \Gamma_0 g)_{\mathcal{G}} - (\Gamma_0 f, \Gamma_1 g)_{\mathcal{G}} \tag{2.1}$$

is valid for all $f, g \in \mathrm{dom}(T)$.

ii) The range of the mapping $\Gamma = (\Gamma_0, \Gamma_1)^\top : \mathrm{dom}(T) \to \mathcal{G} \times \mathcal{G}$ is dense in $\mathcal{G} \times \mathcal{G}$.

iii) The operator $A_0 = T \upharpoonright \ker(\Gamma_0)$ is self-adjoint in $\mathcal{H}$.

Usually quasi boundary triples appear in the context of boundary value problems and therefore the linear operators Γ_0 and Γ_1 are often referred to as abstract boundary maps. As it is stated in [17, Section 1.3] quasi boundary triples exist if and only if S admits self-adjoint extensions. This is equivalent to both defect indices $n_\pm(S) = \dim(\ker(S^* \pm i))$ being equal and in this case $\dim(\mathcal{G}) = n_\pm(S)$ applies.

Let $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ be a quasi boundary triple for $\overline{T} = S^*$ then the restriction $A_0 = T \upharpoonright \ker(\Gamma_0)$ of T is by definition a self-adjoint operator in $\mathcal{H}$ and the direct sum decomposition

$$\mathrm{dom}(T) = \mathrm{dom}(A_0) \dotplus \ker(T - \lambda) = \ker(\Gamma_0) \dotplus \ker(T - \lambda)$$

is valid for all $\lambda \in \rho(A_0)$. A proof of this decomposition can be found for instance in [9, Lem. 4.7]. This implies that $\Gamma_0 \upharpoonright \ker(T - \lambda)$ is an injective linear operator from

$\mathcal{H}$ to $\mathcal{G}$ for all $\lambda \in \rho(A_0)$ and hence the following operator-valued functions associated with the quasi boundary triple $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ are well-defined.

Definition 2.17. Let $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ be a quasi boundary triple for $\overline{T} = S^*$.

i) The γ-field is defined by the values $\gamma(\lambda) = (\Gamma_0 \upharpoonright \ker(T - \lambda))^{-1}$ for all $\lambda \in \rho(A_0)$.

ii) The Weyl function is defined by the values $M(\lambda) = \Gamma_1 \gamma(\lambda) = \Gamma_1 (\Gamma_0 \upharpoonright \ker(T - \lambda))^{-1}$ for all $\lambda \in \rho(A_0)$.

These operator-valued functions will be of great importance in the construction and investigation of certain self-adjoint extensions of the symmetric operator S. The next theorem is is a collection of useful properties concerning the γ-field and the Weyl function. The proofs of these statements can be found for instance in [17, Prop. 1.13 , Prop. 1.14].

Theorem 2.18. Let $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ be a quasi boundary triple for $\overline{T} = S^*$ and $A_0 = T \upharpoonright \ker(\Gamma_0)$, then the following statements are true for all $\lambda, \mu \in \rho(A_0)$.

i) The values of the γ-field $\gamma(\lambda) : \mathrm{dom}(\gamma(\lambda)) \to \mathcal{H}$ are linear, densly defined and bounded operators from $\mathcal{G}$ to $\mathcal{H}$ with $\mathrm{dom}(\gamma(\lambda)) = \mathrm{ran}(\Gamma_0)$ and $\mathrm{ran}(\gamma(\lambda)) = \ker(T - \lambda)$.

ii) For the adjoint operators, one has $\gamma(\lambda)^* \in \mathcal{L}(\mathcal{H}, \mathcal{G})$ and the explicit representation $\gamma(\lambda)^* = \Gamma_1 \left(A_0 - \overline{\lambda}\right)^{-1}$ is valid. In particular, $\mathrm{ran}(\gamma(\lambda)^*) \subseteq \mathrm{ran}(\Gamma_1)$ follows.

iii) The values of the Weyl function $M(\lambda) : \mathrm{dom}(M(\lambda)) \to \mathcal{G}$ are linear and densely defined operators in $\mathcal{G}$ with $\mathrm{dom}(M(\lambda)) = \mathrm{ran}(\Gamma_0)$ and $\mathrm{ran}(M(\lambda)) \subseteq \mathrm{ran}(\Gamma_1)$.

iv) On $\mathrm{dom}(M(\lambda))$

$$M(\lambda) - M(\mu)^* = (\lambda - \overline{\mu})\gamma(\mu)^*\gamma(\lambda)$$

holds true. This implies that $M(\lambda) \subseteq M(\overline{\lambda})^*$ is valid. In particular, $M(\lambda)$ is symmetric if $\lambda \in \rho(A_0) \cap \mathbb{R}$.

Next, we draw our attention to the problem of finding self-adjoint extensions of the symmetric operator S. In its most general form, these considerations require the concept of linear relations as it is discussed for instance in [13] and [69]. However, since we are not going to work with linear relations in this thesis, we leave out their introduction and refer to the mentioned literature for a detailed presentation. For our purposes it will prove to be sufficient to consider the following situation.

Let $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ be a quasi boundary triple for $\overline{T} = S^*$ and $B \in \mathcal{L}(\mathcal{G})$ be a linear and bounded operator in $\mathcal{G}$, then we define a linear operator in $\mathcal{H}$ by

$$A_B = T \upharpoonright \ker(B\Gamma_1 + \Gamma_0) \tag{2.2}$$

as a restriction of the operator T. An application of the abstract Green's identity (2.1) and [16, Prop. 2.2] shows that in this case a symmetric operator B induces a symmetric extension A_B of S. In contrast to ordinary boundary triples, a self-adjoint operator B generally does not lead to a self-adjoint extension A_B of S. This is discussed for instance in [16, Prop. 4.11] for the case of linear relations.

The next theorem allows us to characterize the symmetric extensions A_B of S induced by self-adjoint operators $B \in \mathcal{L}(\mathcal{G})$ according to (2.2) and to study their spectrum. Furthermore, it provides a variant of Krein's formula which enables us to represent the resolvents of the operators A_B in an explicit way. A proof of this result can be found for instance in [16, Thm. 2.8] or [17, Thm. 1.16]. The theorems in the previously mentioned sources are reduced to Theorem 2.19 in the case of linear operators B as it is stated in [18, Thm. 2.8] and [40, Thm. 2.2.6]. This result will be of particular importance in the treatment of Dirac operators with electrostatic and Lorentz scalar δ-shell interactions, since it allows us to obtain an explicit representation of the resolvent.

Theorem 2.19. Let $S : \mathrm{dom}(S) \subseteq \mathcal{H} \to \mathcal{H}$ be a linear, densely defined, closed and symmetric operator in $\mathcal{H}$ and let $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ be a quasi boundary triple for $\overline{T} = S^*$. Furthermore, let $A_0 = T \upharpoonright \ker(\Gamma_0)$ be the self-adjoint extension of S according to Definition 2.16, $B \in \mathcal{L}(\mathcal{G})$ be a linear, bounded and self-adjoint operator in $\mathcal{G}$ and A_B be the symmetric extension of S according to (2.2). Then the following statements are true for all $\lambda \in \rho(A_0)$.

i) $\lambda \in \sigma_p(A_B)$ if and only if $0 \in \sigma_p(I + BM(\lambda))$ and in this case

$$\ker(A_B - \lambda) = \left\{ \gamma(\lambda) f \;\middle|\; f \in \ker(I + BM(\lambda)) \right\}$$

is valid.

ii) If $\lambda \notin \sigma_p(A_B)$ is valid and $f \in \mathcal{H}$ is given, then one has $f \in \mathrm{ran}(A_B - \lambda)$ if and only if $B\gamma(\overline{\lambda})^* f \in \mathrm{ran}(I + BM(\lambda))$.

iii) If $\lambda \notin \sigma_p(A_B)$ is valid, then

$$(A_B - \lambda)^{-1} f = (A_0 - \lambda)^{-1} f - \gamma(\lambda) \left(I + BM(\lambda)\right)^{-1} B\gamma(\overline{\lambda})^* f \tag{2.3}$$

follows for all $f \in \mathrm{ran}(A_B - \lambda)$.

iv) If $\lambda \in \rho(A_0) \cap \rho(A_B)$ is valid, then Krein's formula (2.3) holds true for all $f \in \mathcal{H}$.

We conclude this section with the following observation which follows from Theorem 2.19. As mentioned above, an operator B which is self-adjoint in $\mathcal{G}$ yields a symmetric extension A_B of S in $\mathcal{H}$. Due to Theorem 2.12 and Theorem 2.19 ii) it follows for a given $\lambda \in \rho(A_0)$ with $\lambda \notin \sigma_p(A_B)$ that A_B is even self-adjoint if we can show that $B\gamma(\overline{\lambda})^* f \in \mathrm{ran}(I + BM(\lambda))$ holds true for every $f \in \mathcal{H}$. This is equivalent to the range condition $\mathrm{ran}(B\gamma(\overline{\lambda})^*) \subseteq \mathrm{ran}(I + BM(\lambda))$. In the next section we will use this line of reasoning to show the self-adjointness of Dirac operators electrostatic and Lorentz scalar δ-shell interactions.

2.3 A Krein-like formula

This section deals with the characterization of a self-adjoint operator based on an explicit representation of its resolvent. A situation like this will arise in the next chapter when examining the non-relativistic limit of a Dirac operator with electrostatic and Lorentz scalar δ-shell interactions in the case $\eta + \tau = 0$. In particular, with the result of this section we will be able to identify the limit operator as a Schrödinger operator with oblique jump conditions. Theorem 2.20 can be found in [59] and is formulated here in such a way that it is most convenient to apply for our purposes. For this reason, the notation in this section is based on the one of [59].

Let $A : \mathrm{dom}(A) \subseteq \mathcal{H} \to \mathcal{H}$ be a self-adjoint operator in the Hilbert space $\mathcal{H}$, then we equip $\mathrm{dom}(A)$ with the graph norm

$$\|x\|_A^2 = \|u\|_{\mathcal{H}}^2 + \|Ax\|_{\mathcal{H}}^2$$

for all $x \in \mathrm{dom}(A)$ and thereby obtain a Banach space due to Theorem 2.5. An application of Theorem 2.6 now shows that the resolvent

$$R(z) = (A - z)^{-1} : \mathcal{H} \to \mathrm{dom}(A)$$

is a linear and bounded operator from $(\mathcal{H}, \|\cdot\|_{\mathcal{H}})$ to $(\mathrm{dom}(A), \|\cdot\|_A)$ for all $z \in \rho(A)$. Next we assume that another Hilbert space $\mathcal{G}$ and a linear and bounded operator $\tau : \mathrm{dom}(A) \to \mathcal{G}$ are given. Here, the boundedness of τ is understood with respect to the graph norm on $\mathrm{dom}(A)$. As in our case, A typically corresponds to a differential operator and τ to some trace operator which assigns boundary values to functions in the considered function space.

Our objective now is to explicitly construct a family of self-adjoint operators A_Θ^τ which is parameterized by some quantity Θ and coincides with A on $\ker(\tau)$. If $\ker(\tau)$ is dense in $\mathcal{H}$ then $\mathcal{H}\backslash\ker(\tau)$ can be regarded as a "thin" set and in this case we interpret the operators A_Θ^τ as singular perturbations of the operator A. For each $z \in \rho(A)$, Theorem 2.10 and Theorem 2.15 enable us to define the following linear and bounded operators.

$$\check{G}(z) = \tau R(z) : \mathcal{H} \to \mathcal{G} \qquad \text{and} \qquad \hat{G}(z) = \check{G}(\overline{z})^* : \mathcal{G} \to \mathcal{H}$$

Next we assume that there exists a family of linear, closed and densely defined operators $\Gamma(z) : D \subseteq \mathcal{G} \to \mathcal{G}$ which are parameterized by $z \in \rho(A)$. It is noteworthy to remark that with this assumption we implicitly demand that the domain of definition D of each $\Gamma(z)$ is independent of $z \in \rho(A)$. Furthermore, all operators $\Gamma(z)$ should satisfy the following conditions.

- $\Gamma(z) - \Gamma(w) = (z - w)\check{G}(w)\hat{G}(z)$ on D for all $z, w \in \rho(A)$.
- $\Gamma(\overline{z}) \subseteq \Gamma(z)^*$ for all $z \in \rho(A)$.

Let $\Theta : \mathrm{dom}(\Theta) \subseteq \mathcal{G} \to \mathcal{G}$ be a linear, densely defined and symmetric operator in $\mathcal{G}$, then we define a family of linear operators in $\mathcal{G}$ by

$$\Gamma_\Theta(z) = \Theta + \Gamma(z) : \mathrm{dom}(\Theta) \cap D \subseteq \mathcal{G} \to \mathcal{G} \tag{2.4}$$

for any $z \in \rho(A)$. Next we define the set of all $z \in \rho(A)$ such that $\Gamma_\Theta(z)$ and $\Gamma_\Theta(\overline{z})$ are bijective and the inverse operators are bounded

$$Z_\Theta = \Big\{ z \in \rho(A) \,\Big|\, \exists \Gamma_\Theta(z)^{-1}, \Gamma_\Theta(\overline{z})^{-1} \in \mathcal{L}(\mathcal{G}) \Big\}. \tag{2.5}$$

An application of [59, Rem. 2.9], yields the main result of this section whose proof can be found in [59, Thm. 2.1].

Theorem 2.20. Let Γ_Θ be defined as in (2.4) and Z_Θ according to (2.5). Furthermore it is assumed that $Z_\Theta \neq \emptyset$ is valid and that $\ker(\tau)$ is dense in $\mathcal{H}$. Then, the linear and bounded operator

$$R^\tau_\Theta(z) = R(z) - \hat{G}(z)\Gamma_\Theta(z)^{-1}\check{G}(z) : \mathcal{H} \to \mathcal{H}$$

for $z \in Z_\Theta$ is the resolvent of a self-adjoint operator A^τ_Θ in $\mathcal{H}$. This operator A^τ_Θ coincides with A on $\ker(\tau)$ and can be explicitly represented in the following way

$$\begin{aligned} \mathrm{dom}(A^\tau_\Theta) &= \mathrm{ran}(R^\tau_\Theta(z)) \\ &= \Big\{ x \in \mathcal{H} \,\Big|\, \exists x_z \in \mathrm{dom}(A) \text{ such that } x = x_z - \hat{G}(z)\Gamma_\Theta(z)^{-1}\tau x_z \Big\} \\ (A^\tau_\Theta - z)\, x &= (A - z)\, x_z. \end{aligned}$$

Furthermore, the definition of A^τ_Θ is independent of $z \in Z_\Theta$ and the decomposition of $x \in \mathrm{dom}(A^\tau_\Theta)$ in the representation of the domain of definition $\mathrm{dom}(A^\tau_\Theta)$ is unique.

2.4 Sobolev spaces on a domain

In the context of partial differential equations one is naturally drawn to differentiable functions. But it turns out that differentiable functions are not well suited for dealing with partial differential equations and boundary value problems. For instance to formulate these problems in an appropriate way and to show existence and uniqueness results. In this section we introduce the important concept of Sobolev spaces which generalize differentiable functions in the sense of distributions and which allow a comprehensive treatment of boundary value problems. These function spaces will be the main objects for rigorously defining the formal differential expressions of Dirac operators of chapter 1 by specifying their domain of definition and thereby obtaining self-adjoint realizations. All the material of this section is well known and can for instance be found in the books [22, 24, 53, 77, 84] or the lecture notes [9, 58]. If a result comes from another source text, it is referred to at the respective passage.

In the following we assume that $\Omega \subseteq \mathbb{R}^n$ is an open subset of $\mathbb{R}^n$. We define the space of equivalence classes of complex-valued and p-integrable functions as $L^p(\Omega;\mathbb{C})$. According to Fischer-Riesz's theorem this space is a Banach space for every $1 \leq p \leq \infty$. Furthermore, we define the space of locally p-integrable functions $L^p_{\mathrm{loc}}(\Omega;\mathbb{C})$ as the set of equivalence classes of complex-valued functions $f : \Omega \to \mathbb{C}$ such that $f \restriction K \in L^p(K;\mathbb{C})$ holds true for all compact subsets $K \subseteq \Omega$. Of particular importance in this thesis will be the special case of $p = 2$. We equip the space $L^2(\Omega;\mathbb{C})$ with the inner product

$$(u, v)_{L^2(\Omega;\mathbb{C})} = \int_\Omega u(x)\overline{v(x)}\mathrm{d}x$$

for all $u, v \in L^2(\Omega;\mathbb{C})$ and thereby obtain a Hilbert space.

Next, we introduce spaces of differentiable functions. Let $\alpha = (\alpha_1, \dots, \alpha_n) \in \mathbb{N}_0^n$ be a given multi-index, then we define the α-th derivative of a sufficiently smooth function $f : \Omega \to \mathbb{C}$ in $x \in \Omega$ as

$$\partial^\alpha f(x) = \frac{\partial^{\alpha_1}}{\partial x_1^{\alpha_1}} \cdots \frac{\partial^{\alpha_n}}{\partial x_n^{\alpha_n}} f(x)$$

and $|\alpha| = \alpha_1 + \dots + \alpha_n$ as the order of this derivative. In the special case that $\alpha = e_j$ applies we generally use the notation $\partial^{e_j} f = \partial_j f$ for the partial derivative with respect to the variable x_j as it is common in vector calculus. For a given $k \in \mathbb{N}_0$, we define the set of functions that are k-times continuously differentiable on Ω as

$$C^k(\Omega;\mathbb{C}) = \left\{ f : \Omega \to \mathbb{C} \;\middle|\; \partial^\alpha f \text{ exists and is continuous for every } |\alpha| \leq k \right\}$$

and the set of the infinitely often differentiable functions as

$$C^\infty(\Omega;\mathbb{C}) = \bigcap_{k \in \mathbb{N}_0} C^k(\Omega;\mathbb{C}).$$

The support of a function $f : \Omega \to \mathbb{C}$ is the set

$$\mathrm{supp}(f) = \overline{\left\{ x \in \Omega \;\middle|\; f(x) \neq 0 \right\}}$$

and we define the set of test functions as the set of infinitely often differentiable functions whose support is compact in Ω

$$\mathcal{D}(\Omega;\mathbb{C}) = \left\{ f \in C^\infty(\Omega;\mathbb{C}) \;\middle|\; \mathrm{supp}(f) \text{ is compact in } \Omega \right\}.$$

With the usual definitions of addition and scalar multiplication of functions it can easily be shown that sets $C^k(\Omega;\mathbb{C})$, $C^\infty(\Omega;\mathbb{C})$ and $\mathcal{D}(\Omega;\mathbb{C})$ are vector spaces. Due to technical reasons, we define an additional function space by

$$C^\infty(\overline{\Omega};\mathbb{C}) = \left\{ \psi \restriction \Omega \;\middle|\; \psi \in \mathcal{D}(\mathbb{R}^n;\mathbb{C}) \right\}$$

as restrictions of test functions to the open set $\Omega \subseteq \mathbb{R}^n$.

As a generalization of differentiable functions we follow Schwartz's approach and construct distributions as linear and continuous functionals defined on the space of test functions. For this purpose, a notion of convergence in $\mathcal{D}(\Omega;\mathbb{C})$ has to be introduced.

Definition 2.21. Let $(\varphi_m)_{m\in\mathbb{N}} \subseteq \mathcal{D}(\Omega;\mathbb{C})$ be a sequence of test functions and $\varphi \in \mathcal{D}(\Omega;\mathbb{C})$ be given. We call $(\varphi_m)_{m\in\mathbb{N}}$ convergent to φ in $\mathcal{D}(\Omega;\mathbb{C})$ if the following conditions are met.

i) There exists a compact subset $K \subseteq \Omega$ such that $\operatorname{supp}(\varphi) \subseteq K$ and $\operatorname{supp}(\varphi_m) \subseteq K$ is valid for all $m \in \mathbb{N}$.

ii) For every multi-index $\alpha \in \mathbb{N}_0^n$, $\partial^\alpha \varphi_m$ converges uniformly to $\partial^\alpha \varphi$ on K.

In this case we write $\varphi_m \to \varphi$ in $\mathcal{D}(\Omega;\mathbb{C})$.

Before we define distributions, we introduce a commonly used notation. Let $T : \mathcal{D}(\Omega;\mathbb{C}) \to \mathbb{C}$ be a linear mapping defined on $\mathcal{D}(\Omega;\mathbb{C})$, then we write

$$\langle T, \varphi \rangle = T(\varphi)$$

for the application of T to a test function $\varphi \in \mathcal{D}(\Omega;\mathbb{C})$.

Definition 2.22. A linear functional $T : \mathcal{D}(\Omega;\mathbb{C}) \to \mathbb{C}$ is called a distribution if it is sequentially continuous in the sense of Definition 2.21. In other words, for every sequence $(\varphi_m)_{m\in\mathbb{N}} \subseteq \mathcal{D}(\Omega;\mathbb{C})$ and $\varphi \in \mathcal{D}(\Omega;\mathbb{C})$ with $\varphi_m \to \varphi$ in $\mathcal{D}(\Omega;\mathbb{C})$ it follows that $\langle T, \varphi_m \rangle \to \langle T, \varphi \rangle$ in $\mathbb{C}$ holds true.

With the usual definitions of addition and scalar multiplication it can easily be shown that set of distributions is a vector space. This space is denoted by $\mathcal{D}'(\Omega;\mathbb{C})$ since it is the dual space of $\mathcal{D}(\Omega;\mathbb{C})$ with respect to the topology induced by the notion of convergence of Definition 2.21.

Next, we address the question if sufficiently regular functions can be regarded as distributions. It is easy to see that for a given function $f \in L^1_{\mathrm{loc}}(\Omega;\mathbb{C})$ the assignment

$$\langle T_f, \varphi \rangle = \int\limits_\Omega f(x)\varphi(x)\mathrm{d}x \tag{2.6}$$

for $\varphi \in \mathcal{D}(\Omega;\mathbb{C})$ defines a distribution. Furthermore, with the fundamental lemma of calculus of variations it can be shown that the function $f \in L^1_{\mathrm{loc}}(\Omega;\mathbb{C})$ which characterizes $T = T_f$ is unique and therefore the assignment $f \mapsto T_f$ according to (2.6) corresponds to an embedding of $L^1_{\mathrm{loc}}(\Omega;\mathbb{C})$ in $\mathcal{D}'(\Omega;\mathbb{C})$. Every distribution T for which an $f \in L^1_{\mathrm{loc}}(\Omega;\mathbb{C})$ exists such that $T = T_f$ is valid is called a regular distribution. In this case we identify T with f and using a slight abuse of notation we simply write $T \in L^1_{\mathrm{loc}}(\Omega;\mathbb{C})$ and $\langle T, \cdot \rangle = \langle f, \cdot \rangle$. Similarly we write $T \in L^2(\Omega;\mathbb{C})$ if f is even a L^2-function.

Let $\alpha \in \mathbb{N}_0^n$ be a given multi-index, then we define the α-th derivative of a distribution T by the assignment

$$\langle \partial^\alpha T, \varphi \rangle = (-1)^{|\alpha|} \langle T, \partial^\alpha \varphi \rangle$$

for any test function $\varphi \in \mathcal{D}(\Omega; \mathbb{C})$. It can easily be shown that $\partial^\alpha T$ defines a distribution for all multi-indices $\alpha \in \mathbb{N}_0^n$ and we therefore have $\partial^\alpha T \in \mathcal{D}'(\Omega; \mathbb{C})$. In particular this shows that every distribution is infinitely often differentiable in the above sense.

Next we consider the special case that the α-th derivative $\partial^\alpha T_f$ of a regular distribution T_f induced by the function $f \in L^1_{\text{loc}}(\Omega; \mathbb{C})$ is itself a regular distribution. This implies that there exists a $g \in L^1_{\text{loc}}(\Omega; \mathbb{C})$ such that $\partial^\alpha T_f = T_g$ holds true. In this case we call g the weak derivative of f and we write $g = \partial^\alpha f$ in analogy to the classical derivative for the weak derivative as well. In the entire following thesis we will always assume that $\partial^\alpha f$ represents the weak derivative, unless stated otherwise.

After this preparation we are now able to introduce the important concept of Sobolev spaces on an open set $\Omega \subseteq \mathbb{R}^n$ as subspaces of $\mathcal{D}'(\Omega; \mathbb{C})$. Although it is not the most general setting, we define these function spaces only for the case $p = 2$ as a set of L^2-functions whose distributional derivatives are L^2-functions as well. For a detailed presentation of Sobolev spaces in the case $1 \leq p \leq \infty$, we refer to the literature mentioned in the introduction of this section.

Definition 2.23. Let $\Omega \subseteq \mathbb{R}^n$ be an open set and $k \in \mathbb{N}_0$ be a given integer, then the Sobolev space of order k on Ω is defined as

$$H^k(\Omega; \mathbb{C}) = \Big\{ f \in L^2(\Omega; \mathbb{C}) \,\Big|\, \partial^\alpha f \text{ exists } \text{ for all } |\alpha| \leq k \text{ and } \partial^\alpha f \in L^2(\Omega; \mathbb{C}) \Big\}.$$

Furthermore, we equip the space $H^k(\Omega; \mathbb{C})$ with the inner product

$$(u, v)_{H^k(\Omega;\mathbb{C})} = \sum_{|\alpha| \leq k} (\partial^\alpha u, \partial^\alpha v)_{L^2(\Omega;\mathbb{C})}$$

for $u, v \in H^k(\Omega; \mathbb{C})$.

Since the distributional derivative and thus the weak derivative is a linear operation, it follows that the Sobolev space $H^k(\Omega; \mathbb{C})$ is indeed a subspace of $\mathcal{D}'(\Omega; \mathbb{C})$. Furthermore, it can be shown that Sobolev spaces are Hilbert spaces for all $k \in \mathbb{N}_0$.

In many cases it is not sufficient to consider only integer order Sobolev spaces as for instance the weak formulation of a boundary value problem shows. This leads to the so-called Sobolev-Slobodeckij spaces $H^s(\Omega; \mathbb{C})$ which fill the "gaps" between the integer order Sobolev spaces and allow us to measure the regularity of a function on a continuous scale by introducing a suitable semi-norm.

Definition 2.24. Let $k \in \mathbb{N}_0$ be a given integer and $\sigma \in (0,1)$ be a real number, then the Sobolev space of order $s = k + \sigma$ is defined as

$$H^s(\Omega;\mathbb{C}) = \left\{ f \in H^k(\Omega;\mathbb{C}) \,\middle|\, |\partial^\alpha f|_{H^\sigma(\Omega;\mathbb{C})} < \infty \text{ for all } |\alpha| = k \right\}$$

with semi-norm

$$|f|_{H^\sigma(\Omega;\mathbb{C})} = \left(\int_\Omega \int_\Omega \frac{|f(x) - f(y)|^2}{|x-y|^{n+2\sigma}} \mathrm{d}x\mathrm{d}y \right)^{\frac{1}{2}}.$$

Furthermore, we equip the space $H^s(\Omega;\mathbb{C})$ with the inner product

$$(u,v)_{H^s(\Omega;\mathbb{C})} = (u,v)_{H^k(\Omega;\mathbb{C})} + \sum_{|\alpha|=k} \int_\Omega \int_\Omega \frac{(\partial^\alpha u(x) - \partial^\alpha u(y))(\overline{\partial^\alpha v}(x) - \overline{\partial^\alpha v}(y))}{|x-y|^{n+2\sigma}} \mathrm{d}x\mathrm{d}y$$

for $u, v \in H^s(\Omega;\mathbb{C})$.

It can be easily shown that the Sobolev-Slobodeckij spaces $H^s(\Omega;\mathbb{C})$, such as the integer order Sobolev spaces, are subspaces of $\mathcal{D}'(\Omega;\mathbb{C})$. Furthermore, also the Sobolev-Slobodeckij spaces are Hilbert spaces for all $s \geq 0$.

In order to simplify the presentation and to avoid distinguishing between the cases $s \in \mathbb{N}_0$ and $s \notin \mathbb{N}_0$, we will from now on use Definition 2.23 in the case of $s \in \mathbb{N}_0$ and otherwise Definition 2.24 whenever the space $H^s(\Omega;\mathbb{C})$ is mentioned. In addition, we will also refer to the Sobolev-Slobodeckij spaces in the following as Sobolev spaces.

Next we introduce an important subspace of $H^s(\Omega;\mathbb{C})$, namely the space

$$H_0^s(\Omega;\mathbb{C}) = \overline{\mathcal{D}(\Omega;C)}^{\|\cdot\|_{H^s(\Omega;\mathbb{C})}}$$

which is by definition closed in the Hilbert space $H^s(\Omega;\mathbb{C})$ and thus a Hilbert space itself. In general only $H_0^s(\Omega;\mathbb{C}) \subsetneqq H^s(\Omega;\mathbb{C})$ is valid, which can be easily shown for instance for bounded domains with the help of constant functions. However, an important situation arises in the case of $\Omega = \mathbb{R}^n$ for which $H_0^s(\mathbb{R}^n;\mathbb{C}) = H^s(\mathbb{R}^n;\mathbb{C})$ applies.

At this point it should be noted that in literature the Sobolev-Slobodeckij spaces for $p = 2$ are usually denoted by $W^{s,2}(\Omega;\mathbb{C})$, while $H^s(\Omega;\mathbb{C})$ is used for the so-called Bessel potential spaces, which provide an alternative approach to real order Sobolev spaces. In the following chapters, $\Omega \subseteq \mathbb{R}^n$ will always be at least a Lipschitz domain, and it can be shown in this case that these two function spaces coincide. The same applies to $\Omega = \mathbb{R}^n$. Therefore our labeling is justified. For a more detailed presentation of the Bessel potential spaces and their relationship to the Sobolev-Slobodeckij spaces, we refer to [53, Chapter 3] and [84, Chapter 5].

Finally, we consider vector-valued functions, since they appear in the context of Dirac spinors. The extension of Sobolev spaces to the vector-valued case is done in a straightforward manner by forming the product space of all the occurring function spaces and applying the results of this section component-wise. First, we construct for $m \in \mathbb{N}$ the space $L^2(\Omega;\mathbb{C}^m) = L^2(\Omega;\mathbb{C})^m$ consisting of equivalence classes of functions $f = (f_1,\dots,f_m) : \Omega \to \mathbb{C}^m$ whose components f_k are in $L^2(\Omega;\mathbb{C})$. Using the standard Euclidean inner product in $\mathbb{C}^m$, we define an inner product on $L^2(\Omega;\mathbb{C}^m)$ by

$$(u,v)_{L^2(\Omega;\mathbb{C}^m)} = \sum_{k=1}^{m} (u_k, v_k)_{L^2(\Omega;\mathbb{C})} = \int_\Omega u(x) \cdot \overline{v(x)} \mathrm{d}x$$

for $u = (u_1,\dots,u_m), v = (v_1,\dots,v_m) \in L^2(\Omega;\mathbb{C}^m)$ and thereby turning $L^2(\Omega;\mathbb{C}^m)$ into a Hilbert space. In a similar manner, we define the Sobolev space of order $s \geq 0$ as the set of all equivalence classes of functions $f = (f_1,\dots,f_m) : \Omega \to \mathbb{C}^m$ with components $f_k \in H^s(\Omega;\mathbb{C})$. An inner product on $H^s(\Omega;\mathbb{C}^m)$ is defined by the assignment

$$(u,v)_{H^s(\Omega;\mathbb{C}^m)} = \sum_{k=1}^{m} (u_k, v_k)_{H^s(\Omega;\mathbb{C})}$$

for $u = (u_1,\dots,u_m), v = (v_1,\dots,v_m) \in H^s(\Omega;\mathbb{C}^m)$ and it can now be shown that all the results of this section remain valid also in the vector-valued case, especially the Hilbert space property of the spaces $H^s(\Omega;\mathbb{C}^m)$.

2.5 Sobolev spaces on the boundary

After having defined Sobolev spaces on an open set $\Omega \subseteq \mathbb{R}^n$ in Section 2.4 we now address the question how regularity of functions $f : \partial\Omega \to \mathbb{C}$ defined on the boundary $\partial\Omega$ of Ω can be characterized. This leads to Sobolev spaces on the boundary whose construction is far more technical than the one of Sobolev spaces on an open set. Up to now we have not imposed any regularity conditions on the boundary of an open set, but as it turns out the regularity of the boundary has a great influence on the orders of Sobolev spaces that can be defined. Therefore, we will start this section by introducing Lipschitz domains, which are usually sufficiently regular for our purposes of introducing Sobolev spaces on the boundary. All the material of this section is well known and can be found for instance in the books [53, 77, 84] or the lecture note [58]. If a result comes from another source text, it is referred to at the respective passage.

Definition 2.25. Let $\Omega \subseteq \mathbb{R}^n$ be an open set. If there exists a Lipschitz continuous function $\zeta : \mathbb{R}^{n-1} \to \mathbb{R}$ with a uniform Lipschitz constant such that

$$\Omega = \left\{ x = (x_1,\dots,x_{n-1},x_n) \in \mathbb{R}^n \;\middle|\; x_n < \zeta(x_1,\dots,x_{n-1}) \right\}$$

holds true, then Ω is called a Lipschitz hypograph.

With the function ζ from Definition 2.25, the boundary $\partial\Omega$ of a Lipschitz hypograph can be parameterized explicitly by

$$\partial\Omega = \left\{ (x, \zeta(x)) \in \mathbb{R}^n \,\middle|\, x \in \mathbb{R}^{n-1} \right\}.$$

Using Lipschitz hypographs we now define the more general Lipschitz domains as open sets which can be locally described as Lipschitz hypographs.

Definition 2.26. An open set $\Omega \subseteq \mathbb{R}^n$ is called Lipschitz domain if its boundary $\Gamma = \partial\Omega$ is compact in $\mathbb{R}^n$ and there exist finite families $\{W_i\}_{i\in I}$ and $\{\Omega_i\}_{i\in I}$ consisting of subsets of $\mathbb{R}^n$ such that the following conditions are met.

i) The family $\{W_i\}_{i\in I}$ is an open cover of Γ. In particular, W_i is an open subset of $\mathbb{R}^n$ for every $i \in I$ and $\Gamma \subseteq \bigcup_{i\in I} W_i$ holds true.

ii) For every $i \in I$ there exists a rigid motion κ_i, i.e.: a rotation and a translation, which transforms Ω_i into a Lipschitz hypograph.

iii) $W_i \cap \Omega = W_i \cap \Omega_i$ is valid for every $i \in I$.

At this point it is noteworthy to remark that only the boundary of the Lipschitz domain has to be compact and hence bounded to ensure the finiteness of the families $\{W_i\}_{i\in I}$ and $\{\Omega_i\}_{i\in I}$ in Definition 2.26. The domain itself may very well be unbounded. In particular for a bounded Lipschitz domain $\Omega \subseteq \mathbb{R}^n$ its open complement $\mathbb{R}^n \setminus \overline{\Omega}$ is an unbounded Lipschitz domain.

Occasionally it may be necessary to require more regularity of the boundary and in this case we modify Definition 2.26 as follows. Let $k \in \mathbb{N}$ be a given integer and $\Omega \subseteq \mathbb{R}^n$ an open set for which there exists a function ζ as in Definition 2.25. We call Ω a C^k-hypograph if ζ is a C^k-function and $\partial^\alpha \zeta$ is bounded for all multi-indices $\alpha \in \mathbb{N}_0^n$ with $|\alpha| \le k$. Analogously, we define a C^k-domain by substituting "C^k" for "Lipschitz" in Definition 2.26.

To define Sobolev spaces on the boundary of a Lipschitz domain, a surface integral and therefore a surface measure on an $(n-1)$-dimensional submanifold of $\mathbb{R}^n$ has to be constructed. This will be accomplished by using the next result, also known as Rademacher's theorem, whose proof can be found for instance in [28, Prop. 19.28].

Theorem 2.27. Let $U \subseteq \mathbb{R}^n$ be an open set and $f : U \to \mathbb{R}$ be a Lipschitz continuous function on U, then f is differentiable almost everywhere on U, ∇f is measurable and $\|\nabla f\|_{L^\infty(U;\mathbb{R}^n)} < \infty$ holds true.

A first important consequence of Rademacher's theorem is the following. Let $\Omega \subseteq \mathbb{R}^n$ be a Lipschtz-hypograph according to Definition 2.25 with Lipschitz-continuous function ζ. Theorem 2.27 implies that there exists a unit normal vector field

$$\nu(x, \zeta(x)) = \frac{1}{\sqrt{1 + \|\nabla\zeta(x)\|^2}} \begin{pmatrix} -\nabla\zeta(x) \\ 1 \end{pmatrix} \tag{2.7}$$

on $\Gamma = \partial\Omega$ for almost all $x \in \mathbb{R}^{n-1}$. This result is generalized to Lipschitz domains by using the decomposition from Definition 2.26.

Next we proceed with the construction of a surface integral on the boundary of a Lipschitz domain. Let $\Omega \subseteq \mathbb{R}^n$ be a Lipschitz domain according to Definition 2.26 and let $\zeta_i : \mathbb{R}^{n-1} \to \mathbb{R}$ be the corresponding Lipschitz continuous functions and $\kappa_i : \mathbb{R}^n \to \mathbb{R}^n$ be the corresponding rigid motions. We define the transformation maps

$$\Phi_i(x) = \kappa_i^{-1}(x, \zeta_i(x)) \tag{2.8}$$

for $x \in \mathbb{R}^{n-1}$ and $i \in I$ and choose a partition of unity subordinate to $\{W_i\}_{i\in I}$. This is a family of functions $\{\varphi_i\}_{i\in I}$ such that the following conditions are satisfied.

- $\varphi_i \in \mathcal{D}(\mathbb{R}^n; \mathbb{R})$ and $\operatorname{supp}(\varphi_i) \subseteq W_i$ hold true for every $i \in I$.
- $0 \leq \varphi_i(x) \leq 1$ holds true for every $x \in \mathbb{R}^n$ and every $i \in I$.
- $\sum\limits_{i\in I} \varphi_i(x) = 1$ holds true for every $x \in \Gamma$.

Let $f : \Gamma \to \mathbb{C}$ be a function defined on the boundary of the Lipschitz domain, then we set $\varphi_i f : \Gamma \to \mathbb{C}$ and thereby obtain a family of functions for which $\operatorname{supp}(\varphi_i f) \subseteq W_i \cap \Gamma$ is valid for all $i \in I$. Furthermore it follows that

$$\sum_{i\in I} \varphi_i(x) f(x) = f(x)$$

holds true for every $x \in \Gamma$ and thus $\{\varphi_i f\}_{i\in I}$ is a decomposition of f. Next we define for every $i \in I$ the set $V_i = \Phi_i^{-1}(W_i \cap \partial\Omega_i) = \Phi_i^{-1}(W_i \cap \Gamma) \subseteq \mathbb{R}^{n-1}$ and the mapping $(\varphi_i f) \circ \Phi_i : V_i \to \mathbb{C}$ as the pullback of $\varphi_i f$ to the parameter domain by Φ_i. Since $\operatorname{supp}(\varphi_i f) \subseteq W_i \cap \Gamma$ holds true, we can extend $(\varphi_i f) \circ \Phi_i$ by 0 to all of $\mathbb{R}^{n-1}$ and thus obtain a well-defined mapping $\widetilde{(\varphi_i f)} \circ \Phi_i : \mathbb{R}^{n-1} \to \mathbb{C}$ which has the explicit representation

$$\widetilde{(\varphi_i f)} \circ \Phi_i(x) = \begin{cases} (\varphi_i f) \circ \Phi_i(x) \text{ , if } \Phi_i(x) \in W_i \cap \Gamma \\ 0, \text{ else} \end{cases} \tag{2.9}$$

for all $x \in \mathbb{R}^{n-1}$. At this point it is already apparent that the regularity of the boundary influences the regularity of $\widetilde{(\varphi_i f)} \circ \Phi_i$ via ζ_i. This will be of particular importance when defining the Sobolev spaces on the boundary of a Lipschitz domain.

We call f integrable over Γ, if the mapping

$$x \mapsto \widetilde{(\varphi_i f)} \circ \Phi_i(x) \sqrt{\det(D\Phi_i(x)^\top D\Phi_i(x))}$$

from $\mathbb{R}^{n-1}$ to $\mathbb{C}$ is measurable and integrable with respect to the $(n-1)$-dimensional Lebesgue measure for all $i \in I$, with

$$D\Phi_i(x) = \begin{pmatrix} \frac{\partial}{\partial x_1}\Phi_i^1(x) & \frac{\partial}{\partial x_2}\Phi_i^1(x) & \cdots & \frac{\partial}{\partial x_{n-1}}\Phi_i^1(x) \\ \vdots & \vdots & & \vdots \\ \frac{\partial}{\partial x_1}\Phi_i^n(x) & \frac{\partial}{\partial x_2}\Phi_i^n(x) & \cdots & \frac{\partial}{\partial x_{n-1}}\Phi_i^n(x) \end{pmatrix}$$

being the gradient of Φ_i at $x \in \mathbb{R}^{n-1}$. In this case we define the surface integral of f over the boundary of a Lipschitz domain as the sum of surface integrals over the boundaries of Lipschitz hypographs by

$$\begin{aligned}\int\limits_{\Gamma} f(x)\mathrm{d}\sigma(x) &= \sum_{i\in I} \int\limits_{W_i\cap\Gamma} \varphi_i(x)f(x)\mathrm{d}\sigma(x) \\ &= \sum_{i\in I} \int\limits_{\mathbb{R}^{n-1}} (\widetilde{\varphi_i f}) \circ \Phi_i(x)\sqrt{\det(D\Phi_i(x)^\top D\Phi_i(x))}\mathrm{d}x\end{aligned} \tag{2.10}$$

with σ being the so-called Hausdorff measure. It can be shown that the surface integral on the boundary of a Lipschitz domain is independent of the parameterizations $\{W_i\}_{i\in I}$ and $\{\Omega_i\}_{i\in I}$ and the partition of unity $\{\varphi_i\}_{i\in I}$. For further details we refer to [71, Chapter 3.1] and [27, Rem. 8.10].

With the definition of a surface integral we are now in the position to define L^2-spaces on the boundary $\Gamma = \partial\Omega$ of a Lipschitz domain $\Omega \subseteq \mathbb{R}^n$ as the set of equivalence classes of complex-valued and squadrate-integrable functions with respect to the Hausdorff measure

$$L^2(\Gamma;\mathbb{C}) = \left\{ f : \Gamma \to \mathbb{C} \;\middle|\; \int\limits_{\Gamma} |f(x)|^2 \,\mathrm{d}\sigma(x) < \infty \right\}.$$

Due to the linearity of the Lebesgue integral in $\mathbb{R}^{n-1}$ it follows that $L^2(\Gamma;\mathbb{C})$ is a vector space. Furthermore, by equipping $L^2(\Gamma;\mathbb{C})$ with the inner product

$$(u,v)_{L^2(\Gamma;\mathbb{C})} = \int\limits_{\Gamma} u(x)\overline{v(x)}\mathrm{d}\sigma(x)$$

for $u, v \in L^2(\Gamma;\mathbb{C})$, we obtain a Hilbert space.

Based on the $L^2(\Gamma;\mathbb{C})$-spaces we define now Sobolev spaces on the boundary of a Lipschitz domain by characterizing the regularity of a function $f : \Gamma \to \mathbb{C}$ in terms of the regularity of the pullbacks (2.9) of the decomposition of f on the parameter domain.

Definition 2.28. Let $\Omega \subseteq \mathbb{R}^n$ be a Lipschitz domain with boundary $\Gamma = \partial\Omega$. For $0 \le s \le 1$, the Sobolev space of order s on the boundary of Ω is defined as

$$H^s(\Gamma;\mathbb{C}) = \left\{ f \in L^2(\Gamma;\mathbb{C}) \;\middle|\; (\widetilde{\varphi_i f}) \circ \Phi_i \in H^s(\mathbb{R}^{n-1};\mathbb{C}) \text{ for all } i \in I \right\}.$$

Furthermore we equip $H^s(\Gamma;\mathbb{C})$ with the inner product

$$(u,v)_{H^s(\Gamma;\mathbb{C})} = \sum_{i\in I} ((\widetilde{\varphi_i u}) \circ \Phi_i, (\widetilde{\varphi_i v}) \circ \Phi_i)_{H^s(\mathbb{R}^{n-1};\mathbb{C})} \tag{2.11}$$

for $u, v \in H^s(\Gamma;\mathbb{C})$.

Since $H^s(\mathbb{R}^{n-1};\mathbb{C})$ is a vector space it follows immediately that the sets $H^s(\Gamma;\mathbb{C})$ are vector spaces as well and it can be shown that they are even Hilbert spaces. In the case of C^k-domains, Sobolev spaces of order $0 \leq s \leq k$ can be introduced in a similar way and all the following results remain valid for these spaces if one consistently replaces 1 with k. Although it seems that the spaces $H^s(\Gamma;\mathbb{C})$ and the norm induced by the inner product (2.11) depend on the families $\{W_i\}_{i\in I}$, $\{\Omega_i\}_{i\in I}$ and $\{\varphi_i\}_{i\in I}$ it can be shown that, as in the case of the $L^2(\Gamma;\mathbb{C})$-spaces, another choice yields the same space with an equivalent norm. See [84, Thm. 4.2] for further details.

For technical reasons, we will also consider Sobolev spaces of negative order. We define these as dual spaces and set

$$H^s(\Gamma;\mathbb{C}) = \big(H^{-s}(\Gamma;\mathbb{C})\big)^*$$

for all $-1 \leq s < 0$.

The next result is known as Rellich-Kondrachov theorem and its proof can be found for instance in [84, Thm. 7.9, Thm. 7.10] in combination with Schauder's theorem.

Theorem 2.29. Let $\Omega \subseteq \mathbb{R}^n$ be a Lipschitz domain with boundary $\Gamma = \partial\Omega$ and $s < t$ be given, then the following statements are true.

i) If $0 \leq s$ holds true, then the embedding $H^t(\Omega;\mathbb{C}) \hookrightarrow H^s(\Omega;\mathbb{C})$ is compact.

ii) If $-1 \leq s$ and $t \leq 1$ holds true, then the embedding $H^t(\Gamma;\mathbb{C}) \hookrightarrow H^s(\Gamma;\mathbb{C})$ is compact.

Next, we turn our attention to the calculation of boundary values of Sobolev functions as it is required for boundary value problems. Since the boundary $\Gamma = \partial\Omega$ of a Lipschitz domain $\Omega \subseteq \mathbb{R}^n$ is a Lebesgue zero set, restrictions of L^2-functions to the boundary are not well-defined. To resolve this difficulty, the so-called trace operator is introduced which provides a precise meaning of boundary values of sufficiently regular L^2-functions.

Theorem 2.30. Let $\Omega \subseteq \mathbb{R}^n$ be a Lipschitz domain with boundary $\Gamma = \partial\Omega$ and $\frac{1}{2} < s \leq 1$ be given, then there exists a linear, bounded and surjective operator

$$\tau : H^s(\Omega;\mathbb{C}) \to H^{s-\frac{1}{2}}(\Gamma;\mathbb{C})$$

such that $\tau(f) = f\restriction\Gamma$ is valid for all $f \in C^\infty(\overline{\Omega};\mathbb{C})$.

Using the trace operator of Theorem 2.30 the divergence theorem can be generalized to Sobolev spaces and Lipschitz domains. The proof of this result canbe found in for instance [3, Thm. A.6.8] or [71, Thm. 3.23] and relies heavily on the density of the infinitely often differentiable functions $C^\infty(\overline{\Omega};\mathbb{C})$ in $H^1(\Omega;\mathbb{C})$. Following a common convention, we omit the arguments of the functions under the integrals to simplify the notation.

Theorem 2.31. Let $\Omega \subseteq \mathbb{R}^n$ be a Lipschitz domain with boundary $\Gamma = \partial\Omega$ and let $u, v \in H^1(\Omega;\mathbb{C})$ be two given functions, then

$$\int\limits_{\Omega} \left(\frac{\partial}{\partial x_i} u \cdot v + u \cdot \frac{\partial}{\partial x_i} v \right) \mathrm{d}x = \int\limits_{\Gamma} \tau(u)\tau(v)\nu_i \mathrm{d}\sigma$$

is valid for all $i \in \{1, \dots, n\}$ with ν being the unit normal vector field on Γ.

The next theorem is a collection of useful properties concerning the Sobolev spaces $H^s(\Omega;\mathbb{C})$ and $H^{\frac{1}{2}}(\Gamma;\mathbb{C})$ and the trace operator which are needed in the next chapter. Item ii) is a consequence of [84, Thm. 4.3] and Theorem 2.29, the proof of item iii) can be found in[68, Thm. 46] and [58, Ex. 9] and item iv) is a consequence of [53, Thm. 3.20].

Theorem 2.32. Let $\Omega \subseteq \mathbb{R}^n$ be a Lipschitz domain with boundary $\Gamma = \partial\Omega$, then the following statements are true.

i) $H_0^s(\Omega;\mathbb{C}) = \ker(\tau)$ is valid for all $\frac{1}{2} < s \leq 1$.

ii) $H^s(\Gamma;\mathbb{C})$ is dense in $L^2(\Gamma;\mathbb{C})$ for all $0 \leq s \leq 1$.

iii) If Ω is bounded, then both $\Omega_+ = \Omega$ and $\Omega_- = \mathbb{R}^n \backslash \overline{\Omega}$ are Lipschitz domains with trace operators $\tau_\pm$ according to Theorem 2.30. Let $u \in H^1(\Omega_+ \cup \Omega_-;\mathbb{C})$ with $u_\pm = u \restriction \Omega_\pm \in H^1(\Omega_\pm;\mathbb{C})$ be given, then in this case it follows that $u \in H^1(\mathbb{R}^n;\mathbb{C})$ if and only if $\tau_+ u_+ = \tau_- u_-$ on the common surface $\Gamma = \partial\Omega_\pm$.

iv) If Ω is a C^2-domain with the unit normal vector field ν, then $\nu_i f \in H^{\frac{1}{2}}(\Gamma;\mathbb{C})$ is valid for all $f \in H^{\frac{1}{2}}(\Gamma;\mathbb{C})$ and $i \in \{1, \dots, n\}$.

In this thesis it will be necessary to consider an alternative approach to boundary values, besides the representation in terms of the trace operator of Theorem 2.30. It will turn out that under appropriate conditions both approaches coincide. For this purpose we have to introduce the so-called non-tangential limits.

It is known that every Lipschitz domain satisfies the so-called uniform cone condition. This implies that in each point $x \in \Gamma$ there exists a cone $V(x) \subseteq \mathbb{R}^n$, which has its origin in x, and an open ball $B(x,r) \subseteq \mathbb{R}^n$ such that the set $D(x) = V(x) \cap B(x,r)$ is located entirely in Ω. In this context $D(x)$ is also known as non-tangential approach cone. A function $f : \Omega \to \mathbb{C}$ is said to have a non-tangential limit in $x \in \Gamma$, if the limit

$$(Lf)(x) = \lim_{D(x) \ni y \to x} f(y) = c$$

exists for a $c \in \mathbb{C}$. In the following we will always regard point-wise limits on Σ as non-tangential limits and therefore usually write Ω in the above limit instead of explicitly mentioning the approach cone $D(x)$. In view of the uniform cone condition it is then evident from the context how the limit is performed. With these notions the following result holds true, as it can be found for instance in [33, Thm. 2.5].

Lemma 2.33. Let $\Omega \subseteq \mathbb{R}^n$ be a Lipschitz domain with boundary Γ and let $f \in H^s(\Omega;\mathbb{C})$ with $\frac{1}{2} < s \leq 1$ be a given function. If the non-tangential limit of f exists almost everywhere on Γ, then $Lf = \tau(f)$ is valid in the sense of $H^{s-\frac{1}{2}}(\Gamma;\mathbb{C})$.

Finally, we consider vector-valued functions as in Section 2.4. In order to do so, we assume that a Lipschitz domain $\Omega \subseteq \mathbb{R}^n$ with boundary $\Gamma = \partial\Omega$ is given. The extension of Sobolev spaces to the vector-valued case is done in a straightforward manner by forming the product space of all the occurring function spaces and applying the results of this section component-wise. First we construct for a given $m \in \mathbb{N}$ the space $L^2(\Gamma;\mathbb{C}^m) = L^2(\Gamma;\mathbb{C})^m$ consisting of equivalence classes of functions $f = (f_1,\ldots,f_m) : \Gamma \to \mathbb{C}^m$ whose components f_k are in $L^2(\Gamma;\mathbb{C})$. Using the standard Euclidean inner product in $\mathbb{C}^m$, we define an inner product on $L^2(\Sigma;\mathbb{C}^m)$ by

$$(u,v)_{L^2(\Gamma;\mathbb{C}^m)} = \sum_{k=1}^{m} (u_k,v_k)_{L^2(\Gamma;\mathbb{C})} = \int\limits_{\Gamma} u(x)\cdot\overline{v(x)}\mathrm{d}\sigma(x)$$

for $u = (u_1,\ldots,u_m), v = (v_1,\ldots,v_m) \in L^2(\Gamma;\mathbb{C}^m)$ and thereby turning $L^2(\Gamma;\mathbb{C}^m)$ into a Hilbert space. Furthermore, for $0 \leq s \leq 1$ we define the set of all equivalence classes of function $f = (f_1,\ldots,f_m) : \Gamma \to \mathbb{C}^m$ with components $f_k \in H^s(\Gamma;\mathbb{C})$ as space $H^s(\Gamma;\mathbb{C}^m) = H^s(\Gamma;\mathbb{C})^m$ and equip it with the inner product

$$(u,v)_{H^s(\Gamma;\mathbb{C}^m)} = \sum_{k=1}^{m}(u_k,v_k)_{H^s(\Gamma;\mathbb{C})}$$

for $u = (u_1,\ldots,u_m), v = (v_1,\ldots,v_m) \in H^s(\Gamma;\mathbb{C}^m)$.

Next, by component-wise application of the trace operator of Theorem 2.30, we obtain a linear, bounded and surjective operator $\tau : H^s(\Omega;\mathbb{C}^m) \to H^{s-\frac{1}{2}}(\Gamma;\mathbb{C}^m)$ for all $\frac{1}{2} < s \leq 1$.

As in Section 2.4, all results of this section remain valid for the vector-valued case. Especially the Hilbert space property of the spaces $H^s(\Gamma;\mathbb{C}^m)$, the compact embedding results of $H^s(\Omega;\mathbb{C}^m)$ and $H^s(\Gamma;\mathbb{C}^m)$ of Theorem 2.29 and the properties of the spaces $H^s(\Omega;\mathbb{C}^m)$ and $H^s(\Gamma;\mathbb{C}^m)$ and the trace operator $\tau : H^s(\Omega;\mathbb{C}^m) \to H^{s-\frac{1}{2}}(\Gamma;\mathbb{C}^m)$ of Theorem 2.32.

2.6 Integral operators and operators in $L^2 \times L^2$

This rather technical section deals with results concerning integral operators and operators defined on the Cartesian product of two L^2-spaces which are needed in the next chapters. In particular, the values of the γ-field and Weyl function of the quasi boundary triple used to describe Dirac operators with electrostatic and Lorentz scalar δ-shell interactions will be found to correspond to such integral operators. Therefore, the examination of these operators is of great importance and we will show that for special integral kernels they represent everywhere defined, linear and bounded operators.

We begin with integral operators and follow the presentation of [10] or [40]. Proofs are only provided if the statements are not found in the mentioned literature, but are needed in the course of this thesis. Before we state the theorems, it should be pointed out that on a domain $\Omega \subseteq \mathbb{R}^3$ the Lebesgue measure and on the boundary of a C^2-domain the Hausdorff measure is used. Furthermore, remember that all norms on $\mathbb{R}^n$ and all matrix norms on $\mathbb{C}^{n\times n}$ are equivalent and we therefore do not have to specify a certain norm. The proofs of Theorems 2.34, 2.35 and 2.36 can for instance be found in [10, Prop. A.3 , Prop. A.4 and Prop. A.5] or [40, Prop. 2.4.3 , Prop. 2.4.4 and Prop. 2.4.5] and are based on the so-called Schur-test [81, Chapter 6.3].

Theorem 2.34. Let $\Omega \subseteq \mathbb{R}^3$ be an open set, $n \in \mathbb{N}$ be a given integer and $t : \mathbb{R}^3 \to \mathbb{C}^{n\times n}$ be a measurable, matrix-valued function. Furthermore it is assumed that there exist constants $\kappa_1, \kappa_2 > 0$ and $R > 0$ such that

$$\|t(x)\| \leq \kappa_1 \begin{cases} \|x\|^{-2} , \text{ for } \|x\| < R \\ e^{-\kappa_2\|x\|} , \text{ for } \|x\| \geq R \end{cases}$$

is valid for all $x \in \mathbb{R}^3 \setminus \{0\}$. Then it follows that the assignment

$$(Tf)(x) = \int_\Omega t(x-y)f(y)\mathrm{d}y$$

for $f \in L^2(\Omega;\mathbb{C}^n)$ and $x \in \Omega$ corresponds to a well-defined, linear and bounded operator $T : L^2(\Omega;\mathbb{C}^n) \to L^2(\Omega;\mathbb{C}^n)$ with $\|T\| \leq \kappa_1 K$ for some constant $K > 0$ depending only on κ_2.

Theorem 2.35. Let $\Omega \subseteq \mathbb{R}^3$ be an open set with compact and C^2-smooth boundary Γ, $n \in \mathbb{N}$ be a given integer and $t : \mathbb{R}^3 \to \mathbb{C}^{n\times n}$ be a measurable, matrix-valued function. Furthermore it is assumed that there exist constants $\kappa_1, \kappa_2 > 0$ and $R > 0$ such that

$$\|t(x)\| \leq \kappa_1 \begin{cases} \|x\|^{-2} , \text{ for } \|x\| < R \\ e^{-\kappa_2\|x\|} , \text{ for } \|x\| \geq R \end{cases}$$

is valid for all $x \in \mathbb{R}^3 \setminus \{0\}$. Then it follows that the assignments

$$(T_1 f)(x) = \int_\Gamma t(x-y) f(y) \mathrm{d}\sigma(y)$$

for $f \in L^2(\Gamma; \mathbb{C}^n)$ and $x \in \Omega$ and

$$(T_2 f)(x) = \int_\Omega t(x-y) f(y) \mathrm{d}y$$

for $f \in L^2(\Omega; \mathbb{C}^n)$ and $x \in \Gamma$ correpond to well-defined, linear and bounded operators $T_1 : L^2(\Gamma; \mathbb{C}^n) \to L^2(\Omega; \mathbb{C}^n)$ and $T_2 : L^2(\Omega; \mathbb{C}^n) \to L^2(\Gamma; \mathbb{C}^n)$ with $\|T_1\|, \|T_2\| \leq \kappa_1 K$ for some constant $K > 0$ depending only on κ_2 and on the boundary Γ.

Theorem 2.36. Let $\Sigma \subseteq \mathbb{R}^3$ be a compact, closed and C^2-smooth surface, $n \in \mathbb{N}$ be a given integer and $t : \mathbb{R}^3 \to \mathbb{C}^{n \times n}$ be a measurable, matrix-valued function. Furthermore it is assumed that there exists a constant $\kappa > 0$ such that

$$\|t(x)\| \leq \kappa(1 + \|x\|^{-1})$$

is valid for all $x \in \mathbb{R}^3 \setminus \{0\}$. Then it follows that the assignment

$$(Tf)(x) = \int_\Sigma t(x-y) f(y) \mathrm{d}\sigma(y)$$

for $f \in L^2(\Sigma; \mathbb{C}^n)$ and $x \in \Sigma$ corresponds to a well-defined, linear and bounded operator $T : L^2(\Sigma; \mathbb{C}^n) \to L^2(\Sigma; \mathbb{C}^n)$ with $\|T\| \leq \kappa K$ for some constant $K > 0$ depending only on the surface Σ.

In the derivation of an explicit representation of the resolvent of the free Dirac operator in Theorem 3.4 as well as in other proofs in this thesis it will be necessary to exchange the order of integration of a double integral which arises from an integral operator and an L^2-inner product. The next lemma shows that this is possible under suitable assumptions about the matrix-valued integral kernel. The proof of item ii) is based on a decomposition of the integral kernel, as it can be found in [10, Prop. A.4].

Lemma 2.37. Let $n \in \mathbb{N}$ be a given integer, $\Omega \subseteq \mathbb{R}^3$ be an open set and $t : \mathbb{R}^3 \to \mathbb{C}^{n \times n}$ be a measurable, matrix-valued function, then the following statements are true.

i) If t satisfies the estimate of Theorem 2.34, then

$$\int_\Omega \int_\Omega t(x-y) f(y) \cdot \overline{g(x)} \mathrm{d}x \mathrm{d}y = \int_\Omega \int_\Omega t(x-y) f(y) \cdot \overline{g(x)} \mathrm{d}y \mathrm{d}x \tag{2.12}$$

is valid for all $f, g \in L^2(\Omega; \mathbb{C}^n)$.

ii) If Ω has a compact C^2-smooth boundary Γ and t satisfies the estimate of Theorem 2.35, then

$$\int_\Omega \int_\Gamma t(x-y)f(y)\cdot\overline{g(x)}\mathrm{d}\sigma(x)\mathrm{d}y = \int_\Gamma \int_\Omega t(x-y)f(y)\cdot\overline{g(x)}\mathrm{d}y\mathrm{d}\sigma(x) \tag{2.13}$$

is valid for all $f \in L^2(\Omega;\mathbb{C}^n)$ and $g \in L^2(\Gamma;\mathbb{C}^n)$.

iii) If $\Sigma \subseteq \mathbb{R}^3$ is a compact, closed and C^2-smooth surface and t satisfies the estimate of Theorem 2.36, then

$$\int_\Sigma \int_\Sigma t(x-y)f(y)\cdot\overline{g(x)}\mathrm{d}\sigma(x)\mathrm{d}\sigma(y) = \int_\Sigma \int_\Sigma t(x-y)f(y)\cdot\overline{g(x)}\mathrm{d}\sigma(y)\mathrm{d}\sigma(x) \tag{2.14}$$

is valid for all $f, g \in L^2(\Sigma;\mathbb{C}^n)$.

Proof. *Proof of i):* Due to the similarities of the proofs, we only discuss assertion i) in detail and mention the necessary modifications in the proofs of ii) and iii). We define the functions

$$\tau_1(x) = \tau_2(x) = \kappa_1 \begin{cases} \|x\|^{-2}, & \text{for } \|x\| < R \\ e^{-\kappa_2\|x\|}, & \text{for } \|x\| \geq R \end{cases}$$

for all $x \in \mathbb{R}^3 \setminus \{0\}$ and immediately obtain the estimate $\|t(x)\| \leq \sqrt{\tau_1(x)\tau_2(x)}$. As $r^2 e^{-\frac{\kappa_2 r}{2}} \to 0$ for $r \to \infty$ applies, there exists a constant $\kappa_3 > 0$ such that $r^2 e^{-\kappa_2 r} \leq \kappa_3 e^{-\frac{\kappa_2 r}{2}}$ is valid for all $r > R$. By using spherical coordinates, we obtain

$$\begin{aligned}\int_\Omega \tau_i(x)\mathrm{d}x &\leq \int_{\mathbb{R}^3} \tau_i(x)\mathrm{d}x \\ &= 4\pi\kappa_1 \left(\int_0^R \frac{r^2}{r^2}\mathrm{d}r + \int_R^\infty r^2 e^{-\kappa_2 r}\mathrm{d}r \right) \leq 4\pi \left(R + \kappa_3 \int_R^\infty e^{-\frac{\kappa_2 r}{2}}\mathrm{d}r \right) < \infty\end{aligned} \tag{2.15}$$

for $i \in \{1, 2\}$ with the angle-dependent integrals already being integrated.

Next, we assume that arbitrary functions $f, g \in L^2(\Omega;\mathbb{C}^n)$ are given. Then it follows from Theorem 2.34 and an application of the Cauchy-Schwarz inequality, that the integrals (2.12) exist. With use of (2.15) we find that the integrals

$$\int_\Omega \int_\Omega \tau_1(x-y)\|f(y)\|_2^2\mathrm{d}x\mathrm{d}y = \|f\|^2_{L^2(\Omega;\mathbb{C}^n)} \int_\Omega \tau_1(x)\mathrm{d}x < \infty \tag{2.16}$$

and

$$\int_\Omega \int_\Omega \tau_2(x-y)\|g(x)\|_2^2 \mathrm{d}y\mathrm{d}x = \|g\|^2_{L^2(\Omega;\mathbb{C}^n)} \int_\Omega \tau_2(y)\mathrm{d}y < \infty \tag{2.17}$$

are finite and therefore the order of integration in both integrals can be exchanged due to Fubini's theorem. Using (2.16) and (2.17) and a Cauchy-Schwarz inequality for double integrals as presented in [76, Page 11] results in the finiteness of the following integral

$$\begin{aligned}
&\int_\Omega \int_\Omega \left| t(x-y)f(y) \cdot \overline{g(x)} \right| \mathrm{d}x\mathrm{d}y \\
&\qquad \le \int_\Omega \int_\Omega \|t(x-y)\|_2 \|f(y)\|_2 \|g(x)\|_2 \mathrm{d}x\mathrm{d}y \\
&\qquad \le \int_\Omega \int_\Omega \sqrt{\tau_1(x-y)}\|f(y)\|_2 \sqrt{\tau_2(x-y)}\|g(x)\|_2 \mathrm{d}x\mathrm{d}y \\
&\qquad \le \left(\int_\Omega \int_\Omega \tau_1(x-y)\|f(y)\|_2^2 \mathrm{d}x\mathrm{d}y \right)^{\frac{1}{2}} \left(\int_\Omega \int_\Omega \tau_2(x-y)\|g(x)\|_2^2 \mathrm{d}x\mathrm{d}y \right)^{\frac{1}{2}} \\
&\qquad = \|f\|_{L^2(\Omega;\mathbb{C}^n)} \|g\|_{L^2(\Omega;\mathbb{C}^n)} \left(\int_\Omega \tau_1(x)\mathrm{d}x \right)^{\frac{1}{2}} \left(\int_\Omega \tau_2(y)\mathrm{d}y \right)^{\frac{1}{2}} < \infty.
\end{aligned}$$

A component-wise consideration and a separation into the real and imaginary parts of the integrands, respectively, leads with Fubini's theorem to the equality of the integrals (2.12) and thus to the first assertion of the lemma.

Proof of ii): To prove the claimed property ii) we define for an arbitrary $s \in (0,1)$ the functions

$$\tau_1(x) = \kappa_1 \kappa_3 \|x\|^{-2+s}$$

and

$$\tau_2(x) = \kappa_1 \begin{cases} \|x\|^{-2-s} & \text{, for } \|x\| < R \\ e^{-\kappa_2 \|x\|} & \text{, for } \|x\| \ge R \end{cases}$$

for all $x \in \mathbb{R}^3 \setminus \{0\}$, where the constant $\kappa_3 > 0$ is chosen so that $e^{-\kappa_2\|x\|} \le \kappa_3 \|x\|^{-2+s}$ is valid for all $\|x\| \ge R$. For the choice of κ_3, compare the procedure in the proof of i). By applying [10, Lem. A.2 ii)] we obtain

$$\int_\Gamma \tau_1(x)\mathrm{d}\sigma(x) < \infty$$

while

$$\int_{\Omega} \tau_2(y)\mathrm{d}y < \infty$$

follows with a consideration as in the proof of estimate (2.15). Based on the estimate $\|t(x)\| \leq \sqrt{\tau_1(x)\tau_2(x)}$, we now obtain the assertion about the integral (2.13) with a line of reasoning analogous to the proof of i). In fact, only the integration with respect to the Lebesgue measure $\mathrm{d}x$ has to be replaced by an integration with respect to the Hausdorff measure $\mathrm{d}\sigma(x)$.

Proof of iii): To complete the proof it remains to show item iii). For this purpose we define the functions

$$\tau_1(x) = \tau_2(x) = \kappa(1 + \|x\|^{-1})$$

for all $x \in \mathbb{R}^3 \setminus \{0\}$ and immediately obtain the estimate $\|t(x)\| \leq \sqrt{\tau_1(x)\tau_2(x)}$. Furthermore, from [10, Lem. A.2 ii)] it follows that

$$\int_{\Sigma} \tau_i(x)\mathrm{d}\sigma(x) < \infty$$

is valid for $i \in \{1, 2\}$. With a line of reasoning as in the proof of i), the asserted statement about the integral (2.14) follows. □

Next, we present a result concerning the boundedness of a singular integral operator whose proof can be found in [6, Lem. 3.3] and the references mentioned therein.

Theorem 2.38. Let $\Sigma \subseteq \mathbb{R}^3$ be a compact, closed and C^2-smooth surface and $i \in \{1, 2, 3\}$, then it follows that the assignment

$$(T_i f)(x) = \lim_{\varepsilon \to 0^+} \int_{\Sigma \setminus B(x,\varepsilon)} \frac{x_i - y_i}{\|x - y\|^3} f(y)\mathrm{d}\sigma(y)$$

for $f \in L^2(\Sigma; \mathbb{C})$ and $x \in \Sigma$ corresponds to a well-defined, linear and bounded operator $T_i : L^2(\Sigma; \mathbb{C}) \to L^2(\Sigma; \mathbb{C})$.

We conclude our considerations concerning integral operators with two operators induced by the integral kernel of the resolvent of the free Schrödinger operator. To introduce these operators we assume in the following that a bounded Lipschitz domain $\Omega \subseteq \mathbb{R}^3$ with boundary $\Sigma = \partial\Omega$ is given. We then define the sets $\Omega_+ = \Omega$ and $\Omega_- = \mathbb{R}^3 \setminus \overline{\Omega}$ and thereby obtain two Lipschitz domains which satisfy $\mathbb{R}^3 = \Omega_+ \dot{\cup} \Sigma \dot{\cup} \Omega_-$.
The free Schrödinger operator in $L^2(\mathbb{R}^3; \mathbb{C})$ is defined by the assignment

$$\begin{aligned} \mathrm{dom}(T_0) &= H^2(\mathbb{R}^3; \mathbb{C}) \\ T_0 f &= -\frac{1}{2m}\Delta f \end{aligned} \tag{2.18}$$

and as it is shown in [81, Chapter 11], this is a self-adjoint operator in $L^2(\mathbb{R}^3;\mathbb{C})$ with spectrum $\sigma(T_0) = [0,\infty)$. Furthermore, for all $\lambda \in \rho(T_0)$ the explicit resolvent representation

$$\left((T_0-\lambda)^{-1}f\right)(x) = \int\limits_{\mathbb{R}^3} K_\lambda(x-y)f(y)\mathrm{d}y \tag{2.19}$$

for all $f \in L^2(\mathbb{R}^3;\mathbb{C})$ and for almost all $x \in \mathbb{R}^3$ applies. The integral kernel of the resolvent corresponds to the function

$$K_\lambda(x) = \frac{2m}{4\pi\|x\|}\exp\left(i\sqrt{2m\lambda}\|x\|\right) \tag{2.20}$$

for all $x \in \mathbb{R}^3 \setminus \{0\}$. At this point it is necessary to note that in the following the square root $\sqrt{\mu}$ of a complex number $\mu \in \mathbb{C}$ is always chosen such that $\mathrm{Im}\{\sqrt{\mu}\} \geq 0$ applies. In particular, $\mathrm{Im}\{\sqrt{\mu}\} > 0$ is valid for all $\mu \in \mathbb{C} \setminus [0,\infty)$.

Next, we introduce for $\lambda \in \rho(T_0)$ the so-called single layer potential and the single layer boundary integral operator as they are discussed for instance in [42] and [53]. The single layer potential is defined as the composition of the fundamental solution of the operator $T_0 - \lambda$ and the adjoint trace operator and corresponds to a linear and bounded operator $\mathrm{SL}(\lambda) : H^{-\frac{1}{2}}(\Sigma;\mathbb{C}) \to H^1(\mathbb{R}^3;\mathbb{C})$. Furthermore, we define the single layer boundary integral operator as the trace of the single layer potential and thereby obtain a linear and bounded operator $S(\lambda) : H^{-\frac{1}{2}}(\Sigma;\mathbb{C}) \to H^{\frac{1}{2}}(\Sigma;\mathbb{C})$.

As it is stated in [42], the explicit integral representation

$$\left(\mathrm{SL}(\lambda)f\right)(x) = \int\limits_{\Sigma} K_\lambda(x-y)f(y)\mathrm{d}\sigma(y) \tag{2.21}$$

for all $f \in L^2(\Sigma;\mathbb{C}^4)$ and for almost all $x \in \mathbb{R}^3$ applies to the restriction of the single layer potential $\mathrm{SL}(\lambda) \restriction L^2(\Sigma;\mathbb{C})$. Furthermore, (2.21) in combination with the mapping properties of the single layer potential and Lemma 2.33, results in the representation

$$\left(S(\lambda)f\right)(x) = \int\limits_{\Sigma} K_\lambda(x-y)f(y)\mathrm{d}\sigma(y) \tag{2.22}$$

for all $f \in L^2(\Sigma;\mathbb{C}^4)$ and almost all $x \in \Sigma$ for the restriction of the single layer boundary integral operator $S(\lambda) \restriction L^2(\Sigma;\mathbb{C})$.

The following properties of the single layer potential will be used in Chapter 4.1. The proofs of these statements can be found for instance in [42, Lem. 3.3].

Lemma 2.39. Let $\lambda \in \rho(T_0)$ be given, then the following statements are true for the single layer potential.

i) The jump condition

$$\tau_+\left(\mathrm{SL}(\lambda)f\right)_+ - \tau_-\left(\mathrm{SL}(\lambda)f\right)_- = 0$$

on the surface Σ is valid for all $f \in H^{-\frac{1}{2}}(\Sigma;\mathbb{C})$.

ii) The range condition

$$\operatorname{ran}(\mathrm{SL}(\lambda)) = \left\{ f \in H^1(\mathbb{R}^3;\mathbb{C}) \;\middle|\; \left(-\frac{1}{2m}\Delta - \lambda\right) f_\pm = 0 \right\}$$

applies. In particular, for a given $f \in H^{-\frac{1}{2}}(\Sigma;\mathbb{C})$

$$\Delta\,(\mathrm{SL}(\lambda)f)_\pm = -2m\lambda\,(\mathrm{SL}(\lambda)f)_\pm \in L^2(\Omega_\pm;\mathbb{C})$$

is valid in the sense of distributions.

We conclude this section by considering operators defined on the Cartesian product of two L^2-spaces. In Chapter 3.1, we will require these results when introducing a maximal Dirac operator for functions which do not posses the Sobolev regularity H^1 on the whole of $\mathbb{R}^3$, but only on restrictions of it.

As in the introduction of the single layer potential and the single layer boundary integral operator we assume in the following that $\Omega \subseteq \mathbb{R}^3$ be a bounded Lipschitz domain according to Definition 2.26 with boundary $\Sigma = \partial\Omega$. We define $\Omega_+ = \Omega$ and $\Omega_- = \mathbb{R}^3 \setminus \overline{\Omega}$ and thereby obtain two Lipschitz domains which satisfy $\mathbb{R}^3 = \Omega_+ \dot{\cup} \Sigma \dot{\cup} \Omega_-$. On these two sets we define the spaces $L^2(\Omega_\pm;\mathbb{C}^4)$ and form their Cartesian product $L^2(\Omega_+;\mathbb{C}^4) \times L^2(\Omega_-;\mathbb{C}^4)$. We equip this space with the inner product

$$((f_+, f_-), (g_+, g_-))_{L^2(\Omega_+;\mathbb{C}^4)\times L^2(\Omega_-;\mathbb{C}^4)} = (f_+, g_+)_{L^2(\Omega_+;\mathbb{C}^4)} + (f_-, g_-)_{L^2(\Omega_-;\mathbb{C}^4)} \tag{2.23}$$

for $f_\pm, g_\pm \in L^2(\Omega_\pm;\mathbb{C}^4)$ and thereby turning $L^2(\Omega_+;\mathbb{C}^4) \times L^2(\Omega_-;\mathbb{C}^4)$ into a Hilbert space. Next, we define

$$\iota(f) = (f \restriction \Omega_+, f \restriction \Omega_-)$$

for $f \in L^2(\mathbb{R}^3;\mathbb{C}^4)$ and obtain a linear map $\iota : L^2(\mathbb{R}^3;\mathbb{C}^4) \to L^2(\Omega_+;\mathbb{C}^4) \times L^2(\Omega_-;\mathbb{C}^4)$. Using the inner product (2.23) it is easy to see that ι corresponds to an isometric isomorphism, which will allow us to identify the space $L^2(\mathbb{R}^3;\mathbb{C}^4)$ with the space $L^2(\Omega_+;\mathbb{C}^4) \times L^2(\Omega_-;\mathbb{C}^4)$. At this point it should be noted that the inverse mapping $\iota^{-1} : L^2(\Omega_+;\mathbb{C}^4) \times L^2(\Omega_-;\mathbb{C}^4) \to L^2(\mathbb{R}^3;\mathbb{C}^4)$ can be defined, for instance, by the zero continuation on the Lebesgue zero set Σ by

$$(\iota^{-1} f)(x) = \begin{cases} f_\pm(x)\ , \text{ for } x \in \Omega_\pm \\ 0\ , \text{ for } x \in \Sigma \end{cases}$$

for all $(f_+, f_-) \in L^2(\Omega_+;\mathbb{C}^4) \times L^2(\Omega_-;\mathbb{C}^4)$ and for almost all $x \in \mathbb{R}^3$. The values on Σ are insignificant in the sense of L^2-functions and can be adjusted in accordance with practical needs. However, this choice is advantageous for the treatment of test functions. Due to the isomorphisms

$$L^2(\Omega_+;\mathbb{C}^4) \cong L^2(\Omega_+;\mathbb{C}^4) \times \{0\} \quad \text{and} \quad L^2(\Omega_-;\mathbb{C}^4) \cong \{0\} \times L^2(\Omega_-;\mathbb{C}^4)$$

and since these subspaces are orthogonal with respect to the inner product (2.23), we will from now on write $L^2(\Omega_+;\mathbb{C}^4) \oplus L^2(\Omega_-;\mathbb{C}^4)$ for the Cartesian product $L^2(\Omega_+;\mathbb{C}^4) \times L^2(\Omega_-;\mathbb{C}^4)$ in analogy to the orthogonal sum of Hilbert spaces. Elements $(f_+, f_-) \in L^2(\Omega_+;\mathbb{C}^4) \oplus L^2(\Omega_-;\mathbb{C}^4)$ are usually denoted by $f_+ \oplus f_-$.

In analogy to the L^2-space, we define the Sobolev space $H^1(\Omega_+;\mathbb{C}^4) \oplus H^1(\Omega_-;\mathbb{C}^4)$ and equip it with an inner product similar to (2.23). Again, we obtain a Hilbert space, which in contrast to the L^2-space is not isomorphic to $H^1(\mathbb{R}^3;\mathbb{C}^4)$ but isomprophic to $H^1(\mathbb{R}^3 \setminus \Sigma;\mathbb{C}^4)$. This follows from Theorem 2.32 since a function $f \in H^1(\mathbb{R}^3 \setminus \Sigma;\mathbb{C}^4)$ is only in $H^1(\mathbb{R}^3;\mathbb{C}^4)$ if $\tau_+ f_+ = \tau_- f_-$ is valid on Σ.

For a linear operator T in $L^2(\Omega_+;\mathbb{C}^4) \oplus L^2(\Omega_-;\mathbb{C}^4)$ we obtain a linear operator in $L^2(\mathbb{R}^3;\mathbb{C}^4)$ with $\mathrm{dom}(\iota^{-1}T\iota) = \iota^{-1}(\mathrm{dom}(T))$ by considering $\iota^{-1}T\iota$. It can now be shown that all properties like dense definition, closability, symmetry, etc. are carried over from T to $\iota^{-1}T\iota$. The converse of this statement is true as well and therefore in the following chapters we will often switch back and forth between these two representations without mentioning it explicitly. In particular, to simplify the notation, we will identify the operators T and $\iota^{-1}T\iota$ with each other and use the symbol T for both the operator in $L^2(\Omega_+;\mathbb{C}^4) \oplus L^2(\Omega_-;\mathbb{C}^4)$ and the operator in $L^2(\mathbb{R}^3;\mathbb{C}^4)$. The same applies to elements in the domain of these operators.

3 Dirac operators with electrostatic and Lorentz scalar δ-shell interactions

In this chapter we begin our investigation of Dirac operators. In Section 3.1 we will collect basic properties of the free Dirac operator in $\mathbb{R}^3$ and define operators which we will use in the construction of a quasi boundary triple in Section 3.2. By means of this quasi boundary triple we are able to define Dirac operators with δ-shell interactions in a mathematically rigorous way by imposing certain jump conditions on the common interface Σ of two C^2-domains. Subsequently, the self-adjointness of these operators is shown in the case of non-critical interaction strengths.

3.1 The maximal and free Dirac operator

In this section we will examine the free Dirac operator in $\mathbb{R}^3$ and provide an explicit representation of its resolvent, which will be of great importance in the following sections. Furthermore we define a maximal Dirac operator, which will be needed for the construction of a quasi boundary triple in Section 3.2.

Starting point of this section is the formal differential expression

$$\mathcal{A} = -ic\hbar(\alpha \cdot \nabla) + mc^2\beta \tag{3.1}$$

from Chapter 1 which describes a relativistic quantum particle with spin $1/2$ without the influence of external fields. Here

$$\alpha_k = \begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{pmatrix} \quad \text{and} \quad \beta = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}$$

are the Dirac matrices, which consist of the Pauli spin matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad , \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \text{and} \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

As already mentioned in Chapter 1, these matrices fulfill the anti-commutation relations

- $\alpha_k \alpha_j + \alpha_j \alpha_k = 2\delta_{kj} I_4$
- $\alpha_k \beta + \beta \alpha_k = 0$
- $\beta^2 = I$

for all $k, j \in \{1, 2, 3\}$. Furthermore we use the abbreviation

$$\alpha \cdot x = \sum_{k=1}^{3} \alpha_k x_k$$

for a vector $x \in \mathbb{R}^3$ to simplify the notation. From the above anti-commutation relations it follows by double summation that

$$(\alpha \cdot x)^2 = \sum_{k,j=1}^{3} x_k x_j \alpha_k \alpha_j = \frac{1}{2} \sum_{k,j=1}^{3} x_k x_j (\alpha_k \alpha_j + \alpha_j \alpha_k) = \sum_{k,j=1}^{3} x_k x_j \delta_{kj} = \|x\|^2 \tag{3.2}$$

holds true for all $x \in \mathbb{R}^3$.

The formal differential expression $\mathcal{A}$ of (3.1) will lead us to the maximal and the free Dirac operator on $\mathbb{R}^3$ by choosing suitable domains of definition. In particular, we will obtain the free Dirac operator by closing a Dirac operator defined on the test functions. Furthermore, the maximal operator will turn out to be important when constructing a quasi boundary triple in the next section and the free Dirac operator will serve as the self-adjoint reference operator.

In this section we will follow the presentation of the books [78, 82] for characterizing the free Dirac operator and [14, 40] for the preparation of the construction of the quasi boundary triple in Section 3.2. Although the proofs of the statements of this section can be found in these references, we present some of them in order to provide a self-contained presentation.

We begin our discussion with a realization of the formal differential expression (3.1) and define this operator on the set of the most easily handleable functions, the test functions

$$\begin{aligned} \operatorname{dom}(T_{\mathcal{D}}) &= \mathcal{D}(\mathbb{R}^3; \mathbb{C}^4) = \mathcal{D}(\mathbb{R}^3; \mathbb{C})^4 \\ T_{\mathcal{D}} f &= \mathcal{A} f = (-ic\hbar(\alpha \cdot \nabla) + mc^2 \beta) f. \end{aligned}$$

This linear operator is densely defined since $\mathcal{D}(\mathbb{R}^3; \mathbb{C}^4)$ is dense in $L^2(\mathbb{R}^3; \mathbb{C}^4)$. Furthermore, by using the divergence theorem, it can be easily shown that $T_{\mathcal{D}}$ is symmetric and thus closable.

The next theorem provides a characterization of the closure of the operator $T_{\mathcal{D}}$ and thereby leads to the definition of the free Dirac operator. Furthermore, it shows the self-adjointness of the free Dirac operator and that its spectrum consists exclusively of the essential spectrum. In particular, there are no isolated eigenvalues with a finite-dimensional eigenspace. The proof of this theorem can be found in [82, Theorem 20.1] and relies heavily on the properties of Schwartz functions to reduce the investigation of the free Dirac operator to that of a unitary equivalent multiplication operator in $L^2(\mathbb{R}^3;\mathbb{C}^4)$.

Theorem 3.1. The operator $T_{\mathcal{D}}$ is closable and essentially self-adjoint in $L^2(\mathbb{R}^3;\mathbb{C}^4)$. The free Dirac operator is defined as the self-adjoint operator $A_0 = \overline{T_{\mathcal{D}}}$ and for this operator the following statements are true.

i) For the free Dirac operator the explicit representation

$$\begin{aligned} \operatorname{dom}(A_0) &= H^1(\mathbb{R}^3;\mathbb{C}^4) \\ A_0 f &= (-ic\hbar(\alpha\cdot\nabla) + mc^2\beta)f \end{aligned} \tag{3.3}$$

applies.

ii) There exist constants $C_1, C_2 > 0$ such that

$$C_1\|f\|_{H^1(\mathbb{R}^3;\mathbb{C}^4)} \leq \|A_0 f\|_{L^2(\mathbb{R}^3;\mathbb{C}^4)} \leq C_2\|f\|_{H^1(\mathbb{R}^3;\mathbb{C}^4)}$$

holds true for all $f \in \operatorname{dom}(A_0)$. In particular, the graph norm of A_0 is equivalent to the H^1-norm.

iii) $\sigma(A_0) = (-\infty, -mc^2] \cup [mc^2, \infty)$.

A first observation of Theorem 3.1 is that the Planck's constant $\hbar$ does not influence the spectral properties of the free Dirac operator A_0 and we can therefore set it to $\hbar = 1$ without loss of generality. Furthermore, an important consequence about the square of the free Dirac operator can be deduced from Theorem 3.1, which will be important in the following considerations when deriving an explicit representation of the resolvent for the free Dirac operator. It turns out that A_0^2 corresponds to a shifted, free Laplace operator in $L^2(\mathbb{R}^3;\mathbb{C}^4)$. The proof of this result can be found in [82, Cor. 20.2].

Corollary 3.2. Let A_0 be the free Dirac operator defined as in (3.3), then the following characterization of the square of this operator is valid.

$$\begin{aligned} \operatorname{dom}(A_0^2) &= H^2(\mathbb{R}^3;\mathbb{C}^4) \\ A_0^2 f &= (-c^2\Delta + m^2c^4)I_4 f \end{aligned}$$

Here, the operator on the right side has to be understood in such a way that the operator $-c^2\Delta + m^2c^4$ acts on every component of f.

Next, we show that a certain matrix-valued function which appears in the derivation of the integral kernel of the resolvent of the free Dirac operator satisfies the requirements of Lemma 2.34. At this point it is necessary to note that in the following the square root $\sqrt{\mu}$ of a complex number $\mu \in \mathbb{C}$ is always chosen such that $\operatorname{Im}\{\sqrt{\mu}\} \geq 0$ applies. In particular, $\operatorname{Im}\{\sqrt{\mu}\} > 0$ is valid for all $\mu \in \mathbb{C} \setminus [0,\infty)$.

Lemma 3.3. Let $\lambda \in \rho(A_0)$ and $j \in \{1,2,3\}$ be given and $t_j : \mathbb{R}^3 \setminus \{0\} \to \mathbb{C}^{4\times 4}$ be the matrix-valued function defined by

$$
\begin{aligned}
t_j(x) &= \frac{\partial}{\partial x_j}\left(\frac{1}{4\pi\|x\|}\exp\left(i\sqrt{\frac{\lambda^2}{c^2}-m^2c^2}\|x\|\right)\right) I_4 \\
&= \left(i\sqrt{\frac{\lambda^2}{c^2}-m^2c^2}\|x\|-1\right)\frac{1}{4\pi\|x\|^3}\exp\left(i\sqrt{\frac{\lambda^2}{c^2}-m^2c^2}\|x\|\right) x_j I_4
\end{aligned}
$$

for all $x \in \mathbb{R}^3 \setminus \{0\}$. Then there exist constants $\kappa_1, \kappa_2 > 0$ independent of $x \in \mathbb{R}^3 \setminus \{0\}$ such that

$$
\|t_j(x)\| \leq \kappa_1 \begin{cases} \|x\|^{-2} & , \text{ for } \|x\| < 1 \\ e^{-\kappa_2\|x\|} & , \text{ for } \|x\| \geq 1 \end{cases}
$$

holds true for all $x \in \mathbb{R}^3 \setminus \{0\}$.

Proof. We set

$$
\kappa_2 = \operatorname{Im}\left\{\sqrt{\frac{\lambda^2}{c^2}-m^2c^2}\right\}
$$

and due to the chosen square root $\kappa_2 > 0$ is valid for all $\lambda \in \rho(A_0)$. Since all matrix norms are equivalent, we choose the Frobenius norm for convenience and obtain

$$
\begin{aligned}
\|t_j(x)\|_F &= \frac{2\sqrt{\left|\frac{\lambda^2}{c^2}-m^2c^2\right| \|x\|^2+1}}{4\pi\|x\|^3} e^{-\kappa_2\|x\|}\,|x_j| \\
&\leq \frac{2\sqrt{\left|\frac{\lambda^2}{c^2}-m^2c^2\right| \|x\|^2+1}}{4\pi\|x\|^2} e^{-\kappa_2\|x\|}
\end{aligned} \tag{3.4}
$$

for all $x \in \mathbb{R}^3 \setminus \{0\}$ by direct calculation. If $\|x\| < 1$ holds true, then it follows from (3.4) that

$$
\begin{aligned}
\|t_j(x)\|_F &\leq \frac{2\sqrt{\left|\frac{\lambda^2}{c^2}-m^2c^2\right|+1}}{4\pi\|x\|^2} e^{-\kappa_2\|x\|} \\
&\leq \frac{2\sqrt{\left|\frac{\lambda^2}{c^2}-m^2c^2\right|+1}}{4\pi\|x\|^2}
\end{aligned}
$$

is valid, while for $\|x\| \geq 1$ it follows from (3.4) that the estimation

$$
\begin{aligned}
\|t_j(x)\|_F &\leq \frac{2\sqrt{\left|\frac{\lambda^2}{c^2}-m^2c^2\right|+1}\|x\|}{4\pi\|x\|^2} e^{-\kappa_2\|x\|^2} \\
&\leq \frac{2\sqrt{\left|\frac{\lambda^2}{c^2}-m^2c^2\right|+1}}{4\pi} e^{-\kappa_2\|x\|}
\end{aligned}
$$

applies. Defining

$$\kappa_1 = \frac{2\sqrt{\left|\frac{\lambda^2}{c^2} - m^2c^2\right| + 1}}{4\pi}$$

immediately leads to the validity of the assertion. □

Next, we will discuss the explicit resolvent representation of the free Dirac operator. Although the proof of the next result can be found in [40, Prop. 3.1.1], we will present it here as we will apply a similar line of reasoning again in Section 4.2. The representation of the integral kernel of the resolvent will turn out to be particularly important for the further considerations in this thesis.

Theorem 3.4. Let A_0 be the free Dirac operator defined as in (3.3) and let $\lambda \in \rho(A_0)$ be a given complex number. Then the explicit resolvent representation

$$(A_0 - \lambda)^{-1} f(x) = \int_{\mathbb{R}^3} G_\lambda(x-y) f(y) \mathrm{d}y$$

is valid for all $f \in L^2(\mathbb{R}^3; \mathbb{C}^4)$ and for almost all $x \in \mathbb{R}^3$. The integral kernel G_λ is the matrix-valued function

$$G_\lambda(x) = \left(\frac{\lambda}{c^2} I_4 + m\beta + \left(1 - i\sqrt{\frac{\lambda^2}{c^2} - m^2c^2}\|x\| \right) \frac{i}{c\|x\|^2} (\alpha \cdot x) \right) \frac{1}{4\pi\|x\|} \exp\left(i\sqrt{\frac{\lambda^2}{c^2} - m^2c^2}\|x\| \right) \tag{3.5}$$

for all $x \in \mathbb{R}^3 \setminus \{0\}$.

Proof. *Step 1:* Let $\lambda \in \rho(A_0)$ be given. Then according to Corollary 3.2

$$(A_0 - \lambda)(A_0 + \lambda) = A_0^2 - \lambda^2 = \left(-c^2\Delta + m^2c^4 - \lambda^2\right) I_4 = c^2 \left(-\Delta - \left(\frac{\lambda^2}{c^2} - m^2c^2 \right) \right) I_4 \tag{3.6}$$

is valid on $\mathrm{dom}(A_0^2) = H^2(\mathbb{R}^3; \mathbb{C}^4)$. Here, the operator on the right side has to be understood in such a way that the operator $-c^2\Delta + m^2c^4 - \lambda^2$ acts on every component of a function $f \in H^2(\mathbb{R}^3; \mathbb{C}^4)$.

Due to the choice of λ it follows with [81, Satz 11.25] that

$$\frac{\lambda^2}{c^2} - m^2c^2 \notin [0, \infty) = \sigma(-\Delta)$$

is valid and therefore the resolvent

$$\left(-\Delta - \left(\frac{\lambda^2}{c^2} - m^2c^2 \right) \right)^{-1} : L^2(\mathbb{R}^3; \mathbb{C}) \to H^2(\mathbb{R}^3; \mathbb{C})$$

exists as linear and bounded operator in $L^2(\mathbb{R}^3;\mathbb{C})$. By defining the diagonal operator

$$\frac{1}{c^2}\left(-\Delta-\left(\frac{\lambda^2}{c^2}-m^2c^2\right)\right)^{-1} I_4 : L^2(\mathbb{R}^3;\mathbb{C}^4)\to H^2(\mathbb{R}^3;\mathbb{C}^4)$$

we obtain from the representation (3.6) the inverse operator as

$$\left(\left(-c^2\Delta+m^2c^4-\lambda^2\right)I_4\right)^{-1}=\frac{1}{c^2}\left(-\Delta-\left(\frac{\lambda^2}{c^2}-m^2c^2\right)\right)^{-1} I_4$$

by component-wise consideration. Due to the mapping properties of this operator we can apply the operator $A_0+\lambda$ to it and it follows from (3.6) that

$$(A_0-\lambda)^{-1}f=(A_0+\lambda)\frac{1}{c^2}\left(-\Delta-\left(\frac{\lambda^2}{c^2}-m^2c^2\right)\right)^{-1} I_4 f \tag{3.7}$$

is valid for all $f\in L^2(\mathbb{R}^3;\mathbb{C}^4)$. Our next goal is to determine the expression on the right side to obtain an explicit representation of the resolvent of $A_0-\lambda$.

Step 2: A component-wise application of [81, Satz 11.26] leads to the explicit representation of the resolvent

$$\frac{1}{c^2}\left(-\Delta-\left(\frac{\lambda^2}{c^2}-m^2c^2\right)\right)^{-1} I_4 f(x)= \\ \frac{1}{c^2}\int_{\mathbb{R}^3}\frac{1}{4\pi\|x-y\|}\exp\left(i\sqrt{\frac{\lambda^2}{c^2}-m^2c^2}\|x-y\|\right)f(y)\mathrm{d}y$$

for all $f\in L^2(\mathbb{R}^3;\mathbb{C}^4)$ and for almost all $x\in\mathbb{R}^3$. Here the square root has to be chosen again so that the imaginary part is greater than zero.

If we define the matrix-valued function

$$\tau(x)=\frac{1}{4\pi\|x\|}\exp\left(i\sqrt{\frac{\lambda^2}{c^2}-m^2c^2}\|x\|\right)I_4$$

for all $x\in\mathbb{R}^3\setminus\{0\}$ and the constants

$$k_1=\frac{1}{4\pi}\qquad\text{and}\qquad k_2=\operatorname{Im}\left\{\sqrt{\frac{\lambda^2}{c^2}-m^2c^2}\right\}$$

it follows immediately that

$$\|\tau(x)\|\le k_1\begin{cases}\|x\|^{-1}, & \text{for } \|x\|<1\\ e^{-k_2\|x\|}, & \text{for } \|x\|\ge 1\end{cases}$$

is valid for all $x \in \mathbb{R}^3 \setminus \{0\}$. If $\|x\| < 1$ applies, then obviously $\|x\|^{-1} < \|x\|^{-2}$ follows and therefore we conclude from Theorem 2.34 that the integral operator induced by τ is well-defined and bounded in $L^2(\mathbb{R}^3; \mathbb{C}^4)$. Furthermore an application of Lemma 2.37 shows the interchangeability of the order of integration

$$\int\limits_{\mathbb{R}^3} \int\limits_{\mathbb{R}^3} \tau(x-y) f(y) \cdot \overline{g(x)} \mathrm{d}x \mathrm{d}y = \int\limits_{\mathbb{R}^3} \int\limits_{\mathbb{R}^3} \tau(x-y) f(y) \cdot \overline{g(x)} \mathrm{d}y \mathrm{d}x$$

for all $f, g \in L^2(\mathbb{R}^3; \mathbb{C}^4)$.

Step 3: Let $j \in \{1, 2, 3\}$ be an arbitrary index, then we define a matrix-valued function by

$$\begin{aligned} t_j(x) &= \frac{\partial}{\partial x_j} \left(\frac{1}{4\pi \|x\|} \exp\left(i \sqrt{\frac{\lambda^2}{c^2} - m^2 c^2} \|x\| \right) \right) I_4 \\ &= \left(i \sqrt{\frac{\lambda^2}{c^2} - m^2 c^2} \|x\| - 1 \right) \frac{1}{4\pi \|x\|^3} \exp\left(i \sqrt{\frac{\lambda^2}{c^2} - m^2 c^2} \|x\| \right) x_j I_4 \end{aligned}$$

for all $x \in \mathbb{R}^3 \setminus \{0\}$. Due to Lemma 3.3 and Theorem 2.34 it follows that the assignment

$$(T_j f)(x) = \int\limits_{\mathbb{R}^3} t_j(x-y) f(y) \mathrm{d}y$$

for $f \in L^2(\mathbb{R}^3; \mathbb{C}^4)$ and for $x \in \mathbb{R}^3$ corresponds to a well-defined, linear and bounded operator $T_j : L^2(\mathbb{R}^3; \mathbb{C}^4) \to L^2(\mathbb{R}^3; \mathbb{C}^4)$. Furthermore, Lemma 2.37 yields the interchangeability of the order of integration

$$\int\limits_{\mathbb{R}^3} \int\limits_{\mathbb{R}^3} t_j(x-y) f(y) \cdot \overline{g(x)} \mathrm{d}x \mathrm{d}y = \int\limits_{\mathbb{R}^3} \int\limits_{\mathbb{R}^3} t_j(x-y) f(y) \cdot \overline{g(x)} \mathrm{d}y \mathrm{d}x$$

for all $f, g \in L^2(\mathbb{R}^3; \mathbb{C}^4)$.

Next, we will investigate the relationship between t_j and τ from Step 2. For this purpose we define the function

$$d(x) = \frac{1}{4\pi \|x\|} \exp\left(i \sqrt{\frac{\lambda^2}{c^2} - m^2 c^2} \|x\| \right)$$

for all $x \in \mathbb{R}^3 \setminus \{0\}$ and assume that some arbitrary test function $\Psi \in \mathcal{D}(\mathbb{R}^3; \mathbb{C})$ is given. In the following it will be necessary to transfer a partial derivative $\partial_j d$ to the test function Ψ when performing an integral calculation. It is therefore reasonable to apply the divergence theorem, but since d is not continuously differentiable due to the singularity in $x = 0$, it cannot be applied directly. A solution to this difficulty can be provided by a strategy as in [29, Thm. 1 - Page 23].

We choose an arbitrary $r > 0$ such that $\operatorname{supp}(\Psi) \subseteq B(0,r)$ is valid and also an $0 < \varepsilon < \min\{1, r\}$. With these we define the set $\Omega_\varepsilon = B(0,r)\backslash B(0,\varepsilon)$ and observe that both functions are arbitrarily often differentiable on Ω_ε. A now possible application of the divergence theorem yields

$$\begin{aligned}\int\limits_{\mathbb{R}^3} &\partial_j d(x)\Psi(x)\mathrm{d}x \\ &= -\int\limits_{\Omega_\varepsilon} d(x)\partial_j\Psi(x)\mathrm{d}x + \int\limits_{\partial B(0,\varepsilon)} d(x)\partial_j\Psi(x)\mathrm{d}\sigma(x) + \int\limits_{B(0,\varepsilon)} \partial_j d(x)\Psi(x)\mathrm{d}x \end{aligned} \tag{3.8}$$

due to the choice of $r > 0$. By direct calculation using spherical coordinates one easily shows that the second integral on the right side can be estimated by $4\pi k_1\|\partial_j\Psi\|_{L^\infty(\mathbb{R}^3;\mathbb{C})}\varepsilon$ due to the estimate of τ from Step 2, while the third integral can be estimated by $4\pi\kappa_1\|\Psi\|_{L^\infty(\mathbb{R}^3;\mathbb{C})}\varepsilon$ due to the estimate of Lemma 3.3. Thus the last two integrals on the right side of (3.8) converge to zero for $\varepsilon \to 0$. Furthermore, according to the estimates of Step 2, we have that $f\partial_j\Psi$ is integrable on $\mathbb{R}^3$ and consequently from (3.8) and an application of the dominated convergence theorem

$$\int\limits_{\mathbb{R}^3} \partial_j d(x)\Psi(x)\mathrm{d}x = -\lim_{\varepsilon\to 0}\int\limits_{\Omega_\varepsilon} d(x)\partial_j\Psi(x)\mathrm{d}x = -\int\limits_{\mathbb{R}^3} d(x)\partial_j\Psi(x)\mathrm{d}x$$

follows. Applying this reasoning component-wise leads to the integration by parts formula

$$\int\limits_{\mathbb{R}^3} t_j(x-y)\Psi(x)\mathrm{d}x = -\int\limits_{\mathbb{R}^3} \tau(x-y)\partial_j\Psi(x)\mathrm{d}x$$

for all test functions $\Psi \in \mathcal{D}(\mathbb{R}^3;\mathbb{C}^4)$ and for all $y \in \mathbb{R}^3$.

Step 4: Let $f \in L^2(\mathbb{R}^3;\mathbb{C}^4)$ and $\Psi \in \mathcal{D}(\mathbb{R}^3;\mathbb{C}^4)$ be given, then it follows from the mapping properties of the resolvent of the Laplace operator that

$$\frac{1}{c^2}\left(-\Delta - \left(\frac{\lambda^2}{c^2} - m^2c^2\right)\right)^{-1} I_4 f \in H^2(\mathbb{R}^3;\mathbb{C}^4)$$

applies and thus the weak derivatives of this expression exist. Applying the results from Steps 2 and 3 regarding the interchangeability of the order of integration and the integration by parts formula, we obtain

$$\begin{aligned}
(T_j f, \Psi)_{L^2(\mathbb{R}^3;\mathbb{C}^4)} &= \int\limits_{\mathbb{R}^3}\int\limits_{\mathbb{R}^3} t_j(x-y)f(y)\cdot\overline{\Psi(x)}\mathrm{d}y\mathrm{d}x \\
&= \int\limits_{\mathbb{R}^3} f(y)\cdot\int\limits_{\mathbb{R}^3} t_j(x-y)\overline{\Psi(x)}\mathrm{d}x\mathrm{d}y \\
&= -\int\limits_{\mathbb{R}^3} f(y)\cdot\int\limits_{\mathbb{R}^3} \tau(x-y)\partial_j\overline{\Psi(x)}\mathrm{d}x\mathrm{d}y \\
&= -\int\limits_{\mathbb{R}^3}\int\limits_{\mathbb{R}^3} \tau(x-y)f(y)\cdot\partial_j\overline{\Psi(x)}\mathrm{d}y\mathrm{d}x \\
&= -\left(\left(-\Delta-\left(\frac{\lambda^2}{c^2}-m^2c^2\right)\right)^{-1} I_4 f, \partial_j\Psi\right)_{L^2(\mathbb{R}^3;\mathbb{C}^4)}
\end{aligned}$$

by direct calculation. Since this is valid for all test functions the explicit representation

$$\frac{\partial}{\partial x_j}\left(-\Delta-\left(\frac{\lambda^2}{c^2}-m^2c^2\right)\right)^{-1} I_4 f = T_j f$$

for the weak derivative follows for all $f \in L^2(\mathbb{R}^3;\mathbb{C}^4)$.

Step 5: Let $f \in L^2(\mathbb{R}^3;\mathbb{C}^4)$ be a given function and G_λ be the matrix-valued function defined above. With the result of Step 4 we obtain for the resolvent (3.7) the explicit representation

$$\begin{aligned}
(A_0-\lambda)^{-1}f(x) &= (A_0+\lambda)\frac{1}{c^2}\left(-\Delta-\left(\frac{\lambda^2}{c^2}-m^2c^2\right)\right)^{-1} I_4 f(x) \\
&= \frac{1}{c^2}(-ic\alpha\cdot\nabla+mc^2\beta+\lambda I_4)\left(-\Delta-\left(\frac{\lambda^2}{c^2}-m^2c^2\right)\right)^{-1} I_4 f(x) \\
&= \frac{1}{c^2}\left(-ic\sum_{j=1}^{3}\alpha_j T_j+(mc^2\beta+\lambda I_4)\left(-\Delta-\left(\frac{\lambda^2}{c^2}-m^2c^2\right)\right)^{-1} I_4\right) f(x) \\
&= \frac{1}{c^2}\int\limits_{\mathbb{R}^3}\left(-ic\sum_{j=1}^{3}\alpha_j t_j(x-y)+(mc^2\beta+\lambda I_4)\tau(x-y)\right) f(y)\mathrm{d}y \\
&= \int\limits_{\mathbb{R}^3} G_\lambda(x-y)f(y)\mathrm{d}y
\end{aligned}$$

for almost all $x \in \mathbb{R}^3$ by direct calculation. □

Next, we will define a maximal operator and a restriction of it, which will be of particular importance in the construction of a quasi boundary triple for the Dirac operator. For this purpose it will be necessary to consider functions that do not possess the Sobolev regularity H^1 on the whole of $\mathbb{R}^3$.

In this section we assume that a bounded C^2-domain $\Omega \subseteq \mathbb{R}^3$ according to Definition 2.26 with boundary $\Sigma = \partial\Omega$ is given. Based on this, we define the two sets $\Omega_+ = \Omega$ and $\Omega_- = \mathbb{R}^3 \setminus \overline{\Omega}$ and thus obtain two C^2-domains that satisfy $\mathbb{R}^3 = \Omega_+ \,\dot\cup\, \Sigma \,\dot\cup\, \Omega_-$.

As discussed in Section 2.6, we use the decomposition

$$L^2(\mathbb{R}^3;\mathbb{C}^4) \cong L^2(\Omega_+;\mathbb{C}^4) \oplus L^2(\Omega_-;\mathbb{C}^4)$$

resulting from the isometric isomorphism $\iota : L^2(\mathbb{R}^3;\mathbb{C}^4) \to L^2(\Omega_+;\mathbb{C}^4) \oplus L^2(\Omega_-;\mathbb{C}^4)$. Furthermore, we identify an operator T in $L^2(\Omega_+;\mathbb{C}^4) \oplus L^2(\Omega_-;\mathbb{C}^4)$ with the operator $\iota^{-1}T\iota$ in $L^2(\mathbb{R}^3;\mathbb{C}^4)$, since all properties of T are carried over to $\iota^{-1}T\iota$ and vice versa. In the following we will switch back and forth between these two representations without explicitly mentioning this. In particular, we denote both operators by T and a similar convention is used for elements in their domain of definition.

Similar to the definition of the free Dirac operator, we define another realization of the formal differential expression (3.1) and define this operator on the space of test functions by the assignment

$$\begin{aligned} \operatorname{dom}(A_{\mathcal{D}}) &= \mathcal{D}(\Omega_+;\mathbb{C}^4) \oplus \mathcal{D}(\Omega_-;\mathbb{C}^4) \cong \mathcal{D}(\mathbb{R}^3 \setminus \Sigma;\mathbb{C}^4) \\ A_{\mathcal{D}} f &= (-ic(\alpha\cdot\nabla) + mc^2\beta)f_+ \oplus (-ic(\alpha\cdot\nabla) + mc^2\beta)f_-. \end{aligned}$$

Due to the identification of operators mentioned above we finally obtain a linear operator in $L^2(\mathbb{R}^3;\mathbb{C}^4)$. This operator is densely defined, since $\mathcal{D}(\Omega_+;\mathbb{C}^4) \oplus \mathcal{D}(\Omega_-;\mathbb{C}^4)$ is dense in $L^2(\Omega_+;\mathbb{C}^4) \oplus L^2(\Omega_-;\mathbb{C}^4)$. Furthermore, by a zero extension we obtain $\iota^{-1}\left(\operatorname{dom}(A_{\mathcal{D}})\right) \subseteq \mathcal{D}(\mathbb{R}^3;\mathbb{C}^4)$ and therefore

$$\operatorname{dom}(A_{\mathcal{D}}) \subseteq \mathcal{D}(\mathbb{R}^3;\mathbb{C}^4) \subseteq \operatorname{dom}(A_0)$$

and $A_{\mathcal{D}} \subseteq A_0$ are valid respectively. Thus $A_{\mathcal{D}}$ is itself closable due to the closeness of A_0.

In view of Theorem 3.1 in which we obtained the free Dirac operator A_0 by closing $T_{\mathcal{D}}$ we will also in this case close the operator $A_{\mathcal{D}}$. We have already shown that this is possible and we will characterize this closure in more detail in the next lemma. It will be shown that the domain of definition of the closure contains all functions of $H^1(\mathbb{R}^3;\mathbb{C}^4)$, which vanish on the C^2-surface Σ in the sense of trace operators.

Lemma 3.5. The closure $S = \overline{A_{\mathcal{D}}}$ is a linear, densely defined and symmetric operator in $L^2(\mathbb{R}^3;\mathbb{C}^4)$ and the following explicit representation applies

$$\begin{aligned} \operatorname{dom}(S) &= H_0^1(\Omega_+;\mathbb{C}^4) \oplus H_0^1(\Omega_-;\mathbb{C}^4) \cong H_0^1(\mathbb{R}^3 \setminus \Sigma;\mathbb{C}^4) \\ Sf &= (-ic(\alpha\cdot\nabla) + mc^2\beta)f_+ \oplus (-ic(\alpha\cdot\nabla) + mc^2\beta)f_-. \end{aligned} \tag{3.9}$$

Proof. Since $A_{\mathcal{D}}$ is densely defined we immediately obtain that S is a densely defined operator as well. Furthermore, it follows from the closeness of A_0 and from the inclusion $A_{\mathcal{D}} \subseteq A_0$ that also $S \subseteq A_0$ applies to the closure. Finally, we conclude from this inclusion, the self-adjointness of A_0 and Theorem 2.10

$$S \subseteq A_0 = A_0^* \subseteq S^*$$

which shows the symmetry of S.

Next, we show the claimed property of the domain of S and, as agreed, we omit the isomorphisms ι and ι^{-1} in the following to simplify the notation. Let $f \in \operatorname{dom}(S)$ be given, then it follows immediately from $S \subseteq A_0$ that $f \in H^1(\mathbb{R}^3;\mathbb{C}^4)$ holds true. Furthermore, the definition of S as the closure of $A_{\mathcal{D}}$ implies the existence of a sequence $(f_n)_{n\in\mathbb{N}} \subseteq \mathcal{D}(\mathbb{R}^3;\mathbb{C}^4)$ with $\operatorname{supp}(f_n) \subseteq \Omega_+ \cup \Omega_-$ such that $f_n \to f$ and $A_{\mathcal{D}} f_n \to Sf$ in $L^2(\mathbb{R}^3;\mathbb{C}^4)$ are valid. Due to the inclusions $A_{\mathcal{D}} \subseteq S \subseteq A_0$ this is equivalent to

$$\|f_n - f\|_{L^2(\mathbb{R}^3;\mathbb{C}^4)} + \|A_0 f_n - A_0 f\|_{L^2(\mathbb{R}^3;\mathbb{C}^4)} = \|f_n - f\|_{A_0} \to 0 \quad \text{for } n \to \infty$$

with the graph norm of A_0. According to Theorem 3.1, this norm is equivalent to the H^1-norm and therefore we obtain $f_n \to f$ in $H^1(\mathbb{R}^3;\mathbb{C}^4)$. If we now consider restrictions to $\Omega_\pm$ then it follows that $f_{n,\pm} \to f_\pm$ in $H^1(\Omega_\pm;\mathbb{C}^4)$ is valid. The choice of the sequence $(f_n)_{n\in\mathbb{N}}$ yields $(f_{n,\pm})_{n\in\mathbb{N}} \subseteq \mathcal{D}(\Omega_\pm;\mathbb{C}^4)$ and thus by definition $f_\pm \in H_0^1(\Omega_\pm;\mathbb{C}^4)$. This shows $f \in H_0^1(\Omega_+;\mathbb{C}^4) \oplus H_0^1(\Omega_-;\mathbb{C}^4)$ and consequently the first inclusion.

For the converse inclusion let $f \in H_0^1(\Omega_+;\mathbb{C}^4) \oplus H_0^1(\Omega_-;\mathbb{C}^4)$ be given, then it follows from Theorem 2.32 that $f \in H^1(\mathbb{R}^3;\mathbb{C}^4) = \operatorname{dom}(A_0)$ is valid. Furthermore, by definition of $H_0^1(\Omega_\pm;\mathbb{C}^4)$, there exist sequences $(f_{n,\pm})_{n\in\mathbb{N}} \subseteq \mathcal{D}(\Omega_\pm;\mathbb{C}^4)$ such that $f_{n,\pm} \to f_\pm$ in $H^1(\Omega_\pm;\mathbb{C}^4)$ holds true. In particular, this implies $f_n \to f$ in $H^1(\mathbb{R}^3;\mathbb{C}^4)$. Due to the continuous embedding $H^1(\mathbb{R}^3;\mathbb{C}^4) \hookrightarrow L^2(\mathbb{R}^3;\mathbb{C}^4)$, we therefore obtain $f_n \to f$ and $A_{\mathcal{D}} f_n = A_0 f_n \to A_0 f$ in $L^2(\mathbb{R}^3;\mathbb{C}^4)$. This shows with the definition of the closure of an operator $f \in \operatorname{dom}(S)$ and $Sf = A_0 f$ which completes the proof. □

Next, we will define a maximal operator and for this purpose we have to construct specific subspaces of $L^2(\Omega_\pm;\mathbb{C}^4)$. We define these as the sets of all functions of $L^2(\Omega_\pm;\mathbb{C}^4)$ such that the distributional application of the formal differential expression (3.1) is a regular distribution in $L^2(\Omega_\pm;\mathbb{C}^4)$

$$D_\pm = \left\{ f_\pm \in L^2(\Omega_\pm;\mathbb{C}^4) \;\middle|\; (-ic(\alpha\cdot\nabla) + mc^2) f_\pm \in L^2(\Omega_\pm;\mathbb{C}^4) \right\}.$$

Since the distributional derivative is a linear operation, it immediately follows that the sets $D_\pm$ are vector spaces. Furthermore, we define an inner product on $D_\pm$ by the assignment

$$(f_\pm, g_\pm)_{D_\pm} = (f_\pm, g_\pm)_{L^2(\Omega_\pm;\mathbb{C}^4)} + \big((-ic(\alpha\cdot\nabla) + mc^2) f_\pm, (-ic(\alpha\cdot\nabla) + mc^2) g_\pm\big)_{L^2(\Omega_\pm;\mathbb{C}^4)} \tag{3.10}$$

for $f_\pm, g_\pm \in D_\pm$ and thus obtain pre-Hilbert spaces. This allows us to define the maximal operator as

$$\begin{aligned} \mathrm{dom}(A_{\max}) &= D_+ \oplus D_- \\ A_{\max} f &= (-ic(\alpha\cdot\nabla) + mc^2\beta)f_+ \oplus (-ic(\alpha\cdot\nabla) + mc^2\beta)f_-. \end{aligned}$$

From the definition of $A_{\max}$ it follows immediately that $A_0 \subseteq A_{\max}$ holds true and thus the maximal operator is an extension of the free Dirac operator. Next we will be able to characterize the adjoint of the operator S of Lemma 3.5 as the maximal operator $A_{\max}$. This will be important for constructing a quasi boundary triple for the Dirac operator in the next section.

Lemma 3.6. Let S be the linear operator defined as in (3.9), then $S \subseteq A_{\max}$ and $S^* = A_{\max}$ are valid.

Proof. *Step 1:* By definition, the chain of inclusion

$$A_{\mathcal{D}} \subseteq S \subseteq A_0 \subseteq A_{\max}$$

applies and thus the first assertion. Furthermore, the adjoint operator S^* exists since S is a densely defined linear operator.

Let $f \in \mathrm{dom}(S^*)$ and $g_+ \in \mathcal{D}(\Omega_+;\mathbb{C}^4)$ be given, then we consider the zero extension $g = g_+ \oplus 0 \in \mathrm{dom}(S)$ of g_+ to all of $\mathbb{R}^3$. For this extension, $\partial^\alpha g \in \mathcal{D}(\mathbb{R}^3;\mathbb{C}^4)$ and $\mathrm{supp}(\partial^\alpha g) \subseteq \Omega_+$ are valid for all multi-indices $\alpha \in \mathbb{N}_0^3$ and consequently $g \in \mathrm{dom}(A_{\mathcal{D}})$. This yields $\mathrm{supp}(Sg) = \mathrm{supp}(A_{\mathcal{D}} g) \subseteq \Omega_+$ and further

$$\begin{aligned} \langle (S^*f)_+, g_+\rangle &= ((S^*f)_+, g_+)_{L^2(\Omega_+;\mathbb{C}^4)} = (S^*f, g)_{L^2(\mathbb{R}^3;\mathbb{C}^4)} = (f, Sg)_{L^2(\mathbb{R}^3;\mathbb{C}^4)} \\ &= (f_+, (Sg)_+)_{L^2(\Omega_+;\mathbb{C}^4)} = \big(f_+, (-ic(\alpha\cdot\nabla) + mc^2\beta)g_+\big)_{L^2(\Omega_+;\mathbb{C}^4)} \\ &= \big\langle (-ic(\alpha\cdot\nabla) + mc^2\beta)f_+, g_+\big\rangle \end{aligned}$$

where in the last line the definition of the distributional derivative of a regular distribution was used. Since this is valid for all $g_+ \in \mathcal{D}(\Omega_+;\mathbb{C}^4)$

$$(-ic(\alpha\cdot\nabla) + mc^2\beta)f_+ = (S^*f)_+ \in L^2(\Omega_+;\mathbb{C}^4) \tag{3.11}$$

follows in the sense of distributions. This finally leads to $f_+ \in D_+$ and an analogous lines of reasoning gives $f_- \in D_-$. Altogether we obtain $f \in \mathrm{dom}(A_{\max})$ and with (3.11) the equality $S^*f = A_{\max} f$. This yields the first inclusion $S^* \subseteq A_{\max}$.

Step 2: In order to show the converse inclusion, let $f \in D_+ \oplus D_-$ be given. As a first step we choose an arbitrary $g \in \mathcal{D}(\Omega_+;\mathbb{C}^4) \oplus \mathcal{D}(\Omega_-;\mathbb{C}^4)$ and obtain $g_+ \in \mathcal{D}(\Omega_+;\mathbb{C}^4)$ for its restriction to Ω_+. Therefore

$$\begin{aligned} (f_+, (Sg)_+)_{L^2(\Omega_+;\mathbb{C}^4)} &= \big(f_+, (-ic(\alpha\cdot\nabla) + mc^2\beta)g_+\big)_{L^2(\Omega_+;\mathbb{C}^4)} \\ &= \big\langle (-ic(\alpha\cdot\nabla) + mc^2\beta)f_+, g_+\big\rangle \\ &= \big((-ic(\alpha\cdot\nabla) + mc^2\beta)f_+, g_+\big)_{L^2(\Omega_+;\mathbb{C}^4)} \\ &= ((A_{\max} f)_+, g_+)_{L^2(\Omega_+;\mathbb{C}^4)} \end{aligned}$$

follows, where in the second line the definition of the derivative of a regular distribution was used. Analogously one shows

$$(f_-, (Sg)_-)_{L^2(\Omega_-;\mathbb{C}^4)} = ((A_{\max} f)_-, g_-)_{L^2(\Omega_-;\mathbb{C}^4)}$$

and an addition of these two relations finally leads to

$$(f, Sg)_{L^2(\mathbb{R}^3;\mathbb{C}^4)} = (A_{\max} f, g)_{L^2(\mathbb{R}^3;\mathbb{C}^4)} \tag{3.12}$$

for all $g \in \mathcal{D}(\Omega_+;\mathbb{C}^4) \oplus \mathcal{D}(\Omega_-;\mathbb{C}^4)$.

Next, we are going to extend this result for test functions to all of $\mathrm{dom}(S)$. Let $g \in \mathrm{dom}(S)$ be given, then due to the density of $\mathcal{D}(\Omega_\pm;\mathbb{C}^4)$ in $H_0^1(\Omega_\pm;\mathbb{C}^4)$ there exist sequences $(g_{n,\pm})_{n\in\mathbb{N}} \subseteq \mathcal{D}(\Omega_\pm;\mathbb{C}^4)$ such that $g_{n,\pm} \to g_\pm$ in $H^1(\Omega_\pm;\mathbb{C}^4)$ is valid. In particular, this implies $g_n \to g$ in $H^1(\mathbb{R}^3;\mathbb{C}^4)$. Due to the continuous embedding $H^1(\mathbb{R}^3;\mathbb{C}^4) \hookrightarrow L^2(\mathbb{R}^3;\mathbb{C}^4)$, we therefore obtain $g_n \to g$ and $Sg_n \to Sg$ in $L^2(\mathbb{R}^3;\mathbb{C}^4)$. Using (3.12) , this leads to

$$\begin{aligned}(f, Sg)_{L^2(\mathbb{R}^3;\mathbb{C}^4)} &= \lim_{n\to\infty} (f, Sg_n)_{L^2(\mathbb{R}^3;\mathbb{C}^4)} \\ &= \lim_{n\to\infty} (A_{\max} f, g_n)_{L^2(\mathbb{R}^3;\mathbb{C}^4)} = (A_{\max} f, g)_{L^2(\mathbb{R}^3;\mathbb{C}^4)}\end{aligned}$$

which proves $f \in \mathrm{dom}(S^*)$ and $S^* f = A_{\max} f$. We therefore obtain the inclusion $A_{\max} \subseteq S^*$ and with Step 1 finally $S^* = A_{\max}$ which completes the proof. □

We close this section with an auxiliary result which shows the density of the arbitrarily often differentiable functions in $D_\pm$. This is equivalent to them forming a core of the maximal operator. The proof of this result can be found in [14, Lem. 3.2].

Lemma 3.7. Space $C^\infty(\overline{\Omega_\pm};\mathbb{C}^4)$ is dense in $D_\pm$ with respect to the norm induced by the inner product (3.10).

3.2 A quasi boundary triple for the Dirac operator and δ-shell interactions

In this section we will construct a quasi boundary triple for the Dirac operator and, as discussed in Chapter 1, we will encode the effect of the δ-shell interactions in form of jump conditions at the boundary Σ of the bounded C^2-domain $\Omega \subseteq \mathbb{R}^3$. This will enable us to define self-adjoint realizations $A_{\eta,\tau}$ of the formal expression (1.10) of Chapter 1. We follow the approach described in [14] and [40] and carry out proofs of the results to provide a self-contained presentation.

In the following, as in Chapter 3.1, $\Omega \subseteq \mathbb{R}^3$ is always a bounded C^2-domain according to Definition 2.26 with boundary $\Sigma = \partial\Omega$. We define $\Omega_+ = \Omega$ and $\Omega_- = \mathbb{R}^3 \setminus \overline{\Omega}$ and thereby obtain two C^2-domains which satisfy $\mathbb{R}^3 = \Omega_+ \,\dot\cup\, \Sigma \,\dot\cup\, \Omega_-$. Furthermore, we use the decomposition $L^2(\mathbb{R}^3;\mathbb{C}^4) \cong L^2(\Omega_+;\mathbb{C}^4) \oplus L^2(\Omega_-;\mathbb{C}^4)$ and an analogous decomposition of operators as described in Sections 2.6 and 3.1 without explicitly mentioning the isomorphism ι.

For the definition of a quasi boundary triple for S^* of Section 3.1 it is necessary to specify a closable operator T with $S \subseteq T \subseteq S^*$ and two boundary maps Γ_0 and Γ_1. Due to Lemma 3.6, $S^* = A_{\max}$ applies and consequently $T \subseteq A_{\max}$ has to apply as well. We therefore define the linear operator $T = A_{\max} \upharpoonright H^1(\Omega_+;\mathbb{C}^4) \oplus H^1(\Omega_-;\mathbb{C}^4)$ in $L^2(\mathbb{R}^3;\mathbb{C}^4)$ as a restriction of the maximal operator. For this operator, the explicit representation

$$\begin{aligned} \operatorname{dom}(T) &= H^1(\Omega_+;\mathbb{C}^4) \oplus H^1(\Omega_-;\mathbb{C}^4) \cong H^1(\mathbb{R}^3 \setminus \Sigma;\mathbb{C}^4) \\ Tf &= A_{\max} f = (-ic\alpha \cdot \nabla + mc^2\beta)f_+ \oplus (-ic\alpha \cdot \nabla + mc^2\beta)f_- \end{aligned}$$

is valid and we therefore immediately obtain the chain of inclusions

$$S \subseteq A_0 \subseteq T \subseteq A_{\max} = S^*.$$

To define the boundary maps we assume that an arbitrary $f \in \operatorname{dom}(T)$ is given and obtain $\tau_\pm f_\pm \in H^{\frac{1}{2}}(\Gamma;\mathbb{C}^4) \subseteq L^2(\Sigma;\mathbb{C}^4)$ from the mapping properties of the trace operators according to Theorem 2.30. Furthermore, with the outer unit normal vector field ν on Σ and Theorem 2.32 we find $\nu_j \tau_\pm f_\pm \in H^{\frac{1}{2}}(\Gamma;\mathbb{C}^4) \subseteq L^2(\Sigma;\mathbb{C}^4)$ for all $j \in \{1,2,3\}$. Therefore, the boundary maps $\Gamma_0, \Gamma_1 : \operatorname{dom}(T) \to L^2(\Sigma;\mathbb{C}^4)$, defined by

$$\Gamma_0 f = ic(\alpha \cdot \nu)(\tau_+ f_+ - \tau_- f_-)$$

and

$$\Gamma_1 f = \frac{1}{2}(\tau_+ f_+ + \tau_- f_-)$$

for all $f \in \operatorname{dom}(T)$ are well-defined and linear operators from $\operatorname{dom}(T) \cong H^1(\mathbb{R}^3 \setminus \Sigma;\mathbb{C}^4)$ to $L^2(\Sigma;\mathbb{C}^4)$ which satisfy the range condition

$$\operatorname{ran}(\Gamma_0,\Gamma_1)^\top \subseteq H^{\frac{1}{2}}(\Gamma;\mathbb{C}^4) \times H^{\frac{1}{2}}(\Gamma;\mathbb{C}^4).$$

The reason for this specific choice of the boundary maps will become apparent in the discussion of δ-interactions below. In the next result we will show that the triple $\{L^2(\Sigma;\mathbb{C}^4),\Gamma_0,\Gamma_1\}$ together with the operator T is a quasi boundary triple for S^*.

Theorem 3.8. The triple $\{L^2(\Sigma;\mathbb{C}^4),\Gamma_0,\Gamma_1\}$ is a quasi boundary triple for S^* and satisfies the range condition

$$\operatorname{ran}(\Gamma_0,\Gamma_1)^\top = H^{\frac{1}{2}}(\Gamma;\mathbb{C}^4) \times H^{\frac{1}{2}}(\Gamma;\mathbb{C}^4).$$

Furthermore, there holds

$$T \upharpoonright \ker(\Gamma_0) = A_0$$

with the free Dirac operator A_0 from Theorem 3.1.

Proof. *Step 1:* Due to the definition of T as a restriction of the closed operator $A_{\max}$, it follows immediately that T is closable and the inclusion

$$\overline{T} \subseteq A_{\max} = S^*$$

applies to its closure. To show the converse inclusion let $f \in \operatorname{dom}(A_{\max}) = D_+ \oplus D_-$ be given. Since $C^\infty(\overline{\Omega_+};\mathbb{C}^4) \oplus C^\infty(\overline{\Omega_-};\mathbb{C}^4)$ is dense in $D_+ \oplus D_-$ according to Lemma 3.7, there exists a sequence $(f_n)_{n\in\mathbb{N}} \subseteq C^\infty(\overline{\Omega_+};\mathbb{C}^4) \oplus C^\infty(\overline{\Omega_-};\mathbb{C}^4)$ such that

$$\|f_n - f\|_{A_{\max}} = \|f_n - f\|_{D_+\oplus D_-} \to 0 \quad \text{for } n \to \infty \tag{3.13}$$

holds true. As a consequence of the inclusion

$$C^\infty(\overline{\Omega_+};\mathbb{C}^4) \oplus C^\infty(\overline{\Omega_-};\mathbb{C}^4) \subseteq H^1(\Omega_+;\mathbb{C}^4) \oplus H^1(\Omega_-;\mathbb{C}^4) = \operatorname{dom}(T)$$

and due to (3.13) we find that $(f_n)_{n\in\mathbb{N}}$ is a sequence in $\operatorname{dom}(T)$ for which $f_n \to f$ and $Tf_n = A_{\max} f_n \to A_{\max} f$ in $L^2(\mathbb{R}^3;\mathbb{C}^4)$ are valid. Therefore, we obtain $f \in \operatorname{dom}(\overline{T})$ and $\overline{T}f = A_{\max} f$ by the definition of the closure of an operator. This shows the inclusion

$$A_{\max} \subseteq \overline{T}$$

and with the above consideration, the equality $S^* = \overline{T}$ follows.

Step 2: Let $\nu = \nu_+ = -\nu_-$ be the outer unit normal vector field on Σ. An application of Theorem 2.31 yields by direct calculation

$$\begin{aligned}\big((-ic\alpha\cdot\nabla + mc^2\beta)f_\pm, g_\pm\big)_{L^2(\Omega_\pm;\mathbb{C}^4)} &- \big(f_\pm, (-ic\alpha\cdot\nabla + mc^2\beta)g_\pm\big)_{L^2(\Omega_\pm;\mathbb{C}^4)} \\ &= \pm(-ic(\alpha\cdot\nu)\tau_\pm f_\pm, \tau_\pm g_\pm)_{L^2(\Sigma;\mathbb{C}^4)}\end{aligned}$$

for all $f, g \in \operatorname{dom}(T)$. By adding these two equations and using the hermiticity of the Dirac matrices, the abstract Green's identity

$$\begin{aligned}(\Gamma_1 f, \Gamma_0 g)_{L^2(\Sigma;\mathbb{C}^4)} &- (\Gamma_0 f, \Gamma_1 g)_{L^2(\Sigma;\mathbb{C}^4)} \\ &= \left(\frac{1}{2}(\tau_+ f_+ + \tau_- f_-), ic(\alpha\cdot\nu)(\tau_+ g_+ - \tau_- g_-)\right)_{L^2(\Sigma;\mathbb{C}^4)} \\ &\quad - \left(ic(\alpha\cdot\nu)(\tau_+ f_+ - \tau_- f_-), \frac{1}{2}(\tau_+ g_+ + \tau_- g_-)\right)_{L^2(\Sigma;\mathbb{C}^4)} \\ &= -\left(ic(\alpha\cdot\nu)(\tau_+ f_+ + \tau_- f_-), \frac{1}{2}(\tau_+ g_+ - \tau_- g_-)\right)_{L^2(\Sigma;\mathbb{C}^4)} \\ &\quad - \left(ic(\alpha\cdot\nu)(\tau_+ f_+ - \tau_- f_-), \frac{1}{2}(\tau_+ g_+ + \tau_- g_-)\right)_{L^2(\Sigma;\mathbb{C}^4)} \\ &= (-ic(\alpha\cdot\nu)\tau_+ f_+, \tau_+ g_+)_{L^2(\Sigma;\mathbb{C}^4)} - (-ic(\alpha\cdot\nu)\tau_- f_-, \tau_- g_-)_{L^2(\Sigma;\mathbb{C}^4)} \\ &= (Tf, g)_{L^2(\mathbb{R}^3;\mathbb{C}^4)} - (f, Tg)_{L^2(\mathbb{R}^3;\mathbb{C}^4)}\end{aligned}$$

for all $f, g \in \operatorname{dom}(T)$ follows.

Step 3: Next, we will show the range condition of the mapping

$$(\Gamma_0, \Gamma_1)^\top : \operatorname{dom}(T) \to L^2(\Sigma; \mathbb{C}^4) \times L^2(\Sigma; \mathbb{C}^4)$$

and assume that arbitrary functions $\varphi, \psi \in H^{\frac{1}{2}}(\Gamma; \mathbb{C}^4)$ are given. According to Theorem 2.32 we have $i(\alpha \cdot \nu)\varphi \in H^{\frac{1}{2}}(\Gamma; \mathbb{C}^4)$ and therefore due to the surjectivity of the trace operators $\tau_\pm$ there exist $g_+, h_+ \in H^1(\Omega_+; \mathbb{C}^4)$ and $h_- \in H^1(\Omega_-; \mathbb{C}^4)$ such that

$$\tau_+ g_+ = -\frac{i}{c}(\alpha \cdot \nu)\varphi$$

and

$$\tau_\pm h_\pm = \psi - \frac{1}{2}\tau_+ g_+ \tag{3.14}$$

hold true. We define $h = h_+ \oplus h_- \in H^1(\Omega_+; \mathbb{C}^4) \oplus H^1(\Omega_-; \mathbb{C}^4)$ and by using (3.14) and Theorem 2.32 we obtain that even $h \in H^1(\mathbb{R}^3; \mathbb{C}^4)$ is valid. Next, we define

$$f = g_+ \oplus 0 + h \in H^1(\Omega_+; \mathbb{C}^4) \oplus H^1(\Omega_-; \mathbb{C}^4) = \operatorname{dom}(T)$$

and by applying the relation (3.2) of the Dirac matrices and due to the choice of g_+ and h we find

$$\begin{aligned} \Gamma_0 f &= ic(\alpha \cdot \nu)(\tau_+ f_+ - \tau_- f_-) = ic(\alpha \cdot \nu)(\tau_+ g_+ + \tau_+ h_+ - \tau_- h_-) \\ &= ic(\alpha \cdot \nu)\tau_+ g_+ = (\alpha \cdot \nu)^2 \varphi = \varphi \end{aligned}$$

and

$$\Gamma_1 f = \frac{1}{2}(\tau_+ f_+ + \tau_- f_-) = \frac{1}{2}(\tau_+ g_+ + \tau_+ h_+ + \tau_- h_-) = \psi$$

which shows the claimed range condition. Furthermore, due to Theorem 2.32, the space $H^{\frac{1}{2}}(\Gamma; \mathbb{C}^4)$ is dense in $L^2(\Gamma; \mathbb{C}^4)$ and consequently the mapping $(\Gamma_0, \Gamma_1)^\top$ has dense range.

Step 4: To complete the proof it remains to show that the restriction of T to $\ker(\Gamma_0)$ is a self-adjoint operator in $L^2(\mathbb{R}^3; \mathbb{C}^4)$. For this purpose we assume that an arbitrary $f \in \operatorname{dom}(T)$ is given. From $(\alpha \cdot \nu)^2 = I_4$ and Theorem 2.32 it immediately follows that the equivalence

$$\begin{aligned} f \in \ker(\Gamma_0) &\iff \Gamma_0 f = ic(\alpha \cdot \nu)(\tau_+ f_+ - \tau_- f_-) = 0 \\ &\iff \tau_+ f_+ = \tau_- f_- \\ &\iff f \in H^1(\mathbb{R}^3; \mathbb{C}^4) \end{aligned}$$

applies. This finally leads to

$$\ker(\Gamma_0) = H^1(\mathbb{R}^3; \mathbb{C}^4) = \operatorname{dom}(A_0)$$

and further to the equality

$$T \upharpoonright \ker(\Gamma_0) = A_0$$

in the sense of linear operators. As A_0 is a self-adjoint operator in $L^2(\mathbb{R}^3;\mathbb{C}^4)$ according to Theorem 3.1 we conclude with the previous steps that $\{L^2(\Sigma;\mathbb{C}^4),\Gamma_0,\Gamma_1\}$ is a quasi boundary triple for S^* in the sense of Definition 2.16. $\square$

Next, it is our objective to determine the γ-field and the Weyl function of the quasi boundary triple $\{L^2(\Sigma;\mathbb{C}^4),\Gamma_0,\Gamma_1\}$ in Theorem 3.8. For this purpose, we introduce two families of linear and bounded operators, which are integral operators resulting from the Green's function G_λ of the free Dirac operator. It will turn out that, after being restricted to certain subspaces, they correspond to the values of the γ-field and the Weyl function of the above quasi boundary triple. This will be shown in Theorem 3.11.

Theorem 3.9. Let $\lambda \in \rho(A_0)$ be given and G_λ be the integral kernel of the resolvent of the free Dirac operator defined as in (3.5), then the following statements are true.

i) The assignment

$$(\Phi_\lambda f)(x) = \int_\Sigma G_\lambda(x-y)f(y)\mathrm{d}\sigma(y) \tag{3.15}$$

for $f \in L^2(\Sigma;\mathbb{C}^4)$ and $x \in \mathbb{R}^3$ corresponds to a well-defined, linear and bounded operator $\Phi_\lambda : L^2(\Sigma;\mathbb{C}^4) \to L^2(\mathbb{R}^3;\mathbb{C}^4)$.

ii) The adjoint operator of Φ_λ is given by

$$(\Phi_\lambda^* f)(x) = \int_{\mathbb{R}^3} G_{\overline{\lambda}}(x-y)f(y)\mathrm{d}y \tag{3.16}$$

for all $f \in L^2(\mathbb{R}^3;\mathbb{C}^4)$ and for almost all $x \in \Sigma$ and is a linear and bounded operator $\Phi_\lambda^* : L^2(\mathbb{R}^3;\mathbb{C}^4) \to L^2(\Sigma;\mathbb{C}^4)$ as well.

iii) The assignment

$$(\mathcal{C}_\lambda f)(x) = \lim_{\varepsilon\to 0^+} \int_{\Sigma\setminus B(x,\varepsilon)} G_\lambda(x-y)f(y)\mathrm{d}\sigma(y) \tag{3.17}$$

for $f \in L^2(\Sigma;\mathbb{C}^4)$ and $x \in \Sigma$ corresponds to a well-defined, linear and bounded operator $\mathcal{C}_\lambda : L^2(\Sigma;\mathbb{C}^4) \to L^2(\Sigma;\mathbb{C}^4)$.

Proof. *Proof of i) and ii):* Since all operators are integral operators, we are going to apply the results from Section 2.6. For this we need estimates of the integral kernels. To prove the first two assertions we use the matrix-valued functions

$$t_j(x) = \left(i\sqrt{\frac{\lambda^2}{c^2} - m^2c^2}\|x\| - 1 \right) \frac{1}{4\pi\|x\|^3} \exp\left(i\sqrt{\frac{\lambda^2}{c^2} - m^2c^2}\|x\| \right) x_j I_4$$

of Lemma 3.3 and

$$\tau(x) = \frac{1}{4\pi\|x\|} \exp\left(i\sqrt{\frac{\lambda^2}{c^2} - m^2c^2}\|x\| \right) I_4$$

of Theorem 3.4 for all $x \in \mathbb{R}^3 \backslash \{0\}$. By using these functions we obtain a decomposition of the form

$$G_\lambda(x) = \frac{1}{c^2} \left(-ic \sum_{j=1}^{4} \alpha_j t_j(x) + (mc^2\beta + \lambda I_4)\tau(x) \right)$$

with the Green's function G_λ of the free Dirac operator defined as in (3.5). Furthermore, due to the estimates for t_j and τ from Lemma 3.3 and Theorem 3.4 Step 2 respectively, we obtain the inequality

$$\|G_\lambda(x)\| \le \kappa_1 \begin{cases} \|x\|^{-2} & \text{, for } \|x\| < 1 \\ e^{-\kappa_2\|x\|} & \text{, for } \|x\| \ge 1 \end{cases} \tag{3.18}$$

for all $x \in \mathbb{R}^3 \backslash \{0\}$ and sufficiently large $c > 0$ with constants $\kappa_1, \kappa_2 > 0$. An application of Theorem 2.35 yields with (3.18) the assertion for Φ_λ and that the assignment

$$(Tf)(x) = \int_{\mathbb{R}^3} G_{\overline{\lambda}}(x - y) f(y) \mathrm{d}y$$

for $f \in L^2(\mathbb{R}^3; \mathbb{C}^4)$ and $x \in \Sigma$ corresponds to a well-defined, linear and bounded operator $T : L^2(\mathbb{R}^3; \mathbb{C}^4) \to L^2(\Sigma; \mathbb{C}^4)$. Furthermore, it can be shown by direct calculation that for all $\lambda \in \rho(A_0)$ and for all $x \in \mathbb{R}^3 \setminus \{0\}$ the equality

$$-G_{\overline{\lambda}}(x) = G_\lambda(x)^*$$

applies. Since Φ_λ is a everywhere defined and bounded operator it follows from Theorem 2.10 that $\Phi_\lambda^* \in \mathcal{L}(L^2(\mathbb{R}^3; \mathbb{C}^4), L^2(\Sigma; \mathbb{C}^4))$ holds true. Let $f \in L^2(\mathbb{R}^3; \mathbb{C}^4)$ and $g \in L^2(\Sigma; \mathbb{C}^4)$ be given then, by Lemma 2.37, it follows from Fubini's theorem and the hermiticity of the Dirac matrices that

$$\begin{aligned}(g, \Phi_\lambda^* f)_{L^2(\Sigma;\mathbb{C}^4)} = (\Phi_\lambda g, f)_{L^2(\mathbb{R}^3;\mathbb{C}^4)} &= \int_{\mathbb{R}^3}\int_{\Sigma} G_\lambda(x-y)g(y)\cdot\overline{f(x)}\mathrm{d}\sigma(y)\mathrm{d}x \\ &= \int_{\Sigma}\int_{\mathbb{R}^3} g(y)\cdot G_\lambda(x-y)\overline{f(x)}\mathrm{d}x\mathrm{d}\sigma(y) \\ &= \int_{\Sigma}\int_{\mathbb{R}^3} g(y)\cdot\overline{G_{\overline{\lambda}}(y-x)f(x)}\mathrm{d}x\mathrm{d}\sigma(y) = (g, Tf)_{L^2(\Sigma;\mathbb{C}^4)}\end{aligned}$$

is valid. Since this is true for all $f \in L^2(\mathbb{R}^3;\mathbb{C}^4)$ and $g \in L^2(\Sigma;\mathbb{C}^4)$ we finally obtain $T = \Phi_\lambda^*$ in the sense of operators which proves the assertion ii).

Proof of iii): To investigate $\mathcal{C}_\lambda$ we define the matrix-valued functions

$$\begin{aligned}w_1(x) &= \left(\frac{\lambda}{c^2}I_4 + m\beta + \sqrt{\frac{\lambda^2}{c^2} - m^2c^2}\frac{1}{c\|x\|}\alpha\cdot x\right)\frac{1}{4\pi\|x\|}\exp\left(i\sqrt{\frac{\lambda^2}{c^2}-m^2c^2}\|x\|\right), \\ w_2(x) &= \frac{i}{4\pi c\|x\|^3}\alpha\cdot x\left(\exp\left(i\sqrt{\frac{\lambda^2}{c^2}-m^2c^2}\|x\|\right) - 1\right), \\ w_3(x) &= \frac{i}{4\pi c\|x\|^3}\alpha\cdot x\end{aligned}$$

for all $x \in \mathbb{R}^3 \setminus \{0\}$ and thus obtain by direct calculation the decomposition

$$G_\lambda(x) = w_1(x) + w_2(x) + w_3(x).$$

Since all matrix norms are equivalent, we use the Frobenius norm for convenience and obtain for w_1 the estimate

$$\begin{aligned}\|w_1(x)\|_F &\leq \frac{1}{4\pi\|x\|}\left(2\frac{|\lambda|}{c^2} + 2m + \left|\sqrt{\frac{\lambda^2}{c^2}-m^2c^2}\right|\frac{1}{c\|x\|}\sum_{j=1}^3 \|\alpha_j\|_F\,|x_j|\right) \\ &\leq \frac{1}{4\pi\|x\|}\left(2\frac{|\lambda|}{c^2} + 2m + \left|\sqrt{\frac{\lambda^2}{c^2}-m^2c^2}\right|\frac{1}{c}\sum_{j=1}^3 \|\alpha_j\|_F\right)\end{aligned}$$

for all $x \in \mathbb{R}^3 \setminus \{0\}$. Therefore, according to the Theorem 2.36 the assignment

$$(T_1 f)(x) = \int_\Sigma w_1(x-y)f(y)\mathrm{d}\sigma(y)$$

for $f \in L^2(\Sigma;\mathbb{C}^4)$ and $x \in \Sigma$ corresponds to a well-defined, linear and bounded operator in $L^2(\Sigma;\mathbb{C}^4)$. Since the integral kernel w_1 is integrable over Σ due to the above estimation and [10, Lem. A.2], we obtain

$$\int_\Sigma \int_\Sigma \|w_1(x-y)f(y)\| \mathrm{d}\sigma(y)\mathrm{d}\sigma(x) < \infty$$

as in Lemma 2.37 by choosing $g \equiv 1$. This yields

$$\int_\Sigma \|w_1(x-y)f(y)\| \mathrm{d}\sigma(y) < \infty$$

for almost all $x \in \Sigma$. By applying the dominated convergence theorem we therefore find

$$(T_1 f)(x) = \lim_{\varepsilon \to 0^+} \int_{\Sigma \setminus B(x,\varepsilon)} w_1(x-y) f(y) \mathrm{d}\sigma(y)$$

for all $f \in L^2(\Sigma;\mathbb{C}^4)$ and for almost all $x \in \Sigma$.

In order to analyze w_2 we use the fundamental theorem of calculus and find

$$\begin{aligned}
\left|\exp\left(i\sqrt{\frac{\lambda^2}{c^2} - m^2c^2}\|x\|\right) - 1\right| &= \left|\int_0^1 \frac{\mathrm{d}}{\mathrm{d}t}\exp\left(it\sqrt{\frac{\lambda^2}{c^2} - m^2c^2}\|x\|\right)\mathrm{d}t\right| \\
&= \left|i\sqrt{\frac{\lambda^2}{c^2} - m^2c^2}\|x\| \int_0^1 \exp\left(it\sqrt{\frac{\lambda^2}{c^2} - m^2c^2}\|x\|\right)\mathrm{d}t\right| \\
&\leq \left|\sqrt{\frac{\lambda^2}{c^2} - m^2c^2}\right| \|x\| \int_0^1 \left|\exp\left(it\sqrt{\frac{\lambda^2}{c^2} - m^2c^2}\|x\|\right)\right|\mathrm{d}t \\
&\leq \left|\sqrt{\frac{\lambda^2}{c^2} - m^2c^2}\right| \|x\|
\end{aligned}$$

and furthermore

$$\begin{aligned}
\|w_2(x)\|_F &= \frac{1}{4\pi c\|x\|^3}\left|\exp\left(i\sqrt{\frac{\lambda^2}{c^2} - m^2c^2}\|x\|\right) - 1\right| \sum_{j=1}^3 \|\alpha_j\|_F\,|x_i| \\
&\leq \frac{1}{4\pi c\|x\|}\left|\sqrt{\frac{\lambda^2}{c^2} - m^2c^2}\right| \sum_{j=1}^3 \|\alpha_j\|_F
\end{aligned}$$

for all $x \in \mathbb{R}^3 \setminus \{0\}$. With an analogous line of reasoning as for w_1 we are able to conclude that the assignment

$$(T_2 f)(x) = \lim_{\varepsilon \to 0^+} \int_{\Sigma \setminus B(x,\varepsilon)} w_2(x-y) f(y) \mathrm{d}\sigma(y)$$

for all $f \in L^2(\Sigma;\mathbb{C}^4)$ and almost all $x \in \Sigma$ corresponds to a well-defined, linear and bounded operator in $L^2(\Sigma;\mathbb{C}^4)$ as well.

Finally, by a component-wise application of Theorem 2.38 we obtain that also

$$(T_3 f)(x) = \lim_{\varepsilon \to 0^+} \int\limits_{\Sigma \setminus B(x,\varepsilon)} w_3(x-y) f(y) \mathrm{d}\sigma(y)$$

for $f \in L^2(\Sigma;\mathbb{C}^4)$ and $x \in \Sigma$ corresponds to a well-defined, linear and bounded operator in $L^2(\Sigma;\mathbb{C}^4)$. Consequently, by using the results concerning T_1 and T_2, we obtain that

$$\mathcal{C}_\lambda = T_1 + T_2 + T_3$$

is a well-defined, linear and bounded operator in $L^2(\Sigma;\mathbb{C}^4)$, which proves the assertion iii). □

The next result is a collection of useful properties of the operators Φ_λ and $\mathcal{C}_\lambda$. The proof of item i) can be found in [7, Lem. 2.2] for $\lambda = 0$ and also the general case $\lambda \in \rho(A_0)$ can be shown in a similar manner. Items ii) and iii) follow from the results [40, Prop. 3.2.4] and [40, Prop. 4.1.4] and the compact embeddings

$$H^{\frac{1}{2}}(\Sigma;\mathbb{C}^4) \hookrightarrow L^2(\Sigma;\mathbb{C}^4) \hookrightarrow H^{-\frac{1}{2}}(\Sigma;\mathbb{C}^4)$$

according to Theorem 2.29.

Theorem 3.10. Let $\lambda \in \rho(A_0)$ be given and Φ_λ and $\mathcal{C}_\lambda$ be the linear and bounded operators defined as in (3.15) and (3.17), then the following statements are true.

i) The non-tangential limits

$$(C_\pm f)(x) = \lim_{\Omega_\pm \ni y \to x} (\Phi_\lambda f)(y)$$

exist for all $f \in L^2(\Sigma;\mathbb{C}^4)$ and for almost all $x \in \Sigma$. Furthermore, the relationship

$$C_\pm f = \mathcal{C}_\lambda f \mp \frac{i}{2c}(\alpha \cdot \nu) f$$

with the outer unit normal vector field ν on Σ applies.

ii) The operator

$$\mathcal{C}_\lambda \beta + \beta \mathcal{C}_\lambda : L^2(\Sigma;\mathbb{C}^4) \to L^2(\Sigma;\mathbb{C}^4)$$

is compact and the range condition

$$\operatorname{ran}(\mathcal{C}_\lambda \beta + \beta \mathcal{C}_\lambda) \subseteq H^{\frac{1}{2}}(\Sigma;\mathbb{C}^4)$$

applies.

iii) The operator

$$(\mathcal{C}_\lambda)^2 - \frac{1}{4c^2} I : L^2(\Sigma; \mathbb{C}^4) \to L^2(\Sigma; \mathbb{C}^4)$$

is compact and the range condition

$$\operatorname{ran}\left((\mathcal{C}_\lambda)^2 - \frac{1}{4c^2} I\right) \subseteq H^{\frac{1}{2}}(\Sigma; \mathbb{C}^4).$$

applies.

Based on the results of Theorem 3.9 and Theorem 3.10 we are now able to show an explicit representation of the values of the γ-field and the Weyl function of the quasi boundary triple in Theorem 3.8.

Theorem 3.11. Let $\lambda \in \rho(A_0)$ be given and Φ_λ and $\mathcal{C}_\lambda$ be the linear and bounded operators defined as in (3.15) and (3.17), then for the quasi boundary triple $\{L^2(\Sigma; \mathbb{C}^4), \Gamma_0, \Gamma_1\}$ in Theorem 3.8 the following statements are true.

i) The values of the γ-field are densely defined and bounded operators from $L^2(\Sigma; \mathbb{C}^4)$ to $L^2(\mathbb{R}^3; \mathbb{C}^4)$ with $\operatorname{dom}(\gamma(\lambda)) = H^{\frac{1}{2}}(\Sigma; \mathbb{C}^4)$. Furthermore, $\gamma(\lambda) = \Phi_\lambda \restriction H^{\frac{1}{2}}(\Sigma; \mathbb{C}^4)$ is valid and therefore $\gamma(\lambda)$ is a closable operator with $\overline{\gamma(\lambda)} = \Phi_\lambda$. In particular, the explicit representation

$$(\gamma(\lambda) f)(x) = \int_\Sigma G_\lambda(x - y) f(y) \mathrm{d}\sigma(y)$$

for all $f \in H^{\frac{1}{2}}(\Sigma; \mathbb{C}^4)$ and for almost all $x \in \mathbb{R}^3$ applies.

ii) $\gamma(\lambda)$ as an operator from $H^{\frac{1}{2}}(\Sigma; \mathbb{C}^4)$ to $H^1(\mathbb{R}^3 \setminus \Sigma; \mathbb{C}^4)$ is everywhere defined and bounded.

iii) The values of the Weyl function are densely defined and bounded operators in $L^2(\Sigma; \mathbb{C}^4)$ with $\operatorname{dom}(M(\lambda)) = H^{\frac{1}{2}}(\Sigma; \mathbb{C}^4)$. Furthermore, $M(\lambda) = \mathcal{C}_\lambda \restriction H^{\frac{1}{2}}(\Sigma; \mathbb{C}^4)$ is valid and therefore $M(\lambda)$ is a closable operator with $\overline{M(\lambda)} = \mathcal{C}_\lambda$. In particular, the explicit representation

$$(M(\lambda) f)(x) = \lim_{\varepsilon \to 0^+} \int_{\Sigma \setminus B(x,\varepsilon)} G_\lambda(x - y) f(y) \mathrm{d}\sigma(y)$$

for all $f \in L^2(\Sigma; \mathbb{C}^4)$ and for almost all $x \in \Sigma$ applies.

iv) $M(\lambda)$ as an operator in $H^{\frac{1}{2}}(\Sigma; \mathbb{C}^4)$ is everywhere defined and bounded.

Proof. *Step 1:* Theorem 2.18 and Theorem 3.8 immediately imply

$$\operatorname{dom}(\gamma(\lambda)) = \operatorname{ran}(\Gamma_0) = H^{\frac{1}{2}}(\Sigma;\mathbb{C}^4)$$

and

$$\operatorname{ran}(\gamma(\lambda)) = \ker(T-\lambda) \subseteq \operatorname{dom}(T) = H^1(\Omega_+;\mathbb{C}^4) \oplus H^1(\Omega_-;\mathbb{C}^4) \cong H^1(\mathbb{R}^3\setminus\Sigma;\mathbb{C}^4)$$

which show the mapping properties of $\gamma(\lambda)$ of i) and ii) and its dense definition. Furthermore, according to Theorem 2.18 the representation

$$\gamma(\lambda)^* = \Gamma_1\left(A_0 - \overline{\lambda}\right)^{-1}$$

follows and $\gamma(\lambda)^* \in \mathcal{L}(L^2(\mathbb{R}^3;\mathbb{C}^4), L^2(\Sigma;\mathbb{C}^4))$ applies.

To derive an explicit representation for $\gamma(\lambda)$ we use a strategy as in [6, Lem. 2.10] and assume that arbitrary functions $f \in L^2(\mathbb{R}^3;\mathbb{C}^4)$ and $g \in L^2(\Sigma;\mathbb{C}^4)$ are given. For any $\varepsilon > 0$ we define the bounded sets

$$\Omega_\varepsilon = \left\{x\in\mathbb{R}^3 \;\middle|\; \|x\| < \frac{1}{\varepsilon} \text{ and } \operatorname{dist}(x,\Sigma) > \varepsilon\right\}$$

with the distance function $\operatorname{dist}(\cdot,\Sigma)$ of a point in $\mathbb{R}^3$ to the boundary Σ. Based on the estimate (3.18) of Theorem 3.9 we obtain

$$\|G_{\overline{\lambda}}(x-y)\| \le \kappa_1 \max\left\{\frac{1}{\varepsilon^2}, e^{-\kappa_2\varepsilon}\right\} \tag{3.19}$$

for all $x\in\Sigma$ and all $y\in\Omega_\varepsilon$. As a result of the boundedness of Ω_ε

$$f_\varepsilon = \chi_{\Omega_\varepsilon} f \in L^1(\mathbb{R}^3;\mathbb{C}^3) \cap L^2(\mathbb{R}^3;\mathbb{C}^4) \tag{3.20}$$

follows and we obtain $f_\varepsilon \to f$ in $L^2(\mathbb{R}^3;\mathbb{C}^4)$ for $\varepsilon\to 0$ due to the dominated convergence theorem.

By using (3.19) and (3.20) and the dominated convergence theorem we obtain with the resolvent representation of Theorem 3.4 that the non-tangential limits of $(A_0-\lambda)^{-1} f_\varepsilon$ exist almost everywhere on Σ and are given by

$$(L\,(A_0-\lambda)^{-1} f_\varepsilon)(x) = \int_{\Omega_\varepsilon} G_{\overline{\lambda}}(x-y) f(y)\mathrm{d}y \tag{3.21}$$

for almost all $x\in\Sigma$. Since $(A_0-\lambda)^{-1} f_\varepsilon \in H^1(\mathbb{R}^3;\mathbb{C}^4)$ applies, we deduce from Lemma 2.33 that the non-tangential limits (3.21) coincide with the values of the trace operators $\tau_\pm$ of the functions $\left((A_0-\lambda)^{-1} f_\varepsilon\right)\restriction\Omega_\pm$ and therefore

$$(\gamma(\lambda)^* f_\varepsilon)(x) = \left(\Gamma_1\left(A_0-\overline{\lambda}\right)^{-1} f_\varepsilon\right)(x) = \int_{\Omega_\varepsilon} G_{\overline{\lambda}}(x-y) f(y)\mathrm{d}y \tag{3.22}$$

is valid for almost all $x \in \Sigma$. Using Fubini's theorem as in Lemma 2.37 and (3.22) the equality

$$\begin{aligned}(\Phi_\lambda g, f_\varepsilon)_{L^2(\mathbb{R}^3;\mathbb{C}^4)} &= \int\limits_{\Omega_\varepsilon}\int\limits_{\Sigma} G_\lambda(x-y)g(x)\cdot\overline{f(y)}\mathrm{d}\sigma(x)\mathrm{d}y \\ &= \int\limits_{\Sigma}\int\limits_{\Omega_\varepsilon} g(x)\cdot\overline{G_{\overline{\lambda}}(x-y)f(y)}\mathrm{d}y\mathrm{d}\sigma(x) \\ &= (g, \gamma(\lambda)^* f_\varepsilon)_{L^2(\Sigma;\mathbb{C}^4)}\end{aligned}$$

follows. Consequently, from the boundedness of $\gamma(\lambda)^*$ we deduce

$$\begin{aligned}(g, \Phi_\lambda^* f)_{L^2(\Sigma;\mathbb{C}^4)} &= (\Phi_\lambda g, f)_{L^2(\mathbb{R}^3;\mathbb{C}^4)} = \lim_{\varepsilon\to 0}(\Phi_\lambda g, f_\varepsilon)_{L^2(\mathbb{R}^3;\mathbb{C}^4)} \\ &= \lim_{\varepsilon\to 0}(g, \gamma(\lambda)^* f_\varepsilon)_{L^2(\Sigma;\mathbb{C}^4)} = (g, \gamma(\lambda)^* f)_{L^2(\Sigma;\mathbb{C}^4)}\end{aligned}$$

and since this is true for all $f \in L^2(\mathbb{R}^3;\mathbb{C}^4)$ and all $g \in L^2(\Sigma;\mathbb{C}^4)$ we find the equality $\Phi_{\overline{\lambda}}^* = \gamma(\lambda)^*$ in the sense of linear operators. With Theorem 2.10 and the boundedness of Φ_λ we finally obtain

$$\gamma(\lambda) \subseteq \overline{\gamma(\lambda)} = \gamma(\lambda)^{**} = \Phi_{\overline{\lambda}}^{**} = \Phi_\lambda$$

which shows the claimed representation from i), the boundedness of $\gamma(\lambda)$ and the statement about its closure.

Step 2: We will show that $\gamma(\lambda)$ is closed as an operator from $H^{\frac{1}{2}}(\Sigma;\mathbb{C}^4)$ to $H^1(\mathbb{R}^3\setminus\Sigma;\mathbb{C}^4)$. Then the boundedness follows from the closed graph theorem. For this purpose let $(f_n)_{n\in\mathbb{N}} \subseteq H^{\frac{1}{2}}(\Sigma;\mathbb{C}^4)$ be a sequence such that $f_n \to f \in H^{\frac{1}{2}}(\Sigma;\mathbb{C}^4)$ in $H^{\frac{1}{2}}(\Sigma;\mathbb{C}^4)$ and $\gamma(\lambda)f_n \to g \in H^1(\mathbb{R}^3\setminus\Sigma;\mathbb{C}^4)$ in $H^1(\mathbb{R}^3\setminus\Sigma;\mathbb{C}^4)$. Since the embedding $H^{\frac{1}{2}}(\Sigma;\mathbb{C}^4) \hookrightarrow L^2(\Sigma;\mathbb{C}^4)$ is compact according to Theorem 2.29 there exists a constant $K > 0$ so that

$$\|f_n - f\|_{L^2(\Sigma;\mathbb{C}^4)} \leq K\|f_n - f\|_{H^{\frac{1}{2}}(\Sigma;\mathbb{C}^4)} \to 0$$

holds true and thus the convergence $f_n \to f$ in $L^2(\Sigma;\mathbb{C}^4)$ follows. Due to the boundedness of $\gamma(\lambda)$ as an operator from $L^2(\Sigma;\mathbb{C}^4)$ to $L^2(\mathbb{R}^3;\mathbb{C}^4)$, it follows that $\gamma(\lambda)f_n \to \gamma(\lambda)f$ in $L^2(\mathbb{R}^3;\mathbb{C}^4)$ is valid. On the other hand, from the continuous embedding $H^1(\Omega_\pm;\mathbb{C}^4) \hookrightarrow L^2(\Omega_\pm;\mathbb{C}^4)$ we obtain

$$\begin{aligned}\|\gamma(\lambda)f_n - g\|^2_{L^2(\mathbb{R}^3;\mathbb{C}^4)} &= \|(\gamma(\lambda)f_n)_+ - g_+\|^2_{L^2(\Omega_+;\mathbb{C}^4)} + \|(\gamma(\lambda)f_n)_- - g_-\|^2_{L^2(\Omega_-;\mathbb{C}^4)} \\ &\leq \|(\gamma(\lambda)f_n)_+ - g_+\|^2_{H^1(\Omega_+;\mathbb{C}^4)} + \|(\gamma(\lambda)f_n)_- - g_-\|^2_{H^1(\Omega_-;\mathbb{C}^4)} \\ &= \|\gamma(\lambda)f_n - g\|^2_{H^1(\mathbb{R}^3\setminus\Sigma;\mathbb{C}^4)} \to 0\end{aligned}$$

and thus $\gamma(\lambda)f = g$ in the sense of $L^2(\mathbb{R}^3;\mathbb{C}^4)$. This shows that the value of the γ-field $\gamma(\lambda)$ is closed as an operator from $H^{\frac{1}{2}}(\Sigma;\mathbb{C}^4)$ to $H^1(\mathbb{R}^3\setminus\Sigma;\mathbb{C}^4)$ and with Theorem 2.6 the claimed boundedness follows.

Step 3: From Theorem 2.18 and Theorem 3.8 it immediately follows that

$$\operatorname{dom}(M(\lambda)) = \operatorname{ran}(\Gamma_0) = H^{\frac{1}{2}}(\Sigma;\mathbb{C}^4)$$

and

$$\operatorname{ran}(M(\lambda)) \subseteq \operatorname{ran}(\Gamma_1) = H^{\frac{1}{2}}(\Sigma;\mathbb{C}^4)$$

are valid. This shows the mapping properties of $M(\lambda)$ from iii) and iv) and its dense definition.

Let $f \in H^{\frac{1}{2}}(\Sigma;\mathbb{C}^4)$ be given, then it follows from ii) that

$$\Phi_\lambda f = \gamma(\lambda)f \in H^1(\mathbb{R}^3\setminus\Sigma;\mathbb{C}^4)$$

holds true. By using Lemma 2.33 we therefore obtain that the non-tangential limits $C_\pm f$, which exist according to Theorem 3.10, coincide with the image of the trace operators $\tau_\pm(\gamma(\lambda)f)_\pm$. Consequently, it follows from the definition of the Weyl function, item i) and Theorem 3.10 that

$$M(\lambda)f = \Gamma_1\gamma(\lambda)f = \frac{1}{2}\left(\tau_+(\gamma(\lambda)f)_+ + \tau_-(\gamma(\lambda)f)_-\right) = \mathcal{C}_\lambda f$$

is valid, which shows the relationship $M(\lambda) = \mathcal{C}_\lambda \upharpoonright H^{\frac{1}{2}}(\Sigma;\mathbb{C}^4)$. This yields the claimed representation from iii) and the boundedness of $M(\lambda)$ on its domain of definition.

As $H^{\frac{1}{2}}(\Sigma;\mathbb{C}^4)$ is dense in $L^2(\Sigma;\mathbb{C}^4)$ and $M(\lambda)$ is bounded, we obtain

$$\operatorname{dom}\big(\overline{M(\lambda)}\big) = \overline{\operatorname{dom}\left(M(\lambda)\right)} = L^2(\Sigma;\mathbb{C}^4)$$

for the closure of $M(\lambda)$ and therefore immediately $\overline{M(\lambda)} = \mathcal{C}_\lambda$ follows.

To show the boundedness of $M(\lambda)$ as an operator in $H^{\frac{1}{2}}(\Sigma;\mathbb{C}^4)$ we first observe that $\gamma(\lambda)$ as an operator from $H^{\frac{1}{2}}(\Sigma;\mathbb{C}^4)$ to $H^1(\mathbb{R}^3\setminus\Sigma;\mathbb{C}^4)$ according to item ii) and the trace operators $\tau_\pm$ from $H^1(\Omega_\pm;\mathbb{C}^4)$ to $H^{\frac{1}{2}}(\Sigma;\mathbb{C}^4)$ according to Theorem 2.30 are bounded operators. Thus, the representation $M(\lambda) = \Gamma_1\gamma(\lambda)$ immediately leads to the claimed boundedness of $M(\lambda)$ as an operator in $H^{\frac{1}{2}}(\Sigma;\mathbb{C}^4)$. □

Next, we draw our attention to Dirac operators with electrostatic and Lorentz scalar δ-shell interactions. We intend to define these as self-adjoint operators $A_{\eta,\tau}$ in $L^2(\mathbb{R}^3;\mathbb{C}^4)$, which result from the formal differential expression

$$\mathcal{A}_{\eta,\tau} = A_0 + (\eta I_4 + \tau\beta)\,\langle\delta_\Sigma,\cdot\rangle\delta_\Sigma$$

with constant interaction strengths $\eta, \tau \in \mathbb{R}$. As mentioned in Chapter 1, we will construct these operators by using the quasi boundary triple of Theorem 3.8 as restrictions of the operator T and by imposing suitable jump conditions on the surface Σ. To find these jump conditions we proceed as in [12].

Since $C^\infty(\overline{\Omega_+}; \mathbb{C}^4) \oplus C^\infty(\overline{\Omega_-}; \mathbb{C}^4)$ is dense in $\mathrm{dom}(T) = H^1(\Omega_+; \mathbb{C}^4) \oplus H^1(\Omega_-; \mathbb{C}^4)$ we assume in the first step that an arbitrary function $f \in C^\infty(\overline{\Omega_+}; \mathbb{C}^4) \oplus C^\infty(\overline{\Omega_-}; \mathbb{C}^4)$ is given. In this case it is possible to consider point evaluations of the functions f. We define the effect of the δ-distribution on the function f in a symmetrical way as

$$\delta_\Sigma f = \frac{1}{2}\left(f_+ \upharpoonright \Sigma + f_- \upharpoonright \Sigma\right)$$

on Σ and thereby the assignment

$$\delta_\Sigma f \langle \delta_\Sigma, \varphi \rangle = \int\limits_\Sigma \frac{1}{2}\left(f_+ + f_-\right) \cdot \overline{\varphi} \mathrm{d}\sigma$$

for $\varphi \in \mathcal{D}(\mathbb{R}^3; \mathbb{C}^4)$ becomes a distribution. By this definition, $\mathcal{A}_{\eta,\tau} f$ can be regarded as a distribution and we find its effect on any test function $\varphi \in \mathcal{D}(\mathbb{R}^3; \mathbb{C}^4)$ as

$$\langle \mathcal{A}_{\eta,\tau} f, \varphi \rangle = \int\limits_{\mathbb{R}^3} f \cdot \overline{(-ic\alpha \cdot \nabla + mc^2\beta)\varphi} \mathrm{d}x + \int\limits_\Sigma \frac{1}{2}\left(\eta I_4 + \tau\beta\right)\left(f_+ + f_-\right) \cdot \overline{\varphi} \mathrm{d}\sigma. \quad (3.23)$$

On the other hand, it is expected that the effect of the δ-potentials for $x \notin \Sigma$ will not appear, as they are supported on Σ. Thus, using the divergence theorem and the fact that Σ is a zero set leads to

$$\begin{aligned}
\langle \mathcal{A}_{\eta,\tau} f, \varphi \rangle &= \int\limits_{\Omega_+ \cup \Omega_-} (-ic\alpha \cdot \nabla + mc^2\beta) f \cdot \overline{\varphi} \mathrm{d}x \\
&= \int\limits_{\Omega_+ \cup \Omega_-} f \cdot \overline{(-ic\alpha \cdot \nabla + mc^2\beta)\varphi} \mathrm{d}x - \int\limits_\Sigma ic(\alpha \cdot \nu)\left(f_+ - f_-\right) \cdot \overline{\varphi} \mathrm{d}\sigma \qquad (3.24) \\
&= \int\limits_{\mathbb{R}^3} f \cdot \overline{(-ic\alpha \cdot \nabla + mc^2\beta)\varphi} \mathrm{d}x - \int\limits_\Sigma ic(\alpha \cdot \nu)\left(f_+ - f_-\right) \cdot \overline{\varphi} \mathrm{d}\sigma
\end{aligned}$$

for all $\varphi \in \mathcal{D}(\mathbb{R}^3; \mathbb{C}^4)$ with the outer unit normal vector field $\nu = \nu_+ = -\nu_-$ on Σ.

A comparison of (3.23) and (3.24) and the density of the arbitrarily often differentiable functions suggests that the ansatz for the jump conditions

$$-ic(\alpha \cdot \nu)\left(\tau_+ f_+ - \tau_- f_-\right) = \frac{1}{2}\left(\eta I_4 + \tau\beta\right)\left(\tau_+ f_+ + \tau_- f_-\right) \quad (3.25)$$

for all functions $f \in \mathrm{dom}(A_{\eta,\tau}) \subseteq \mathrm{dom}(T) \cong H^1(\mathbb{R}^3 \setminus \Sigma; \mathbb{C}^4)$ on Σ seems plausible.

It should be pointed out that although the derivation of the jump conditions was not done in a mathematically rigorous way, Theorem 4.4 with the non-relativistic limit will show that the operators $A_{\eta,\tau}$ can be regarded as a relativistic counterpart of Schrödinger operators with δ-potentials. Therefore it can be expected that these jump conditions correctly model δ-potentials of Dirac operators.

To formulate the above jump conditions in a more compact form, we define the multiplication operator

$$\begin{aligned} \mathrm{dom}(B) &= L^2(\Sigma;\mathbb{C}^4) \\ Bf &= (\eta I_4 + \tau\beta)\, f \end{aligned} \tag{3.26}$$

in $L^2(\Sigma;\mathbb{C}^4)$. It can be shown by a component-wise consideration, as in [81, Satz 6.1], that B is a well-defined, linear, bounded and self-adjoint operator in $L^2(\Sigma;\mathbb{C}^4)$. Using the boundary maps Γ_0 and Γ_1 of the quasi boundary triple in Theorem 3.8, the above jump conditions are equivalent to

$$\Gamma_0 f + B\Gamma_1 f = 0$$

and we therefore define

$$A_{\eta,\tau} = T \upharpoonright \ker\left(\Gamma_0 + B\Gamma_1\right)$$

as our model operator for a Dirac operator with electrostatic and Lorentz scalar δ-shell interactions. It follows immediately from the considerations of Section 2.2 that $A_{\eta,\tau}$ is a symmetric extension of the operator S since B is self-adjoint.

At this point, it is noteworthy to remark that already the definition of the operator $A_{\eta,\tau}$ leads to an interesting observation. In the case of $\eta^2 - \tau^2 = -4c^2$, it can be shown as in [12, Lem. 3.1] that the operator $A_{\eta,\tau}$ decouples into two independent Dirac operators defined on $\Omega_\pm$. For the parameter combination $\eta = 0$ and $\tau = 2c$ the operator defined on Ω_+ corresponds to the MIT bag model operator of the quark confinement. Roughly speaking, this has the effect that a particle being inside Ω_+ remains in Ω_+ for all times and the δ-potential makes the surface Σ impenetrable for it. Since we will not consider these operators separately in this thesis, we refer to [56] and [40, Chapter 5.1] for a more detailed presentation.

Before we are able to further investigate the operators $A_{\eta,\tau}$, two more auxiliary results are required. The proof of the first result is based on the one of [12, Lem. 3.3], whereas we explicitly use the mapping properties of the values of the Weyl function from Theorem 3.11.

Lemma 3.12. Let $\lambda \in \rho(A_0)$ and $\eta, \tau \in \mathbb{R}$ with $\eta^2 - \tau^2 \neq 4c^2$ be given, then for a function $f \in L^2(\Sigma;\mathbb{C}^4)$ with

$$\left(I_4 + (\eta I_4 + \tau\beta)\,\mathcal{C}_\lambda\right) f \in H^{\frac{1}{2}}(\Sigma;\mathbb{C}^4)$$

it follows that $f \in H^{\frac{1}{2}}(\Sigma;\mathbb{C}^4)$ holds true.

Proof. Let $f \in L^2(\Sigma; \mathbb{C}^4)$ with the mentioned property be given, then it follows from Theorem 3.11 and the mapping properties of $M(\lambda)$ that

$$\begin{aligned}\Psi &= (I_4 - (\eta I_4 - \tau\beta)\,\mathcal{C}_\lambda)\,(I_4 + (\eta I_4 + \tau\beta)\,\mathcal{C}_\lambda)\,f \\ &= (I_4 - (\eta I_4 - \tau\beta M(\lambda)))\,(I_4 + (\eta I_4 + \tau\beta)\,\mathcal{C}_\lambda)\,f \in H^{\frac{1}{2}}(\Sigma; \mathbb{C}^4)\end{aligned}$$

holds true. On the other hand, we obtain

$$\Psi = \left(1 - \frac{\eta^2 - \tau^2}{4c^2}\right) f + \tau\,(\mathcal{C}_\lambda \beta + \beta \mathcal{C}_\lambda)\,f - \left(\eta^2 - \tau^2\right)\left((\mathcal{C}_\lambda)^2 - \frac{1}{4c^2} I\right) f$$

by explicit calculation of the expression for Ψ. A rearrangement of this equation with $\Psi \in H^{\frac{1}{2}}(\Sigma; \mathbb{C}^4)$ and the mapping properties of Theorem 3.10 leads to

$$f = \frac{4c^2}{4c^2 - \eta^2 + \tau^2}\left(\Psi - \tau\,(\mathcal{C}_\lambda\beta + \beta\mathcal{C}_\lambda)\,f + \left(\eta^2 - \tau^2\right)\left((\mathcal{C}_\lambda)^2 - \frac{1}{4c^2} I\right) f\right) \in H^{\frac{1}{2}}(\Sigma; \mathbb{C}^4)$$

which completes the proof. □

At this point it is important to remark that the difficulty in dealing with the critical case $\eta^2 - \tau^2 = 4c^2$ results from the requirement $\eta^2 - \tau^2 \neq 4c^2$ in Lemma 3.12, and we will therefore restrict ourselves in the following exclusively to the case of non-critical interaction strengths $\eta, \tau \in \mathbb{R}$ with $\eta^2 - \tau^2 \neq 4c^2$. At the end of this section we will briefly comment on the critical case.

The next result is of particular importance for the proof of the self-adjointness and an explicit representation of the resolvent of the operator $A_{\eta,\tau}$. For the proof of Lemma 3.13 we follow a line of reasoning as it can be found in [14, Prop. 5.2] and [40, Prop. 4.1.7].

Lemma 3.13. Let $\lambda \in \rho(A_0)$ with $\lambda \notin \sigma_p(A_{\pm\eta,\pm\tau})$ and interaction strengths $\eta, \tau \in \mathbb{R}$ which satisfy $\eta^2 - \tau^2 \neq 4c^2$ be given. Then the bounded operator $I + B\mathcal{C}_\lambda$ is bijective as a mapping in $L^2(\Sigma; \mathbb{C}^4)$ and the inverse operator is bounded as well. Furthermore, the bounded operator $I + BM(\lambda)$ as a mapping in $H^{\frac{1}{2}}(\Sigma; \mathbb{C}^4)$ is also continuously invertable.

Proof. *Step 1:* Suppose there exists an $f \in L^2(\Sigma; \mathbb{C}^4) \setminus \{0\}$ such that

$$(I + B\mathcal{C}_\lambda)f = 0$$

applies. Since $0 \in H^{\frac{1}{2}}(\Sigma; \mathbb{C}^4)$ holds true, Lemma 3.12 implies that $f \in H^{\frac{1}{2}}(\Sigma; \mathbb{C}^4)$ holds as well and thus we obtain

$$(I + BM(\lambda))f = 0$$

by Theorem 3.11. This shows $0 \in \sigma_p(I+BM(\lambda))$. In this case it follows from Theorem 2.19 that $\lambda \in \sigma_p(A_{\eta,\tau})$ is valid, which is a contradiction to the choice of λ. This shows the injectivity of the operator $I + B\mathcal{C}_\lambda : L^2(\Sigma;\mathbb{C}^4) \to L^2(\Sigma;\mathbb{C}^4)$.

Step 2: Next, we show the surjectivity of the operator $I+B\mathcal{C}_\lambda : L^2(\Sigma;\mathbb{C}^4) \to L^2(\Sigma;\mathbb{C}^4)$. For this purpose we consider the operator

$$I - (B\mathcal{C}_\lambda)^2 = (I + B\mathcal{C}_\lambda)(I - B\mathcal{C}_\lambda)$$

in $L^2(\Sigma;\mathbb{C}^4)$ and immediately obtain the range condition

$$\operatorname{ran}\left(I - (B\mathcal{C}_\lambda)^2\right) \subseteq \operatorname{ran}(I + B\mathcal{C}_\lambda) \tag{3.27}$$

from its definition. As the first step, we show the injectivity of the operator $I-(B\mathcal{C}_\lambda)^2$ and therefore assume that there exists an $f \in L^2(\Sigma;\mathbb{C}^4) \setminus \{0\}$ such that

$$0 = \left(I - (B\mathcal{C}_\lambda)^2\right) f = (I + B\mathcal{C}_\lambda)(I - B\mathcal{C}_\lambda) f$$

is valid. In this case $(I - B\mathcal{C}_\lambda) f \in \ker(I + B\mathcal{C}_\lambda)$ holds true and since $I + B\mathcal{C}_\lambda$ is injective according to Step 1 we obtain

$$(I - B\mathcal{C}_\lambda) f = 0.$$

With a line of reasoning as in Step 1, applied to $-B$, it then follows that $\lambda \in \sigma_p(A_{-\eta,-\tau})$ is valid which is a contradiction to the choice of λ. Thus, $I - (B\mathcal{C}_\lambda)^2$ is an injective operator.

An explicit computation now shows

$$I - (B\mathcal{C}_\lambda)^2 = \left(1 - \frac{\eta^2 - \tau^2}{4c^2}\right) I + \mathcal{K}_\lambda$$

with the linear and bounded operator

$$\mathcal{K}_\lambda = -\tau\left(\mathcal{C}_\lambda\beta + \beta\mathcal{C}_\lambda\right) B\mathcal{C}_\lambda - \left(\eta^2 - \tau^2\right)\left((\mathcal{C}_\lambda)^2 - \frac{1}{4c^2} I\right)$$

in $L^2(\Sigma;\mathbb{C}^4)$. Since $\mathcal{C}_\lambda$ is a bounded operator according to Theorem 3.9 and B is bounded as well, it follows from Theorem 3.10 and the properties of compact operators that $\mathcal{K}_\lambda$ is a compact operator in $L^2(\Sigma;\mathbb{C}^4)$. Fredholm's alternative, Theorem 2.3, therefore yields that $I-(B\mathcal{C}_\lambda)^2$ is a surjective operator in $L^2(\Sigma;\mathbb{C}^4)$ for $\eta^2 - \tau^2 \neq 4c^2$. By using the range condition (3.27) the surjectivity of the operator $I + B\mathcal{C}_\lambda$ follows and with Step 1 finally its bijectivity. The boundedness of the inverse operator then follows from Theorem 2.6 or the open mapping theorem.

Step 3: To complete this proof, we show the bijectivity of $I + BM(\lambda)$ as an operator in $H^{\frac{1}{2}}(\Sigma;\mathbb{C}^4)$ and its continuous invertibility. Since $I + B\mathcal{C}_\lambda$ is injective according to Step 1, this is also carried over to $I + BM(\lambda)$ due to $M(\lambda) = \mathcal{C}_\lambda \upharpoonright H^{\frac{1}{2}}(\Sigma;\mathbb{C}^4)$. To show its surjectivity we assume that a $g \in H^{\frac{1}{2}}(\Sigma;\mathbb{C}^4)$ is given. Due to the surjectivity of $I + B\mathcal{C}_\lambda$ according to Step 2 there exists an $f \in L^2(\Sigma;\mathbb{C}^4)$ such that

$$(I + B\mathcal{C}_\lambda)\, f = g$$

holds true. Furthermore, it follows from Lemma 3.12 and $g \in H^{\frac{1}{2}}(\Sigma;\mathbb{C}^4)$ that $f \in H^{\frac{1}{2}}(\Sigma;\mathbb{C}^4)$ is valid and therefore we obtain

$$(I + BM(\lambda)\, f = g$$

which shows the surjectivity of $I + BM(\lambda)$. The boundedness of the inverse operator follows from the boundedness of $I + BM(\lambda)$ as operator in $H^{\frac{1}{2}}(\Sigma;\mathbb{C}^4)$ according to Theorem 3.11 and from Theorem 2.6 or the open mapping theorem. □

As in the case of Lemma 3.12, the validity of Lemma 3.13 follows only in the case of non-critical interaction strengths $\eta, \tau \in \mathbb{R}$. If $\eta^2 - \tau^2 = 4c^2$ would be true, then Fredholm's alternative could not be applied in Step 2 in the proof of Lemma 3.13.

Now we will discuss to the main result of this section and show the self-adjointness of the operators $A_{\eta,\tau}$ in case of non-critical interaction strengths.

Theorem 3.14. Let non-critical interaction strengths $\eta, \tau \in \mathbb{R}$ with $\eta^2 - \tau^2 \neq 4c^2$ be given, then the symmetric operator

$$\begin{aligned} \operatorname{dom}(A_{\eta,\tau}) &= \Big\{ f \in H^1(\Omega_+;\mathbb{C}^4) \oplus H^1(\Omega_-;\mathbb{C}^4) \;\Big|\; \\ &\qquad ic\alpha\cdot\nu\,(\tau_+ f_+ - \tau_- f_-) + \frac{1}{2}\,(\eta I_4 + \tau\beta)\,(\tau_+ f_+ + \tau_- f_-) = 0 \Big\} \\ A_{\eta,\tau} f &= \big(-ic\alpha\cdot\nabla + mc^2\beta\big)\, f_+ \oplus \big(-ic\alpha\cdot\nabla + mc^2\beta\big)\, f_- \end{aligned} \tag{3.28}$$

is self-adjoint in $L^2(\mathbb{R}^3;\mathbb{C}^4)$. Furthermore $\lambda \in \rho(A_{\eta,\tau})$ applies to all $\lambda \in \rho(A_0)$ with $\lambda \notin \sigma_p(A_{\pm\eta,\pm\tau})$ and in this case the explicit resolvent representation

$$(A_{\eta,\tau} - \lambda)^{-1} f = (A_0 - \lambda)^{-1} f - \gamma(\lambda)\,(I + BM(\lambda))^{-1}\, B\gamma(\overline{\lambda})^* f \tag{3.29}$$

for all $f \in L^2(\mathbb{R}^3;\mathbb{C}^4)$ is valid.

Proof. Let $\lambda \in \rho(A_0)$ with $\lambda \notin \sigma_p(A_{\pm\eta,\pm\tau})$ be given. It follows immediately from Theorem 2.19 that the representation (3.29) is valid for all $f \in \operatorname{ran}(A_{\eta,\tau} - \lambda)$ and therefore it is sufficient to show the surjectivity of the operator $A_{\eta,\tau} - \lambda$. From Theorem 2.18 the range condition

$$\operatorname{ran}(\gamma(\lambda)^*) \subseteq \operatorname{ran}(\Gamma_1) = H^{\frac{1}{2}}(\Sigma;\mathbb{C}^4)$$

follows and thus, due to the definition of B as a multiplication operator with constants, also $B\gamma(\lambda)^* f \in H^{\frac{1}{2}}(\Sigma; \mathbb{C}^4)$ for all $f \in L^2(\mathbb{R}^3; \mathbb{C}^4)$. By using the bijectivity of $I + BM(\lambda)$ according to Lemma 3.13 we obtain

$$\operatorname{ran}(B\gamma(\lambda)^*) \subseteq \operatorname{ran}(I + BM(\lambda))$$

which in combination with Theorem 2.19 shows the range condition

$$\operatorname{ran}(A_{\eta,\tau} - \lambda) = L^2(\mathbb{R}^3; \mathbb{C}^4). \tag{3.30}$$

Consequently, $A_{\eta,\tau} - \lambda$ is a surjective operator from $\operatorname{dom}(A_{\eta,\tau})$ to $L^2(\mathbb{R}^3; \mathbb{C}^4)$. Furthermore, the choice $\lambda \notin \sigma_p(A_{\eta,\tau})$ shows the injectivity of $A_{\eta,\tau} - \lambda$ and thus all together its bijectivity. This shows $\lambda \in \rho(A_{\eta,\tau})$ and from Theorem 2.19 the resolvent representation (3.29) follows for all $f \in L^2(\mathbb{R}^3; \mathbb{C}^4)$.

To show the self-adjointness of the operator $A_{\eta,\tau}$ we choose an arbitrary $\lambda \in \mathbb{C} \setminus \mathbb{R}$. With Theorem 2.15, the self-adjointness of A_0 and the symmetry of $A_{\pm\eta,\pm\tau}$ we obtain that $\lambda \in \rho(A_0)$ and $\lambda \notin \sigma_p(A_{\pm\eta,\pm\tau})$ are valid. Therefore the range condition (3.30) is also valid in this case and an application of Theorem 2.12 then yields the claimed self-adjointness of $A_{\eta,\tau}$. □

Next, for the sake of completeness, we characterize the spectrum of the operators $A_{\eta,\tau}$ without providing any proofs. Item i) of the following result can be shown as in [40, Thm. 3.2.3] by using [62, Thm. XIII.14], while the proof of item iii) can be found in [12, Thm. 4.1 , Cor. 4.3]. For the proof of item ii) we refer to [12, Thm. 4.1] and [40, Thm. 3.2.3] with a slight modification of the argumentation as its carried out for instance in [15, Prop. 3.9].

Theorem 3.15. Let non-critical interactions strengths $\eta, \tau \in \mathbb{R}$ with $\eta^2 - \tau^2 \neq 4c^2$ be given, then the following statements are true.

i) $\sigma_{\mathrm{ess}}(A_{\eta,\tau}) = (-\infty, -mc^2] \cup [mc^2, \infty)$.

ii) $\sigma_{\mathrm{disc}}(A_{\eta,\tau}) \subseteq (-mc^2, mc^2)$ is a finite set.

iii) There exists a constant $K > 0$ independent of η and τ such that $\sigma_{\mathrm{disc}}(A_{\eta,\tau}) = \emptyset$ is valid if $|\eta \pm \tau| < K$ applies. If the interaction strengths additionally satisfy $\eta^2 - \tau^2 \neq 0$, then $\sigma_{\mathrm{disc}}(A_{\eta,\tau}) = \emptyset$ is valid as well if $|\eta \pm \tau| > \frac{4c^2}{K}$ applies.

To conclude this section, we will briefly discuss the case of critical interaction strengths $\eta, \tau \in \mathbb{R}$ with $\eta^2 - \tau^2 = 4c^2$ although they do not appear explicitly in this thesis. The reason for non-occurring critical interaction strengths is that the condition $\eta^2 - \tau^2 = 4c^2$ is valid only in a single point $c > 0$ and therefore does not influence the non-relativistic limit $c \to \infty$ which is of interest to us.

The case of critical interaction strengths is investigated for instance in [14] and [40, Chapter 4.3] and it turns out that the properties of Dirac operators with critical interaction strengths differ significantly from those with non-critical interaction strengths.

In particular, it can be shown that in the case of critical interaction strengths, the symmetric operator $A_{\eta,\tau}$ is not self-adjoint but only essentially self-adjoint in $L^2(\mathbb{R}^3;\mathbb{C}^4)$. In order to deduce properties of its self-adjoint closure $\overline{A_{\eta,\tau}}$ the decisive step is to consider the jump condition for functions in its domain of definition not in the sense of $L^2(\Sigma;\mathbb{C}^4)$ but in the larger space $H^{-\frac{1}{2}}(\Sigma;\mathbb{C}^4)$. This can be accomplished by transforming the quasi boundary triple of Theorem 3.8 into an ordinary boundary triple. By using this ordinary boundary triple it can be shown that the domain of definition of the self-adjoint operator $\overline{A_{\eta,\tau}}$ is not contained in $H^1(\mathbb{R}^3 \setminus \Sigma;\mathbb{C}^4)$ and depending on the geometry of the boundary $\Sigma = \partial\Omega$ it is possible that spectral values of the essential spectrum are located in the gap $(-mc^2, mc^2)$. For a more detailed presentation of these results we refer to the literature mentioned above.

Finally, it is noteworthy to remark that in case of two-dimensional Dirac operators with singular electrostatic and Lorentz scalar interactions supported on closed loops, a complete treatment is presented in [15]. In particular, a reduction of the regularity of the functions in the domain of the self-adjoint realizations is observed, as well as an additional point in the essential spectrum, which can be specified explicitly and can take any value within the spectral gap depending on the interaction strengths.

4 The non-relativistic limit

In this chapter we investigate the non-relativistic limit of the operators $A_{\eta,\tau}$ with constant interaction strengths $\eta, \tau \in \mathbb{R}$. The case $\eta + \tau \neq 0$ is considered in Section 4.1 and it is shown that the limit operator of the resolvent of $A_{\eta,\tau} - mc^2$ is the resolvent of a Schrödinger operator with a δ-interaction of strength $\eta + \tau$. Finally in the main part of this thesis, in Section 4.2, we investigate the case of interaction strengths which satisfy $\eta + \tau = 0$. It is shown that also in this case a Schrödinger operator is obtained as the limit operator. However, it turns out that this Schrödinger operator differs significantly in the characterization of the domain of definition from the one in the case of $\eta + \tau \neq 0$. In particular, on the interface Σ there are no jump conditions describing δ-interactions but oblique jump conditions.

4.1 The non-relativistic limit for $\eta + \tau \neq 0$

In this section we will investigate the behavior of the resolvents of the operators $A_{\eta,\tau}$ for $c \to \infty$ in the case of interaction strengths which satisfy $\eta + \tau \neq 0$. This will prove to be less complicated than the case $\eta + \tau = 0$, which we will investigate in the next section, since we will be able to apply results concerning Schrödinger operators from [18]. The cases $\eta = 0$ or $\tau = 0$ have already been investigated in [10, 12, 40] and the same line of reasoning can also be applied in the general case.

For interaction strengths $\eta, \tau \in \mathbb{R}$ with $\eta + \tau \neq 0$ we will be able to relate the resolvent of $A_{\eta,\tau} - mc^2$ to the one of a Schrödinger operator. In particular, it will be shown that there is a convergence to the resolvent of a Schrödinger operator with a δ-interaction of strength $\eta + \tau$ supported on Σ times a projection onto the first two components of the Dirac spinors. Furthermore, a convergence rate of $\mathcal{O}\left(c^{-1}\right)$ is found.

For this purpose, we first have to introduce a few concepts. In this section we will assume that $\Omega \subseteq \mathbb{R}^3$ is a bounded C^2-domain with boundary $\Sigma = \partial\Omega$ and we set $\Omega_+ = \Omega$ and $\Omega_- = \mathbb{R}^3 \setminus \overline{\Omega}$ to obtain two C^2-domains which satisfy $\mathbb{R}^3 = \Omega_+ \dot{\cup} \Sigma \dot{\cup} \Omega_-$. Furthermore, we choose the outer unit normal vector field $\nu = \nu_+ = -\nu_-$ on Σ and therewith define the normal derivative of a function $f \in H^2(\Omega_\pm; \mathbb{C})$ in analogy to the classical normal derivative of a differentiable function as

$$\partial_{\nu_\pm} f_\pm = \nu_\pm \cdot \tau(\nabla f_\pm) = \pm \nu \cdot \tau(\nabla f_\pm)$$

with $\tau_\pm$ being the trace operators on $\Omega_\pm$ from Theorem 2.30.

Next, we are going to discuss Schrödinger operators with δ-interactions, as we considered them for Dirac operators in the previous chapter. For a scalar quantity $a \in \mathbb{R}$, these interactions are modeled by the formal expression

$$\mathcal{T} = -\frac{1}{2m}\Delta + a\langle \delta_\Sigma, \cdot \rangle \delta_\Sigma \tag{4.1}$$

and also in the case of Schrödinger operators we can give rigorous meaning to this formal expression by imposing suitable jump conditions on Σ. We therefore define the linear operator

$$\begin{aligned} \operatorname{dom}(T_a) &= \Big\{ f \in H^2(\Omega_+;\mathbb{C}) \oplus H^2(\Omega_-;\mathbb{C}) \,\Big|\, \tau_+ f_+ = \tau_- f_- \text{ and} \\ &\qquad \frac{a}{2}(\tau_+ f_+ + \tau_- f_-) = \frac{1}{2m}(\partial_\nu f_+ - \partial_\nu f_-) \Big\} \\ T_a f &= \left(-\frac{1}{2m}\Delta f_+\right) \oplus \left(-\frac{1}{2m}\Delta f_-\right) \end{aligned} \tag{4.2}$$

and interpret it as a realization of the formal expression (4.1). As in the previous chapter, this operator can be regarded as an operator in $L^2(\mathbb{R}^3;\mathbb{C})$ by using the decomposition $L^2(\mathbb{R}^3;\mathbb{C}) \cong L^2(\Omega_+;\mathbb{C}) \oplus L^2(\Omega_-;\mathbb{C})$ from Section 2.6.

Next, we define the operator $\widetilde{\gamma}(\lambda) = \mathrm{SL}(\lambda) \restriction L^2(\Sigma;\mathbb{C})$ for $\lambda \in \mathbb{C} \setminus [0,\infty)$ with the single layer potential of the free Schrödinger operator (2.18) and, based on the considerations of Section 2.6, we obtain the explicit representation

$$\left(\widetilde{\gamma}(\lambda) f\right)(x) = \int_\Sigma K_\lambda(x-y) f(y) \mathrm{d}\sigma(y) \tag{4.3}$$

for all $f \in L^2(\Sigma;\mathbb{C})$ and almost all $x \in \mathbb{R}^3$. The integral kernel of $\widetilde{\gamma}(\lambda)$ corresponds to the function

$$K_\lambda(x) = \frac{2m}{4\pi\|x\|}\exp\left(i\sqrt{2m\lambda}\|x\|\right)$$

for all $x \in \mathbb{R}^3 \setminus \{0\}$. Due to the compact embedding $H^{-\frac{1}{2}}(\Gamma;\mathbb{C}) \hookrightarrow L^2(\Gamma;\mathbb{C})$ according to Theorem 2.29 and the continuous embedding $H^1(\mathbb{R}^3;\mathbb{C}) \hookrightarrow L^2(\mathbb{R}^3;\mathbb{C})$ it follows immediately that $\widetilde{\gamma}(\lambda)$ is a linear and bounded operator from $L^2(\Sigma;\mathbb{C})$ to $L^2(\mathbb{R}^3;\mathbb{C})$.

Analogous to $\widetilde{\gamma}(\lambda)$, we define the operator $\widetilde{M}(\lambda) = S(\lambda) \restriction L^2(\Sigma;\mathbb{C})$ with the single layer boundary integral operator and are led to the explicit representation

$$\left(\widetilde{M}(\lambda) f\right)(x) = \int_\Sigma K_\lambda(x-y) f(y) \mathrm{d}\sigma(y) \tag{4.4}$$

for all $f \in L^2(\Sigma;\mathbb{C})$ and allmost all $x \in \Sigma$. Furthermore, with the same line of reasoning as for $\widetilde{\gamma}(\lambda)$, we find that $\widetilde{M}(\lambda)$ is a linear and bounded operator in $L^2(\Sigma;\mathbb{C})$.

Applying the results [18, Thm. 3.5 , Thm. 3.6], which remain valid for the case of a C^2-domain, the following theorem can be shown.

Theorem 4.1. Let $a \in \mathbb{R}$ be a real number, then the following statements are true.

i) The operator T_a is self-adjoint in $L^2(\mathbb{R}^3; \mathbb{C})$.

ii) For all $\lambda \in \rho(T_a) \cap \rho(T_0)$ the explicit resolvent representation

$$(T_a - \lambda)^{-1} = (T_0 - \lambda)^{-1} - \widetilde{\gamma}(\lambda)(I + a\widetilde{M}(\lambda))^{-1} a \widetilde{\gamma}(\overline{\lambda})^*$$

in $L^2(\mathbb{R}^3; \mathbb{C})$ with $(I + a\widetilde{M}(\lambda))^{-1} \in \mathcal{L}(L^2(\Sigma; \mathbb{C}))$ is valid.

Before we discuss the non-relativistic limit of the operators $A_{\eta,\tau}$ we need to prove two more auxiliary results. We begin with an uniform boundedness result of a function which will appear in Theorem 4.3 and several times in the further course of this thesis.

Lemma 4.2. Let $\lambda \in \mathbb{C} \setminus \mathbb{R}$ be given, then for sufficiently large $c > 0$ the estimates

$$0 < \frac{1}{2}\left|\sqrt{2m\lambda}\right| \leq \left|\sqrt{t\frac{\lambda^2}{c^2} + 2m\lambda}\right| \leq \frac{3}{2}\left|\sqrt{2m\lambda}\right|$$

and

$$-\operatorname{Im}\left\{\sqrt{t\frac{\lambda^2}{c^2} + 2m\lambda}\right\} \leq -\frac{1}{2}\operatorname{Im}\left\{\sqrt{2m\lambda}\right\}$$

are valid for all $t \in [0, 1]$.

Proof. *Step 1:* For a given $\lambda \in \mathbb{C} \setminus \mathbb{R}$ we define the functions

$$f_c(t) = t\frac{\lambda^2}{c^2} + 2m\lambda$$

for $t \in [0, 1]$ and find that these functions converge uniformly on $[0, 1]$ to the constant function $f(t) = 2m\lambda$ for $c \to \infty$. Furthermore, for sufficiently large $c > 0$ the values of f_c and f are located in the same complex half-plane and with the continuity of the complex root on the latter we obtain the uniform convergence of the sequence of functions

$$g_c(t) = \sqrt{f_c(t)} = \sqrt{t\frac{\lambda^2}{c^2} + 2m\lambda}$$

on $[0, 1]$ to the constant function $g(t) = \sqrt{2m\lambda}$ with $\operatorname{Im}\{g\} > 0$ as well. By using the reversed triangle inequality we are therefore led to the inequalities

$$\begin{aligned}\frac{1}{2}\left|\sqrt{2m\lambda}\right| &= \frac{1}{2}\|g\|_{L^\infty([0,1],\mathbb{C})} \leq \|g\|_{L^\infty([0,1],\mathbb{C})} - \|g - g_c\|_{L^\infty([0,1],\mathbb{C})} \\ &\leq |g(t)| - |g(t) - g_c(t)| \leq |g_c(t)|\end{aligned}$$

and

$$\begin{aligned}|g_c(t)| &\leq |g(t)| + |g(t) - g_c(t)| \leq \|g\|_{L^\infty([0,1],\mathbb{C})} + \|g - g_c\|_{L^\infty([0,1],\mathbb{C})} \\ &\leq \frac{3}{2}\|g\|_{L^\infty([0,1],\mathbb{C})} = \frac{3}{2}\left|\sqrt{2m\lambda}\right|.\end{aligned}$$

for all $t \in [0,1]$ and sufficiently large $c > 0$. Combining these two estimates we finally obtain

$$0 < \frac{1}{2}\left|\sqrt{2m\lambda}\right| \leq \left|\sqrt{t\frac{\lambda^2}{c^2} + 2m\lambda}\right| \leq \frac{3}{2}\left|\sqrt{2m\lambda}\right|$$

for all $t \in [0,1]$ which proves the first inequality.

Step 2: As in Step 1 it follows from the continuity of the imaginary part that the sequence of functions $h_c = \mathrm{Im}\{g_c\}$ defined on $[0,1]$ converges uniformly to the constant function $h = \mathrm{Im}\{g\} = \mathrm{Im}\left\{\sqrt{2m\lambda}\right\} > 0$ and therefore the inequality

$$\begin{aligned}\frac{1}{2}\mathrm{Im}\left\{\sqrt{2m\lambda}\right\} &= \frac{1}{2}\|h\|_{L^\infty([0,1],\mathbb{C})} \leq \|h\|_{L^\infty([0,1],\mathbb{C})} - \|h - h_c\|_{L^\infty([0,1],\mathbb{C})} \\ &\leq h(t) - |h(t) - h_c(t)| \leq |h_c(t)| = h_c(t).\end{aligned}$$

is valid for all $t \in [0,1]$ and sufficiently large $c > 0$. In particular, we find

$$-\mathrm{Im}\left\{\sqrt{t\frac{\lambda^2}{c^2} + 2m\lambda}\right\} \leq -\frac{1}{2}\mathrm{Im}\left\{\sqrt{2m\lambda}\right\}$$

for all $t \in [0,1]$ which also shows the second inequality. □

Next, we draw our attention to a result which is crucial for the investigation of the non-relativistic limit in the case of $\eta + \tau \neq 0$. It is shown that if we perform the limit $c \to \infty$ the integral operators $\Phi_{\lambda+mc^2}$ and $\mathcal{C}_{\lambda+mc^2}$, defined as in (3.15) and (3.17), converge to the operators $\widetilde{\gamma}(\lambda)$ and $\widetilde{M}(\lambda)$ from (4.3) and (4.4). This enables us to determine the limit operator of $(A_{\eta,\tau} - (\lambda + mc^2))^{-1}$ for $c \to \infty$ using the resolvent representation from Theorem 3.14. Although a proof of the next result can be found in [10, Prop. 5.2] and [40, Lem. 4.4.2], we present it here to emphasize the necessity of a separate analysis of the case $\eta + \tau = 0$ in the non-relativistic limit.

Theorem 4.3. Let $\lambda \in \mathbb{C} \setminus \mathbb{R}$ be given and $\Phi_{\lambda+mc^2}$ and $\mathcal{C}_{\lambda+mc^2}$ be the linear and bounded integral operators defined as in (3.15) and (3.17). Furthermore, let $\widetilde{\gamma}(\lambda)$ and $\widetilde{M}(\lambda)$ the linear and bounded integral operators according to (4.3) and (4.4) and $P_+ = \mathrm{diag}(1,1,0,0)$ be a diagonal matrix. Then there exists a constant $\kappa(m,\lambda,\Sigma) > 0$ only depending on m, λ and Σ such that the following inequalities apply to sufficiently large $c > 0$

$$\left\|(A_0 - (\lambda + mc^2))^{-1} - (T_0 - \lambda)^{-1}P_+\right\| \leq \frac{\kappa}{c}, \tag{4.5}$$

$$\|\Phi_{\lambda+mc^2} - \widetilde{\gamma}(\lambda)P_+\| \leq \frac{\kappa}{c}, \tag{4.6}$$

$$\left\| \Phi^*_{\lambda+mc^2} - \widetilde{\gamma}(\lambda)^* P_+ \right\| \leq \frac{\kappa}{c}, \tag{4.7}$$

$$\left\| \mathcal{C}_{\lambda+mc^2} - \widetilde{M}(\lambda) P_+ \right\| \leq \frac{\kappa}{c}. \tag{4.8}$$

Proof. *Step 1:* Let $\lambda \in \mathbb{C} \setminus \mathbb{R}$ be given. Then it follows from the self-adjointness of the operators A_0 and T_0 that $\lambda, \lambda + mc^2 \in \rho(A_0) \cap \rho(T_0)$ is valid and therefore the operators $(A_0 - (\lambda + mc^2))^{-1}$ and $(T_0 - \lambda)^{-1}$ are well defined. Since all the occurring operators are integral operators, it is our approach to apply the results of Section 2.6. For this purpose we require estimates of the integral kernels.

By direct calculation one shows that the integral kernel of $(A_0 - (\lambda + mc^2))^{-1}$ of Theorem 3.4 is represented by

$$G_{\lambda+mc^2}(x) =$$
$$\left(\frac{\lambda}{c^2} I_4 + 2mP_+ + \left(1 - i\sqrt{\frac{\lambda^2}{c^2} + 2m\lambda}\|x\|\right) \frac{i}{c\|x\|^2}(\alpha \cdot x) \right) \frac{1}{4\pi\|x\|} \exp\left(i\sqrt{\frac{\lambda^2}{c^2} + 2m\lambda}\|x\| \right)$$

for all $x \in \mathbb{R}^3 \setminus \{0\}$. Furthermore, we define the matrix-valued functions

$$t_1(x) = \left(\frac{\lambda}{c^2} I_4 + \left(1 - i\sqrt{\frac{\lambda^2}{c^2} + 2m\lambda}\|x\|\right) \frac{i}{c\|x\|^2}(\alpha \cdot x) \right) \frac{1}{4\pi\|x\|} \exp\left(i\sqrt{\frac{\lambda^2}{c^2} + 2m\lambda}\|x\| \right)$$

and

$$t_2(x) = \frac{2m}{4\pi\|x\|} \left(\exp\left(i\sqrt{\frac{\lambda^2}{c^2} + 2m\lambda}\|x\| \right) - \exp\left(i\sqrt{2m\lambda}\|x\| \right) \right) P_+$$

for all $x \in \mathbb{R}^3 \setminus \{0\}$. By using that

$$K_\lambda(x) = \frac{2m}{4\pi\|x\|} \exp\left(i\sqrt{2m\lambda}\|x\| \right)$$

and due to the definition of the functions t_1 and t_2 we obtain the relation

$$G_{\lambda+mc^2}(x) - K_\lambda(x) P_+ = t_1(x) + t_2(x)$$

for all $x \in \mathbb{R}^3 \setminus \{0\}$.

Step 2: By using the Frobenius norm and Lemma 4.2 with $t = 1$ we obtain

$$\begin{aligned}
\|t_1(x)\|_F &\le \frac{1}{4\pi\|x\|}\exp\left(-\mathrm{Im}\left\{\sqrt{\frac{\lambda^2}{c^2}+2m\lambda}\right\}\|x\|\right)\cdot \\
&\qquad \left(\frac{2|\lambda|}{c^2}+\frac{1}{c\|x\|^2}\left(1+\left|\sqrt{\frac{\lambda^2}{c^2}+2m\lambda}\right|\|x\|\right)\sum_{j=1}^{3}\|\alpha_j\|_F|x_j|\right) \\
&\le \frac{1}{4\pi\|x\|}\exp\left(-\frac{1}{2}\mathrm{Im}\left\{\sqrt{2m\lambda}\right\}\|x\|\right)\cdot \\
&\qquad \left(\frac{2|\lambda|}{c^2}+\frac{1}{c\|x\|}\left(1+\frac{3}{2}\left|\sqrt{2m\lambda}\right|\|x\|\right)\right)\sum_{j=1}^{3}\|\alpha_j\|_F
\end{aligned} \tag{4.9}$$

for sufficiently large $c > 0$. In the case of $\|x\| < 1$ the inequality (4.9) implies the estimate

$$\begin{aligned}
\|t_1(x)\|_F &\le \frac{1}{4\pi\|x\|}\left(\frac{2|\lambda|}{c^2}+\frac{1}{c\|x\|}+\frac{3}{2c}\left|\sqrt{2m\lambda}\right|\right)\sum_{j=1}^{3}\|\alpha_j\|_F \\
&\le \frac{1}{4c\pi\|x\|^2}\left(1+\left(\frac{2|\lambda|}{c}+\frac{3}{2}\left|\sqrt{2m\lambda}\right|\right)\|x\|\right)\sum_{j=1}^{3}\|\alpha_j\|_F \\
&\le \frac{1}{4c\pi\|x\|^2}\left(1+2|\lambda|+\frac{3}{2}\left|\sqrt{2m\lambda}\right|\right)\sum_{j=1}^{3}\|\alpha_j\|_F
\end{aligned}$$

for all $c \ge 1$. On the other hand, in the case of $\|x\| \ge 1$ it follows from (4.9) that

$$\begin{aligned}
\|t_1(x)\|_F &\le \frac{1}{4\pi}\left(\frac{2|\lambda|}{c^2}+\frac{1}{c\|x\|}+\frac{3}{2c}\left|\sqrt{2m\lambda}\right|\right)\left(\sum_{j=1}^{3}\|\alpha_j\|_F\right)\exp\left(-\frac{1}{2}\mathrm{Im}\left\{\sqrt{2m\lambda}\right\}\|x\|\right) \\
&\le \frac{1}{4c\pi}\left(1+\frac{2|\lambda|}{c}+\frac{3}{2}\left|\sqrt{2m\lambda}\right|\right)\left(\sum_{j=1}^{3}\|\alpha_j\|_F\right)\exp\left(-\frac{1}{2}\mathrm{Im}\left\{\sqrt{2m\lambda}\right\}\|x\|\right) \\
&\le \frac{1}{4c\pi}\left(1+2|\lambda|+\frac{3}{2}\left|\sqrt{2m\lambda}\right|\right)\left(\sum_{j=1}^{3}\|\alpha_j\|_F\right)\exp\left(-\frac{1}{2}\mathrm{Im}\left\{\sqrt{2m\lambda}\right\}\|x\|\right)
\end{aligned}$$

applies to sufficiently large $c > 0$. Consequently, if we define the constants

$$k_1 = \frac{1}{4\pi}\left(1+2|\lambda|+\frac{3}{2}\left|\sqrt{2m\lambda}\right|\right)\sum_{j=1}^{3}\|\alpha_j\|_F \qquad \text{and} \qquad k_2 = \frac{1}{2}\mathrm{Im}\left\{\sqrt{2m\lambda}\right\}$$

which depend only on m and λ, then the estimation

$$\|t_1(x)\| \leq \frac{k_1}{c}\begin{cases}\|x\|^{-2} & \text{, for } \|x\| < 1 \\ e^{-k_2\|x\|} & \text{, for } \|x\| \geq 1\end{cases}$$

applies to all $x \in \mathbb{R}^3 \setminus \{0\}$ and sufficiently large $c > 0$.

Step 3: Let $x \in \mathbb{R}^3$ and $t \in [0,1]$ be given, then

$$\frac{\mathrm{d}}{\mathrm{d}t}\exp\left(i\sqrt{t\frac{\lambda^2}{c^2} + 2m\lambda}\|x\|\right) = \frac{i\lambda^2\|x\|}{2c^2}\frac{1}{\sqrt{t\frac{\lambda^2}{c^2} + 2m\lambda}}\exp\left(i\sqrt{t\frac{\lambda^2}{c^2} + 2m\lambda}\|x\|\right)$$

is valid and by applying Lemma 4.2 we find the estimate

$$\begin{aligned}\left|\frac{\mathrm{d}}{\mathrm{d}t}\exp\left(i\sqrt{t\frac{\lambda^2}{c^2} + 2m\lambda}\|x\|\right)\right| &= \frac{|\lambda|^2\|x\|}{2c^2}\frac{1}{\left|\sqrt{t\frac{\lambda^2}{c^2} + 2m\lambda}\right|}\exp\left(-\mathrm{Im}\left\{\sqrt{t\frac{\lambda^2}{c^2} + 2m\lambda}\right\}\|x\|\right) \\ &\leq \frac{|\lambda|^2\|x\|}{c^2}\frac{1}{\left|\sqrt{2m\lambda}\right|}\exp\left(-\frac{1}{2}\mathrm{Im}\left\{\sqrt{2m\lambda}\right\}\|x\|\right)\end{aligned}$$

for all $x \in \mathbb{R}^3$ and all $t \in [0,1]$. If we now define the constants

$$k_3 = \frac{|\lambda|^2}{\left|\sqrt{2m\lambda}\right|} \qquad \text{and} \qquad k_4 = -\frac{1}{2}\mathrm{Im}\left\{\sqrt{2m\lambda}\right\}$$

which depend only on m and λ, we are led to the estimate

$$\begin{aligned}\left|\exp\left(i\sqrt{\frac{\lambda^2}{c^2} + 2m\lambda}\|x\|\right) - \exp\left(i\sqrt{2m\lambda}\|x\|\right)\right| &\leq \int_0^1\left|\frac{\mathrm{d}}{\mathrm{d}t}\exp\left(i\sqrt{t\frac{\lambda^2}{c^2} + 2m\lambda}\|x\|\right)\right|\mathrm{d}t \\ &\leq \frac{k_3\|x\|}{c^2}\exp\left(-k_4\|x\|\right)\end{aligned}$$

for all $x \in \mathbb{R}^3$ by using the fundamental theorem of calculus. From the definition of t_2 we therefore obtain the estimation of the Frobenius norm

$$\begin{aligned}\|t_2(x)\|_F &= \frac{2\sqrt{2}m}{4\pi\|x\|}\left|\exp\left(i\sqrt{\frac{\lambda^2}{c^2} + 2m\lambda}\|x\|\right) - \exp\left(i\sqrt{2m\lambda}\|x\|\right)\right| \\ &\leq \frac{mk_3}{\sqrt{2}c^2\pi}e^{-k_4\|x\|} \leq \frac{mk_3}{\sqrt{2}c\pi}e^{-k_4\|x\|}\end{aligned}$$

for all $x \in \mathbb{R}^3 \setminus \{0\}$ and sufficiently large $c > 0$.

Step 4: We define the constants

$$k_5 = 2\max\left\{k_1, \frac{mk_3}{\sqrt{2\pi}}\right\} \qquad \text{and} \qquad k_6 = \min\{k_2, k_4\}$$

which depend only on m and λ and obtain with Steps 1,2 and 3 the estimate

$$\|G_{\lambda+mc^2}(x) - K_\lambda(x)P_+\| \leq \|t_1(x)\| + \|t_2(x)\| \leq \frac{k_5}{c}\begin{cases}\|x\|^{-2}, & \text{for } \|x\| < 1\\ e^{-k_6\|x\|}, & \text{for } \|x\| \geq 1\end{cases}$$

for all $x \in \mathbb{R}^3 \setminus \{0\}$ and sufficiently large $c > 0$. Since this is an estimation of the integral kernel of the value of the operator

$$\begin{aligned}\left(\left((A_0 - (\lambda + mc^2))^{-1} - (T_0 - \lambda)^{-1}P_+\right) f\right)(x)&\\ = \int_{\mathbb{R}^3} \left(G_{\lambda+mc^2}(x-y) - K_\lambda(x-y)P_+\right) f(y)\mathrm{d}y&\end{aligned}$$

for all $f \in L^2(\mathbb{R}^3;\mathbb{C}^4)$ and almost all $x \in \mathbb{R}^3$, an application of Theorem 2.34 yields the estimate

$$\left\|(A_0 - (\lambda + mc^2))^{-1} - (T_0 - \lambda)^{-1}P_+\right\| \leq \frac{k}{c}$$

for sufficiently large $c > 0$ with a constant $k(m, \lambda) > 0$ depending only on m and λ. This shows the first inequality (4.5).

Step 5: From the representation of $\Phi_{\lambda+mc^2}$ as in Theorem 3.9 and the one of $\widetilde{\gamma}(\lambda)$ according to (4.3) we obtain

$$\left(\left(\Phi_{\lambda+mc^2} - \widetilde{\gamma}(\lambda)P_+\right) f\right)(x) = \int_\Sigma \left(G_{\lambda+mc^2}(x-y) - K_\lambda(x-y)P_+\right) f(y)\mathrm{d}\sigma(y)$$

for all $f \in L^2(\Sigma;\mathbb{C}^4)$ and almost all $x \in \mathbb{R}^3$. In conclusion, by using the result of Step 4 and Theorem 2.36 the estimate

$$\|\Phi_{\lambda+mc^2} - \widetilde{\gamma}(\lambda)P_+\| \leq \frac{k}{c}$$

for sufficiently large $c > 0$ follows with a constant $k(m, \lambda, \Sigma) > 0$ only depending on m, λ and Σ. This shows the second inequality (4.6).

Step 6: Due to the boundedness of the occurring operators, Theorem 2.10 and Step 5 we are led to

$$\left\|\Phi^*_{\lambda+mc^2} - \widetilde{\gamma}(\lambda)^*P_+\right\| = \|\Phi_{\lambda+mc^2} - \widetilde{\gamma}(\lambda)P_+\| \leq \frac{k}{c}$$

by component-wise consideration. This shows the third inequality (4.7).

Step 7: Finally, let us consider the convergence of $\mathcal{C}_{\lambda+mc^2}$ for $c \to \infty$. By the definition of the integral kernel K_λ we immediately obtain the estimate

$$\|K_\lambda(x)\| \leq \frac{k}{\|x\|}$$

for all $x \in \Sigma \setminus \{0\}$ with a constant $k(m, \lambda) > 0$ only depending on m and λ. A line of reasoning as in Lemma 2.37 and the choice $g \equiv 1$ leads to

$$\int_\Sigma \int_\Sigma |K_\lambda(x-y)| \, \|f(y)\| \mathrm{d}\sigma(y) \mathrm{d}\sigma(x) < \infty$$

for all $f \in L^2(\Sigma; \mathbb{C}^4)$ and thus

$$\int_\Sigma |K_\lambda(x-y)| \, \|f(y)\| \mathrm{d}\sigma(y) < \infty$$

follows for almost all $x \in \Sigma$. Consequently, the dominated convergence theorem can be applied and we obtain the representation

$$\left(\left(\mathcal{C}_{\lambda+mc^2} - \widetilde{M}(\lambda) P_+\right) f\right)(x) = \lim_{\varepsilon \to 0^+} \int_{\Sigma \setminus B(x,\varepsilon)} \left(G_{\lambda+mc^2}(x-y) - K_\lambda(x-y) P_+\right) f(y) \mathrm{d}\sigma(y)$$

for all $f \in L^2(\Sigma; \mathbb{C}^4)$ and for almost all $x \in \Sigma$. Next, we define the matrix-valued functions

$$\begin{aligned}
u_1(x) &= \left(\frac{\lambda}{c^2} I_4 + \sqrt{\frac{\lambda^2}{c^2} + 2m\lambda} \frac{1}{c\|x\|} \alpha \cdot x\right) \frac{1}{4\pi\|x\|} \exp\left(i\sqrt{\frac{\lambda^2}{c^2} + 2m\lambda} \|x\|\right) \\
u_2(x) &= \frac{2m}{4\pi\|x\|} \left(\exp\left(i\sqrt{\frac{\lambda^2}{c^2} + 2m\lambda} \|x\|\right) - \exp\left(i\sqrt{2m\lambda}\|x\|\right)\right) P_+ = t_2(x) \\
u_3(x) &= \frac{i}{4\pi c\|x\|^3} \alpha \cdot x \left(\exp\left(i\sqrt{\frac{\lambda^2}{c^2} + 2m\lambda} \|x\|\right) - 1\right) \\
u_4(x) &= \frac{i}{4\pi c\|x\|^3} \alpha \cdot x
\end{aligned}$$

for $x \in \mathbb{R}^3 \setminus \{0\}$ and immediately obtain

$$\|u_2(x)\| = \|t_2(x)\| \leq \frac{k_1}{c} e^{-k_2\|x\|} \leq \frac{k_1}{c}$$

due to Step 3 with a constant $k_1(m,\lambda) > 0$ only depending on m and λ.

For u_1 we proceed as in the proof of Theorem 3.9 Step 2 and obtain with Lemma 4.2 and $t = 1$ the estimation of the Frobenius norm

$$\begin{aligned} \|u_1(x)\|_F &\le \frac{1}{4\pi\|x\|}\left(2\frac{|\lambda|}{c^2} + \left|\sqrt{\frac{\lambda^2}{c^2} + 2m\lambda}\right| \frac{1}{c}\sum_{j=1}^{3}\|\alpha_j\|_F\right) \\ &\le \frac{1}{4\pi\|x\|}\left(2\frac{|\lambda|}{c^2} + \frac{3}{2}\left|\sqrt{2m\lambda}\right| \frac{1}{c}\sum_{j=1}^{3}\|\alpha_j\|_F\right) \\ &\le \frac{1}{4c\pi\|x\|}\left(2\,|\lambda| + \frac{3}{2}\left|\sqrt{2m\lambda}\right| \sum_{j=1}^{3}\|\alpha_j\|_F\right) \\ &= \frac{k_2}{c\|x\|} \end{aligned}$$

for sufficiently large $c > 0$ with the constant

$$k_2 = \frac{1}{4\pi}\left(2\,|\lambda| + \frac{3}{2}\left|\sqrt{2m\lambda}\right| \sum_{j=1}^{3}\|\alpha_j\|_F\right)$$

which depends only on m and λ.

To estimate u_3 we again apply the same procedure as in the proof of Theorem 3.9 Step 2 and obtain with Lemma 4.2 and $t = 1$ the estimation of the Frobenius norm

$$\begin{aligned} \|u_3(x)\|_F &\le \frac{1}{4\pi c\|x\|^2}\left|\exp\left(i\sqrt{\frac{\lambda^2}{c^2} + 2m\lambda}\|x\|\right) - 1\right| \sum_{j=1}^{3}\|\alpha_j\|_F \\ &\le \frac{1}{4\pi c\|x\|}\left|\sqrt{\frac{\lambda^2}{c^2} + 2m\lambda}\right| \sum_{j=1}^{3}\|\alpha_j\|_F \\ &\le \frac{1}{4\pi c\|x\|}\frac{3}{2}\left|\sqrt{2m\lambda}\right| \sum_{j=1}^{3}\|\alpha_j\|_F \\ &= \frac{k_3}{c\|x\|} \end{aligned}$$

for sufficiently large $c > 0$ with the constant

$$k_3 = \frac{3}{8\pi}\left|\sqrt{2m\lambda}\right| \sum_{j=1}^{3}\|\alpha_j\|_F$$

which depends only on m and λ.

It now follows from Theorem 2.36 that the assignments

$$\left(U_j f\right)(x) = \int\limits_{\Sigma} u_j(x-y) f(y) \mathrm{d}y$$

for $f \in L^2(\Sigma; \mathbb{C}^4)$ and $x \in \Sigma$ correspond to well-defined, linear and bounded operators $U_j : L^2(\Sigma; \mathbb{C}^4) \to L^2(\Sigma; \mathbb{C}^4)$ for all $j \in \{1, 2, 3\}$. Furthermore there exists a constant $k(m, \lambda, \Sigma) > 0$ only depending on m, λ and Σ such that the estimate

$$\|U_j\| \leq \frac{k}{c}$$

is valid for all $j \in \{1, 2, 3\}$. By using a similar reasoning as at the beginning of Step 7, we obtain the representation

$$\left(U_j f\right)(x) = \lim_{\varepsilon \to 0+} \int\limits_{\Sigma \setminus B(x,\varepsilon)} u_j(x-y) f(y) \mathrm{d}y$$

for all $f \in L^2(\Sigma; \mathbb{C}^4)$ and almost all $x \in \Sigma$ based on the above estimates of u_j and the dominated convergence theorem.

Step 8: To conclude the proof of this theorem we will show the boundedness of the integral operator generated by u_4. By component-wise consideration it follows from Theorem 2.38 that the assignment

$$\left(U_4 f\right)(x) = \lim_{\varepsilon \to 0+} \int\limits_{\Sigma \setminus B(x,\varepsilon)} u_4(x-y) f(y) \mathrm{d}\sigma(y)$$

for $f \in L^2(\Sigma; \mathbb{C}^4)$ and $x \in \Sigma$ corresponds to a well-defined, linear and bounded operator $U_4 : L^2(\Sigma; \mathbb{C}^4) \to L^2(\Sigma; \mathbb{C}^4)$. Furthermore, the estimate

$$\|U_4\| \leq \frac{K}{c}$$

with a constant $K(\Sigma) > 0$ only dependent on Σ applies to this operator. As the decomposition

$$G_{\lambda+mc^2}(x) - K_\lambda(x) P_+ = u_1(x) + u_2(x) + u_3(x) + u_4(x)$$

is valid for all $x \in \Sigma \setminus \{0\}$ we obtain

$$\mathcal{C}_{\lambda+mc^2} - \widetilde{M}(\lambda) P_+ = \sum_{j=1}^{4} U_j$$

and thus finally

$$\left\| \mathcal{C}_{\lambda+mc^2} - \widetilde{M}(\lambda)P_+ \right\| \le \sum_{j=1}^{4} \|U_j\| \le \frac{\kappa}{c}$$

with a constant $\kappa(m, \lambda, \Sigma) > 0$ only depending on m, λ and Σ. This proves the fourth inequality (4.8) and completes the proof of the theorem. □

Finally we draw our attention to the main result of this section, the non-relativistic limit for the parameter combination $\eta+\tau \neq 0$ of the interaction strengths. Our ansatz for the limit operator is motivated by the following physical consideration. Intuitively we expect that by removing the limiting speed c for relativistic quantum particles with spin $1/2$, the description by a Dirac operator changes to the description by a Schrödinger operator. Since no energy states with negative energy are possible for non-relativistic quantum particles, the spinor wave functions for these must be zero. As shown in [78, Chapter 1.4.5] the wave functions of the negative energy states correspond precisely to the last two components of a four-element Dirac spinor after a spectral transformation. Therefore, taking the δ-shell interactions into account, the formal ansatz

$$\mathcal{T} = -\frac{1}{2m}\Delta + (\eta + \tau)\langle \delta_\Sigma, \cdot \rangle \delta_\Sigma \tag{4.10}$$

for the limit operator for the first two components of the Dirac spinors seems plausible. The next result will show that this formal differential expression actually generates an operator in $L^2(\mathbb{R}^3; \mathbb{C}^2)$ which is the limit operator. The proof for $\tau = 0$ can be found in [10, Thm. 5.3] and [40, Thm. 4.4.3] and also for the general case of constant interaction strengths $\eta, \tau \in \mathbb{R}$ with $\eta+\tau \neq 0$ the strategy followed there can be applied. It should be noted that in the following we will always assume that $c > 0$ is sufficiently large so that $\eta^2 - \tau^2 \neq 4c^2$ applies and therefore no critical interaction strengths are given. This requirement can always be met, since the interaction strengths are constant.

Theorem 4.4. Let $\lambda \in \mathbb{C} \setminus \mathbb{R}$ and non-critical interaction strengths $\eta, \tau \in \mathbb{R}$ with $\eta + \tau \neq 0$ and $\eta^2 - \tau^2 \neq 4c^2$ be given. Furthermore, let $A_{\eta,\tau}$ be the self-adjoint Dirac operator defined as in (3.28) and $T_{\eta+\tau}$ be the self-adjoint Schrödinger operator according to (4.2), then there exists a constant $\kappa(m, \lambda, \eta, \tau, \Sigma) > 0$ only dependent on m, λ, η, τ and Σ such that the following estimate is valid for sufficiently large $c > 0$,

$$\left\| \left(A_{\eta,\tau} - (\lambda + mc^2)\right)^{-1} - \left(T_{\eta+\tau} - \lambda\right)^{-1} P_+ \right\| \le \frac{\kappa}{c}.$$

In particular, the convergence

$$\left(A_{\eta,\tau} - (\lambda + mc^2)\right)^{-1} \to \begin{pmatrix} \left(T_{\eta+\tau} - \lambda\right)^{-1} I_2 & 0 \\ 0 & 0 \end{pmatrix} \quad \text{for } c \to \infty$$

in the operator norm applies as well as a convergence rate of $\mathcal{O}\left(\frac{1}{c}\right)$.

Proof. *Step 1:* Due to the choice of $\lambda \in \mathbb{C} \setminus \mathbb{R}$ we conclude from the self-adjointness of the operators $A_{\eta,\tau}$ and $T_{\eta+\tau}$ and Theorem 2.15 that $\lambda + mc^2 \in \rho(A_0) \cap \rho(A_{\eta,\tau})$ and $\lambda \in \rho(T_0) \cap \rho(T_{\eta+\tau})$ are valid. According to Theorem 4.3 there exists a constant $\kappa_1(m, \lambda, \Sigma) > 0$ only dependent on m, λ and Σ such that for sufficiently large $c > 0$

$$\left\| \mathcal{C}_{\lambda+mc^2} - \widetilde{M}(\lambda) P_+ \right\| \leq \frac{\kappa_1}{c}$$

holds true. As before, we define B as the self-adjoint multiplication operator in $L^2(\Sigma; \mathbb{C}^4)$ by the matrix $\eta I_4 + \tau\beta$ and therefore, from the boundedness of all the occurring operators, we obtain the estimate

$$\begin{aligned} &\left\| (I + B\mathcal{C}_{\lambda+mc^2}) - \left(I + B\widetilde{M}(\lambda) P_+ \right) \right\| \\ &= \left\| B \left(\mathcal{C}_{\lambda+mc^2} - \widetilde{M}(\lambda) P_+ \right) \right\| \leq \|B\| \left\| \mathcal{C}_{\lambda+mc^2} - \widetilde{M}(\lambda) P_+ \right\| \leq \|B\| \frac{\kappa_1}{c} = \frac{\kappa_2}{c} \end{aligned} \tag{4.11}$$

with the constant $\kappa_2(m, \lambda, \eta, \tau, \Sigma) = \|B\| \kappa_1(m, \lambda, \Sigma)$ only dependent on m, λ, η , τ and Σ. Due to Theorem 4.1

$$\left(I + B\widetilde{M}(\lambda) P_+ \right)^{-1} \in \mathcal{L}(L^2(\Sigma; \mathbb{C}^4))$$

follows by component-wise consideration and by setting

$$T = I + B\widetilde{M}(\lambda) P_+$$

and

$$A = (I + B\mathcal{C}_{\lambda+mc^2}) - \left(I + B\widetilde{M}(\lambda) P_+ \right) = B \left(\mathcal{C}_{\lambda+mc^2} - \widetilde{M}(\lambda) P_+ \right)$$

we obtain with (4.11) the estimate $\|A\| \|T^{-1}\| < 1$ for sufficiently large $c > 0$. If we now define the operator

$$S = A + T = I + B\mathcal{C}_{\lambda+mc^2}$$

then it follows from Theorem 2.8 and (4.11) that

$$\begin{aligned} \left\| (I + B\mathcal{C}_{\lambda+mc^2})^{-1} - \left(I + B\widetilde{M}(\lambda) P_+ \right)^{-1} \right\| &\leq \frac{\|T^{-1}\|^2 \|A\|}{1 - \|A\| \|T^{-1}\|} \\ &\leq \frac{\frac{\kappa_2}{c} \|T^{-1}\|^2}{1 - \frac{\kappa_2}{c} \|T^{-1}\|} \\ &\leq \frac{2\kappa_2 \|T^{-1}\|^2}{c} \end{aligned}$$

is valid for sufficiently large $c > 0$ with $\frac{\kappa_2}{c} \|T^{-1}\| \leq \frac{1}{2}$.

Step 2: From Theorem 4.3 and Step 1 the estimates

$$\|\Phi_{\lambda+mc^2}\| \le 1 + \|\widetilde{\gamma}(\lambda)P_+\| = K_1 \tag{4.12}$$

and

$$\left\|(I + B\mathcal{C}_{\lambda+mc^2})^{-1}\right\| \le 1 + \left\|\left(I + B\widetilde{M}(\lambda)P_+\right)^{-1}\right\| = K_2 \tag{4.13}$$

follow for sufficiently large $c > 0$ due to the triangle inequality. The constants $K_1(m, \lambda, \Sigma) \ge 1$ and $K_2(m, \lambda, \eta, \tau, \Sigma) \ge 1$ are only dependent on m, λ, η, τ and Σ.

Next, we use the explicit resolvent representations of the operators $A_{\eta,\tau}$ and $T_{\eta+\tau}$. For the Dirac operator it is given by

$$\begin{aligned}
&\left(A_{\eta,\tau} - (\lambda + mc^2)\right)^{-1} \\
&= \left(A_0 - (\lambda + mc^2)\right)^{-1} - \gamma(\lambda + mc^2)\left(I + BM(\lambda + mc^2)\right)^{-1} B\gamma(\overline{\lambda} + mc^2)^* \\
&= \left(A_0 - (\lambda + mc^2)\right)^{-1} - \Phi_{\lambda+mc^2}\left(I + B\mathcal{C}_{\lambda+mc^2}\right)^{-1} B\Phi^*_{\overline{\lambda}+mc^2}
\end{aligned}$$

according to Theorem 3.11 and Theorem 3.14 and for the Schrödinger operator by

$$\begin{aligned}
(T_{\eta+\tau} - \lambda)^{-1}P_+ &= (T_0 - \lambda)^{-1}P_+ - \widetilde{\gamma}(\lambda)P_+\left(I + (\eta+\tau)\widetilde{M}(\lambda)P_+\right)^{-1}(\eta+\tau)\widetilde{\gamma}(\overline{\lambda})^*P_+ \\
&= (T_0 - \lambda)^{-1}P_+ - \widetilde{\gamma}(\lambda)P_+\left(I + B\widetilde{M}(\lambda)P_+\right)^{-1} B\widetilde{\gamma}(\overline{\lambda})^*P_+
\end{aligned}$$

due to Theorem 4.1. By using (4.12) and (4.13) and applying the triangle inequality several times, these two resolvent representations lead to the estimate

$$\begin{aligned}
&\left\|\left(A_{\eta,\tau} - (\lambda + mc^2)\right)^{-1} - (T_{\eta+\tau} - \lambda)^{-1}P_+\right\| \le \left\|\left(A_0 - (\lambda + mc^2)\right)^{-1} - (T_0 - \lambda)^{-1}P_+\right\| \\
&\qquad + \max\{K_1, K_2\}^2\|B\|\Bigg(\|\Phi_{\lambda+mc^2} - \widetilde{\gamma}(\lambda)P_+\| + \left\|\Phi^*_{\overline{\lambda}+mc^2} - \widetilde{\gamma}(\overline{\lambda})^*P_+\right\| \\
&\qquad + \left\|(I + B\mathcal{C}_{\lambda+mc^2})^{-1} - \left(I + B\widetilde{M}(\lambda)P_+\right)^{-1}\right\|\Bigg)
\end{aligned}$$

for sufficiently large $c > 0$. Finally combining Theorem 4.3 and Step 1 yields

$$\left\|(A_{\eta,\tau} - \lambda)^{-1} - (T_{\eta+\tau} - \lambda)^{-1}P_+\right\| \le \frac{K}{c}$$

with a constant $K(m, \lambda, \eta, \tau, \Sigma) > 0$ only depending on m, λ, η, τ and Σ. This completes the proof. □

We conclude this section with a comment on the case of interaction strengths $\eta, \tau \in \mathbb{R}$ which satisfy $\eta + \tau = 0$. If one examines the proof of Theorem 4.4, then it is evident that it relies heavily on the result of Theorem 4.3. In fact, for each value $\lambda \in \mathbb{C} \setminus \mathbb{R}$ the integral kernel of the resolvent of the Dirac operator $A_{\eta,\tau}$ is represented as

$$G_{\lambda+mc^2}(x) =$$
$$\left(\frac{\lambda}{c^2} I_4 + 2mP_+ + \left(1 - i\sqrt{\frac{\lambda^2}{c^2} + 2m\lambda}\|x\|\right) \frac{i}{c\|x\|^2}(\alpha \cdot x)\right) \frac{1}{4\pi\|x\|} \exp\left(i\sqrt{\frac{\lambda^2}{c^2} + 2m\lambda}\|x\|\right)$$

and as the proof of Theorem 4.3 shows, the integral kernel of the limit operator must have a form such as $K_\lambda P_+$. If we define the diagonal matrix $P_- = \operatorname{diag}(0,0,1,1)$, then for interaction strengths $\eta, \tau \in \mathbb{R}$ with $\eta + \tau = 0$ and $\eta - \tau \neq 0$

$$B\widetilde{\gamma}(\overline{\lambda})^* P_+ = (\eta - \tau)\widetilde{\gamma}(\overline{\lambda})^* P_- P_+ = 0$$

would would be valid. As in the proof of Theorem 4.4, we therefore obtain the convergence

$$\left(A_{\eta,\tau} - (\lambda + mc^2)\right)^{-1} \to (T_0 - \lambda)^{-1} P_+$$

for $c \to \infty$ which is also suggested by the formal differential expression (4.10).

However, this description of the δ-shell interactions and the execution of the limiting process $c \to \infty$ are strongly connected to the scaling of the interaction strengths by the chosen quasi boundary triple of Section 3.2 and therefore it cannot be ruled out that a different description of the δ-shell interactions might give a different result. We will address this question in the next section, using a different approach than the one described in this section. Roughly speaking, we will investigate interaction strengths $\eta, \tau \in \mathbb{R}$ whose difference is located on the parabola εc^2 for an $\varepsilon \in \mathbb{R}$ and consider the limit $c \to \infty$ for these. This means that we change the strength of interaction along with the constant c. This approach is strongly motivated by known results for Dirac operators with electrostatic and Lorentz scalar δ-point interactions in one dimension.

4.2 The non-relativistic limit for $\eta + \tau = 0$

In this last section we will investigate the non-relativistic limit of Dirac operators $A_{\eta,\tau}$ in the case of constant interaction strengths $\eta, \tau \in \mathbb{R}$ which satisfy $\eta + \tau = 0$. While the case of interaction strengths $\eta, \tau \in \mathbb{R}$ with $\eta + \tau \neq 0$ has already been investigated in [10, 12, 40] and in Section 4.1, the case $\eta + \tau = 0$ has not yet been considered.

The procedure in this section is as follows. First, the explicit resolvent representation of $A_{\eta,\tau} - mc^2$ according to Theorem 3.14 is rewritten by suitable multiplication operators. This is inspired by a technique in [11]. Furthermore, a rescaling of the interaction strengths is performed. Next, it is shown with the results of Section 2.6 that the modified resolvent of $A_{\eta,\tau} - mc^2$ converges to the resolvent of the free Schrödinger operator and a perturbation term which is composed of certain integral operators. By applying the result of Section 2.3, this bounded limit operator can be characterized as the resolvent of a self-adjoint Schrödinger operator. It turns out that this Schrödinger operator differs significantly in the characterization of the domain of definition from the one in the case of $\eta + \tau \neq 0$. In particular, on the interface Σ there are no jump conditions describing δ-interactions but oblique jump conditions.

As in the previous sections, we will always assume in the following that a bounded C^2-domain $\Omega \subseteq \mathbb{R}^3$ with boundary $\Sigma = \partial\Omega$ is given. We set $\Omega_+ = \Omega$ and $\Omega_- = \mathbb{R}^3 \setminus \overline{\Omega}$ and thereby obtain two C^2-domains which satisfy $\mathbb{R}^3 = \Omega_+ \dot\cup \Sigma \dot\cup \Omega_-$. Furthermore, we choose the outer unit normal vector field $\nu = \nu_+ = -\nu_-$on Σ.

In order to motivate our procedure in this section we change the quasi boundary triple of Section 3.2 by the assignment

$$\widetilde{\Gamma}_0 = \frac{1}{c}\Gamma_0 \quad \text{and} \quad \widetilde{\Gamma}_1 = c\Gamma_1$$

with the boundary maps Γ_0 and Γ_1 from Theorem 3.8. Analogous to the proof of Theorem 3.8 it can now be shown that these boundary maps and $L^2(\Sigma;\mathbb{C}^4)$ provide a quasi boundary triple for the Dirac operator S^* as well and all results from the previous sections remain valid if we replace the operators Φ_λ and $\mathcal{C}_\lambda$ defined as in (3.15) and (3.17) by the operators

$$\widetilde{\Phi}_\lambda = c\Phi_\lambda \quad \text{and} \quad \widetilde{\mathcal{C}}_\lambda = c^2\mathcal{C}_\lambda.$$

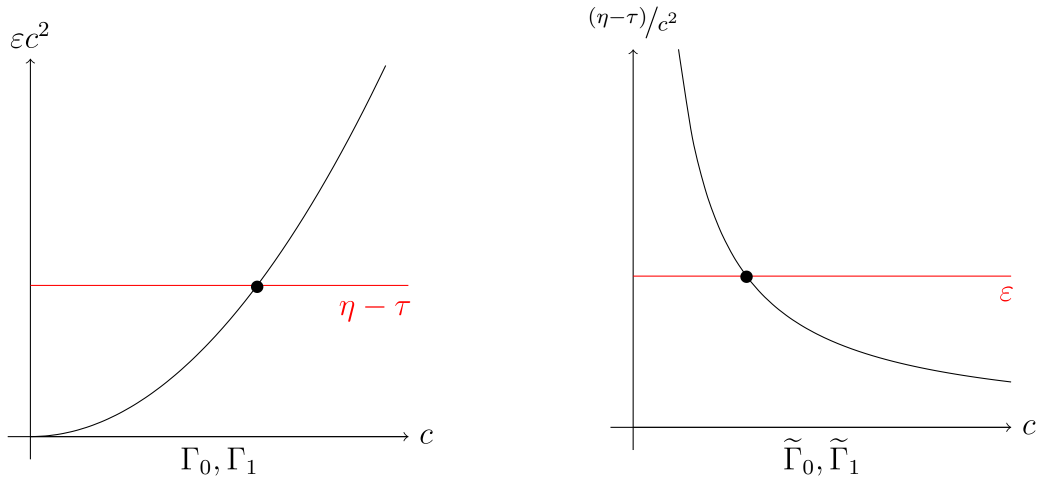
Thus, for a given $f \in L^2(\mathbb{R}^3;\mathbb{C}^4)$

$$f \in \ker(\Gamma_0 + B\Gamma_1) \iff f \in \ker(\widetilde{\Gamma}_0 + \widetilde{B}\widetilde{\Gamma}_1)$$

with the multiplication operator $\widetilde{B}$ in $L^2(\Sigma;\mathbb{C}^4)$, defined as multiplication by the matrix $\frac{1}{c^2}(\eta I_4 + \tau\beta)$, is valid. In particular, we obtain for the constant interaction strengths $\eta, \tau \in \mathbb{R}$ with $\eta + \tau = 0$

$$\frac{1}{c^2}(\eta I_4 + \tau\beta) = \frac{\eta - \tau}{c^2} P_-$$

with the diagonal matrix $P_- = \operatorname{diag}(0,0,1,1)$. Therefore we may equivalently describe electrostatic and Lorentz scalar δ-shell interactions in this situation by the parameter $\varepsilon = \frac{\eta-\tau}{c^2}$. At this point it should be noted that both descriptions only give the same Dirac operator $A_{\eta,\tau}$ for a certrain c-value, marked by the dot in the following graph, and therefore provide an equivalent way of defining electrostatic and Lorentz scalar δ-shell interactions.



By changing the speed of light c, as we will do in the calculation of the non-relativistic limit, we generally obtain different operators. In particular, the interaction strengths in the description in terms of the boundary maps Γ_0, Γ_1 change according to the red line in the left graph, while the red line in the right graph represents the change of the interactions strengths described in terms of $\widetilde{\Gamma}_0, \widetilde{\Gamma}_1$. The behavior of the interaction strengths in the receptive other description is indicated by the black line. Recalling the last remarks of the previous section, we observe in the description in terms of the boundary maps $\widetilde{\Gamma}_0, \widetilde{\Gamma}_1$ that for constant interaction strengths $\eta - \tau = \text{const}$ the influence of the δ-potentials becomes insignificant for increasing c-values and therefore the convergence to the free Schrödinger operator seems plausible.

In spite of these observations, we stick to the original boundary maps Γ_0 and Γ_1 of Theorem 3.8 and the operators Φ_λ und $\mathcal{C}_\lambda$ defined as in (3.15) and (3.17) due to frequent references to the previous sections. In particular, in this section we will always assume that the constant interaction strengths $\eta, \tau \in \mathbb{R}$ satisfy the relation $\eta + \tau = 0$ and in this case we set

$$\varepsilon = \frac{\eta - \tau}{c^2}.$$

With this assignment we obtain $\eta - \tau = \varepsilon c^2$ which leads to

$$\eta I_4 + \tau\beta = (\eta - \tau)P_- = \varepsilon c^2 P_-.$$

Next, we define the matrices

$$A_1 = \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \text{and} \quad A_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}$$

and thereby obtain a decomposition of the form $\eta I_4 + \tau\beta = \varepsilon c^2 A_1 A_1^\top$.

By using these matrices, we define linear and bounded multiplication operators $M_i : L^2(\Sigma; \mathbb{C}^2) \to L^2(\Sigma; \mathbb{C}^4)$ by the assignment

$$M_i f = A_i f$$

for $f \in L^2(\Sigma; \mathbb{C}^2)$ and $i \in \{1, 2\}$. A direct calculation shows that the adjoint operators $M_i^* : L^2(\Sigma; \mathbb{C}^4) \to L^2(\Sigma; \mathbb{C}^2)$ are given as the multiplication operators with the matrices $A_i^\top$. Furthermore, due to the above relation of the matrices $\eta I_4 + \tau\beta$ and A_1

$$B = \varepsilon c^2 M_1 M_1^* \tag{4.14}$$

follows with the multiplication operator B defined as in (3.26).

Let $\lambda \in \mathbb{C} \setminus \mathbb{R}$ be given and $\mathcal{C}_\lambda$ be the linear and bounded operator in $L^2(\Sigma; \mathbb{C}^4)$ defined as in (3.17), then the operator $I + B\mathcal{C}_\lambda$ is bijective for all $\eta, \tau \in \mathbb{R}$ with $\eta^2 - \tau^2 \neq 4c^2$ according to the Theorem 3.13. This applies in particular to interaction strengths which satisfy $\eta + \tau = 0$ and $\eta - \tau = \varepsilon c^2$, since in this case $\eta^2 - \tau^2 = 0$ holds true. We will now show that this bijectivity is preserved even if we modify the operator $I + B\mathcal{C}_\lambda$ by the multiplication operator M_1 .

Lemma 4.5. Let $\lambda \in \mathbb{C} \setminus \mathbb{R}$ be given, then the linear and bounded operator

$$I + \varepsilon c^2 M_1^* \mathcal{C}_\lambda M_1 : L^2(\Sigma; \mathbb{C}^2) \to L^2(\Sigma; \mathbb{C}^2)$$

is bijective. Furthermore, the inverse operator is bounded as well and satisfies the relation

$$(I + B\mathcal{C}_\lambda)^{-1} M_1 = M_1 \left(I + \varepsilon c^2 M_1^* \mathcal{C}_\lambda M_1\right)^{-1}$$

in $L^2(\Sigma; \mathbb{C}^2)$.

Proof. *Step 1:* Let $\lambda \in \mathbb{C} \setminus \mathbb{R}$ be given, then $\lambda \in \rho(A_0)$ follows and thus the operator $\mathcal{C}_\lambda$ is well defined according to Theorem 3.9. Since all occurring operators are linear and bounded, we find that $I + \varepsilon c^2 M_1^* \mathcal{C}_\lambda M_1$ is a linear and bounded operator as well. Obviously M_1 is bijective as an operator from $L^2(\Sigma; \mathbb{C}^2)$ to

$$\operatorname{ran}(M_1) = \left\{ (0, 0, f_1, f_2)^\top \in L^2(\Sigma; \mathbb{C}^4) \;\middle|\; (f_1, f_2)^\top \in L^2(\Sigma; \mathbb{C}^2) \right\}.$$

First, we show that $I + \varepsilon c^2 M_1^* \mathcal{C}_\lambda M_1$ is injective and therefore assume that the condition

$$\left(I + \varepsilon c^2 M_1^* \mathcal{C}_\lambda M_1\right) f = 0$$

is satisfied for a function $f \in L^2(\Sigma; \mathbb{C}^2)$. Since $\eta^2 - \tau^2 = 0$ holds true, we deduce from Theorem 3.13 that $I + B\mathcal{C}_\lambda$ is bijective and therefore we can apply the operator $(I + B\mathcal{C}_\lambda)^{-1} M_1$. This yields with (4.14)

$$\begin{aligned}
0 &= (I + B\mathcal{C}_\lambda)^{-1} M_1 \left(I + \varepsilon c^2 M_1^* \mathcal{C}_\lambda M_1\right) f \\
&= (I + B\mathcal{C}_\lambda)^{-1} \left(M_1 + \varepsilon c^2 M_1 M_1^* \mathcal{C}_\lambda M_1\right) f \\
&= (I + B\mathcal{C}_\lambda)^{-1} (I + B\mathcal{C}_\lambda) M_1 f \\
&= M_1 f
\end{aligned}$$

and since M_1 is injective according to the above consideration, $f = 0$ follows. This shows the injectivity of $I + \varepsilon c^2 M_1^* \mathcal{C}_\lambda M_1$.

Step 2: Next, we show the surjectivity of $I+\varepsilon c^2 M_1^* \mathcal{C}_\lambda M_1$ and assume that an arbitrary $f \in L^2(\Sigma; \mathbb{C}^2)$ is given. It then follows from the definition of M_1 that $M_1 f \in L^2(\Sigma; \mathbb{C}^4)$ is valid and due to the surjectivity of $I + B\mathcal{C}_\lambda$ there exists a $g \in L^2(\Sigma; \mathbb{C}^4)$ such that

$$(I + B\mathcal{C}_\lambda)\, g = M_1 f$$

applies. With the definition of B and by using $\eta I_4 + \tau\beta = \varepsilon c^2 P_-$ we obtain

$$\begin{pmatrix} 0 \\ 0 \\ f_1 \\ f_2 \end{pmatrix} = M_1 f = (I + B\mathcal{C}_\lambda)\, g = \begin{pmatrix} g_1 \\ g_2 \\ g_3 \\ g_4 \end{pmatrix} + \varepsilon c^2 \begin{pmatrix} 0 \\ 0 \\ (\mathcal{C}_\lambda g)_3 \\ (\mathcal{C}_\lambda g)_4 \end{pmatrix}$$

by component-wise consideration and consequently $g_1 = g_2 = 0$. This leads to $g \in \operatorname{ran}(M_1)$ and therefore there exists an $h \in L^2(\Sigma; \mathbb{C}^2)$, namely $h = (g_3, g_4)^\top$, which satisfies $g = M_1 h$. Hence, the choice of g leads to

$$\begin{aligned} M_1 f &= (I + B\mathcal{C}_\lambda)\, g = (I + B\mathcal{C}_\lambda)\, M_1 h \\ &= \left(M_1 + \varepsilon c^2 M_1 M_1^* \mathcal{C}_\lambda M_1\right) h = M_1 \left(I + \varepsilon c^2 M_1^* \mathcal{C}_\lambda M_1\right) h \end{aligned}$$

and finally

$$f = \left(I + \varepsilon c^2 M_1^* \mathcal{C}_\lambda M_1\right) h$$

due to the injectivity of M_1. This shows the surjectivity of $I + \varepsilon c^2 M_1^* \mathcal{C}_\lambda M_1$.

Step 3: According to Step 1 and 2 we have that $I + \varepsilon c^2 M_1^* \mathcal{C}_\lambda M_1$ is a bounded and bijective operator and therefore it follows from Theorem 2.6 or the open mapping theorem that the inverse operator is bounded as well. A direct calculation finally shows

$$\begin{aligned} &(I + B\mathcal{C}_\lambda)^{-1} M_1 - M_1 \left(I + \varepsilon c^2 M_1^* \mathcal{C}_\lambda M_1\right)^{-1} \\ &= (I + B\mathcal{C}_\lambda)^{-1} \left(M_1 \left(I + \varepsilon c^2 M_1^* \mathcal{C}_\lambda M_1\right) - \left(I + \varepsilon c^2 M_1 M_1^* \mathcal{C}_\lambda\right) M_1\right) \left(I + \varepsilon c^2 M_1^* \mathcal{C}_\lambda M_1\right)^{-1} \\ &= 0 \end{aligned}$$

what completes the proof. □

Next, we define integral operators which will prove to be important in the following. For this purpose we define the matrix-valued function

$$H_\lambda(x) = \left(1 - i\sqrt{2m\lambda}\|x\|\right) \frac{i}{4\pi\|x\|^3} (\sigma \cdot x) \exp\left(i\sqrt{2m\lambda}\|x\|\right) \tag{4.15}$$

for all $x \in \mathbb{R}^3 \setminus \{0\}$ and all $\lambda \in \mathbb{C} \setminus \mathbb{R}$ with σ_k being the Pauli spin matrices. As in the previous sections, the square root of a complex number $\mu \in \mathbb{C} \setminus [0, \infty)$ is chosen such that $\operatorname{Im}\left\{\sqrt{\mu}\right\} > 0$ applies.

Theorem 4.6. Let $\lambda \in \mathbb{C} \setminus \mathbb{R}$ be given, then the following statements are true.

i) The assignment
$$(\Psi_\lambda f)(x) = \int_\Sigma H_\lambda(x-y) f(y) \mathrm{d}\sigma(y) \tag{4.16}$$
for $f \in L^2(\Sigma; \mathbb{C}^2)$ and $x \in \mathbb{R}^3$ corresponds to a well-defined, linear and bounded operator $\Psi_\lambda : L^2(\Sigma; \mathbb{C}^2) \to L^2(\mathbb{R}^3; \mathbb{C}^2)$.

ii) The adjoint operator of Ψ_λ is given by
$$(\Psi_\lambda^* f)(x) = \int_{\mathbb{R}^3} H_{\overline{\lambda}}(x-y) f(y) \mathrm{d}y \tag{4.17}$$
for all $f \in L^2(\mathbb{R}^3; \mathbb{C}^2)$ and for almost all $x \in \Sigma$ and is a linear and bounded operator $\Psi_\lambda^* : L^2(\mathbb{R}^3; \mathbb{C}^2) \to L^2(\Sigma; \mathbb{C}^2)$ as well.

iii) The assignment
$$(\mathcal{D}_\lambda f)(x) = \int_\Sigma \frac{\lambda}{4\pi\|x-y\|} \exp\left(i\sqrt{2m\lambda}\|x\|\right) f(y) \mathrm{d}\sigma(y) \tag{4.18}$$
for $f \in L^2(\Sigma; \mathbb{C}^2)$ and $x \in \Sigma$ corresponds to a well-defined, linear and compact operator $\mathcal{D}_\lambda : L^2(\Sigma; \mathbb{C}^2) \to L^2(\Sigma; \mathbb{C}^2)$ with $\operatorname{ran}(\mathcal{D}_\lambda) \subseteq H^{\frac{1}{2}}(\Sigma; \mathbb{C}^2)$.

Proof. *Step 1:* Since all operators are integral operators, we are going to apply the results from Section 2.6. For this we need estimates of the integral kernels. Let $x \in \mathbb{R}^3 \setminus \{0\}$ be given, then the estimation
$$\begin{aligned} \|H_\lambda(x)\|_F &\leq \frac{\left|1 - i\sqrt{2m\lambda}\|x\|\right|}{4\pi\|x\|^3} \left(\sum_{j=1}^3 \|\sigma_j\|_F |x_j|\right) \exp\left(-\operatorname{Im}\left\{\sqrt{2m\lambda}\right\}\|x\|\right) \\ &\leq \frac{1 + \left|\sqrt{2m\lambda}\right| \|x\|}{4\pi\|x\|^2} \left(\sum_{j=1}^3 \|\sigma_j\|_F\right) \exp\left(-\operatorname{Im}\left\{\sqrt{2m\lambda}\right\}\|x\|\right). \end{aligned} \tag{4.19}$$
follows for the Frobenius norm. If $\|x\| < 1$ holds true, then it follows from (4.19) that
$$\begin{aligned} \|H_\lambda(x)\|_F &\leq \frac{1 + \left|\sqrt{2m\lambda}\right|}{4\pi\|x\|^2} \left(\sum_{j=1}^3 \|\sigma_j\|_F\right) \exp\left(-\operatorname{Im}\left\{\sqrt{2m\lambda}\right\}\|x\|\right) \\ &\leq \frac{1 + \left|\sqrt{2m\lambda}\right|}{4\pi\|x\|^2} \left(\sum_{j=1}^3 \|\sigma_j\|_F\right) \end{aligned}$$

is valid, while for $\|x\| \geq 1$ it follows from (4.19) that the estimate

$$\begin{aligned}\|H_\lambda(x)\|_F &\leq \frac{1 + \left|\sqrt{2m\lambda}\right|}{4\pi\|x\|}\left(\sum_{j=1}^{3}\|\sigma_j\|_F\right)\exp\left(-\operatorname{Im}\left\{\sqrt{2m\lambda}\right\}\|x\|\right)\\ &\leq \frac{1 + \left|\sqrt{2m\lambda}\right|}{4\pi}\left(\sum_{j=1}^{3}\|\sigma_j\|_F\right)\exp\left(-\operatorname{Im}\left\{\sqrt{2m\lambda}\right\}\|x\|\right)\end{aligned}$$

applies. Setting

$$\kappa_1 = \frac{1 + \left|\sqrt{2m\lambda}\right|}{4\pi}\left(\sum_{j=1}^{3}\|\sigma_j\|_F\right) \qquad \text{and} \qquad \kappa_2 = -\operatorname{Im}\left\{\sqrt{2m\lambda}\right\}$$

then immediately leads to

$$\|H_\lambda(x)\|_F \leq \kappa_1 \begin{cases} \|x\|^{-2}, & \text{for } \|x\| < 1 \\ e^{-\kappa_2\|x\|}, & \text{for } \|x\| \geq 1 \end{cases}$$

for all $x \in \mathbb{R}^3 \setminus \{0\}$. An application of Theorem 2.35 results in the validity of the assertion for Ψ_λ.

Step 2: As Ψ_λ is an everywhere defined and bounded operator according to Step 1 it follows from Theorem 2.10 that $\Psi_\lambda^* \in \mathcal{L}(L^2(\mathbb{R}^3;\mathbb{C}^2), L^2(\Sigma;\mathbb{C}^2))$ holds true. Next, we define an integral operator by

$$(Tf)(x) = \int_{\mathbb{R}^3} H_{\overline{\lambda}}(x-y)f(y)\mathrm{d}y$$

for $f \in L^2(\mathbb{R}^3;\mathbb{C}^2)$ and $x \in \Sigma$ and conclude from Step 1 and Theorem 2.35 that this assignment corresponds to a well-defined, linear and bounded operator $T : L^2(\mathbb{R}^3;\mathbb{C}^2) \to L^2(\Sigma;\mathbb{C}^2)$. Furthermore, it can be shown by direct calculation that

$$-H_{\overline{\lambda}}(x) = H_\lambda(x)^*$$

is valid for all $\lambda \in \mathbb{C} \setminus \mathbb{R}$ and all $x \in \mathbb{R}^3 \setminus \{0\}$.

To prove assertion ii) we assume that arbitrary functions $f \in L^2(\mathbb{R}^3;\mathbb{C}^2)$ and $g \in L^2(\Sigma;\mathbb{C}^2)$ are given. Then it follows from Lemma 2.37 with Fubini 's theorem and the hermiticity of the Pauli spin matrices that

$$\begin{aligned}(g, \Psi_\lambda^* f)_{L^2(\Sigma;\mathbb{C}^2)} = (\Psi_\lambda g, f)_{L^2(\mathbb{R}^3;\mathbb{C}^2)} &= \int_{\mathbb{R}^3}\int_{\Sigma} H_\lambda(x-y)g(y)\cdot\overline{f(x)}\mathrm{d}\sigma(y)\mathrm{d}x\\ &= \int_{\Sigma}\int_{\mathbb{R}^3} g(y)\cdot\overline{H_{\overline{\lambda}}(y-x)f(x)}\mathrm{d}x\mathrm{d}\sigma(y) = (g, Tf)_{L^2(\Sigma;\mathbb{C}^2)}\end{aligned}$$

applies. Since this holds true for all $f \in L^2(\mathbb{R}^3;\mathbb{C}^2)$ and $g \in L^2(\Sigma;\mathbb{C}^2)$, the equality $T = \Psi_\lambda^*$ follows in the sense of linear operators which shows the assertion ii).

Step 3: Let $\widetilde{M}(\lambda)$ be the linear and bounded operator defined in (4.4), then it follows immediately from the definition of $\mathcal{D}_\lambda$ that

$$\mathcal{D}_\lambda = \frac{\lambda}{2m}\widetilde{M}(\lambda)I_2 = \frac{\lambda}{2m}S(\lambda)I_2 \restriction L^2(\Sigma;\mathbb{C}^2)$$

with the single layer boundary integral operator $S(\lambda)$ is valid. The latter is a linear and bounded operator from $H^{-\frac{1}{2}}(\Sigma;\mathbb{C})$ to $H^{\frac{1}{2}}(\Sigma;\mathbb{C})$. Due to the compact embeddings

$$H^{\frac{1}{2}}(\Sigma;\mathbb{C}) \hookrightarrow L^2(\Sigma;\mathbb{C}^2) \hookrightarrow H^{-\frac{1}{2}}(\Sigma;\mathbb{C})$$

according to Theorem 2.29 the claimed properties of $\mathcal{D}_\lambda$ follow. □

The reason for the definition of the operators Ψ_λ and $\mathcal{D}_\lambda$ is provided by the following theorem, which is of particular importance for the investigation of the non-relativistic limit in Theorem 4.12. It is shown that the operators $c\Phi_\lambda$ and $c^2\mathcal{C}_\lambda$ converge to modified operators Ψ_λ and $\mathcal{D}_\lambda$ after a suitable transformation by multiplication operators. Furthermore, an important relationship between the operators Ψ_λ and $\mathcal{D}_\lambda$ is derived from this theorem in Lemma 4.8.

Theorem 4.7. Let $\lambda \in \mathbb{C}\backslash\mathbb{R}$ be given, Φ_λ and $\mathcal{C}_\lambda$ be the linear and bounded operators defined as in (3.15) and (3.17) and Ψ_λ and $\mathcal{D}_\lambda$ be the linear and bounded operators according to (4.16) and (4.18). Then there exists a constant $\kappa(m,\lambda,\Sigma) > 0$ only dependent on m, λ and Σ such that the following estimates are valid for sufficiently large $c > 0$

$$\|c\Phi_{\lambda+mc^2}M_1 - M_2\Psi_\lambda\| \leq \frac{\kappa}{c}, \tag{4.20}$$

$$\left\|cM_1^*\Phi_{\lambda+mc^2}^* - \Psi_\lambda^* M_2^*\right\| \leq \frac{\kappa}{c}, \tag{4.21}$$

$$\left\|c^2 M_1^*\mathcal{C}_{\lambda+mc^2}M_1 - \mathcal{D}_\lambda\right\| \leq \frac{\kappa}{c}. \tag{4.22}$$

Proof. *Step 1:* Let $\lambda \in \mathbb{C}\backslash\mathbb{R}$ be given, then it immediately follows that $\lambda + mc^2 \in \mathbb{C}\backslash\mathbb{R}$ applies and therefore all occurring operators are well defined according to Theorem 3.9 and Theorem 4.6. Since these are integral operators, it is our approach to apply the results of Section 2.6. For this purpose we require estimates of the integral kernels.

We begin with the integral kernel of the resolvent of the free Dirac operator and conclude by direct calculation that

$$G_{\lambda+mc^2}(x) =$$
$$\left(\frac{\lambda}{c^2}I_4 + 2mP_+ + \left(1 - i\sqrt{\frac{\lambda^2}{c^2} + 2m\lambda}\|x\|\right)\frac{i}{c\|x\|^2}(\alpha\cdot x)\right)\frac{1}{4\pi\|x\|}\exp\left(i\sqrt{\frac{\lambda^2}{c^2} + 2m\lambda}\|x\|\right)$$

is valid for all $x \in \mathbb{R}^3 \setminus \{0\}$. Consequently, we obtain from $P_+ A_1 = 0$ with the diagonal matrix $P_+ = \mathrm{diag}(1,1,0,0)$

$$\begin{aligned} &cG_{\lambda+mc^2}(x)A_1 = \\ &\left(\frac{\lambda}{c}I_4 + \left(1 - i\sqrt{\frac{\lambda^2}{c^2} + 2m\lambda}\|x\|\right)\frac{i}{\|x\|^2}(\alpha\cdot x)\right)\frac{1}{4\pi\|x\|}\exp\left(i\sqrt{\frac{\lambda^2}{c^2}+2m\lambda}\|x\|\right)A_1 \end{aligned} \tag{4.23}$$

for all $x \in \mathbb{R}^3 \setminus \{0\}$. Furthermore, the definition of the matrices A_1 and A_2 yields

$$A_2 H_\lambda(x) = \left(1 - i\sqrt{2m\lambda}\|x\|\right)\frac{i}{4\pi\|x\|^3}(\alpha\cdot x)\exp\left(i\sqrt{2m\lambda}\|x\|\right)A_1 \tag{4.24}$$

for all $x \in \mathbb{R}^3 \setminus \{0\}$. Next, we define the matrix-valued functions

$$\begin{aligned} t_1(x) &= \frac{\lambda}{c}\frac{1}{4\pi\|x\|}\exp\left(i\sqrt{\frac{\lambda^2}{c^2}+2m\lambda}\|x\|\right)I_4 \\ t_2(x) &= \frac{i}{4\pi\|x\|^3}(\alpha\cdot x)\left(\exp\left(i\sqrt{\frac{\lambda^2}{c^2}+2m\lambda}\|x\|\right) - \exp\left(i\sqrt{2m\lambda}\|x\|\right)\right) \\ t_3(x) &= \frac{1}{4\pi\|x\|^2}\left(\sqrt{\frac{\lambda^2}{c^2}+2m\lambda} - \sqrt{2m\lambda}\right)(\alpha\cdot x)\exp\left(i\sqrt{\frac{\lambda^2}{c^2}+2m\lambda}\|x\|\right) \\ t_4(x) &= \frac{\sqrt{2m\lambda}}{4\pi\|x\|^2}(\alpha\cdot x)\left(\exp\left(i\sqrt{\frac{\lambda^2}{c^2}+2m\lambda}\|x\|\right) - \exp\left(i\sqrt{2m\lambda}\|x\|\right)\right) \end{aligned}$$

and thus, by combining (4.23) and (4.24), we obtain the relationship

$$cG_{\lambda+mc^2}(x)A_1 - A_2 H_\lambda(x) = \left(\sum_{j=1}^{4} t_j(x)\right)A_1$$

between the integral kernels $G_{\lambda+mc^2}$ and H_λ for all $x \in \mathbb{R}^3 \setminus \{0\}$.

Step 2: In order to derive an estimate for t_1 we use the Frobnenius norm and find with Lemma 4.2 and $t = 1$

$$\begin{aligned} \|t_1(x)\|_F &= \frac{2\,|\lambda|}{4\pi c\|x\|}\exp\left(-\mathrm{Im}\left\{\sqrt{\frac{\lambda^2}{c^2}+2m\lambda}\right\}\|x\|\right) \\ &\le \frac{1}{c}\frac{|\lambda|}{2\pi\|x\|}\exp\left(-\frac{1}{2}\mathrm{Im}\left\{\sqrt{2m\lambda}\right\}\|x\|\right) \end{aligned} \tag{4.25}$$

for all $x \in \mathbb{R}^3 \setminus \{0\}$. If $\|x\| < 1$ holds true, then it follows from (4.25) that

$$\|t_1(x)\|_F \leq \frac{1}{c}\frac{|\lambda|}{2\pi\|x\|} < \frac{1}{c}\frac{|\lambda|}{2\pi\|x\|^2}$$

is valid, while for $\|x\| \geq 1$ it follows from (4.25) that the estimation

$$\|t_1(x)\|_F \leq \frac{1}{c}\frac{|\lambda|}{2\pi}\exp\left(-\frac{1}{2}\mathrm{Im}\left\{\sqrt{2m\lambda}\right\}\|x\|\right)$$

applies. Defining

$$\kappa_1 = \frac{|\lambda|}{2\pi} \qquad \text{and} \qquad \kappa_2 = \frac{1}{2}\mathrm{Im}\left\{\sqrt{2m\lambda}\right\}$$

leads to the estimate

$$\|t_1(x)\| \leq \frac{\kappa_1}{c}\begin{cases}\|x\|^{-2} & \text{, for } \|x\| < 1\\ e^{-\kappa_2\|x\|} & \text{, for } \|x\| \geq 1\end{cases}$$

for all $x \in \mathbb{R}^3 \setminus \{0\}$ and sufficiently large $c > 0$ with the constants κ_1 and κ_2, which depend only on m and λ.

Step 3: Let $x \in \mathbb{R}^3 \setminus \{0\}$ be given, then it follows as in the proof of Theorem 4.3 Step 3 that there exist constants $k_1, k_2 > 0$ depending only on m and λ such that

$$\left|\exp\left(i\sqrt{\frac{\lambda^2}{c^2} + 2m\lambda}\|x\|\right) - \exp\left(i\sqrt{2m\lambda}\|x\|\right)\right| \leq \frac{k_1\|x\|}{c^2}e^{-k_2\|x\|}$$

holds true. Consequently, for t_2 the estimate

$$\begin{aligned}\|t_2(x)\|_F &\leq \frac{1}{4\pi\|x\|^3}\left(\sum_{j=1}^{3}\|\alpha_j\|_F\,|x_j|\right)\left|\exp\left(i\sqrt{\frac{\lambda^2}{c^2} + 2m\lambda}\|x\|\right) - \exp\left(i\sqrt{2m\lambda}\|x\|\right)\right|\\ &\leq \frac{1}{4\pi\|x\|^2}\left(\sum_{j=1}^{3}\|\alpha_j\|_F\right)\left|\exp\left(i\sqrt{\frac{\lambda^2}{c^2} + 2m\lambda}\|x\|\right) - \exp\left(i\sqrt{2m\lambda}\|x\|\right)\right|\\ &\leq \frac{k_1}{4c^2\pi\|x\|}\left(\sum_{j=1}^{3}\|\alpha_j\|_F\right)e^{-k_2\|x\|}\\ &\leq \frac{k_1}{4c\pi\|x\|}\left(\sum_{j=1}^{3}\|\alpha_j\|_F\right)e^{-k_2\|x\|}\end{aligned}$$

follows for sufficiently large $c > 0$. As in Step 2, we obtain constants $\kappa_3, \kappa_4 > 0$ only dependent on m and λ such that

$$\|t_2(x)\| \leq \frac{\kappa_3}{c} \begin{cases} \|x\|^{-2} &, \text{ for } \|x\| < 1 \\ e^{-\kappa_4 \|x\|} &, \text{ for } \|x\| \geq 1 \end{cases}$$

applies to all $x \in \mathbb{R}^3 \setminus \{0\}$ and sufficiently large $c > 0$.

Step 4: Next, we consider t_3. From the convergence

$$\sqrt{\frac{\lambda^2}{c^2} + 2m\lambda} \to \sqrt{2m\lambda} \qquad \text{for } c \to \infty$$

and an application of the triangle inequality we obtain

$$\left| \left| \sqrt{\frac{\lambda^2}{c^2} + 2m\lambda} + \sqrt{2m\lambda} \right| - 2 \left| \sqrt{2m\lambda} \right| \right| \leq \left| \sqrt{\frac{\lambda^2}{c^2} + 2m\lambda} - \sqrt{2m\lambda} \right| \leq \left| \sqrt{2m\lambda} \right|$$

for sufficiently large $c > 0$. This yields the chain of inequalities

$$\left| \sqrt{2m\lambda} \right| \leq \left| \sqrt{\frac{\lambda^2}{c^2} + 2m\lambda} + \sqrt{2m\lambda} \right| \leq 3 \left| \sqrt{2m\lambda} \right|. \tag{4.26}$$

Furthermore, it follows from the convergence $\frac{\lambda^2}{c} \to 0$ for $c \to \infty$ that

$$\frac{|\lambda|^2}{c} \leq 1 \tag{4.27}$$

applies to sufficiently large $c > 0$. If $x \in \mathbb{R}^3 \setminus \{0\}$ is given, then we conclude from Lemma 4.2 with $t = 1$ in combination with (4.26) and (4.27) that the estimate

$$\begin{aligned}
\|t_3(x)\|_F &\leq \frac{1}{4\pi \|x\|^2} \left| \sqrt{\frac{\lambda^2}{c^2} + 2m\lambda} - \sqrt{2m\lambda} \right| \left(\sum_{j=1}^{3} \|\alpha_j\|_F |x_j| \right) \cdot \\
&\qquad\qquad \exp\left(-\mathrm{Im}\left\{ \sqrt{\frac{\lambda^2}{c^2} + 2m\lambda} \right\} \|x\| \right) \\
&\leq \frac{1}{4\pi \|x\|} \left| \sqrt{\frac{\lambda^2}{c^2} + 2m\lambda} - \sqrt{2m\lambda} \right| \left(\sum_{j=1}^{3} \|\alpha_j\|_F \right) \exp\left(-\frac{1}{2} \mathrm{Im}\left\{ \sqrt{2m\lambda} \right\} \|x\| \right) \\
&= \frac{1}{4\pi \|x\|} \frac{\frac{|\lambda|^2}{c^2}}{\left| \sqrt{\frac{\lambda^2}{c^2} + 2m\lambda} + \sqrt{2m\lambda} \right|} \left(\sum_{j=1}^{3} \|\alpha_j\|_F \right) \exp\left(-\frac{1}{2} \mathrm{Im}\left\{ \sqrt{2m\lambda} \right\} \|x\| \right) \\
&\leq \frac{1}{4c\pi \|x\|} \frac{1}{\left| \sqrt{2m\lambda} \right|} \left(\sum_{j=1}^{3} \|\alpha_j\|_F \right) \exp\left(-\frac{1}{2} \mathrm{Im}\left\{ \sqrt{2m\lambda} \right\} \|x\| \right)
\end{aligned}$$

is valid for sufficiently large $c > 0$. Finally, as in Step 2, we obtain constants $\kappa_5, \kappa_6 > 0$ only dependent on m and λ such that

$$\|t_3(x)\| \le \frac{\kappa_5}{c} \begin{cases} \|x\|^{-2} & \text{, for } \|x\| < 1 \\ e^{-\kappa_6 \|x\|} & \text{, for } \|x\| \ge 1 \end{cases}$$

applies to all $x \in \mathbb{R}^3 \setminus \{0\}$ and sufficiently large $c > 0$.

Step 5: For a given $x \in \mathbb{R}^3 \setminus \{0\}$ we use the same estimation as in Step 3 and obtain

$$\begin{aligned}
\|t_4(x)\|_F &\le \frac{\left|\sqrt{2m\lambda}\right|}{4\pi\|x\|^2} \left(\sum_{j=1}^{3} \|\alpha_j\|_F\, |x_j|\right) \left|\exp\left(i\sqrt{\frac{\lambda^2}{c^2} + 2m\lambda}\|x\|\right) - \exp\left(i\sqrt{2m\lambda}\|x\|\right)\right| \\
&\le \frac{\left|\sqrt{2m\lambda}\right|}{4\pi\|x\|} \left(\sum_{j=1}^{3} \|\alpha_j\|_F\right) \left|\exp\left(i\sqrt{\frac{\lambda^2}{c^2} + 2m\lambda}\|x\|\right) - \exp\left(i\sqrt{2m\lambda}\|x\|\right)\right| \\
&\le \frac{k_1\left|\sqrt{2m\lambda}\right|}{4\pi c^2} \left(\sum_{j=1}^{3} \|\alpha_j\|_F\right) e^{-k_2\|x\|} \\
&\le \frac{k_1\left|\sqrt{2m\lambda}\right|}{4\pi c} \left(\sum_{j=1}^{3} \|\alpha_j\|_F\right) e^{-k_2\|x\|}
\end{aligned}$$

for sufficiently large $c > 0$. Defining the constants

$$\kappa_7 = \frac{k_1\left|\sqrt{2m\lambda}\right|}{4\pi} \left(\sum_{j=1}^{3} \|\alpha_j\|_F\right) \qquad \text{and} \qquad \kappa_8 = k_2$$

which depend only on m and λ, immediately leads to

$$\|t_4(x)\| \le \frac{\kappa_7}{c} \begin{cases} \|x\|^{-2} & \text{, for } \|x\| < 1 \\ e^{-\kappa_8 \|x\|} & \text{, for } \|x\| \ge 1 \end{cases}$$

for all $x \in \mathbb{R}^3 \setminus \{0\}$ and sufficiently large $c > 0$.

Step 6: From the previous steps it follows that there exist constants $\widetilde{\kappa}_1(m,\lambda) > 0$ and $\widetilde{\kappa}_2(m,\lambda) > 0$ only dependent on m and λ such that

$$\|t_j(x)\| \le \frac{\widetilde{\kappa}_1}{c} \begin{cases} \|x\|^{-2} & \text{, for } \|x\| < 1 \\ e^{-\widetilde{\kappa}_2 \|x\|} & \text{, for } \|x\| \ge 1 \end{cases}$$

is valid for all $j\in\{1,\dots,4\}$, all $x\in\mathbb{R}^3\setminus\{0\}$ and sufficiently large $c>0$. This leads to the estimate

$$\|cG_{\lambda+mc^2}(x)A_1-A_2H_\lambda(x)\|\leq\left(\sum_{j=1}^{4}\|t_j(x)\|\right)\|A_1\|\leq\frac{4\|A_1\|\widetilde{\kappa}_1}{c}\begin{cases}\|x\|^{-2}, & \text{for } \|x\|<1\\ e^{-\widetilde{\kappa}_2\|x\|}, & \text{for } \|x\|\geq 1\end{cases}$$

for all $x\in\mathbb{R}^3\setminus\{0\}$ and sufficiently large $c>0$ for the integral kernel of the operator $c\Phi_{\lambda+mc^2}M_1-M_2\Psi_\lambda$. An application of Theorem 2.35 finally results in

$$\|c\Phi_{\lambda+mc^2}M_1-M_2\Psi_\lambda\|\leq\frac{4\|A_1\|\widetilde{\kappa}_1K}{c}$$

with a constant $K(\widetilde{\kappa}_2,\Sigma)>0$ only dependent on $\widetilde{\kappa}_2(m,\lambda)$ and Σ. This proves the first inequality (4.20).

Step 7: Due to the boundedness of all the occurring operators we obtain with Theorem 2.10 and Step 6 the estimation

$$\left\|cM_1^*\Phi_{\lambda+mc^2}^*-\Psi_\lambda^*M_2^*\right\|=\|c\Phi_{\lambda+mc^2}M_1-M_2\Psi_\lambda\|\leq\frac{4\|A_1\|\widetilde{\kappa}_1K}{c}$$

for sufficiently large $c>0$ which proves the second inequality (4.21).

Step 8: Finally, we prove the last inequality and find by direct calculation that $P_+A_1=0$ and $A_1^\top\alpha_jA_1=0$ for all $j\in\{1,2,3\}$ are valid. Therefore, it follows from the representation of $G_{\lambda+mc^2}$ that

$$\begin{aligned}c^2A_1^\top G_{\lambda+mc^2}(x)A_1&=\frac{\lambda}{4\pi\|x\|}\exp\left(i\sqrt{\frac{\lambda^2}{c^2}+2m\lambda}\|x\|\right)A_1^\top A_1\\&=\frac{\lambda}{4\pi\|x\|}\exp\left(i\sqrt{\frac{\lambda^2}{c^2}+2m\lambda}\|x\|\right)I_2\end{aligned}$$

holds true for all $x\in\mathbb{R}^3\setminus\{0\}$. The definition of this integral kernel immediately leads to the estimate

$$\left\|c^2A_1^\top G_{\lambda+mc^2}(x)A_1\right\|\leq\frac{k}{\|x\|}$$

for all $x\in\mathbb{R}^3\setminus\{0\}$ with a constant $k(\lambda)>0$ only dependent on λ. With a reasoning as in Lemma 2.37 and the choice $g\equiv 1$ we find that

$$\int_\Sigma\int_\Sigma\left\|c^2A_1^\top G_{\lambda+mc^2}(x-y)A_1\right\|\|f(y)\|\mathrm{d}\sigma(y)\mathrm{d}\sigma(x)<\infty$$

is valid for all $f \in L^2(\Sigma;\mathbb{C}^2)$. This leads to

$$\int_\Sigma \left\|c^2 A_1^\top G_{\lambda+mc^2}(x-y)A_1\right\| \|f(y)\| \mathrm{d}\sigma(y) < \infty$$

for almost all $x \in \Sigma$ and an application of the dominated convergence theorem then yields

$$\begin{aligned}
\left(c^2 M_1^* \mathcal{C}_{\lambda+mc^2} M_1 f\right)(x) &= \lim_{\delta\to 0^+} \int_{\Sigma\setminus B(x,\delta)} c^2 A_1^\top G_{\lambda+mc^2}(x-y)A_1 f(y)\mathrm{d}\sigma(y) \\
&= \lim_{\delta\to 0^+} \int_{\Sigma\setminus B(x,\delta)} \frac{\lambda}{4\pi\|x-y\|} \exp\left(i\sqrt{\frac{\lambda^2}{c^2}+2m\lambda}\|x-y\|\right) f(y)\mathrm{d}\sigma(y) \\
&= \int_\Sigma \frac{\lambda}{4\pi\|x-y\|} \exp\left(i\sqrt{\frac{\lambda^2}{c^2}+2m\lambda}\|x-y\|\right) f(y)\mathrm{d}\sigma(y)
\end{aligned}$$

for all $f \in L^2(\Sigma;\mathbb{C}^2)$ and almost all $x \in \Sigma$. Defining the matrix-valued function

$$t(x) = \frac{\lambda}{4\pi\|x\|}\left(\exp\left(i\sqrt{\frac{\lambda^2}{c^2}+2m\lambda}\|x\|\right) - \exp\left(i\sqrt{2m\lambda}\|x\|\right)\right) I_2$$

for all $x \in \mathbb{R}^3 \setminus \{0\}$ we obtain with the same estimate as in Step 3

$$\begin{aligned}
\|t(x)\|_F &= \frac{2\,|\lambda|}{4\pi\|x\|}\left|\exp\left(i\sqrt{\frac{\lambda^2}{c^2}+2m\lambda}\|x\|\right) - \exp\left(i\sqrt{2m\lambda}\|x\|\right)\right| \\
&\le \frac{k_1\,|\lambda|}{4\pi c^2} e^{-k_2\|x\|} \le \frac{k_1\,|\lambda|}{4\pi c}
\end{aligned}$$

for sufficiently large $c > 0$. Therefore, with the representation of $\mathcal{D}_\lambda$ and Theorem 2.36

$$\left\|c^2 M_1^* \mathcal{C}_{\lambda+mc^2} M_1 - \mathcal{D}_\lambda\right\| \le \frac{k_1 K\,|\lambda|}{4\pi c}$$

follows for sufficiently large $c > 0$ with a constant $K(\Sigma) > 0$ only depending on Σ. This shows the third inequality (4.22) and completes the proof. $\square$

Theorem 4.7 enables us to show an important relationship between the operators Ψ_λ, $\Psi_{\overline{\lambda}}^*$ and $\mathcal{D}_\lambda$ which will be used in the proof of Theorem 4.12. Note the striking similarity to Theorem 2.18 for quasi boundary triples.

Lemma 4.8. Let $\lambda, \mu \in \mathbb{C} \setminus \mathbb{R}$ be given, then

$$\mathcal{D}_\lambda - \mathcal{D}_\mu^* = (\lambda - \overline{\mu})\, \Psi_\mu^* \Psi_\lambda$$

holds on the domain of definition $L^2(\Sigma;\mathbb{C}^2)$ of the operators. In particular, it follows that $\mathcal{D}_\lambda = \mathcal{D}_{\overline{\lambda}}^*$ applies.

Proof. According to Theorem 3.11 we have that the values of the Weyl function are closable operators and $\overline{M(\lambda + mc^2)} = \mathcal{C}_{\lambda+mc^2}$ applies. Due to Theorem 2.10 we therefore obtain

$$M(\lambda + mc^2)^* = \mathcal{C}^*_{\lambda+mc^2}$$

and with Theorem 4.7 the convergence

$$c^2 M_1^* \mathcal{C}^*_{\lambda+mc^2} M_1 \to \mathcal{D}^*_\lambda \qquad \text{for } c \to \infty.$$

Let $f \in H^{\frac{1}{2}}(\Sigma; \mathbb{C}^2)$ be given then $M_1 f \in H^{\frac{1}{2}}(\Sigma; \mathbb{C}^4)$ follows and an application of Theorem 2.18 leads to

$$\begin{aligned} M_1^* \mathcal{C}_{\lambda+mc^2} M_1 f - M_1^* \mathcal{C}^*_{\mu+mc^2} M_1 f &= M_1^* M(\lambda + mc^2) M_1 f - M_1^* M(\mu + mc^2)^* M_1 f \\ &= (\lambda - \overline{\mu})\, M_1^* \gamma(\mu + mc^2)^* \gamma(\lambda + mc^2) M_1 f \\ &= (\lambda - \overline{\mu})\, M_1^* \Phi^*_{\mu+mc^2} \Phi_{\lambda+mc^2} M_1 f \end{aligned}$$

for all $\lambda, \mu \in \mathbb{C} \setminus \mathbb{R}$. Since $H^{\frac{1}{2}}(\Sigma; \mathbb{C}^2)$ is dense in $L^2(\Sigma; \mathbb{C}^2)$ and since all occurring operators are bounded, it can be shown by a simple approximation argument that this equality is even valid for all $f \in L^2(\Sigma; \mathbb{C}^2)$. By multiplying with c^2 and executing the limit $c \to \infty$ we finally obtain the relationship

$$\mathcal{D}_\lambda - \mathcal{D}^*_\mu = (\lambda - \overline{\mu})\, \Psi^*_\mu \Psi_\lambda$$

on $L^2(\Sigma; \mathbb{C}^2)$ due to Theorem 4.7 and the definition of the multiplication operator M_2. $\square$

Next, we will show mapping properties and an alternative representation of the operators Ψ_λ and Ψ^*_λ which will be needed in the following. For this purpose it will be necessary to define another trace operator, which we construct by the following consideration.

Let $f \in H^1(\mathbb{R}^3; \mathbb{C}^2)$ be given, then it follows from Theorem 2.32 that $\tau_+ f_+ = \tau_- f_-$ applies and therefore by assigning

$$\tau f = \frac{1}{2} (\tau_+ f_+ + \tau_- f_-) = \tau_+ f_+ \tag{4.28}$$

we obtain a well-defined, linear and bounded operator $\tau : H^1(\mathbb{R}^3; \mathbb{C}^2) \to H^{\frac{1}{2}}(\Sigma; \mathbb{C}^2)$.

Furthermore, it should be remembered that for a given operator S in $L^2(\mathbb{R}^3; \mathbb{C})$, an expression of the form $S I_2 f$ is always understood in such a way that the operator S acts on every component of a $\mathbb{C}^2$-valued function f.

Theorem 4.9. Let $\lambda \in \mathbb{C}\backslash\mathbb{R}$ be given, Ψ_λ and $\Psi_{\overline{\lambda}}^*$ be the linear and bounded operators defined as in (4.16) and (4.17) and τ be the trace operator according to (4.28), then the following statements are true.

i) With the resolvent of the free Schrödinger operator in (2.19) the representation

$$\Psi_{\overline{\lambda}}^* f = \tau\left(-\frac{i}{2m}(\sigma\cdot\nabla)\right)\left(-\frac{1}{2m}\Delta-\lambda\right)^{-1} I_2 f$$

is valid for all $f \in L^2(\mathbb{R}^3;\mathbb{C}^2)$. In particular, $\Psi_{\overline{\lambda}}^* f \in H^{\frac{1}{2}}(\Sigma;\mathbb{C}^2)$ applies to all $f \in L^2(\mathbb{R}^3;\mathbb{C}^2)$.

ii) With the single layer potential of the free Schrödinger operator, the representation

$$\Psi_\lambda f = -\frac{i}{2m}(\sigma\cdot\nabla)\mathrm{SL}(\lambda)I_2 f.$$

is valid for all $f \in L^2(\Sigma;\mathbb{C}^2)$. Furthermore

$$i(\sigma\cdot\nabla)\Psi_\lambda f = -\lambda\mathrm{SL}(\lambda)I_2 f \in H^1(\mathbb{R}^3;\mathbb{C}^2)$$

and

$$\Delta\Psi_\lambda f = i\lambda(\sigma\cdot\nabla)\mathrm{SL}(\lambda)I_2 f = -2m\lambda\Psi_\lambda f \in L^2(\mathbb{R}^3;\mathbb{C}^2)$$

are valid in the distributional sense for all $f \in L^2(\Sigma;\mathbb{C}^2)$.

iii) $\Psi_\lambda f \in H^1(\mathbb{R}^3\setminus\Sigma;\mathbb{C}^2)$ is valid for all $f \in H^{\frac{1}{2}}(\Sigma;\mathbb{C}^2)$ and the jump condition

$$i(\sigma\cdot\nu)\left(\tau_+\left(\Psi_\lambda f\right)_+ - \tau_-\left(\Psi_\lambda f\right)_-\right) = f$$

on the surface Σ holds true.

Proof. *Step 1:* As the reasoning of this proof is analogous to the one of Theorem 3.4, we will not present all the details, but refer to the proof of Theorem 3.4. In fact, only the dimension of the matrices needs to be changed from 4×4 to 2×2 without modifying the other arguments.

First, we define for $\lambda \in \mathbb{C}\setminus\mathbb{R}$ the matrix-valued functions

$$K_\lambda(x) = \frac{2m}{4\pi\|x\|}\exp\left(i\sqrt{2m\lambda}\|x\|\right)I_2$$

and

$$\begin{aligned} t_j(x) &= \frac{\partial}{\partial x_j}\left(\frac{2m}{4\pi\|x\|}\exp\left(i\sqrt{2m\lambda}\|x\|\right)\right)I_2 \\ &= \left(i\sqrt{2m\lambda}\|x\|-1\right)\frac{2m}{4\pi\|x\|^3}\exp\left(i\sqrt{2m\lambda}\|x\|\right)x_j I_2 \end{aligned}$$

for all $x \in \mathbb{R}^3 \setminus \{0\}$ and all $j \in \{1,2,3\}$. By using a line of reasoning as in the proof of Lemma 3.3 it can be shown that there exist constants $k_1, k_2 > 0$ such that

$$\|K_\lambda(x)\|, \|t_j(x)\| \leq k_1 \begin{cases} \|x\|^{-2} & , \text{ for } \|x\| < 1 \\ e^{-k_2\|x\|} & , \text{ for } \|x\| \geq 1 \end{cases}$$

is valid for all $x \in \mathbb{R}^3 \setminus \{0\}$ and all $j \in \{1,2,3\}$. Consequently, due to Theorem 2.34, we find that the assignment

$$(T_j f)(x) = \int\limits_{\mathbb{R}^3} t_j(x-y) f(y) \mathrm{d}y$$

for $f \in L^2(\mathbb{R}^3;\mathbb{C}^2)$ and $x \in \mathbb{R}^3$ corresponds to a well-defined, linear and bounded operator $T_j : L^2(\mathbb{R}^3;\mathbb{C}^2) \to L^2(\mathbb{R}^3;\mathbb{C}^2)$. Furthermore, as shown in Theorem 3.4 Step 3, the integration by parts formula

$$\int\limits_{\mathbb{R}^3} t_j(x-y)\Psi(x)\mathrm{d}x = -\int\limits_{\mathbb{R}^3} K_\lambda(x-y)\partial_j \Psi(x)\mathrm{d}x$$

is valid for all test functions $\Psi \in \mathcal{D}(\mathbb{R}^3;\mathbb{C}^2)$ and almost all $y \in \mathbb{R}^3$. This yields, as in Theorem 3.4 Step 5 with Fubini's theorem

$$\begin{aligned}
(T_j f, \Psi)_{L^2(\mathbb{R}^3;\mathbb{C}^2)} &= \int\limits_{\mathbb{R}^3}\int\limits_{\mathbb{R}^3} t_j(x-y) f(y) \cdot \overline{\Psi(x)} \mathrm{d}y \mathrm{d}x \\
&= \int\limits_{\mathbb{R}^3} f(y) \cdot \int\limits_{\mathbb{R}^3} t_j(x-y) \overline{\Psi(x)} \mathrm{d}x \mathrm{d}y \\
&= -\int\limits_{\mathbb{R}^3} f(y) \cdot \int\limits_{\mathbb{R}^3} K_\lambda(x-y) \partial_j \overline{\Psi(x)} \mathrm{d}x \mathrm{d}y \\
&= -\int\limits_{\mathbb{R}^3}\int\limits_{\mathbb{R}^3} K_\lambda(x-y) f(y) \cdot \partial_j \overline{\Psi(x)} \mathrm{d}y \mathrm{d}x \\
&= -\left(\left(-\frac{1}{2m}\Delta - \lambda \right)^{-1} I_2 f, \partial_j \Psi \right)_{L^2(\mathbb{R}^3;\mathbb{C}^2)}
\end{aligned}$$

and since this holds true for all test functions Ψ we obtain the explicit representation

$$\frac{\partial}{\partial x_j} \left(-\frac{1}{2m}\Delta - \lambda \right)^{-1} I_2 f = T_j f$$

for the weak derivative with respect to the variable x_j. As a result, it follows immediately by direct calculation that

$$\begin{aligned}&\left(-\frac{i}{2m}(\sigma\cdot\nabla)\right)\left(-\frac{1}{2m}\Delta-\lambda\right)^{-1}I_2f(x)=-\frac{i}{2m}\sum_{j=1}^{3}\sigma_j\frac{\partial}{\partial x_j}\left(-\frac{1}{2m}\Delta-\lambda\right)^{-1}I_2f(x)\\&=-\frac{i}{2m}\sum_{j=1}^{3}\sigma_jT_jf(x)=\int_{\mathbb{R}^3}-\frac{i}{2m}\sum_{j=1}^{3}\sigma_jt_j(x-y)f(y)\mathrm{d}y=\int_{\mathbb{R}^3}H_\lambda(x-y)f(y)\mathrm{d}y\end{aligned}$$

is valid for all $f\in L^2(\mathbb{R}^3;\mathbb{C}^2)$ and almost all $x\in\mathbb{R}^3$ with the integral kernel H_λ defined as in (4.15). Furthermore, the definition of the free Schrödinger operator leads to

$$\left(-\frac{i}{2m}(\sigma\cdot\nabla)\right)\left(-\frac{1}{2m}\Delta-\lambda\right)^{-1}I_2f\in H^1(\mathbb{R}^3;\mathbb{C}^2)$$

for all $f\in L^2(\mathbb{R}^3;\mathbb{C}^2)$ and therefore the trace operator τ can be applied. By proceeding as in the proof of Theorem 3.11 Step 1 it can now be shown that the non-tangential limits for this function exist as well and we therefore obtain

$$\tau\left(-\frac{i}{2m}(\sigma\cdot\nabla)\right)\left(-\frac{1}{2m}\Delta-\lambda\right)^{-1}I_2f(x)=\int_{\mathbb{R}^3}H_\lambda(x-y)f(y)\mathrm{d}y=\left(\Psi_{\overline{\lambda}}^*f\right)(x)$$

for all $f\in L^2(\mathbb{R}^3;\mathbb{C}^2)$ and almost all $x\in\Sigma$. This shows item i) of this lemma by using the mapping property of the trace operator τ.

Step 2: Assertion ii) can be proven analogously to i) by defining a linear and bounded operator $\widetilde{T}_j:L^2(\Sigma;\mathbb{C}^2)\to L^2(\mathbb{R}^3;\mathbb{C}^2)$ by the assignment

$$(\widetilde{T}_jf)(x)=\int_\Sigma t_j(x-y)f(y)\mathrm{d}\sigma(y)$$

for $f\in L^2(\Sigma;\mathbb{C}^2)$ and $x\in\mathbb{R}^3$ according to Step 1 and Theorem 2.36. Due to Theorem 2.39 it follows that $\mathrm{SL}(\lambda)I_2f\in H^1(\mathbb{R}^3;\mathbb{C}^2)$ is valid for all $f\in L^2(\Sigma;\mathbb{C}^2)$ and thus the weak derivatives of this function exist. Consequently, with the representation of the single layer potential for L^2-functions according to (4.3) there follows the explicit representation of the weak derivatives as

$$\begin{aligned}-\frac{i}{2m}(\sigma\cdot\nabla)\mathrm{SL}(\lambda)I_2f(x)&=-\frac{i}{2m}\sum_{j=1}^{3}\sigma_j\frac{\partial}{\partial x_j}\mathrm{SL}(\lambda)I_2f(x)=-\frac{i}{2m}\sum_{j=1}^{3}\sigma_j\widetilde{T}_jf(x)\\&=\int_\Sigma-\frac{i}{2m}\sum_{j=1}^{3}\sigma_jt_j(x-y)f(y)\mathrm{d}y=\int_\Sigma H_\lambda(x-y)f(y)\mathrm{d}y\\&=\left(\Psi_\lambda f\right)(x)\end{aligned}\tag{4.29}$$

for all $f \in L^2(\Sigma; \mathbb{C}^2)$ and almost all $x \in \mathbb{R}^3$, as in Step 1. This shows the first assertion of item ii).

Furthermore, this representation and Lemma 2.39 leads to

$$\begin{aligned} -i(\sigma \cdot \nabla)\left(\Psi_\lambda f\right)_\pm &= -\frac{1}{2m}(\sigma \cdot \nabla)^2 \left(\mathrm{SL}(\lambda) I_2 f\right)_\pm = -\frac{1}{2m}\Delta \left(\mathrm{SL}(\lambda) I_2 f\right)_\pm \\ &= \lambda \left(\mathrm{SL}(\lambda) I_2 f\right)_\pm \in H^1(\Omega_\pm; \mathbb{C}^2) \end{aligned}$$

on $\Omega_\pm$ in the distributional sense. It should be noted that for the second equal sign, the definition of the distributional Laplace operator and the validity of Schwarz's theorem for test functions was used. Another application of Lemma 2.39 yields the jump condition

$$\begin{aligned} \tau_+ \left(i(\sigma \cdot \nabla)\left(\Psi_\lambda f\right)_+\right) - \tau_- \left(i(\sigma \cdot \nabla)\left(\Psi_\lambda f\right)_-\right) &= -\lambda \left(\tau_+ \left(\mathrm{SL}(\lambda) I_2 f\right)_+ - \tau_- \left(\mathrm{SL}(\lambda) I_2 f\right)_-\right) \\ &= 0 \end{aligned}$$

on Σ which, in combination with Theorem 2.32 shows

$$i(\sigma \cdot \nabla)\Psi_\lambda f = -\lambda \mathrm{SL}(\lambda) I_2 f \in H^1(\mathbb{R}^3; \mathbb{C}^2). \tag{4.30}$$

Therefore, the weak derivatives of this expression exist and by using (4.29) and (4.30) we obtain

$$\begin{aligned} \Delta \Psi_\lambda f &= -i(\sigma \cdot \nabla) i(\sigma \cdot \nabla)\Psi_\lambda f = \lambda i(\sigma \cdot \nabla)\mathrm{SL}(\lambda) I_2 f \\ &= -2m\lambda \Psi_\lambda f \in L^2(\mathbb{R}^3; \mathbb{C}^2) \end{aligned}$$

in the distributional sense. This shows the claimed property concerning the distributional Laplace operator and completes the proof of ii).

Step 3: To prove assertion iii) we choose a complex number $\mu \in \mathbb{C} \setminus \mathbb{R}$ and an $c > 0$ such that

$$\frac{\mu^2}{c^2} - m^2 c^2 = 2m\lambda$$

is satisfied. By direct calculation the relation

$$\begin{aligned} A_2 H_\lambda(x) &= \left(1 - i\sqrt{2m\lambda}\|x\|\right) \frac{i}{4\pi\|x\|^3}(\alpha \cdot x)\exp\left(i\sqrt{2m\lambda}\|x\|\right) A_1 \\ &= \left(cG_\mu(x) - \left(\frac{\mu}{c} + mc\beta\right) K_\lambda(x)\right) A_1 \end{aligned}$$

for all $x \in \mathbb{R}\backslash\{0\}$ follows with the integral kernel G_μ defined as in (3.5) and the integral kernel of the resolvent of the free Schrödinger operator K_λ according to (2.20).

Obviously $M_1 f \in H^{\frac{1}{2}}(\Sigma; \mathbb{C}^4) = \mathrm{dom}(\gamma(\mu))$ is valid for a given $f \in H^{\frac{1}{2}}(\Sigma; \mathbb{C}^2)$ with the γ-field for the Dirac operator. Thus, by using the representation of the operator

Φ_μ defined as in (3.15) and the one of the single layer potential according to (2.21) we obtain

$$\begin{aligned} M_2\Psi_\lambda f &= \Big(c\Phi_\mu - \Big(\frac{\mu}{c} + mc\beta\Big)\,\mathrm{SL}(\lambda)\Big)\, M_1 f \\ &= \Big(c\gamma(\mu) - \Big(\frac{\mu}{c} + mc\beta\Big)\,\mathrm{SL}(\lambda)\Big)\, M_1 f \end{aligned} \tag{4.31}$$

by applying Theorem 3.11. This, in combination with the mapping properties of the values of the γ-field of Theorem 3.11 and those of the single layer potential of Lemma 2.39 shows that $\Psi_\lambda f \in H^1(\mathbb{R}^3 \setminus \Sigma; \mathbb{C}^2)$ is valid for all $f \in H^{\frac{1}{2}}(\Sigma; \mathbb{C}^2)$.

From the definition of the boundary maps of the quasi boundary triple of Theorem 3.8

$$M_1 f = \Gamma_0 \gamma(\mu) M_1 f = ic(\alpha\cdot\nu)\left(\tau_+\left(\gamma(\mu)M_1 f\right)_+ - \tau_-\left(\gamma(\mu)M_1 f\right)_-\right)$$

follows and with $(\alpha\cdot\nu)^2 = I_4$ furthermore that

$$-\,i(\alpha\cdot\nu)M_1 f = c\left(\tau_+\left(\gamma(\mu)M_1 f\right)_+ - \tau_-\left(\gamma(\mu)M_1 f\right)_-\right) \tag{4.32}$$

applies. By applying Lemma 2.39 we conclude from (4.31) and (4.32)

$$M_2\left(\tau_+\left(\Psi_\lambda f\right)_+ - \tau_-\left(\Psi_\lambda f\right)_-\right) = c\left(\tau_+\left(\gamma(\mu)M_1 f\right)_+ - \tau_-\left(\gamma(\mu)M_1 f\right)_-\right) = -i(\alpha\cdot\nu)M_1 f$$

for all $f \in H^{\frac{1}{2}}(\Sigma; \mathbb{C}^2)$. A component-wise consideration, the definition of the multiplication operators M_1 and M_2 and $(\sigma\cdot\nu)^2 = I_2$ finally results in

$$i(\sigma\cdot\nu)\left(\tau_+\left(\Psi_\lambda f\right)_+ - \tau_-\left(\Psi_\lambda f\right)_-\right) = f$$

for all $f \in H^{\frac{1}{2}}(\Sigma; \mathbb{C}^2)$. This shows the jump condition on Σ and completes the proof of the theorem. □

Next, we define a linear operator in $L^2(\mathbb{R}^3; \mathbb{C}^2)$, which will be important for the subsequent considerations, by the following observation. Let $f \in H^1(\Omega_+; \mathbb{C}^2) \oplus H^1(\Omega_-; \mathbb{C}^2)$ with $(\sigma\cdot\nabla)f_+ \oplus (\sigma\cdot\nabla)f_- \in H^1(\mathbb{R}^3; \mathbb{C}^2)$ be given, then it can be shown by using the definition of the distributional derivative and Schwarz's theorem for test functions that the relation

$$\Delta f = (\sigma\cdot\nabla)(\sigma\cdot\nabla) f \in L^2(\mathbb{R}^3; \mathbb{C}^2)$$

is valid for the distributional Laplace operator. Therefore, for an arbitrary $\varepsilon \in \mathbb{R}$ the linear operator

$$\begin{aligned} \mathrm{dom}(T_\varepsilon) = \Bigg\{ f \in H^1(\Omega_+; \mathbb{C}^2) \oplus H^1(\Omega_-; \mathbb{C}^2) \,\Bigg|\, & (\sigma\cdot\nabla)f_+ \oplus (\sigma\cdot\nabla)f_- \in H^1(\mathbb{R}^3; \mathbb{C}^2) \\ & \text{and } i(\sigma\cdot\nu)\left(\tau_+ f_+ - \tau_- f_-\right) = \varepsilon\tau\left(\frac{i}{2m}(\sigma\cdot\nabla)f\right) \Bigg\} \\ T_\varepsilon f = -\frac{1}{2m}\Delta f \qquad & \end{aligned} \tag{4.33}$$

with the trace operator τ from (4.28) is well-defined. As in the previous sections, we use the isomorphism $\iota : L^2(\mathbb{R}^3;\mathbb{C}^4) \to L^2(\Omega_+;\mathbb{C}^4) \oplus L^2(\Omega_-;\mathbb{C}^4)$ of Section 2.6 to regard T_ε as a linear operator in $L^2(\mathbb{R}^3;\mathbb{C}^2)$ with domain of definition $\mathrm{dom}(T_\varepsilon) \subseteq H^1(\mathbb{R}^3 \setminus \Sigma;\mathbb{C}^2)$. Furthermore, this linear operator is densely defined since $\mathcal{D}(\mathbb{R}^3 \setminus \Sigma;\mathbb{C}^2) \subseteq \mathrm{dom}(T_\varepsilon)$ holds true.

Lemma 4.10. The operator T_ε defined as in (4.33) is a symmetric operator in $L^2(\mathbb{R}^3;\mathbb{C}^2)$.

Proof. Let $f, g \in \mathrm{dom}(T_\varepsilon)$ be given, then from the divergence theorem and the hermiticity of the Pauli spin matrices it follows that

$$\begin{aligned}
&\left(-\frac{1}{2m}\Delta f_\pm, g_\pm\right)_{L^2(\Omega_\pm;\mathbb{C}^2)} = \left(\frac{1}{2m} i(\sigma\cdot\nabla) i(\sigma\cdot\nabla) f_\pm, g_\pm\right)_{L^2(\Omega_\pm;\mathbb{C}^2)}\\
&= \frac{1}{2m}(i(\sigma\cdot\nabla)f_\pm, i(\sigma\cdot\nabla)g_\pm)_{L^2(\Omega_\pm;\mathbb{C}^2)} \pm \left(\frac{i}{2m}(\sigma\cdot\nu)\tau_\pm\left(i(\sigma\cdot\nabla)f_\pm\right), \tau_\pm g_\pm\right)_{L^2(\Sigma;\mathbb{C}^2)}\\
&= \frac{1}{2m}(i(\sigma\cdot\nabla)f_\pm, i(\sigma\cdot\nabla)g_\pm)_{L^2(\Omega_\pm;\mathbb{C}^2)} \mp \left(\tau_\pm\left(\frac{i}{2m}(\sigma\cdot\nabla)f_\pm\right), i(\sigma\cdot\nu)\tau_\pm g_\pm\right)_{L^2(\Sigma;\mathbb{C}^2)}\\
&= \frac{1}{2m}(i(\sigma\cdot\nabla)f_\pm, i(\sigma\cdot\nabla)g_\pm)_{L^2(\Omega_\pm;\mathbb{C}^2)} \mp \left(\tau\left(\frac{i}{2m}(\sigma\cdot\nabla)f\right), i(\sigma\cdot\nu)\tau_\pm g_\pm\right)_{L^2(\Sigma;\mathbb{C}^2)}.
\end{aligned}$$

applies. If we add these two equations and use the jump condition on Σ for functions from the domain of definition of T_ε we obtain the following equality.

$$\begin{aligned}
&\left(-\frac{1}{2m}\Delta f, g\right)_{L^2(\mathbb{R}^3;\mathbb{C}^2)} = \left(-\frac{1}{2m}\Delta f_+, g\right)_{L^2(\Omega_+;\mathbb{C}^2)} + \left(-\frac{1}{2m}\Delta f_-, g_-\right)_{L^2(\Omega_-;\mathbb{C}^2)}\\
&= \frac{1}{2m}(i(\sigma\cdot\nabla)f_+, i(\sigma\cdot\nabla)g_+)_{L^2(\Omega_+;\mathbb{C}^2)} + \frac{1}{2m}(i(\sigma\cdot\nabla)f_-, i(\sigma\cdot\nabla)g_-)_{L^2(\Omega_-;\mathbb{C}^2)}\\
&\quad - \left(\tau\left(\frac{i}{2m}(\sigma\cdot\nabla)f\right), i(\sigma\cdot\nu)\left(\tau_+ g_+ - \tau_- g_-\right)\right)_{L^2(\Sigma;\mathbb{C}^2)}\\
&= \frac{1}{2m}(i(\sigma\cdot\nabla)f, i(\sigma\cdot\nabla)g)_{L^2(\mathbb{R}^3;\mathbb{C}^2)} - \varepsilon\left(\tau\left(\frac{i}{2m}(\sigma\cdot\nabla)f\right), \tau\left(\frac{i}{2m}(\sigma\cdot\nabla)g\right)\right)_{L^2(\Sigma;\mathbb{C}^2)}
\end{aligned}$$

In the same way it can be shown that

$$\begin{aligned}
&\left(f, -\frac{1}{2m}\Delta g\right)_{L^2(\mathbb{R}^3;\mathbb{C}^2)}\\
&= \frac{1}{2m}(i(\sigma\cdot\nabla)f, i(\sigma\cdot\nabla)g)_{L^2(\mathbb{R}^3;\mathbb{C}^2)} - \varepsilon\left(\tau\left(\frac{i}{2m}(\sigma\cdot\nabla)f\right), \tau\left(\frac{i}{2m}(\sigma\cdot\nabla)g\right)\right)_{L^2(\Sigma;\mathbb{C}^2)}
\end{aligned}$$

is valid as well. Finally, this leads to

$$(T_\varepsilon f, g)_{L^2(\mathbb{R}^3;\mathbb{C}^2)} - (f, T_\varepsilon g)_{L^2(\mathbb{R}^3;\mathbb{C}^2)} = \left(-\frac{1}{2m}\Delta f, g\right)_{L^2(\mathbb{R}^3;\mathbb{C}^2)} - \left(f, -\frac{1}{2m}\Delta g\right)_{L^2(\mathbb{R}^3;\mathbb{C}^2)} = 0$$

for all $f, g \in \mathrm{dom}(T_\varepsilon)$ which shows the symmetry of T_ε. $\square$

Before we finally discuss the non-relativistic limit we require a further auxiliary result, which shows the continuous invertibility of the operator $I + \varepsilon\mathcal{D}_\lambda$.

Lemma 4.11. The operator $I + \varepsilon\mathcal{D}_\lambda$ is bijective in $L^2(\Sigma; \mathbb{C}^2)$ for all $\varepsilon \in \mathbb{R}$ and all $\lambda \in \mathbb{C} \setminus \mathbb{R}$ and also the inverse operator is bounded. Furthermore, the restriction $(I + \varepsilon\mathcal{D}_\lambda) \upharpoonright H^{\frac{1}{2}}(\Sigma; \mathbb{C}^2)$ as a linear operator in $H^{\frac{1}{2}}(\Sigma; \mathbb{C}^2)$ is bijective as well.

Proof. *Step 1:* Since $\mathcal{D}_\lambda$ is compact according to Theorem 4.6, it is sufficient to show that the operator $I + \varepsilon\mathcal{D}_\lambda$ is injective due to Fredholm's alternative. For this purpose we assume that there exists an $f \in \ker(I + \varepsilon\mathcal{D}_\lambda) \setminus \{0\}$. Due to the mapping properties of $\mathcal{D}_\lambda$ according to Theorem 4.6 one obtains

$$f = -\varepsilon\mathcal{D}_\lambda f \in H^{\frac{1}{2}}(\Sigma; \mathbb{C}^2)$$

which leads with Theorem 4.9 to $\Psi_\lambda f \in H^1(\mathbb{R}^3 \setminus \Sigma; \mathbb{C}^2)$ and $i(\sigma \cdot \nabla)\Psi_\lambda f \in H^1(\mathbb{R}^3; \mathbb{C}^2)$. Furthermore, we conclude from Theorem 4.9, the definition of $\mathcal{D}_\lambda$ as a restriction of the single layer boundary integral operator and the connection of the latter with the single layer potential

$$\begin{aligned} i(\sigma \cdot \nu)\left(\tau_+ (\Psi_\lambda f)_+ - \tau_- (\Psi_\lambda f)_-\right) = f = -\varepsilon\mathcal{D}_\lambda f &= -\frac{\varepsilon\lambda}{2m} S(\lambda) f \\ &= -\frac{\varepsilon\lambda}{2m}\tau\left(\mathrm{SL}(\lambda) I_2 f\right) = \varepsilon\tau\left(\frac{i}{2m}(\sigma \cdot \nabla)\Psi_\lambda f\right) \end{aligned}$$

with the trace operator τ from (4.28). Overall, $\Psi_\lambda f \in \mathrm{dom}(T_\varepsilon)$ follows and therefore we are able to apply the operator T_ε to $\Psi_\lambda f$.

With Theorem 4.9 we obtain

$$T_\varepsilon \Psi_\lambda f = -\frac{1}{2m}\Delta\Psi_\lambda f = -\frac{\lambda}{2m} i(\sigma \cdot \nabla)\mathrm{SL}(\lambda) f = \lambda\Psi_\lambda f$$

and therefore $\Psi_\lambda f$ is a eigenfunction of T_ε to the complex eigenvalue $\lambda \in \mathbb{C} \setminus \mathbb{R}$. This is a contradiction due to the symmetry of T_ε and Theorem 2.15. Consequently, $I + \varepsilon\mathcal{D}_\lambda$ is injective and according to Theorem 2.3 even bijective. Finally, from Theorem 2.6 the boundedness of the inverse operator follows.

Step 2: As $I + \varepsilon\mathcal{D}_\lambda$ is injective according to Step 1, this also carries over to the restriction to $H^{\frac{1}{2}}(\Sigma; \mathbb{C}^2)$. Thus the surjectivity of the latter remains to be shown. Let an arbitrary $g \in H^{\frac{1}{2}}(\Sigma; \mathbb{C}^2)$ be given, then due to Step 1 there exists an $f \in L^2(\Sigma; \mathbb{C}^2)$ such that

$$g = (I + \varepsilon\mathcal{D}_\lambda) f$$

applies. From the mapping properties of $\mathcal{D}_\lambda$ according to Theorem 4.6 we immediately deduce that

$$f = g - \varepsilon\mathcal{D}_\lambda f \in H^{\frac{1}{2}}(\Sigma; \mathbb{C}^2)$$

is valid and thus the operator $I + \varepsilon\mathcal{D}_\lambda$ is bijective as an operator in $H^{\frac{1}{2}}(\Sigma; \mathbb{C}^2)$. $\square$

Now we are in the position to show the main result of this section. It turns out that for the c-dependent interaction strengths $\eta, \tau \in \mathbb{R}$ the resolvents of the Dirac operators $A_{\eta,\tau}$ converge to the resolvents of T_ε modified by the multiplication operator M_2.

Theorem 4.12. Let $\lambda \in \mathbb{C} \setminus \mathbb{R}$ and c-dependent interaction strengths $\eta, \tau \in \mathbb{R}$ with $\eta + \tau = 0$ and $\eta - \tau = \varepsilon c^2$ for an $\varepsilon \in \mathbb{R}$ be given. Furthermore, let T_ε be the linear operator defined as in (4.33), then there exists a constant $\kappa(m, \lambda, \varepsilon, \Sigma) > 0$ only dependent on m, λ, ε and Σ such that the following estimate is valid for sufficiently large $c > 0$

$$\left\| \left(A_{\eta,\tau} - \left(\lambda + mc^2\right)\right)^{-1} - M_2 \left(T_\varepsilon - \lambda\right)^{-1} M_2^* \right\| \leq \frac{\kappa}{c}.$$

In particular, the convergence

$$\left(A_{\eta,\tau} - \left(\lambda + mc^2\right)\right)^{-1} \to \begin{pmatrix} \left(T_\varepsilon - \lambda\right)^{-1} & 0 \\ 0 & 0 \end{pmatrix} \quad \text{for } c \to \infty$$

in the operator norm applies as well as a convergence rate of $\mathcal{O}\left(\frac{1}{c}\right)$.

Proof. *Step 1:* Let $\lambda \in \mathbb{C} \setminus \mathbb{R}$ be given, then it follows from Lemma 4.5 and Lemma 4.11 that the operators $I + \varepsilon c^2 M_1^* \mathcal{C}_{\lambda+mc^2} M_1$ and $I + \varepsilon \mathcal{D}_\lambda$ are invertible and their inverse operators are bounded. Furthermore, according to Theorem 4.7 there exists a constant $k(m, \lambda) > 0$ only dependent on m and λ such that for sufficiently large $c > 0$ the estimate

$$\left\| c^2 M_1^* \mathcal{C}_{\lambda+mc^2} M_1 - \mathcal{D}_\lambda \right\| \leq \frac{k}{c}$$

applies. If we define the operators

$$T = I + \varepsilon \mathcal{D}_\lambda$$

and

$$A = \left(I + \varepsilon c^2 M_1^* \mathcal{C}_{\lambda+mc^2} M_1\right) - \left(I + \varepsilon \mathcal{D}_\lambda\right) = \varepsilon \left(c^2 M_1^* \mathcal{C}_{\lambda+mc^2} M_1 - \mathcal{D}_\lambda\right)$$

then the estimate $\|A\| \|T^{-1}\| < 1$ is valid for sufficiently large $c > 0$. Thus by applying Theorem 2.8 we obtain

$$\begin{aligned} \left\| \left(I + \varepsilon c^2 M_1^* \mathcal{C}_{\lambda+mc^2} M_1\right)^{-1} - \left(I + \varepsilon \mathcal{D}_\lambda\right)^{-1} \right\| &\leq \frac{\|T^{-1}\|^2 \|A\|}{1 - \|A\| \|T^{-1}\|} \\ &\leq \frac{\frac{|\varepsilon| k}{c} \|T^{-1}\|^2}{1 - \frac{|\varepsilon| k}{c} \|T^{-1}\|} \\ &\leq \frac{2 \left|\varepsilon\right| k \|T^{-1}\|^2}{c} \end{aligned}$$

for sufficiently large $c > 0$. In addition, Theorem 4.7 provides us with the estimates

$$\|c \Phi_{\lambda+mc^2} M_1\| \leq 1 + \|M_2 \Psi_\lambda\| = K_1 \tag{4.34}$$

and
$$\left\| \left(I + \varepsilon c^2 \mathcal{C}_{\lambda+mc^2}\right)^{-1} \right\| \leq 1 + \left\| (I + \varepsilon \mathcal{D}_\lambda)^{-1} \right\| = K_2 \tag{4.35}$$
for sufficiently large $c > 0$ due to the triangle inequality. The two constants $K_1(m, \lambda, \Sigma) \geq 1$ and $K_2(m, \lambda, \varepsilon, \Sigma) \geq 1$ are only dependent on m, λ, ε and Σ.

Next, from Theorem 3.14 and Lemma 4.5 the resolvent representation of $A_{\eta,\tau}$ as

$$\begin{aligned}
\left(A_{\eta,\tau} - (\lambda + mc^2)\right)^{-1} &= \left(A_0 - (\lambda + mc^2)\right)^{-1} \\
&\quad - \gamma(\lambda + mc^2) \left(I + BM(\lambda + mc^2)\right)^{-1} B\gamma(\overline{\lambda} + mc^2)^* \\
&= \left(A_0 - (\lambda + mc^2)\right)^{-1} - \Phi_{\lambda+mc^2} \left(I + B\mathcal{C}_{\lambda+mc^2}\right)^{-1} B\Phi^*_{\overline{\lambda}+mc^2} \\
&= \left(A_0 - (\lambda + mc^2)\right)^{-1} \\
&\quad - c\Phi_{\lambda+mc^2} M_1 \left(I + \varepsilon c^2 M_1^* \mathcal{C}_{\lambda+mc^2} M_1\right)^{-1} \varepsilon c M_1^* \Phi^*_{\overline{\lambda}+mc^2}
\end{aligned}$$

is obtained. By using (4.34) and (4.35) and applying the triangle inequality several times, this leads to

$$\begin{aligned}
&\left\| \left(A_{\eta,\tau} - (\lambda + mc^2)\right)^{-1} - (T_0 - \lambda)^{-1} P_+ + M_2 \Psi_\lambda \left(I + \varepsilon \mathcal{D}_\lambda\right)^{-1} \varepsilon \Psi^*_{\overline{\lambda}} M_2^* \right\| \\
&\qquad \leq \left\| \left(A_0 - (\lambda + mc^2)\right)^{-1} - (T_0 - \lambda)^{-1} P_+ \right\| \\
&\qquad\quad + |\varepsilon| \max\{K_1, K_2\}^2 \Bigg(\|c\Phi_{\lambda+mc^2} M_1 - M_2 \Psi_\lambda\| \\
&\qquad\quad + \|c\Phi_{\lambda+mc^2} M_1 - M_2 \Psi_\lambda\| + \left\| \left(I + \varepsilon c^2 \mathcal{C}_{\lambda+mc^2}\right)^{-1} - (I + \varepsilon)^{-1} \mathcal{D}_\lambda \right\| \Bigg)
\end{aligned}$$

for sufficiently large $c > 0$ with the free Schrödinger operator T_0 defined as in (2.18). Finally, with Theorem 4.3 and Theorem 4.7 the estimate

$$\left\| \left(A_{\eta,\tau} - (\lambda + mc^2)\right)^{-1} - (T_0 - \lambda)^{-1} P_+ + M_2 \Psi_\lambda \left(I + \varepsilon \mathcal{D}_\lambda\right)^{-1} \varepsilon \Psi^*_{\overline{\lambda}} M_2^* \right\| \leq \frac{\kappa}{c}$$

follows for sufficiently large $c > 0$. The constant $\kappa(m, \lambda, \varepsilon, \Sigma) > 0$ is only dependent on m, λ, ε and Σ. Furthermore, a direct calculation involving the definition of the multiplication operator M_2 shows that

$$M_2 \Psi_\lambda \left(I + \varepsilon \mathcal{D}_\lambda\right)^{-1} \varepsilon \Psi^*_{\overline{\lambda}} M_2^* = \begin{pmatrix} \Psi_\lambda \left(I + \varepsilon \mathcal{D}_\lambda\right)^{-1} \varepsilon \Psi^*_{\overline{\lambda}} & 0 \\ 0 & 0 \end{pmatrix}$$

applies.

Step 2: Next, we will show that the linear and bounded operator

$$R(\lambda) = (T_0 - \lambda)^{-1} I_2 - \Psi_\lambda (I + \varepsilon \mathcal{D}_\lambda)^{-1} \varepsilon \Psi_{\overline{\lambda}}^*$$

from Step 1 corresponds to the resolvent of a self-adjoint operator in $L^2(\mathbb{R}^3; \mathbb{C}^2)$. For this purpose we will apply the result of Section 2.3.

By using the trace operator $\tau : H^1(\mathbb{R}^3; \mathbb{C}^2) \to H^{\frac{1}{2}}(\Sigma; \mathbb{C}^2)$ of (4.28) we now define a mapping $\widetilde{\tau} : H^2(\mathbb{R}^3; \mathbb{C}^2) \to H^{\frac{1}{2}}(\Sigma; \mathbb{C}^2)$ by the assignment

$$\widetilde{\tau} f = \tau \left(-\frac{i}{2m} (\sigma \cdot \nabla) \right) f$$

for $f \in H^2(\mathbb{R}^3; \mathbb{C}^2)$ and thus obtain a linear and bounded operator. It can now be shown with the help of the Fourier transform that the H^2-norm is equivalent to the graph norm induced by the Laplace operator and therefore $\widetilde{\tau}$ is bounded as a mapping from $\left(\mathrm{dom}(T_0 I_2), \|\cdot\|_{T_0 I_2}\right)$ to $L^2(\mathbb{R}^3; \mathbb{C}^2)$. Furthermore, its kernel is dense in $L^2(\mathbb{R}^3; \mathbb{C}^2)$, since $\widetilde{\tau} f = 0$ applies to all test functions $f \in \mathcal{D}(\mathbb{R}^3 \setminus \Sigma; \mathbb{C}^2)$. An application of Theorem 4.9 eventually leads to the relationship

$$\Psi_{\overline{\lambda}}^* = \widetilde{\tau} \left(-\frac{1}{2m} \Delta - \lambda \right)^{-1} I_2$$

on $L^2(\mathbb{R}^3; \mathbb{C}^2)$ between the resolvent of the free Schrödinger operator and the linear operator $\Psi_{\overline{\lambda}}^*$.

Next, we restrict ourselves to the case that $\varepsilon \neq 0$ applies, otherwise Theorem 4.3 shows the convergence of the free Dirac operator to a free Schrödinger operator with the claimed properties. We define the mapping

$$\Gamma_\varepsilon(\lambda) = \frac{1}{\varepsilon} I + \mathcal{D}_\lambda : L^2(\Sigma; \mathbb{C}^2) \to L^2(\Sigma; \mathbb{C}^2)$$

for $\lambda \in \mathbb{C} \setminus \mathbb{R}$ and thus obtain a family of linear and bounded operators which are continuously invertible due to Lemma 4.11.

Finally, an application of Lemma 4.8 yields that the operators $\Gamma_\varepsilon(\lambda)$, $\mathcal{D}_\lambda$, $\Psi_{\overline{\lambda}}^*$ and Ψ_λ satisfy the conditions of Theorem 2.20 and therefore there exists a self-adjoint operator $\widetilde{T}_\varepsilon$ in $L^2(\mathbb{R}^3; \mathbb{C}^2)$ which coincides on $\ker(\widetilde{\tau})$ with the free Schrödinger operator $T_0 I_2$ defined as in (2.18). This operator has the following explicit representation for all $\lambda \in \mathbb{C} \setminus \mathbb{R}$.

$$\begin{aligned} \mathrm{dom}(\widetilde{T}_\varepsilon) &= \mathrm{ran}\left((T_0 - \lambda)^{-1} I_2 - \Psi_\lambda (I + \varepsilon \mathcal{D}_\lambda) \varepsilon \Psi_{\overline{\lambda}}^* \right) \\ &= \left\{ f \in L^2(\mathbb{R}^3; \mathbb{C}^2) \,\middle|\, \exists f_\lambda \in H^2(\mathbb{R}^3; \mathbb{C}^2) \text{ with } f = f_\lambda - \Psi_\lambda (I + \varepsilon \mathcal{D}_\lambda)^{-1} \varepsilon \widetilde{\tau} f_\lambda \right\} \end{aligned}$$

$$(\widetilde{T}_\varepsilon - \lambda) f = (T_0 - \lambda) I_2 f_\lambda$$

Furthermore, the definition of $\widetilde{T}_\varepsilon$ is independent of $\lambda \in \mathbb{C} \setminus \mathbb{R}$ and the decomposition of $f \in \operatorname{dom}(\widetilde{T}_\varepsilon)$ in the representation of the domain of definition $\operatorname{dom}(\widetilde{T}_\varepsilon)$ is unique.

Step 3: To complete the proof it remains to show that $T_\varepsilon = \widetilde{T}_\varepsilon$ is valid in the sense of linear operators. In the first step we will show that $\operatorname{dom}(\widetilde{T}_\varepsilon) \subseteq \operatorname{dom}(T_\varepsilon)$ holds true and therefore we assume that an arbitrary $f \in \operatorname{dom}(\widetilde{T}_\varepsilon)$ is given. Due to the explicit representation of the operator $\widetilde{T}_\varepsilon$ of Step 2 there exists a unique $f_\lambda \in L^2(\mathbb{R}^3;\mathbb{C}^2)$ for any $\lambda \in \mathbb{C} \setminus \mathbb{R}$ such that

$$\begin{aligned} f &= (T_0 - \lambda)^{-1} I_2 f_\lambda - \Psi_\lambda \left(I + \varepsilon \mathcal{D}_\lambda\right)^{-1} \varepsilon \Psi_{\overline{\lambda}}^* f_\lambda \\ &= g_\lambda - \Psi_\lambda h_\lambda. \end{aligned}$$

with functions $g_\lambda \in L^2(\mathbb{R}^3;\mathbb{C}^2)$ and $h_\lambda \in L^2(\Sigma;\mathbb{C}^2)$ applies.

From the definition of the resolvent of the free Schrödinger operator we obtain $g_\lambda \in H^2(\mathbb{R}^3;\mathbb{C}^2)$ whereas due to Theorem 4.9 and Lemma 4.11 $h_\lambda \in H^{\frac{1}{2}}(\Sigma;\mathbb{C}^2)$ follows. This yields with Theorem 4.9 that $\Psi_\lambda h_\lambda \in H^1(\mathbb{R}^3 \setminus \Sigma;\mathbb{C}^2)$ and finally that $f \in H^1(\mathbb{R}^3 \setminus \Sigma;\mathbb{C}^2)$ applies. Consequently, $\operatorname{dom}(\widetilde{T}_\varepsilon) \subseteq H^1(\mathbb{R}^3 \setminus \Sigma;\mathbb{C}^2)$ is valid.

To derive further properties of f we first observe that

$$(\sigma \cdot \nabla) g_\lambda \in H^1(\mathbb{R}^3;\mathbb{C}^2)$$

is valid for $g_\lambda \in H^2(\mathbb{R}^3;\mathbb{C}^2)$ while according to Theorem 4.9

$$(\sigma \cdot \nabla)(\Psi_\lambda h_\lambda)_+ \oplus (\sigma \cdot \nabla)(\Psi_\lambda h_\lambda)_- \in H^1(\mathbb{R}^3;\mathbb{C}^2)$$

follows for $h_\lambda \in H^{\frac{1}{2}}(\Sigma;\mathbb{C}^2)$. Thus, due to the linearity of the weak derivative, we obtain $(\sigma \cdot \nabla) f \in H^1(\mathbb{R}^3;\mathbb{C}^2)$.

Next, by using Theorem 2.32 for $g_\lambda \in H^2(\mathbb{R}^3;\mathbb{C}^2)$ we obtain the jump condition

$$i(\sigma \cdot \nu)\left(\tau_+ (g_\lambda)_+ - \tau_- (g_\lambda)_-\right) = 0 \tag{4.36}$$

on Σ while Theorem 4.9 provides the jump condition

$$i(\sigma \cdot \nu)\left(\tau_+ (\Psi_\lambda h_\lambda)_+ - \tau_- (\Psi_\lambda h_\lambda)_-\right) = h_\lambda \tag{4.37}$$

on Σ for $h_\lambda \in H^{\frac{1}{2}}(\Sigma;\mathbb{C}^2)$. If we now combine (4.36) and (4.37) we obtain

$$\begin{aligned} &i(\sigma \cdot \nu)\left(\tau_+ f_+ - \tau_- f_-\right) \\ &\quad= i(\sigma \cdot \nu)\left(\tau_+ (g_\lambda)_+ - \tau_- (g_\lambda)_-\right) - i(\sigma \cdot \nu)\left(\tau_+ (\Psi_\lambda h_\lambda)_+ - \tau_- (\Psi_\lambda h_\lambda)_-\right) \\ &\quad= -i(\sigma \cdot \nu)\left(\tau_+ (\Psi_\lambda h_\lambda)_+ - \tau_- (\Psi_\lambda h_\lambda)_-\right) \\ &\quad= -h_\lambda = -\left(\frac{1}{\varepsilon} I + \mathcal{D}_\lambda\right)^{-1} \Psi_{\overline{\lambda}}^* f_\lambda \end{aligned} \tag{4.38}$$

for the behavior of f on the surface Σ.

On the other hand, with Theorem 4.9, the definition of the operator $\mathcal{D}_\lambda$ and the trace operator $\tau : H^1(\mathbb{R}^3; \mathbb{C}^2) \to H^{\frac{1}{2}}(\Sigma; \mathbb{C}^2)$ according to (4.28) we find

$$\begin{aligned}
\tau\left(\frac{i}{2m}(\sigma\cdot\nabla)f\right) &= \tau\left(\frac{i}{2m}(\sigma\cdot\nabla)g_\lambda\right) - \tau\left(\frac{i}{2m}(\sigma\cdot\nabla)\Psi_\lambda h_\lambda\right)\\
&= \tau\left(\frac{i}{2m}(\sigma\cdot\nabla)\left(T_0-\lambda\right)^{-1} I_2 f_\lambda\right) + \frac{\lambda}{2m}\tau\left(\mathrm{SL}(\lambda) I_2 h_\lambda\right)\\
&= -\Psi_{\overline{\lambda}}^* f_\lambda + \mathcal{D}_\lambda h_\lambda\\
&= -\Psi_{\overline{\lambda}}^* f_\lambda + \mathcal{D}_\lambda\left(\frac{1}{\varepsilon}I + \mathcal{D}_\lambda\right)^{-1}\Psi_{\overline{\lambda}}^* f_\lambda
\end{aligned} \tag{4.39}$$

due to the definition of h_λ. Combining (4.38) and (4.39) finally leads to

$$\begin{aligned}
&\tau\left(\frac{i}{2m}(\sigma\cdot\nabla)f\right) - \frac{i}{\varepsilon}(\sigma\cdot\nu)\left(\tau_+ f_+ - \tau_- f_-\right)\\
&\quad= -\Psi_{\overline{\lambda}}^* f_\lambda + \mathcal{D}_\lambda\left(\frac{1}{\varepsilon}I + \mathcal{D}_\lambda\right)^{-1}\Psi_{\overline{\lambda}}^* f_\lambda + \frac{1}{\varepsilon}\left(\frac{1}{\varepsilon}I + \mathcal{D}_\lambda\right)^{-1}\Psi_{\overline{\lambda}}^* f_\lambda\\
&\quad= \left(-I + \left(\frac{1}{\varepsilon}I + \mathcal{D}_\lambda\right)\left(\frac{1}{\varepsilon}I + \mathcal{D}_\lambda\right)^{-1}\right)\Psi_{\overline{\lambda}}^* f_\lambda\\
&\quad= 0
\end{aligned}$$

which after a multiplication with ε shows the jump condition of f on Σ. Altogether we therefore obtain $f \in \mathrm{dom}(T_\varepsilon)$ and further $\mathrm{dom}(\widetilde{T}_\varepsilon) \subseteq \mathrm{dom}(T_\varepsilon)$.

Step 4: After we have already shown $\mathrm{dom}(\widetilde{T}_\varepsilon) \subseteq \mathrm{dom}(T_\varepsilon)$ in Step 3 we will now show $\widetilde{T}_\varepsilon f = T_\varepsilon f$ for all $f \in \mathrm{dom}(\widetilde{T}_\varepsilon)$. This then yields the inclusion $\widetilde{T}_\varepsilon \subseteq T_\varepsilon$ in the sense of linear operators.

For this purpose we choose arbitrary $f \in \mathrm{dom}(\widetilde{T}_\varepsilon)$ and $\lambda \in \mathbb{C} \setminus \mathbb{R}$ with the unique element $f_\lambda \in L^2(\mathbb{R}^3; \mathbb{C}^2)$ as in Step 3 such that

$$\begin{aligned}
f &= \left(T_0-\lambda\right)^{-1} I_2 f_\lambda - \Psi_\lambda\left(I + \varepsilon\mathcal{D}_\lambda\right)^{-1}\varepsilon\Psi_{\overline{\lambda}}^* f_\lambda\\
&= g_\lambda - \Psi_\lambda h_\lambda.
\end{aligned}$$

with $g_\lambda \in H^2(\mathbb{R}^3; \mathbb{C}^2)$ and $h_\lambda \in H^{\frac{1}{2}}(\Sigma; \mathbb{C}^2)$ applies. Due to Theorem 4.9 we obtain

$$-\frac{1}{2m}\Delta\Psi_\lambda h_\lambda = \lambda\Psi_\lambda h_\lambda$$

and therefore, after rearranging this equation

$$\left(-\frac{1}{2m}\Delta - \lambda\right)\Psi_\lambda h_\lambda = 0 \tag{4.40}$$

in the distributional sense. Consequently, with (4.40), the definition of the operator $\widetilde{T}_\varepsilon$ from Step 2 and the linearity of the distributional Laplace operator we obtain

$$\begin{aligned}(T_\varepsilon - \lambda) f = (T_\varepsilon - \lambda)(g_\lambda - \Psi_\lambda h_\lambda) &= \left(-\frac{1}{2m}\Delta - \lambda\right) I_2 (g_\lambda - \Psi_\lambda h_\lambda) \\ &= \left(-\frac{1}{2m}\Delta - \lambda\right) I_2 g_\lambda - \left(-\frac{1}{2m}\Delta - \lambda\right) I_2 \Psi_\lambda h_\lambda \\ &= \left(-\frac{1}{2m}\Delta - \lambda\right) I_2 g_\lambda = (T_0 - \lambda) I_2 g_\lambda = \left(\widetilde{T}_\varepsilon - \lambda\right) f\end{aligned}$$

which finally leads to $T_\varepsilon f = \widetilde{T}_\varepsilon f$. This is equivalent to $\widetilde{T}_\varepsilon \subseteq T_\varepsilon$ and due to Theorem 2.10, the symmetry of T_ε and the self-adjointness of $\widetilde{T}_\varepsilon$ we find the following chain of inclusions.

$$\widetilde{T}_\varepsilon \subseteq T_\varepsilon \subseteq T_\varepsilon^* \subseteq \widetilde{T}_\varepsilon^* = \widetilde{T}_\varepsilon$$

Thus $T_\varepsilon = \widetilde{T}_\varepsilon$ in the sense of linear operators follows which completes the proof. □

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