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Spectral Analysis of Transmission and Boundary Value Problems for Dirac Operators

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Abstract

The present thesis is devoted to the spectral analysis of transmission and boundary value problems for Dirac operators. Dirac operators are one of the main mathematical tools in relativistic quantum mechanics to describe the propagation of spin $\frac{1}{2}$ particles taking relativistic effects into account. In the first part of the thesis Dirac operators with singular δ-shell interactions which are combinations of electrostatic and Lorentz scalar potentials are studied. Such operators are associated to transmission problems for the Dirac equation. The second part of the thesis is then devoted to self-adjoint Dirac operators in domains. With the aid of boundary triples the self-adjointness of the corresponding operators is shown and some of the spectral data are computed. An interesting property is the existence of critical interaction strengths and boundary values, respectively, for which the associated operators have significantly different spectral properties. Eventually, for Dirac operators with singular interactions also the nonrelativistic limit is computed.

Zusammenfassung

In der vorliegenden Dissertation werden Transmissions- und Randwertprobleme für Dirac-Operatoren behandelt. Dirac-Operatoren sind eines der wichtigsten mathematischen Werkzeuge in der relativistischen Quantenmechanik zur Beschreibung von Teilchen mit Spin $\frac{1}{2}$, sodass auch Effekte der Relativitätstheorie eingebunden werden. Im ersten Teil der Doktorarbeit geht es um Dirac-Operatoren mit singulären δ-Interaktionen, welche Kombinationen von elektrostatischen und Lorentz-skalaren Potentialen sind. Solche Operatoren können zur Behandlung von bestimmten Transmissionsproblemen verwendet werden. Im zweiten Teil der Arbeit werden selbstadjungierte Dirac-Operatoren in Gebieten studiert. Mithilfe von Randtripeln wird die Selbstadjungiertheit der Operatoren gezeigt und es werden einige spektrale Kenngrößen berechnet. Ein interessanter Aspekt ist die Existenz von kritischen Interaktionsstärken und Randwerten, für welche die spektralen Eigenschaften der zugehörigen Operatoren signifikant unterschiedlich sind. Schließlich wird für Dirac-Operatoren mit singulären Interaktionen der nichtrelativistische Grenzwert berechnet.

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1 INTRODUCTION

The Dirac equation is one of the main mathematical tools in relativistic quantum mechanics. While nonrelativistic quantum mechanics, which is based on the Schrödinger equation, led some new light into fundamental physics, it is not compatible with Einstein's theory of relativity. In order to find a theory that combines these two ideas in a more compatible way Paul Dirac suggested to replace Schrödinger's equation by another partial differential equation, that shall be discussed now. Assume that $\hbar = 1$ and denote the speed of light by c. Then the Dirac equation whose solution describes the propagation of a spin-$\frac{1}{2}$ particle with mass m in $\mathbb{R}^3$ under the influence of an external electrostatic potential V_e and a scalar potential V_s, which are both functions $V_\mathrm{e}, V_\mathrm{s} : \mathbb{R}^3 \to \mathbb{R}$, is

$$i\partial_t \Psi(t,x) = \left[-ic \sum_{j=1}^{3} \alpha_j \partial_{x_j} + V_\mathrm{e} I_4 + (mc^2 + V_\mathrm{s})\beta \right] \Psi(t,x), \quad \Psi(0,x) = \psi_0(x). \tag{1.1}$$

In the above equation the wave function Ψ is required to fulfill $\Psi(t,\cdot) \in L^2(\mathbb{R}^3;\mathbb{C}^4)$ for almost every $t > 0$, that means Ψ is a vector valued function with four components, I_d is the $d \times d$ identity matrix, and the Dirac matrices $\alpha_j, \beta \in \mathbb{C}^{4\times 4}$ satisfy the anti-commutation relations

$$\alpha_j \alpha_k + \alpha_k \alpha_j = 2\delta_{jk}, \quad \beta^2 = I_4, \quad \text{and} \quad \alpha_j \beta + \beta \alpha_j = 0, \quad j,k \in \{1,2,3\}; \tag{1.2}$$

see (3.1) for their definition. The Dirac equation describes the same physical problems as the Schrödinger equation and there is also a similar interpretation, see [68] and the explanations below.

Following [68] there were several motivations for Paul Dirac to introduce the equation (1.1) in 1928 in his famous paper [40]:

(i) It is a first order equation in time, which is required to have a meaningful quantum mechanical evolution equation.

(ii) The spin of the particle is modelled automatically in a natural way.

(iii) Employing the replacement relations

$$E \to i\partial_t, \qquad p \to -i\nabla_x,$$

where E denotes the energy of a particle and p its momentum, then we see that the free Dirac equation (for vanishing external potentials $V_e = V_s = 0$) formally fulfills, in contrast to Schrödinger's equation, the energy-momentum relation

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

predicted in Einstein's special theory of relativity.

Although Dirac designed the equation (1.1) only by theoretical arguments, it turned out that with its help the hydrogen atom could be described with an impressive exactness.

To get a quantum mechanical observable one associates to the right hand side of the Dirac equation (1.1) a self-adjoint partial differential operator in $L^2(\mathbb{R}^3;\mathbb{C}^4)$

$$A = -ic\sum_{j=1}^{3} \alpha_j \partial_{x_j} f + V_e I_4 + (mc^2 + V_s)\beta,$$

which is the Dirac operator. An important special case is $V_e = V_s = 0$, which yields the free Dirac operator. It is the relativistic counterpart of the free Laplacian and it often has the role of a reference operator. As the Dirac operator describes the same physics as the Schrödinger operator, one would expect similar (spectral) properties. Nevertheless, there are several unexpected features of A. The most important one is that A is not bounded from below. For the interpretation of this interesting property the existence of anti-particles was postulated. From the mathematical point of view the lack of semi-boundedness makes the analysis more complicated and it is one of the reasons why several problems which are solved for Schrödinger operators are still open for Dirac operators. It is one of the main goals in this thesis to make a contribution to this field. In particular, we want to study transmission problems for the Dirac equation which can be reformulated to the spectral study of Dirac operators in $L^2(\mathbb{R}^3;\mathbb{C}^4)$ with singular interactions that are formally given by

$$A^{\Sigma}_{\eta_e,\eta_s} = -ic(\alpha\cdot\nabla) + mc^2\beta + (\eta_e I_4 + \eta_s\beta)\delta_\Sigma, \tag{1.3}$$

where Σ is a compact and sufficiently smooth surface in $\mathbb{R}^3$ and $\eta_e, \eta_s : \Sigma \to \mathbb{R}$ are Lipschitz continuous functions. The second main topic of this thesis are Dirac operators acting in a domain $\Omega \subset \mathbb{R}^3$ that are related to boundary value problems for the Dirac equation with boundary conditions of the form

$$\tau\big(I_4 + i\beta(\alpha\cdot\nu)\big)f|_{\partial\Omega} = \big(I_4 + i\beta(\alpha\cdot\nu)\big)\beta f|_{\partial\Omega}, \tag{1.4}$$

where τ is a Lipschitz continuous function on $\partial\Omega$ and ν is the unit normal vector field on $\partial\Omega$. In the above equations (1.3) and (1.4) we used for vectors $x = (x_1,x_2,x_3)^\top \in \mathbb{R}^3$ the notation

$$\alpha\cdot x := \sum_{j=1}^{3} \alpha_j x_j. \tag{1.5}$$

Our main mathematical instrument to study the operators associated to the above problems are quasi and ordinary boundary triples. Boundary triples are a powerful tool in the extension and spectral theory of symmetric and self-adjoint operators. They will allow us to study the operators with non trivial transmission and boundary conditions as self-adjoint extensions of operators with zero transmission and boundary conditions, respectively. While quasi boundary triples were introduced in [17] in particular to investigate boundary value problems for partial differential operators, the application of ordinary boundary triples for partial differential operators is more complicated, but they have the advantage that with their help one can describe *all* self-adjoint extensions of a given symmetry. For our purposes a combination of quasi and ordinary boundary triple techniques will be convenient. Note that these tools were successfully applied in similar problems for the Laplace and Schrödinger operator [12, 13, 17–19, 22]. Let us describe our problems and results now in a more detailed way and let us have a look on the existing literature:

The first main part of this thesis is devoted to Dirac operators with δ-shell potentials. Singular δ-type potentials are often used in mathematical physics as idealized models for strongly located electric potentials, as the spectral and scattering data as well as the location of eigenfunctions of the corresponding differential operators are then approximately the same. For Schrödinger operators such ideas are well established, see the monographs [3,27,44], the review article [43], and the references therein. In the relativistic setting first the Dirac operator in 1D with point interactions was investigated, compare [46] and [3, Appendix J]. Using some standard techniques the resolvents and the complete spectral data could be computed explicitly. Moreover, in [66] Šeba showed that these Hamiltonians can be approximated in the norm resolvent sense by Dirac operators with squeezed potentials. In this procedure the interaction strength of the limit operator depends in a nonlinear way on the approximating potentials – this corresponds to a phenomenon known in the physical literature as Klein's paradox. Eventually, based on [46] and a decomposition to spherical harmonics Dittrich, Exner, and Šeba investigated in [41] Dirac operators with singular interactions supported on a sphere in $\mathbb{R}^3$. With this technique the self-adjointness for a wide class of parameters was shown and the resolvent and some spectral data could be computed, but due to this decomposition to spherical harmonics many of the interesting properties of $A^{\Sigma}_{\eta_e,\eta_s}$ were still hidden.

After a longer period without much progress a breakthrough was then the seminal paper [5] from 2014, where Arrizabalaga, Mas and Vega studied the operator $A^{\Sigma}_{\eta_e,0}$ in 3D for constant η_e and Σ being the boundary of a bounded C^2-domain using a modern approach from extension theory for symmetric operators. There, the δ-shell potential was modelled via a jump condition for functions in the domain of $A^{\Sigma}_{\eta_e,0}$ along Σ. Such ideas are well known from the study of Schrödinger operators with singular interactions, see for instance [3, 19, 43]. Using some integral operators related to the resolvent of the free Dirac operator the authors managed to prove the self-adjointness of $A^{\Sigma}_{\eta_e,0}$ for $\eta_e \neq \pm 2c$; the case $\eta_e = \pm 2c$ remained open and it seemed that the corresponding operator has different properties. The study was then continued in [6,7,54], where among other things a Birman-Schwinger principle and an isoperimetric inequality for $A^{\Sigma}_{\eta_e,0}$ were shown. Furthermore, in [6] an interesting confinement phenomenon for $A^{\Sigma}_{\eta_e,\eta_s}$ was obtained: if $\eta_e^2 - \eta_s^2 = -4c^2$, then the operator $A^{\Sigma}_{\eta_e,\eta_s}$ decouples to two independent operators acting in the interior and the exterior domain with boundary Σ; such effects are not known for the corresponding Schrödinger operators. Other recent papers related to the approach in [5] are [56] and [57], where it is shown that $A^{\Sigma}_{\eta_e,0}$ and A^{Σ}_{0,η_s} can be approximated in the strong resolvent sense by Dirac operators with squeezed electrostatic and scalar potentials, respectively, supposed that the interaction strengths η_e and η_s fulfill a certain smallness condition, and where similar as in 1D Klein's paradox appears.

Then in [11] the approach from [5] was translated to the framework of quasi boundary triples. Since boundary triple techniques do not require semi-boundedness of the operators they are suitable for the application to Dirac operators with singular interactions, as it was done in 1D for instance in [30, 33, 58]. In [11] again $A^{\Sigma}_{\eta_e,0}$ with constant $\eta_e \neq \pm 2c$ was considered and with the aid of the above mentioned quasi boundary triple a Krein type resolvent formula for $A^{\Sigma}_{\eta_e,0}$ was derived. It turned out that the spectral properties of $A^{\Sigma}_{\eta_e,0}$ are encoded in a family of boundary integral operators appearing also in [5]. With the help of these operators some spectral properties and the nonrelativistic limit of $A^{\Sigma}_{\eta_e,0}$ were studied in [11]. The analysis was continued in [14], where the quasi boundary triple from [11] was transformed to an ordinary boundary triple, which allowed to prove the self-adjointness and to deduce some spectral properties of $A^{\Sigma}_{\eta_e,0}$ also in the critical case $\eta_e = \pm 2c$. Other notable publications in this direction are [55], where the self-adjointness of $A^{\Sigma}_{\pm 2c,0}$ was shown via some Calderon projectors, and [48], where the discrete eigenvalues of A^{Σ}_{0,η_s} were studied for fixed constant η_s and large masses m.

Let us turn the discussion to the main results of this thesis on Dirac operators with singular interactions. These are generalizations of results in [11, 14, 48] to combinations of electrostatic and scalar shell-potentials with non-constant strengths. Let $\Sigma \subset \mathbb{R}^3$ be the boundary of a sufficiently smooth bounded domain Ω_+, let ν be the unit normal vector field on Σ pointing outwards Ω_+, and let $\eta_e, \eta_s : \Sigma \to \mathbb{R}$ be Lipschitz continuous. We set $\Omega_- := \mathbb{R}^3 \setminus \overline{\Omega_+}$ and use for $f \in L^2(\mathbb{R}^3;\mathbb{C}^4)$ the notation $f_\pm := f \upharpoonright \Omega_\pm$. Then the (formal) operator $A^{\Sigma}_{\eta_e,\eta_s}$ from (1.3) is rigorously defined by

$$\begin{aligned} A^{\Sigma}_{\eta_e,\eta_s} f &:= (-ic\alpha\cdot\nabla + mc^2\beta) f_+ \oplus (-ic\alpha\cdot\nabla + mc^2\beta) f_-, \\ \mathrm{dom}\, A^{\Sigma}_{\eta_e,\eta_s} &:= \Big\{ f = f_+ \oplus f_- \in H^1(\Omega_+;\mathbb{C}^4) \oplus H^1(\Omega_-;\mathbb{C}^4) : \\ &\qquad ic(\alpha\cdot\nu)(f_+|_\Sigma - f_-|_\Sigma) = -\frac{1}{2}(\eta_e I_4 + \eta_s\beta)(f_+|_\Sigma + f_-|_\Sigma) \Big\}. \end{aligned} \tag{1.6}$$

Here $H^1(\Omega_\pm;\mathbb{C}^4)$ denotes the Sobolev space of once weakly differentiable functions in $\Omega_\pm$. As for δ-shell potentials with constant coupling it turns out that interaction strengths with

$$\eta_{\mathrm{e}}(x)^2 - \eta_{\mathrm{s}}(x)^2 = 4c^2 \quad \text{for some} \quad x \in \Sigma \tag{1.7}$$

are in some sense critical. For the noncritical case we obtain in Section 4.2 the following basic properties of $A^{\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}}$

Theorem 1. *Assume that* (1.7) *does not hold. Then $A^{\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}}$ is self-adjoint and the following is true:*

(i) *The essential spectrum of $A^{\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}}$ is $(-\infty, -mc^2] \cup [mc^2, \infty)$.*

(ii) *The discrete spectrum of $A^{\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}}$ is finite.*

(iii) $\left(A^{\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}} - \lambda\right)^{-3} - \left(A^{\Sigma}_{0,0} - \lambda\right)^{-3}$ *is a trace class operator for any $\lambda \in \mathbb{C} \setminus \mathbb{R}$.*

The proof of Theorem 1 is based on a Krein type resolvent formula that relates the resolvent of $A^{\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}}$ to the resolvent of the free Dirac operator and some perturbation term that contains the spectral properties of $A^{\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}}$. Item (ii) can be shown by a standard trick using that functions in $\operatorname{dom} A^{\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}}$ have some Sobolev regularity and that the interaction is compactly supported. Eventually, assertion (iii) in Theorem 1 is interesting, because it provides a basis to do scattering theory for the operators $A^{\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}}$ and the free Dirac operator $A^{\Sigma}_{0,0}$.

The spectral properties of $A^{\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}}$ change significantly, if the interaction strength is critical, that means if (1.7) is fulfilled. It turns out in Proposition 4.3.1 that $A^{\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}}$ defined as in (1.6) is symmetric, but not self-adjoint. Following the strategy of [14] we compute then the self-adjoint realization of $A^{\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}}$ for constant interaction strengths η_{e} and η_{s} with $\eta_{\mathrm{e}}^2 - \eta_{\mathrm{s}}^2 = 4c^2$. The crucial point is to consider the jump condition in the definition of $A^{\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}}$ not in $L^2(\Sigma;\mathbb{C}^4)$, but in the larger Sobolev space of negative order $H^{-1/2}(\Sigma;\mathbb{C}^4)$. Using this we show in Section 4.3 the following results:

Theorem 2. *Assume that $\eta_{\mathrm{e}}, \eta_{\mathrm{s}} \in \mathbb{R}$ such that $\eta_{\mathrm{e}}^2 - \eta_{\mathrm{s}}^2 = 4c^2$. Then $A^{\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}}$ defined by* (1.6) *is essentially self-adjoint, the domain of its self-adjoint closure is not contained in the space $H^1(\mathbb{R}^3 \setminus \Sigma;\mathbb{C}^4)$, the set $(-\infty, -mc^2] \cup [mc^2, \infty)$ is contained in the essential spectrum of $\overline{A^{\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}}}$ and there can be essential spectrum in $(-mc^2, mc^2)$.*

We would like to point out that in the critical case $\overline{A^{\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}}}$ can have essential spectrum in $(-mc^2, mc^2)$; this is shown in Theorem 4.3.6 for $\eta_{\mathrm{e}} = \pm 2c$ and $\eta_{\mathrm{s}} = 0$ under the assumption that there is a flat part contained in Σ. This is closely related to a similar effect known for indefinite Laplacians, compare [16, 31]. In particular it seems that this phenomenon is related to the geometry of Σ, that means we do not expect that it appears for all Σ.

Eventually, we compute in Section 4.4 the nonrelativistic limit of $A^{\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}}$ in the purely electrostatic and purely scalar case, that means that $\eta_{\mathrm{s}} = 0$ and $\eta_{\mathrm{e}} = 0$, respectively. For this, one subtracts/adds the energy of the resting particle mc^2 to the total energy and computes the limit of the resolvent in the operator norm for $c \to \infty$. The expected result is (the resolvent of) a Schrödinger operator describing the same physics times a projection onto the upper/lower component of the Dirac wave function. The two different considerations correspond to the limit of the positive and the negative part of the Dirac operators. In our case it turns out that the nonrelativistic limit is a Schrödinger operator with an electric δ-potential of the same strength. This yields then finally a justification to call $A^{\Sigma}_{\eta_e,\eta_s}$ a Dirac operator with a δ-shell potential. Note that the critical interaction strength is no limitation here, as for any fixed Lipschitz continuous η_e we have $\eta_e < 4c^2$ on Σ for all sufficiently large c. Moreover, since the spectral properties of Schrödinger operators with δ-potentials are well studied, see for instance [3,43,44] and the references therein, one can deduce from this approximation analysis some of the spectral properties of $A^{\Sigma}_{\eta_e,0}$ and A^{Σ}_{0,η_s} for large values of c, as it is shown in one model example in Proposition 4.4.5. The theorem on the nonrelativistic limit reads (in a simplified form) as follows:

Theorem 3. *Let $\eta : \Sigma \to \mathbb{R}$ be a Lipschitz continuous function. Then it holds for any $\lambda \in \mathbb{C} \setminus \mathbb{R}$*

$$\lim_{c\to\infty} \big(A^{\Sigma}_{\eta,0} - (\lambda + mc^2)\big)^{-1} = \lim_{c\to\infty} \big(A^{\Sigma}_{0,\eta} - (\lambda + mc^2)\big)^{-1} = \left(-\frac{1}{2m}\Delta + \eta\,\delta_\Sigma - \lambda\right)^{-1} \begin{pmatrix} I_2 & 0 \\ 0 & 0 \end{pmatrix}$$

and

$$\lim_{c\to\infty} \big(A^{\Sigma}_{0,\eta} - (\lambda - mc^2)\big)^{-1} = \left(\frac{1}{2m}\Delta - \eta\,\delta_\Sigma - \lambda\right)^{-1} \begin{pmatrix} 0 & 0 \\ 0 & I_2 \end{pmatrix},$$

where all limits are in the operator norm.

Let us discuss now the second main topic of this thesis. The motivation for studying Dirac operators in domains $\Omega \subset \mathbb{R}^3$ with some boundary conditions that make them self-adjoint arise from several aspects: from the mathematical point of view they can be seen as the counterpart of Laplacians with Robin type boundary conditions. Hence, one can expect interesting spectral properties of these operators. From the physical point of view Dirac operators with special boundary conditions are used to describe in relativistic quantum mechanics particles (like gluons) that are confined to a predefined area or box. The most important model in this context is the MIT bag model suggested in the 1970s by physicists at the MIT to study the quark-gluon confinement, see [34–37, 49]; the MIT bag model corresponds to the boundary condition (1.4) with $\tau = 0$. Moreover, in 2D Dirac operators with special boundary conditions similar to the MIT bag boundary conditions are used in the description of graphene, compare [25, 26].

The mathematical literature on Dirac operators in domains contains different approaches. In differential geometry there are several articles dealing with self-adjoint Dirac operators on smooth manifolds, see for instance [8,9,59]. In dimension two the paper [64] from 1995 is remarkable, where Schmidt studied the Dirac operator with so-called zigzag boundary conditions and showed, that (in the massless case) these operators are self-adjoint and that zero is an eigenvalue of infinite multiplicity. This indicates that similar as for Dirac operators with singular interactions there are some critical boundary values, for which the associated operators have different spectral properties. Other publications in this field are [25, 26] where the self-adjointness of Dirac operators for a wide class of boundary conditions is shown. Note that the papers [25,26,64] have in common that a transformation of $\mathbb{R}^2$ to $\mathbb{C}$ and some methods from complex analysis are used. A recent paper on the MIT bag operator in $\mathbb{R}^3$ is [4], where the self-adjointness of the corresponding operator is shown via operator theoretic arguments and the asymptotics of the discrete eigenvalues are computed for large masses.

Our motivation is to study the self-adjointness and the spectral properties of Dirac operators on domains in $\mathbb{R}^3$ with boundary conditions of the form (1.4) using boundary triple techniques. The strategy used here is very similar as for Dirac operators with singular interactions in Chapter 4 and we get comparable results. Assume that $\Omega \subset \mathbb{R}^3$ is a bounded and sufficiently smooth domain or the complement of such a set, let $\tau : \partial\Omega \to \mathbb{R}$ be Lipschitz continuous, and define

$$\begin{aligned} A_\tau^\Omega f &:= (-ic\alpha\cdot\nabla + mc^2\beta)f, \\ \mathrm{dom} A_\tau^\Omega &:= \big\{ f \in H^1(\Omega;\mathbb{C}^4) : \tau\big(I_4 + i\beta(\alpha\cdot\nu)\big) f|_{\partial\Omega} = \big(I_4 + i\beta(\alpha\cdot\nu)\big)\beta f|_{\partial\Omega} \big\}. \end{aligned} \tag{1.8}$$

There are two reasons why we are interested in boundary conditions of the form (1.4): on the one hand the orthogonal sum $A_\tau^\Omega \oplus A_\tau^{\Omega^c}$ is of the form $A_{\eta_e,\eta_s}^{\partial\Omega}$ with η_e and η_s depending on τ in a suitable form, compare Section 5.3.1. Hence A_τ^Ω can be seen as a Dirac operator describing a particle actually living in $\mathbb{R}^3$, but which is confined to Ω, which is of interest in particle physics. On the other hand, the boundary condition (1.4) is a translation of the boundary condition used in [25] to a boundary triple framework. In fact, in [25] similar operators in $\mathbb{R}^2$ with boundary conditions

$$\big[I_2 + i\sigma_3(\sigma\cdot\nu)\cos\eta - \sin\eta\,\sigma_3\big] u|_{\partial\Omega} = 0$$

for a Lipschitz continuous function $\eta : \partial\Omega \to \mathbb{R}$ are studied. Here $\sigma = (\sigma_1, \sigma_2)$ and σ_3 are the Pauli spin matrices, see (3.2), and the notation $\sigma\cdot\nu$ is the 2D analogue of (1.5). Using a splitting

$$u|_{\partial\Omega} = \frac{1}{2}(I_2 + i\sigma_3(\sigma\cdot\nu))u|_{\partial\Omega} + \frac{1}{2}(I_2 - i\sigma_3(\sigma\cdot\nu))u|_{\partial\Omega} =: P_+ u|_{\partial\Omega} + P_- u|_{\partial\Omega},$$

$i\sigma_3(\sigma\cdot\nu)P_\pm = \pm P_\pm$, and $P_- = \sigma_3 P_+ \sigma_3$ we see that these boundary conditions are the 2D analogue of (1.4) for $\tau = -\frac{\sin(2\eta)}{2\cos\eta(1-\cos\eta)}$, if $\cos\eta(x) \notin \{0,1\}$ for all $x \in \partial\Omega$.

As already mentioned above, in a similar manner as for Dirac operators with singular interactions there exist critical boundary values for which the spectral properties of the corresponding operators A_τ^Ω are significantly different, namely

$$\tau(x)^2 = 1 \quad \text{for some} \quad x \in \partial\Omega. \tag{1.9}$$

In the case of noncritical boundary values the basic spectral properties of A_τ^Ω are investigated in Section 5.3. Clearly, they are significantly different whether Ω is bounded or unbounded and hence, we discuss them separately. In the following we will denote the Dirac operator in Ω with MIT bag boundary conditions by T_{MIT}^Ω, compare Section 5.1 for its properties. If Ω is the complement of a bounded domain then the basic properties of A_τ^Ω are the following:

Theorem 4. *Let $\Omega \subset \mathbb{R}^3$ be the complement of a bounded and sufficiently smooth domain and assume that* (1.9) *does not hold. Then A_τ^Ω is self-adjoint and the following is true:*

(i) *The essential spectrum of A_τ^Ω is $(-\infty, -mc^2] \cup [mc^2, \infty)$.*

(ii) *The discrete spectrum of A_τ^Ω is finite.*

(iii) $\big(A_\tau^\Omega - \lambda\big)^{-3} - \big(T_{\mathrm{MIT}}^\Omega - \lambda\big)^{-3}$ *is a trace class operator for any $\lambda \in \mathbb{C} \setminus \mathbb{R}$.*

The strategy for the proof of Theorem 4 is very similar as for Theorem 1: we prove a Krein type resolvent formula that relates, in this case, the resolvent of A_τ^Ω to the resolvent of T_{MIT}^Ω. Then, the claims follow from perturbation arguments and of the regularity of functions in $\mathrm{dom} A_\tau^\Omega$. Moreover, it is worth to mention that we can characterize the eigenvalues of A_τ^Ω in $(-mc^2, mc^2)$ with an abstract version of the Birman Schwinger principle.

If Ω is a bounded domain, then $\mathrm{dom} A_\tau^\Omega \subset H^1(\Omega; \mathbb{C}^4)$ is compactly embedded in $L^2(\Omega; \mathbb{C}^4)$ and hence, the spectrum of A_τ^Ω is purely discrete:

Theorem 5. *Let $\Omega \subset \mathbb{R}^3$ be a bounded and sufficiently smooth domain and assume that the condition* (1.9) *does not hold. Then A_τ^Ω is self-adjoint and $\sigma(A_\tau^\Omega)$ is purely discrete.*

If we are in the situation of Theorem 5 then one can compute all eigenvalues of A_τ^Ω with the help of a modified Birman-Schwinger principle described in Proposition 5.3.5.

In the investigation of A_τ^Ω in the case of critical boundary values (1.9) we use similar ideas as in the study of A_{η_s,η_s}^Σ for critical interaction strengths described above. First, it turns out that A_τ^Ω is symmetric, but not self-adjoint. Then we conclude, if $\tau \in \{\pm 1\}$ is constant, that the operator A_τ^Ω given as in (1.8) is essentially self-adjoint and we obtain some of the basic spectral properties of the self-adjoint realization:

Theorem 6. *Assume that $\tau \in \{\pm 1\}$. Then $A_{\pm 1}^\Omega$ defined by* (1.8) *is essentially self-adjoint, the domain of its self-adjoint closure is not contained in $H^1(\Omega; \mathbb{C}^4)$, and $\pm mc^2$ is an eigenvalue of $\overline{A_{\pm 1}^\Omega}$ of infinite multiplicity.*

We would like to draw the attention of the reader to the last claim of Theorem 6. The effect that $\overline{A_{\pm 1}^\Omega}$ has an eigenvalue of infinite multiplicity appears for bounded and unbounded domains Ω, although for unbounded Ω this eigenvalue is embedded in $(-\infty, -mc^2] \cup$

$[mc^2, \infty)$. Moreover, at a first glance the result seems to be comparable to Theorem 2, but a deeper look does not confirm this: in fact a super-symmetry in $\overline{A_\tau^\Omega}$ is responsible for the appearance of the eigenvalue with infinite multiplicity and in contrast to what we had for $\overline{A_{\eta_e,\eta_s}^\Sigma}$ it appears for any geometry. Thus it seems that the reason for these effects is different

Let us shortly describe the structure of the present thesis. In Chapter 2 we provide some preliminary material which is needed to formulate and prove our main results. We summarize some basic notions of the spectral theory for linear operators in Hilbert spaces, discuss quasi and ordinary boundary triples, introduce some function spaces, in particular Sobolev spaces on the boundary of a bounded and sufficiently smooth domain, and collect results on integral operators and mappings that are associated to the multiplication with a Lipschitz continuous function. Then, in Chapter 3 we introduce the free Dirac operator in $\mathbb{R}^3$ and a minimal and a maximal Dirac operator on a domain $\Omega \subset \mathbb{R}^3$. In particular, we will discuss several families of integral operators that are associated to Green's function for the free Dirac operator that will play a crucial role in the study of A_{η_e,η_s}^Σ and A_τ^Ω.

In Chapters 4 and 5 we prove then the main results of this thesis. Chapter 4 is devoted to A_{η_e,η_s}^Σ. After introducing boundary triples that are convenient to study Dirac operators with singular interactions, we define in Section 4.2 the operator A_{η_e,η_s}^Σ rigorously and prove for noncritical interaction strengths the basic properties, that means Theorem 1. Next, in Section 4.3 we study A_{η_e,η_s}^Σ for critical interaction strengths and show Theorem 2. Eventually, Section 4.4 is devoted to the proof of Theorem 3.

The topic of Chapter 5 is then the operator A_τ^Ω, where we use a similar approach as in Chapter 4. After collecting some properties of the MIT bag operator in Section 5.1 we introduce in Section 5.2 boundary triples that we use later to define and study self-adjoint Dirac operators on domains with boundary conditions. Next, in Section 5.3 we investigate the operator A_τ^Ω in the case of noncritical boundary values and prove Theorems 4 and 5. Finally, in Section 5.4 we verify Theorem 6 on Dirac operators on domains with critical boundary values.

2 PRELIMINARIES AND NOTATIONS

In this chapter we provide some preliminary material that is needed to formulate and prove the main results of this thesis. On the one hand we introduce some basic notions on the spectral theory for linear operators in Hilbert spaces, quasi and ordinary boundary triples and Schatten-von Neumann ideals. On the other hand, we discuss several function spaces and results on the boundedness of special integral operators and mappings that are associated to the multiplication with Lipschitz continuous functions.

2.1 Linear operators and their spectra

In this section we collect several notations and properties of bounded and unbounded linear operators in Banach and Hilbert spaces that will be used in this thesis. In particular, we introduce the adjoint of an unbounded operator and fix notations concerning the spectral properties of self-adjoint operators in Hilbert spaces. Most of the results presented in this section are standard knowledge and can be found, for instance, in [50, 60, 65, 69].

Throughout this section let X and Y be separable Banach spaces over the complex numbers. If $T : \operatorname{dom} T \to Y$, where $\operatorname{dom} T$ is a linear subspace of X, is a linear operator then $\operatorname{dom} T$ is its domain of definition and we denote the range and kernel by $\operatorname{ran} T$ and $\ker T$, respectively. The set of all bounded linear operators $T : X \to Y$ is denoted by $\mathfrak{B}(X,Y)$. If $X = Y$, then we simply write $\mathfrak{B}(X) := \mathfrak{B}(X,X)$.

If T is a closed operator in X, then the resolvent set and the spectrum of T are defined by

$$\rho(T) := \big\{\lambda \in \mathbb{C} : T - \lambda \text{ is injective and } (T-\lambda)^{-1} \in \mathfrak{B}(X)\big\}$$

and $\sigma(T) := \mathbb{C} \setminus \rho(T)$. If $T - \lambda$ is not injective, then λ is called eigenvalue of T and the set of all eigenvalues is denoted by $\sigma_{\mathrm{p}}(T)$.

Let $\mathfrak{M}$ be an open subset of $\mathbb{C}$ and let $F : \mathfrak{M} \to X$. We say that F is holomorphic in $\lambda \in \mathfrak{M}$ if the limit

$$\frac{\mathrm{d}}{\mathrm{d}\lambda} F(\lambda) := \lim_{\mu \to \lambda} \frac{F(\lambda) - F(\mu)}{\lambda - \mu}$$

exists in X. In the case that $X = \mathfrak{B}(Y,Z)$ for some Banach spaces Y and Z, then many well-known rules from complex analysis can be translated in a suitable way. In particular, if $A(\cdot), B(\cdot)$ and $C(\cdot)$ are holomorphic operator-valued functions defined in a neighborhood of $\lambda \in \mathbb{C}$, then it holds by [20, equation (2.7)] for any $k \in \mathbb{N}$

$$\frac{\mathrm{d}^k}{\mathrm{d}\lambda^k}\big(A(\lambda)B(\lambda)C(\lambda)\big) = \sum_{p+q+r=k} \frac{k!}{p!q!r!} \frac{\mathrm{d}^p}{\mathrm{d}\lambda^p}A(\lambda)\frac{\mathrm{d}^q}{\mathrm{d}\lambda^q}B(\lambda)\frac{\mathrm{d}^r}{\mathrm{d}\lambda^r}C(\lambda). \tag{2.1}$$

Furthermore, if $A(\cdot)$ is boundedly invertible in a neighborhood of λ, then it holds by [20, equation (2.8)]

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}\big(A(\lambda)^{-1}\big) = -A(\lambda)^{-1}\frac{\mathrm{d}}{\mathrm{d}\lambda}A(\lambda)A(\lambda)^{-1}. \tag{2.2}$$

Next, let $\big(\mathcal{H}, (\cdot,\cdot)_{\mathcal{H}}\big)$ and $\big(\mathcal{K}, (\cdot,\cdot)_{\mathcal{K}}\big)$ be separable Hilbert spaces. Then the adjoint of a densely defined operator A from $\mathcal{H}$ to $\mathcal{K}$ is defined on the set

$$\operatorname{dom} A^* := \big\{x \in \mathcal{K} : \exists x^* \in \mathcal{H} : (x, Ay)_{\mathcal{K}} = (x^*, y)_{\mathcal{H}} \text{ for all } y \in \operatorname{dom} A\big\}$$

and acts as $A^*x = x^*$. Note that A^* is well defined, as $\operatorname{dom} A$ is dense in $\mathcal{H}$. It is well-known that if A^* is densely defined, then $(A^*)^* = \overline{A}$ and if $A \in \mathfrak{B}(\mathcal{H},\mathcal{K})$ or $\overline{A} \in \mathfrak{B}(\mathcal{H},\mathcal{K})$, then $A^* \in \mathfrak{B}(\mathcal{K},\mathcal{H})$.

A densely defined operator in a Hilbert space $\mathcal{H}$ is called *symmetric*, if $A \subset A^*$, and *self-adjoint*, if $A = A^*$. If A is self-adjoint, then $\sigma(A) \subset \mathbb{R}$, for a symmetric symmetric operator S the same holds true only for $\sigma_{\mathrm{p}}(S)$. Moreover, a symmetric operator is self-adjoint if and only if

$$\operatorname{ran}(A - \lambda) = \mathcal{H} \quad \text{for all} \quad \lambda \in \mathbb{C} \setminus \mathbb{R}. \tag{2.3}$$

The last statement remains correct, if (2.3) holds for one $\lambda_0 \in \mathbb{R}$. For a self-adjoint operator A the spectrum can be split into the *discrete spectrum*

$$\sigma_{\mathrm{disc}}(A) := \big\{\lambda \in \sigma_{\mathrm{p}}(A) : \lambda \text{ is isolated in } \sigma(A)\big\}$$

and the *essential spectrum*

$$\sigma_{\mathrm{ess}}(A) := \sigma(A) \setminus \sigma_{\mathrm{disc}}(A).$$

An important result from perturbation theory of linear operators says that the essential spectrum is stable under (weak) compact perturbations, that means if A and B are self-adjoint operators such that

$$(A - \lambda)^{-1} - (B - \lambda)^{-1}$$

is compact for some $\lambda \in \rho(A) \cap \rho(B)$, then $\sigma_{\mathrm{ess}}(A) = \sigma_{\mathrm{ess}}(B)$.

Finally, we introduce a special class of symmetric operators, the so called simple or completely non self-adjoint operators. Let S be a symmetric operator in a Hilbert space $\mathcal{H}$ and let $\mathcal{H}_1$ be a closed subspace of $\mathcal{H}$. Then $\mathcal{H}_1$ is called invariant under S, if $S(\mathcal{H}_1) \subset \mathcal{H}_1$. We say that S is *simple*, if for any orthogonal decomposition $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2$ such that $\mathcal{H}_1$

and $\mathcal{H}_2$ are invariant under S and $S_1 := S \upharpoonright \mathcal{H}_1$ is self-adjoint in $\mathcal{H}_1$ it follows $\mathcal{H}_1 = \{0\}$. It is clear by this definition that a simple operator can not have eigenvalues, as $S \upharpoonright \ker(S-\lambda)$ is self-adjoint in $\ker(S-\lambda)$ for any $\lambda \in \mathbb{R}$. A useful criteria to check whether a given symmetry is simple is the following: a symmetric operator S is simple if and only if

$$\overline{\operatorname{span}\big\{f \in \operatorname{dom} S^* : (S^* - \lambda)f = 0 \text{ for a } \lambda \in \mathbb{C} \setminus \mathbb{R}\big\}} = \mathcal{H}, \tag{2.4}$$

see for instance [23].

2.2 Quasi and ordinary boundary triples

In this section we give a short introduction to the theory of quasi and ordinary boundary triples and their associated Weyl functions. Boundary triples are an important concept in the extension and spectral theory of symmetric and self-adjoint operators in Hilbert spaces. The presentation of the results in this chapter is chosen in a way such that they can be applied directly in the main part of this thesis to define and study Dirac operators with singular interactions and Dirac operators with boundary conditions on domains. For a more general and detailed survey and proofs we refer the reader for instance to [17, 18, 29, 38, 39, 47, 65].

Throughout this section $\mathcal{H}$ is always a complex Hilbert space with inner product $(\cdot,\cdot)_{\mathcal{H}}$; if no confusion arises, we skip the index in the inner product. We start with the definition of quasi and ordinary boundary triples.

Definition 2.2.1. *Let S be a densely defined closed symmetric operator in $\mathcal{H}$ and assume that T is a linear operator in $\mathcal{H}$ such that $\overline{T} = S^*$. Moreover, let $\mathcal{G}$ be another complex Hilbert space and let $\Gamma_0, \Gamma_1 : \operatorname{dom} T \to \mathcal{G}$ be linear mappings. Then $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ is called a quasi boundary triple for S^* if the following conditions are fulfilled:*

(i) *For all $f, g \in \operatorname{dom} T$ there holds the abstract Green's identity*

$$(Tf, g)_{\mathcal{H}} - (f, Tg)_{\mathcal{H}} = (\Gamma_1 f, \Gamma_0 g)_{\mathcal{G}} - (\Gamma_0 f, \Gamma_1 g)_{\mathcal{G}}. \tag{2.5}$$

(ii) $\Gamma := (\Gamma_0, \Gamma_1) : \operatorname{dom} T \to \mathcal{G} \times \mathcal{G}$ *has dense range.*

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

If additionally the mapping $\Gamma = (\Gamma_0, \Gamma_1)$ is surjective in $\mathcal{G} \times \mathcal{G}$, then $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ is called ordinary boundary triple for S^*.

If $\{\mathcal{G},\Gamma_0,\Gamma_1\}$ is a quasi boundary triple for $\overline{T}=S^*$, then the symmetry S can be recovered by

$$S = T \upharpoonright (\ker\Gamma_0 \cap \ker\Gamma_1),$$

see [17, Proposition 2.2], and the mappings $\Gamma_0,\Gamma_1 : \operatorname{dom} T \to \mathcal{G}$ are closable, if $\{\mathcal{G},\Gamma_0,\Gamma_1\}$ is an ordinary boundary triple, then Γ_0 and Γ_1 are even continuous. Note that the above non-standard definition of ordinary boundary triples is equivalent to the usual one given for instance in [29,47,65], see [17, Corollary 3.2]. Moreover, if $\{\mathcal{G},\Gamma_0,\Gamma_1\}$ is an ordinary boundary triple, then the operator T in Definition 2.2.1 coincides with S^*. In contrast to that, the operator T is in general not unique, if the dimension of $\mathcal{G}$ is infinite. Eventually we remark that a quasi or ordinary boundary triple exists, if and only if $\dim\ker(S^*-i) = \dim\ker(S^*+i)$, that means if and only if S admits self-adjoint extensions.

The main idea of boundary triples is to define self-adjoint extensions of the underlying symmetry S with suitable boundary/interface conditions in terms of the boundary mappings Γ_0 and Γ_1 and to study the spectral properties of these self-adjoint extensions. As we will see the spectrum of an extension of S is encoded in the so-called Weyl function associated to the boundary triple. This family of operators shall be introduced next.

Let $\{\mathcal{G},\Gamma_0,\Gamma_1\}$ be a quasi boundary triple for $\overline{T}=S^*$ and let $A_0 := T \upharpoonright \ker\Gamma_0$. The definition of the γ-field and the Weyl function is based on the direct sum decomposition

$$\operatorname{dom} T = \operatorname{dom} A_0 \dot{+} \ker(T-\lambda) = \ker\Gamma_0 \dot{+} \ker(T-\lambda), \quad \lambda \in \rho(A_0), \tag{2.6}$$

and it follows the definition of these objects for ordinary boundary triples from [38]. Note that (2.6) implies, in particular, that $\Gamma_0 \upharpoonright \ker(T-\lambda)$ is injective for $\lambda \in \rho(A_0)$.

Definition 2.2.2. *Let S be a densely defined, closed and symmetric operator in $\mathcal{H}$, let T be a linear operator such that $\overline{T}=S^*$ and let $\{\mathcal{G},\Gamma_0,\Gamma_1\}$ be a quasi boundary triple for S^*.*

(i) *The γ-field associated to the triple $\{\mathcal{G},\Gamma_0,\Gamma_1\}$ is the mapping*

$$\rho(A_0) \ni \lambda \mapsto \gamma(\lambda) := (\Gamma_0 \upharpoonright \ker(T-\lambda))^{-1}.$$

(ii) *The Weyl function associated to the triple $\{\mathcal{G},\Gamma_0,\Gamma_1\}$ is the mapping*

$$\rho(A_0) \ni \lambda \mapsto M(\lambda) := \Gamma_1(\Gamma_0 \upharpoonright \ker(T-\lambda))^{-1} = \Gamma_1\gamma(\lambda).$$

The γ-field is a densely defined operator in $\mathcal{G}$ and it maps boundary values $\varphi \in \operatorname{ran}\Gamma_0 \subset \mathcal{G}$ onto a solution $f_\lambda = \gamma(\lambda)\varphi$ of the boundary value problem

$$(T-\lambda)f_\lambda = 0, \quad \Gamma_0 f_\lambda = \varphi. \tag{2.7}$$

In this sense $\gamma(\lambda)$ is a potential operator as it is often seen in applications, compare for instance in [53]. In a similar flavour the Weyl function is a densely defined operator in $\mathcal{G}$

and it maps boundary values $\varphi \in \operatorname{ran}\Gamma_0$ onto the second boundary value $\Gamma_1 f_\lambda$, where f_λ is again the solution of the boundary value problem (2.7). In this sense $M(\lambda)$ can be seen as a generalized Dirichlet to Neumann map.

Some basic properties of the γ-field which will be used later in the main part of this thesis are summarized in the following proposition. The proofs of these statements can be found in [17, Proposition 2.6] and [20, Lemma 2.4].

Proposition 2.2.3. *Let S be a densely defined, closed and symmetric operator in $\mathcal{H}$, let T be a linear operator such that $\overline{T} = S^*$, let $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ be a quasi boundary triple for S^*, set $A_0 := T \restriction \ker\Gamma_0$ and let γ be the associated γ-field. Then the following assertions are true:*

(i) *For any $\lambda \in \rho(A_0)$ the mapping $\gamma(\lambda)$ is densely defined on* $\operatorname{ran}\Gamma_0$ *and bounded from $\mathcal{G}$ into $\mathcal{H}$.*

(ii) *Let $\lambda, \mu \in \rho(A_0)$ and $\varphi \in \operatorname{ran}\Gamma_0$. Then*

$$\gamma(\lambda)\varphi = \big(I + (\lambda - \mu)(A_0 - \lambda)^{-1}\big)\gamma(\mu)\varphi.$$

In particular, the mapping $\rho(A_0) \ni \lambda \mapsto \gamma(\lambda)\varphi$ is holomorphic and

$$\frac{\mathrm{d}^k}{\mathrm{d}\lambda^k}\gamma(\lambda)\varphi = k!(A_0 - \lambda)^{-k}\gamma(\lambda)\varphi, \quad k \in \mathbb{N}.$$

(iii) *The adjoint $\gamma(\lambda)^* : \mathcal{H} \to \mathcal{G}$ is given by $\gamma(\lambda)^* = \Gamma_1(A_0 - \overline{\lambda})^{-1}$. In particular $\gamma(\lambda)^* \in \mathcal{B}(\mathcal{H}, \mathcal{G})$, the mapping $\rho(A_0) \ni \lambda \mapsto \gamma(\overline{\lambda})^*$ is holomorphic and*

$$\frac{\mathrm{d}^k}{\mathrm{d}\lambda^k}\gamma(\overline{\lambda})^* = k!\Gamma_1(A_0 - \lambda)^{-k-1}, \quad k \in \mathbb{N}.$$

In the next proposition we state some useful properties of the Weyl function. For the proof see for instance [17, Proposition 2.6] and [20, Lemma 2.4].

Proposition 2.2.4. *Let S be a densely defined, closed and symmetric operator in $\mathcal{H}$, let T be a linear operator such that $\overline{T} = S^*$, let $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ be a quasi boundary triple for S^*, set $A_0 := T \restriction \ker\Gamma_0$ and let M be the associated Weyl function. Then the following assertions are true:*

(i) *For any $\lambda \in \rho(A_0)$ the mapping $M(\lambda)$ is densely defined on* $\operatorname{ran}\Gamma_0$ *with* $\operatorname{ran} M(\lambda) \subset \operatorname{ran}\Gamma_1$.

(ii) *For $\lambda \in \rho(A_0)$ and $f_\lambda \in \ker(T - \lambda)$ it holds $M(\lambda)\Gamma_0 f_\lambda = \Gamma_1 f_\lambda$.*

(iii) *Let $\lambda, \mu \in \rho(A_0)$ and $\varphi \in \operatorname{ran}\Gamma_0$. Then*

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

In particular, the operator $M(\lambda)$ is closable, $M(\lambda) \subset M(\overline{\lambda})^*$ and $M(\lambda)$ is symmetric for $\lambda \in \rho(A_0) \cap \mathbb{R}$.

(iv) *Let* $\lambda, \mu \in \rho(A_0)$ *and* $\varphi \in \operatorname{ran}\Gamma_0$. *Then*

$$M(\lambda)\varphi = M(\overline{\mu})\varphi + (\lambda - \overline{\mu})\gamma(\mu)^*\big(I + (\lambda-\mu)(A_0-\lambda)^{-1}\big)\gamma(\mu)\varphi.$$

In particular, the mapping $\rho(A_0) \ni \lambda \mapsto M(\lambda)\varphi$ *is holomorphic and*

$$\frac{\mathrm{d}^k}{\mathrm{d}\lambda^k} M(\lambda)\varphi = k!\Gamma_1(A_0-\lambda)^{-k}\gamma(\lambda)\varphi, \quad k \in \mathbb{N}.$$

Moreover, the mapping $\rho(A_0) \cap \mathbb{R} \ni \lambda \mapsto (M(\lambda)\varphi, \varphi)_{\mathcal{G}}$ *is monotonously increasing.*

In the main part of this thesis we will use boundary triples to introduce special extensions of a symmetric operator S. For that let $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ be a quasi boundary triple for $\overline{T} = S^*$ and let ϑ be a symmetric operator in $\mathcal{G}$. Then we define the operator A_ϑ acting in $\mathcal{H}$ by

$$A_\vartheta := T \upharpoonright \ker(\Gamma_1 - \vartheta\Gamma_0). \tag{2.8}$$

In other words, a vector $f \in \operatorname{dom} T$ belongs to $\operatorname{dom} A_\vartheta$ if it satisfies the abstract boundary condition $\Gamma_1 f = \vartheta\Gamma_0 f$. It follows immediately from Green's identity (2.5) that A_ϑ is symmetric, as it holds for $f, g \in \operatorname{dom} A_\vartheta$

$$\begin{aligned}(A_\vartheta f, g)_{\mathcal{H}} - (f, A_\vartheta g)_{\mathcal{H}} &= (\Gamma_1 f, \Gamma_0 g)_{\mathcal{G}} - (\Gamma_0 f, \Gamma_1 g)_{\mathcal{G}} \\ &= (\vartheta\Gamma_0 f, \Gamma_0 g)_{\mathcal{G}} - (\Gamma_0 f, \vartheta\Gamma_0 g)_{\mathcal{G}} = 0\end{aligned} \tag{2.9}$$

due to the symmetry of ϑ in $\mathcal{G}$. Of course, one would be mostly interested in the self-adjointness of A_ϑ. But for general quasi boundary triples it does not hold that A_ϑ is self-adjoint, if ϑ is self-adjoint in $\mathcal{G}$; such a statement is just true for ordinary boundary triples, see Proposition 2.2.7 below. But it holds the very efficient theorem below which induces a sufficient condition to show the self-adjointness of A_ϑ and which gives us an explicit Krein-type resolvent formula; for a proof of this result see for instance [17, Theorem 2.8].

Theorem 2.2.5. *Let* S *be a densely defined, closed and symmetric operator in* $\mathcal{H}$*, let* $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ *be a quasi boundary triple for* $\overline{T} = S^*$*, set* $A_0 := T \upharpoonright \ker\Gamma_0$*, and let* γ *and* M *be the associated* γ*-field and Weyl function, respectively. Moreover, let* ϑ *be a symmetric operator in* $\mathcal{G}$ *and let the associated operator* A_ϑ *be defined by* (2.8). *Then the following assertions are true for* $\lambda \in \rho(A_0)$*:*

(i) $\lambda \in \sigma_\mathrm{p}(A_\vartheta)$ *if and only if* $0 \in \sigma_\mathrm{p}(\vartheta - M(\lambda))$. *Furthermore, it holds*

$$\ker(A_\vartheta - \lambda) = \{\gamma(\lambda)\varphi : \varphi \in \ker(\vartheta - M(\lambda))\}.$$

(ii) *If* $\lambda \notin \sigma_\mathrm{p}(A_\vartheta)$*, then* $f \in \operatorname{ran}(A_\vartheta - \lambda)$ *if and only if* $\gamma(\overline{\lambda})^* f \in \operatorname{ran}(\vartheta - M(\lambda))$.

(iii) *If* $\lambda \notin \sigma_p(A_\vartheta)$, *then*

$$(A_\vartheta - \lambda)^{-1} f = (A_0 - \lambda)^{-1} f + \gamma(\lambda)(\vartheta - M(\lambda))^{-1}\gamma(\overline{\lambda})^* f$$

is true for all $f \in \operatorname{ran}(A_\vartheta - \lambda)$.

We would like to point out that assertion (ii) in Theorem 2.2.5 gives an efficient tool to check the self-adjointness of A_ϑ. Since A_ϑ is symmetric by (2.9) it suffices to check that $\operatorname{ran}(A_\vartheta - \lambda) = \mathcal{H}$ for $\lambda \in \mathbb{C} \setminus \mathbb{R}$. According to Theorem 2.2.5 (ii) this is true, if $\operatorname{ran}\gamma(\overline{\lambda})^* \subset \operatorname{ran}(\vartheta - M(\lambda))$.

In some applications it is more convenient to introduce self-adjoint extensions of S via $A_{[B]} := T \upharpoonright \ker(\Gamma_0 + B\Gamma_1)$, where B is a symmetric operator in $\mathcal{G}$. Formally, one can write $A_{[B]} = A_\vartheta$ with $\vartheta = -B^{-1}$. In the same way as in (2.9) one sees that also $A_{[B]}$ is symmetric. Moreover, one can show the following counterpart to Theorem 2.2.5, see for instance [19, Theorem 2.8].

Theorem 2.2.6. *Let S be a densely defined, closed and symmetric operator in $\mathcal{H}$, let $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ be a quasi boundary triple for $\overline{T} = S^*$, set $A_0 := T \upharpoonright \ker\Gamma_0$, and let γ and M be the associated γ-field and Weyl function, respectively. Moreover, let $B = B^* \in \mathcal{B}(\mathcal{G})$ and set $A_{[B]} := T \upharpoonright \ker(\Gamma_0 + B\Gamma_1)$. Then the following assertions are true for $\lambda \in \rho(A_0)$:*

(i) $\lambda \in \sigma_p(A_{[B]})$ *if and only if* $0 \in \sigma_p(I + BM(\lambda))$. *Furthermore, it holds*

$$\ker(A_{[B]} - \lambda) = \{\gamma(\lambda)\varphi : \varphi \in \ker(I + BM(\lambda))\}.$$

(ii) *If* $\lambda \notin \sigma_p(A_{[B]})$, *then* $f \in \operatorname{ran}(A_{[B]} - \lambda)$ *if and only if* $B\gamma(\overline{\lambda})^* f \in \operatorname{ran}(I + BM(\lambda))$.

(iii) *If* $\lambda \notin \sigma_p(A_{[B]})$, *then*

$$(A_{[B]} - \lambda)^{-1} f = (A_0 - \lambda)^{-1} f - \gamma(\lambda)(I + BM(\lambda))^{-1} B\gamma(\overline{\lambda})^* f$$

is true for all $f \in \operatorname{ran}(A_{[B]} - \lambda)$.

Eventually, if $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ is an ordinary boundary triple, then proving self-adjointness of extensions A_ϑ is simpler as in the case of quasi boundary triples. Some important statements, that are used later in this thesis, are summarized in the following proposition; for a proof of this result see for instance [38, 39] and [29, Theorem 1.29 and Theorem 3.3].

Proposition 2.2.7. *Let S be a densely defined, closed and symmetric operator in $\mathcal{H}$, let $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ be an ordinary boundary triple for S^*, set $A_0 := T \upharpoonright \ker\Gamma_0$, and let γ and M be the associated γ-field and Weyl function, respectively. Moreover, let ϑ be a symmetric operator in $\mathcal{G}$ and let the associated operator A_ϑ be defined by* (2.8). *Then ϑ is (essentially) self-adjoint in $\mathcal{G}$, if and only if A_ϑ is (essentially) self-adjoint in $\mathcal{H}$. Moreover, if ϑ is self-adjoint, then the following items are true:*

(i) $\lambda \in \sigma(A_\vartheta)$ *if and only if* $0 \in \sigma(\vartheta - M(\lambda))$.

(ii) $\lambda \in \sigma_p(A_\vartheta)$ *if and only if* $0 \in \sigma_p(\vartheta - M(\lambda))$. *Furthermore, it holds*

$$\ker(A_\vartheta - \lambda) = \{\gamma(\lambda)\varphi : \varphi \in \ker(\vartheta - M(\lambda))\}.$$

(iii) $\lambda \in \sigma_{disc}(A_\vartheta)$ *if and only if* $0 \in \sigma_{disc}(\vartheta - M(\lambda))$.

If $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ is a quasi boundary triple for S^*, then Theorem 2.2.5, Theorem 2.2.6 and Proposition 2.2.7 show how the eigenvalues $\lambda \notin \rho(A_0)$ of self-adjoint extensions of S can be characterized by the Weyl function M. If the symmetry S is simple, then one can do something similar for *all* eigenvalues, that means also for those that are embedded in $\sigma(A_0)$, compare [23, Corollary 3.4]. Note that there are also similar characterizations for the other types of the spectrum available in [23], but in our applications we restrict ourselves to find the eigenvalues.

Proposition 2.2.8. *Let S be a densely defined, closed and simple symmetric operator in $\mathcal{H}$, let $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ be a quasi boundary triple for $\overline{T} = S^*$, set $A_0 := T \upharpoonright \ker \Gamma_0$, and let γ and M be the associated γ-field and Weyl function, respectively. Moreover, let ϑ be a bounded and self-adjoint operator in $\mathcal{G}$ and assume that the associated operator A_ϑ defined by* (2.8) *is self-adjoint. Then λ is an eigenvalue of A_ϑ if and only if there exists $\varphi \in \operatorname{ran}(M(\lambda) - \vartheta)$ satisfying*

$$\lim_{\varepsilon \searrow 0} i\varepsilon \big(M(\lambda + i\varepsilon) - \vartheta\big)^{-1} \varphi \neq 0.$$

Proof. Define the boundary mappings $\Gamma_0^\vartheta, \Gamma_1^\vartheta : \operatorname{dom} T \to \mathcal{G}$ by

$$\Gamma_0^\vartheta f := \Gamma_1 - \vartheta \Gamma_0 \quad \text{and} \quad \Gamma_1^\vartheta f = -\Gamma_0 f, \quad f \in \operatorname{dom} T.$$

We claim that $\{\mathcal{G}, \Gamma_0^\vartheta, \Gamma_1^\vartheta\}$ is a quasi boundary triple for S^* with the additional property $T \upharpoonright \ker \Gamma_0^\vartheta = A_\vartheta$. In fact, using that ϑ is bounded and self-adjoint we deduce from the Green's identity for $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ and for $f, g \in \operatorname{dom} T$

$$\begin{aligned}(Tf, g)_{\mathcal{H}} - (f, Tg)_{\mathcal{H}} &= (\Gamma_1 f, \Gamma_0 g)_{\mathcal{G}} - (\Gamma_0 f, \Gamma_1 g)_{\mathcal{G}} - (\vartheta \Gamma_0 f, \Gamma_0 g)_{\mathcal{G}} + (\Gamma_0 f, \vartheta \Gamma_0 g)_{\mathcal{G}} \\ &= \big(-\Gamma_0 f, (\Gamma_1 - \vartheta \Gamma_0) g\big)_{\mathcal{G}} - \big((\Gamma_1 - \vartheta \Gamma_0) f, -\Gamma_0 g\big)_{\mathcal{G}} \\ &= \big(\Gamma_1^\vartheta f, \Gamma_0^\vartheta g\big)_{\mathcal{G}} - \big(\Gamma_0^\vartheta f, \Gamma_1^\vartheta g\big)_{\mathcal{G}},\end{aligned} \tag{2.10}$$

that means Green's identity holds also for the triple $\{\mathcal{G}, \Gamma_0^\vartheta, \Gamma_1^\vartheta\}$.

Next, the definition of $\Gamma_0^\vartheta, \Gamma_1^\vartheta$ can be written equivalently as

$$\begin{pmatrix} \Gamma_0^\vartheta \\ \Gamma_1^\vartheta \end{pmatrix} = B \begin{pmatrix} \Gamma_0 \\ \Gamma_1 \end{pmatrix}, \qquad B := \begin{pmatrix} -\vartheta & 1 \\ -1 & 0 \end{pmatrix}.$$

Since ϑ is bounded, we deduce that B is boundedly invertible with

$$B^{-1} := \begin{pmatrix} 0 & -1 \\ 1 & -\vartheta \end{pmatrix}.$$

Since $\operatorname{ran}(\Gamma_0, \Gamma_1)$ is dense in $\mathcal{G} \times \mathcal{G}$ this implies that also $\operatorname{ran}(\Gamma_0^\vartheta, \Gamma_1^\vartheta)$ is dense. Finally, $T \upharpoonright \ker(\Gamma_0^\vartheta) = T \upharpoonright \ker(\Gamma_1 - \vartheta\Gamma_0) = A_\vartheta$ is self-adjoint by assumption. Therefore $\{\mathcal{G}, \Gamma_0^\vartheta, \Gamma_1^\vartheta\}$ is a quasi boundary triple for S^*.

Next, we compute on $\mathbb{C} \setminus \mathbb{R}$ the Weyl function M^ϑ corresponding to the triple $\{\mathcal{G}, \Gamma_0^\vartheta, \Gamma_1^\vartheta\}$. For a fixed $\lambda \in \mathbb{C} \setminus \mathbb{R}$ this is the mapping which is determined uniquely by the relation $M^\vartheta(\lambda)\Gamma_0^\vartheta f_\lambda = \Gamma_1^\vartheta f_\lambda$ for $f_\lambda \in \ker(T - \lambda)$. We compute for such an $f_\lambda \in \ker(T - \lambda)$

$$\Gamma_0^\vartheta f_\lambda = (\Gamma_1 - \vartheta\Gamma_0) f_\lambda = \big(M(\lambda) - \vartheta\big)\Gamma_0 f_\lambda = -\big(M(\lambda) - \vartheta\big)\Gamma_1^\vartheta f_\lambda. \tag{2.11}$$

Note that $M(\lambda) - \vartheta$ is invertible by Theorem 2.2.5, as otherwise the self-adjoint operator A_ϑ would have the non-real eigenvalue λ. Thus, we conclude

$$M^\vartheta(\lambda) = -\big(M(\lambda) - \vartheta\big)^{-1}.$$

After all these preparations the claim of this proposition follows from [23, Corollary 3.4] applied to the quasi boundary triple $\{\mathcal{G}, \Gamma_0^\vartheta, \Gamma_1^\vartheta\}$, as S is simple. □

In the next proposition we state a similar result as in Proposition 2.2.8 for ordinary boundary triples and unbounded parameters ϑ:

Proposition 2.2.9. *Let S be a densely defined, closed and simple symmetric operator in $\mathcal{H}$, let $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ be an ordinary boundary triple for S^*, set $A_0 := T \upharpoonright \ker \Gamma_0$, and let γ and M be the associated γ-field and Weyl function, respectively. Moreover, let ϑ be a self-adjoint operator in $\mathcal{G}$. Then λ is an eigenvalue of A_ϑ if and only if there exists $\varphi \in \operatorname{ran}(M(\lambda) - \vartheta)$ satisfying*

$$\lim_{\varepsilon \searrow 0} i\varepsilon\big(M(\lambda + i\varepsilon) - \vartheta\big)^{-1}\varphi \neq 0.$$

Proof. The proof of this result is very similar as the one of Proposition 2.2.8, hence, we only indicate the differences in the verification. We set $T_\vartheta := S^* \upharpoonright (\operatorname{dom} A_0 + \operatorname{dom} A_\vartheta)$ and define the mappings $\Gamma_0^\vartheta, \Gamma_1^\vartheta : \operatorname{dom} T^\vartheta \to \mathcal{G}$ by

$$\Gamma_0^\vartheta f := \Gamma_1 - \vartheta\Gamma_0 \quad \text{and} \quad \Gamma_1^\vartheta f = -\Gamma_0 f, \quad f \in \operatorname{dom} T^\vartheta.$$

We claim that $\{\mathcal{G}, \Gamma_0^\vartheta, \Gamma_1^\vartheta\}$ is a quasi boundary triple for S^* with the additional property $T \upharpoonright \ker \Gamma_0^\vartheta = A_\vartheta$.

It is simple to see that $S = S^* \upharpoonright (\operatorname{dom} A_0 \cap \operatorname{dom} A_\vartheta)$. Hence, it follows from [21, Proposition 2.9] that $\overline{T^\vartheta} = S^*$. Next, Green's identity for $\{\mathcal{G}, \Gamma_0^\vartheta, \Gamma_1^\vartheta\}$ can be shown in exactly the same way as in (2.10). Furthermore, $T^\vartheta \upharpoonright \ker \Gamma_0^\vartheta = A_\vartheta$ is self-adjoint by Proposition 2.2.7.

So it remains to show that $\operatorname{ran}\big(\Gamma_0^\vartheta, \Gamma_1^\vartheta\big)$ is dense in $\mathcal{G} \times \mathcal{G}$. Assume that $(\varphi, \psi) \in \mathcal{G} \times \mathcal{G}$ fulfills for all $f \in \operatorname{dom} T^\vartheta$

$$0 = \big(\varphi, \Gamma_0^\vartheta f\big)_{\mathcal{G}} + \big(\psi, \Gamma_1^\vartheta f\big)_{\mathcal{G}} = (\varphi, (\Gamma_1 - \vartheta\Gamma_0) f)_{\mathcal{G}} - (\psi, \Gamma_0 f)_{\mathcal{G}}. \tag{2.12}$$

This implies, in particular, $(\varphi, \Gamma_1 f)_{\mathcal{G}} = 0$ for all $f \in \ker \Gamma_0$. Since $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ is an ordinary boundary triple it holds $\Gamma_1(\ker \Gamma_0) = \mathcal{G}$ and therefore $\varphi = 0$. Thus (2.12) reduces to $(\psi, \Gamma_0 f)_{\mathcal{G}} = 0$ for all $f \in \operatorname{dom} T^\vartheta$. Using now that $\operatorname{dom} T^\vartheta$ is dense in $\operatorname{dom} S^*$ with respect to the graph norm induced by S^* and Γ_0 is continuous, it follows from the surjectivity of Γ_0 that also $\psi = 0$. Therefore $\operatorname{ran}\big(\Gamma_0^\vartheta, \Gamma_1^\vartheta\big)$ is dense in $\mathcal{G} \times \mathcal{G}$ and we have shown that $\{\mathcal{G}, \Gamma_0^\vartheta, \Gamma_1^\vartheta\}$ is indeed a quasi boundary triple for S^*.

Finally, in the same way as in (2.11) one shows that the value of the Weyl function associated to the triple $\{\mathcal{G}, \Gamma_0^\vartheta, \Gamma_1^\vartheta\}$ for $\lambda \in \mathbb{C} \setminus \mathbb{R}$ is

$$M^\vartheta(\lambda) = -\big(M(\lambda) - \vartheta\big)^{-1}.$$

Hence, since S is simple by assumption, we deduce the claim of this proposition again from [23, Corollary 3.4] applied to $\{\mathcal{G}, \Gamma_0^\vartheta, \Gamma_1^\vartheta\}$. □

In the rest of this section we describe a construction introduced in [22] which allows under some assumptions to transform and extend a given quasi boundary triple to an ordinary boundary triple. This procedure will be very useful to study Dirac operators with critical interaction strengths or boundary values. Assume that S is a densely defined, closed and symmetric operator in $\mathcal{H}$ and that $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ be a quasi boundary triple for $\overline{T} = S^*$. We define the sets

$$\mathscr{G}_0 := \operatorname{ran}(\Gamma_0 \upharpoonright \ker \Gamma_1) \quad \text{and} \quad \mathscr{G}_1 := \operatorname{ran}(\Gamma_1 \upharpoonright \ker \Gamma_0). \tag{2.13}$$

The main idea from [22] is the following: under the assumption that $\mathscr{G}_1$ (or $\mathscr{G}_0$) is dense in $\mathcal{G}$ one endows this space with a suitable topology and extends then the boundary mapping Γ_0 (or Γ_1) to a mapping having values in the anti-dual space $\mathscr{G}_1'$ (or $\mathscr{G}_0'$, respectively). The first important step in this construction is to find a suitable topology on $\mathscr{G}_1$, see [22, Proposition 2.9 and Proposition 2.10]. We set

$$\Lambda := \overline{\operatorname{Im} M(i)} = \frac{1}{2i}\big(\overline{M(i)} - \overline{M(-i)}\big) = \gamma(i)^* \overline{\gamma(i)}, \tag{2.14}$$

where the last equality follows from Proposition 2.2.4 (iii) and the operator on the right hand side is non-negative.

Proposition 2.2.10. *Let S be a densely defined, closed and symmetric operator in $\mathcal{H}$, let $\{\mathcal{G},\Gamma_0,\Gamma_1\}$ be a quasi boundary triple for $\overline{T}=S^*$ with Weyl function M and let Λ be given by* (2.14). *Assume additionally that $\mathscr{G}_1$ given by* (2.13) *is dense in $\mathcal{G}$. Then $\Lambda^{1/2}:\mathcal{G}\to\mathscr{G}_1$ is an isometry and $\mathscr{G}_1$ endowed with the inner product*

$$(\varphi,\psi)_{\mathscr{G}_1} := \big(\Lambda^{-1/2}\varphi,\Lambda^{-1/2}\psi\big)_{\mathcal{G}}, \quad \varphi,\psi\in\mathscr{G}_1, \tag{2.15}$$

is a Hilbert space. Moreover, all norms $\|\cdot\|$ such that $(\mathscr{G}_1,\|\cdot\|)$ is a reflexive Banach space continuously embedded into $\mathcal{G}$ are equivalent to the norm induced by (2.15).

In the following we assume that $\mathscr{G}_1$ is dense in $\mathcal{G}$. Then $\{\mathscr{G}_1,\mathcal{G},\mathscr{G}_1'\}$ forms a Gelfand triple and making use of the operator Λ we can find suitable expressions also for the duality product in $\mathscr{G}_1'\times\mathscr{G}_1$. We set

$$\iota_+ := \Lambda^{-1/2}:\mathscr{G}_1\to\mathcal{G}. \tag{2.16}$$

Via some standard constructions for Gelfand triples, see ???, the operator $\Lambda^{1/2}$ can be extended to an isometry

$$\iota_-:\mathscr{G}_1'\to\mathcal{G}, \quad \iota_-\restriction\mathcal{G}=\Lambda^{1/2}. \tag{2.17}$$

Eventually, the duality product in $\mathscr{G}_1'\times\mathscr{G}_1$ can be expressed by

$$(\varphi,\psi)_{\mathscr{G}_1'\times\mathscr{G}_1} := (\iota_-\varphi,\iota_+\psi)_{\mathcal{G}}, \quad \varphi\in\mathscr{G}_1',\psi\in\mathscr{G}_1. \tag{2.18}$$

This choice of the duality product has for $\varphi\in\mathcal{G}\subset\mathscr{G}_1'$ and $\psi\in\mathscr{G}_1$ the useful property

$$(\varphi,\psi)_{\mathscr{G}_1'\times\mathscr{G}_1} = (\Lambda^{1/2}\varphi,\Lambda^{-1/2}\psi)_{\mathcal{G}} = (\varphi,\psi)_{\mathcal{G}}, \tag{2.19}$$

as $\Lambda^{1/2}$ is a bounded and self-adjoint operator in $\mathcal{G}$.

After these preliminary considerations about the space $\mathscr{G}_1$ and its topology we extend now the boundary mappings Γ_0 and Γ_1 to bounded mappings from $\operatorname{dom} S^*$ onto $\mathscr{G}_1'$ and $\mathscr{G}_0'$, respectively. This result is proven in [22, Proposition 2.10 and Corollary 2.11].

Proposition 2.2.11. *Let S be a densely defined, closed and symmetric operator in $\mathcal{H}$, let $\{\mathcal{G},\Gamma_0,\Gamma_1\}$ be a quasi boundary triple for $\overline{T}=S^*$, and let $\mathscr{G}_0$ and $\mathscr{G}_1$ be given by* (2.13). *Then the following assertions are true:*

(i) *If $\mathscr{G}_1$ is dense in $\mathcal{G}$, then Γ_0 has a unique surjective and bounded extension*

$$\widetilde{\Gamma}_0:\big(\operatorname{dom} S^*,\|\cdot\|_{S^*}\big)\to\mathscr{G}_1'.$$

(ii) *If $\mathscr{G}_0$ is dense in $\mathcal{G}$ and the operator $A_\infty := T\restriction\ker\Gamma_1$ is self-adjoint in $\mathcal{H}$, then Γ_1 has a unique surjective and bounded extension*

$$\widetilde{\Gamma}_1:\big(\operatorname{dom} S^*,\|\cdot\|_{S^*}\big)\to\mathscr{G}_0'.$$

Under the assumptions of the previous proposition also the γ-field and the Weyl function associated to the quasi boundary triple $\{\mathcal{G},\Gamma_0,\Gamma_1\}$ have natural extensions, see [22, Definition 2.14] and the following discussion.

Proposition 2.2.12. *Let S be a densely defined, closed and symmetric operator in $\mathcal{H}$, let $\{\mathcal{G},\Gamma_0,\Gamma_1\}$ be a quasi boundary triple for $\overline{T} = S^*$ with γ-field γ and Weyl function M, set $A_0 := T \upharpoonright \ker\Gamma_0$, and let $\mathscr{G}_0$ and $\mathscr{G}_1$ be given by* (2.13). *Then the following is true:*

(i) *Assume that $\mathscr{G}_1$ is dense in $\mathcal{G}$ and let $\lambda \in \rho(A_0)$. Then $\gamma(\lambda)$ has a bounded extension*

$$\widetilde{\gamma}(\lambda) := \big(\widetilde{\Gamma}_0 \upharpoonright \ker(S^* - \lambda)\big)^{-1} : \mathscr{G}_1' \to \mathcal{H}.$$

(ii) *Assume that $\mathscr{G}_0$ and $\mathscr{G}_1$ are dense in $\mathcal{G}$, that $A_\infty := T \upharpoonright \ker\Gamma_1$ is self-adjoint in $\mathcal{H}$, and let $\lambda \in \rho(A_0)$. Then $M(\lambda)$ has a bounded extension*

$$\widetilde{M}(\lambda) := \widetilde{\Gamma}_1\widetilde{\gamma}(\lambda) = \widetilde{\Gamma}_1\big(\widetilde{\Gamma}_0 \upharpoonright \ker(S^* - \lambda)\big)^{-1} : \mathscr{G}_1' \to \mathscr{G}_0'.$$

Finally, making use of the extended boundary mapping $\widetilde{\Gamma}_0$ one can transform the originally given quasi boundary triple to an ordinary boundary triple, compare [22, Theorem 2.12]. Recall that for $A_0 = T \upharpoonright \ker\Gamma_0$ and $\mu \in \rho(A_0)$ there holds the direct sum decomposition

$$\operatorname{dom} S^* = \operatorname{dom} A_0 \dotplus \ker(S^* - \mu).$$

Theorem 2.2.13. *Let S be a densely defined, closed and symmetric operator in $\mathcal{H}$, let $\{\mathcal{G},\Gamma_0,\Gamma_1\}$ be a quasi boundary triple for $\overline{T} = S^*$ such that $\mathscr{G}_0$ given by* (2.13) *is dense in $\mathcal{G}$, and set $A_0 := T \upharpoonright \ker\Gamma_0$. Moreover, let ι_+ and ι_- be defined by* (2.16) *and* (2.17), *respectively, and assume that there exists some $\mu \in \rho(A_0) \cap \mathbb{R}$. Let $\widetilde{\Gamma}_0$ be the extension of Γ_0 from Proposition 2.2.11 and define the mappings $\Upsilon_0, \Upsilon_1 : \operatorname{dom} S^* \to \mathcal{G}$ by*

$$\Upsilon_0 f := \iota_-\widetilde{\Gamma}_0 f, \quad \Upsilon_1 f := \iota_+\Gamma_1 f_0, \quad f = f_0 + g \in \operatorname{dom} A_0 \dotplus \ker(S^* - \mu) = \operatorname{dom} S^*.$$

Then $\{\mathcal{G},\Upsilon_0,\Upsilon_1\}$ is an ordinary boundary triple for S^* with the additional property that $S^* \upharpoonright \ker\widetilde{\Gamma}_0 = T \upharpoonright \Gamma_0 = A_0$.

Let $\{\mathcal{G},\Gamma_0,\Gamma_1\}$ be a quasi boundary triple for S^*, assume that $\mathscr{G}_0$ and $\mathscr{G}_1$ are dense in $\mathcal{G}$ and that $A_\infty := T \upharpoonright \ker\Gamma_1$ is self-adjoint in $\mathcal{H}$. Then the γ-field β and the Weyl function $\mathcal{M}$ associated to the ordinary boundary triple $\{\mathcal{G},\Upsilon_0,\Upsilon_1\}$ from Theorem 2.2.13 are given by

$$\beta(\lambda) = \widetilde{\gamma}(\lambda)\iota_-^{-1} \quad \text{and} \quad \mathcal{M}(\lambda) = \iota_+\big(\widetilde{M}(\lambda) - \widetilde{M}(\mu)\big)\iota_-^{-1} \tag{2.20}$$

for $\lambda \in \rho(A_0)$ and $\mu \in \rho(A_0) \cap \mathbb{R}$ chosen as in Theorem 2.2.13, where $\widetilde{\gamma}$ and $\widetilde{M}$ are given as in Proposition 2.2.12, compare [22, equation (2.17)].

Eventually, assume that S is a densely defined, closed and symmetric operator in $\mathcal{H}$, that $\{\mathcal{G},\Gamma_0,\Gamma_1\}$ is a quasi boundary triple for $\overline{T}=S^*$ and that all assumptions of Theorem 2.2.13 are fulfilled. Choose $\mu\in\rho(A_0)\cap\mathbb{R}$ as in Theorem 2.2.13, let ϑ be a symmetric operator in $\mathcal{G}$, and define

$$\begin{aligned}\Theta(\vartheta)\varphi &:= \iota_+(\vartheta-M(\mu))\iota_-^{-1}\varphi,\\ \operatorname{dom}\Theta(\vartheta) &= \big\{\varphi\in\mathcal{G}:\iota_-^{-1}\varphi\in\operatorname{dom}(\vartheta-M(\mu)) \text{ and } (\vartheta-M(\mu))\iota_-^{-1}\varphi\in\mathscr{G}_1\big\}.\end{aligned}\tag{2.21}$$

Then by [22, Corollary 3.5] it holds

$$\ker(\Gamma_1-\vartheta\Gamma_0)=\ker(\Upsilon_1-\Theta(\vartheta)\Upsilon_0).\tag{2.22}$$

In view of Proposition 2.2.7 this yields that $A_\vartheta := T\upharpoonright\ker(\Gamma_1-\vartheta\Gamma_0)$ is (essentially) self-adjoint, if and only if $\Theta(\vartheta)$ is (essentially) self-adjoint.

2.3 Sobolev spaces

In this section we introduce the function spaces which are used to formulate and prove the main results of the present thesis. First, we state the notations for classical function spaces how they are used here. Then, we introduce Sobolev spaces of weakly differentiable functions on domains. Finally, we also discuss spaces for functions acting on the boundary of bounded and sufficiently regular domains. The presentation in this section follows [53]; more details can be found for instance also in [1,52].

Let $\Omega\subset\mathbb{R}^d$, $d\in\mathbb{N}$, be an open set and $k\in\mathbb{N}\cup\{\infty\}$. Moreover, assume that $\mathbb{K}$ is either $\mathbb{R}^n,\mathbb{C}^n$, $n\in\mathbb{N}$, or any space which is isomorphic to one of these sets. Then we denote the space of k times continuously differentiable functions $f:\Omega\to\mathbb{K}$ by $C^k(\Omega;\mathbb{K})$. The symbol $C_0^\infty(\Omega;\mathbb{K})$ stands for the space of infinitely many times differentiable and compactly supported functions. Moreover, we define

$$C^\infty(\overline{\Omega};\mathbb{K}):=\{f\upharpoonright\Omega: f\in C_0^\infty(\mathbb{R}^3;\mathbb{K})\}.$$

For a multi index $\alpha=(\alpha_1,\dots,\alpha_d)^\top\in\mathbb{N}_0^d$ we write $|\alpha|:=\sum_{k=1}^d\alpha_k$ and for $f\in C^k(\Omega;\mathbb{K})$ and $\alpha\in\mathbb{N}_0^d$ with $|\alpha|\le k$ we set

$$D^\alpha f:=\frac{\partial^{\alpha_1}}{\partial x_1^{\alpha_1}}\cdots\frac{\partial^{\alpha_d}}{\partial x_d^{\alpha_d}}f.$$

As usual $L^2(\Omega;\mathbb{K})$ is the Hilbert space (of equivalence classes) of square integrable functions defined on Ω with values in $\mathbb{K}$ endowed with the inner product

$$(f,g)_\Omega:=\int_\Omega f(x)\cdot\overline{g(x)}\mathrm{d}x;$$

the corresponding norm is denoted by $\|\cdot\|_\Omega$.

We say that a function $f \in L^2(\Omega;\mathbb{K})$ is weakly differentiable of order $\alpha \in \mathbb{N}_0^d$ or differentiable in the distributional sense if there exists some $g \in L^2(\Omega;\mathbb{K})$ such that

$$\int_\Omega f \cdot D^\alpha \varphi \mathrm{d}x = (-1)^{|\alpha|} \int_\Omega g \cdot \varphi \mathrm{d}x$$

holds for all $\varphi \in C_0^\infty(\Omega;\mathbb{K})$. In this case we write $D^\alpha f = g$. The Sobolev space of order $k \in \mathbb{N}$ is then defined as

$$H^k(\Omega;\mathbb{K}) := \left\{ f \in L^2(\Omega;\mathbb{K}) : D^\alpha f \in L^2(\Omega;\mathbb{K}) \ \forall \alpha \in \mathbb{N}_0^d : |\alpha| \leq k \right\}. \tag{2.23}$$

If one endows $H^k(\Omega;\mathbb{K})$ with the inner product

$$(f,g)_{H^k(\Omega;\mathbb{K})} := \sum_{|\alpha| \leq k} (D^\alpha f, D^\alpha g)_\Omega, \qquad f,g \in H^k(\Omega;\mathbb{K}), \tag{2.24}$$

then $H^k(\Omega;\mathbb{K})$ is a Hilbert space; the corresponding norm is denoted by $\|\cdot\|_{H^k(\Omega;\mathbb{K})}$. An important subspace of $H^k(\Omega;\mathbb{K})$ is given by

$$H_0^k(\Omega;\mathbb{K}) := \overline{C_0^\infty(\Omega;\mathbb{K})}^{\|\cdot\|_{H^k(\Omega;\mathbb{K})}}.$$

Roughly speaking $H_0^k(\Omega;\mathbb{K})$ consists of functions in $H^k(\Omega;\mathbb{K})$ with vanishing boundary values (a justification for this is given in Proposition 2.3.3 below).

In order to introduce Sobolev spaces of real order recall that the Fourier transform is the unitary operator $\mathcal{F} : L^2(\mathbb{R}^d;\mathbb{K}) \to L^2(\mathbb{R}^d;\mathbb{K})$ which acts on $f \in C_0^\infty(\mathbb{R}^d;\mathbb{K})$ as

$$\mathcal{F}f(x) = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} e^{-ix\cdot y} f(y) \mathrm{d}y, \qquad x \in \mathbb{R}^d.$$

Then we define for a real $s \geq 0$

$$H^s(\mathbb{R}^d;\mathbb{K}) := \left\{ f \in L^2(\mathbb{R}^d;\mathbb{K}) : (1+|\cdot|^2)^{s/2}\mathcal{F}f \in L^2(\mathbb{R}^d;\mathbb{K}) \right\}. \tag{2.25}$$

If we endow $H^s(\mathbb{R}^d;\mathbb{K})$ with the inner product

$$(f,g)_{H^s(\mathbb{R}^d;\mathbb{K})} := \int_{\mathbb{R}^d} (1+|x|^2)^s \mathcal{F}f(x) \cdot \overline{\mathcal{F}g(x)} \mathrm{d}x, \qquad f,g \in H^s(\mathbb{R}^d;\mathbb{K}), \tag{2.26}$$

then $H^s(\mathbb{R}^d;\mathbb{K})$ is a Hilbert space. We point out that for $s \in \mathbb{N}$ the definitions of $H^s(\mathbb{R}^d;\mathbb{K})$ in (2.23) and (2.25) are the same and the associated norms induced by (2.24) and (2.26) are equivalent.

In the rest of this section we discuss suitable function spaces on the boundary $\partial\Omega$ of a domain $\Omega \subset \mathbb{R}^d$. This is only possible, if the domain satisfies some further smoothness condition. For $k \in \mathbb{N}$ we say that a set $\Omega \subset \mathbb{R}^d$, $d \geq 2$, is a *C^k-hypograph*, if there exists a function $\Lambda \in C^k(\mathbb{R}^{d-1};\mathbb{R})$ such that

$$\Omega = \{x = (x', x_d) \in \mathbb{R}^d : x' \in \mathbb{R}^{d-1},\ x_d < \Lambda(x')\}.$$

In a similar way we say that Ω is a *Lipschitz hypograph*, if Λ is Lipschitz continuous. With the help of this notion we are prepared to introduce Lipschitz and C^k-domains.

Definition 2.3.1. *Let $d,k \in \mathbb{N}$ with $d \geq 2$. Then $\Omega \subset \mathbb{R}^d$ is called a C^k-domain or a C^k-smooth domain, if $\partial\Omega$ is compact and if there exist an $l \in \mathbb{N}$ and open sets $\Omega_1, \dots, \Omega_l$ and $W_1, \dots, W_l$ with the following properties:*

(i) $\partial\Omega \subset \bigcup_{j=1}^{l} W_j$.

(ii) *Ω_j can be transformed by a rotation to a C^k-hypograph, $j \in \{1, \dots, l\}$.*

(iii) $W_j \cap \Omega_j = W_j \cap \Omega$, $j \in \{1, \dots, l\}$.

In a similar way as in Definition 2.3.1 one defines Lipschitz domains by replacing C^k-hypographs by Lipschitz hypographs.

The boundary of a C^k-domain Ω can be parametrized in the following sense: by point (ii) in Definition 2.3.1 there exists for any $j \in \{1, \dots, l\}$ a C^k-mapping $\widetilde{\Lambda}_j : \mathbb{R}^{d-1} \to \mathbb{R}^d$ such that $\widetilde{\Lambda}_j(\mathbb{R}^{d-1}) = \partial\Omega_j$. We define $U_j := \widetilde{\Lambda}_j^{-1}(\partial\Omega)$ and $\Lambda_j := \widetilde{\Lambda}_j \restriction U_j$. Then $\Lambda_j(U_j) \subset W_j$ by Definition 2.3.1 (iii). We say that $\{\Lambda_j, U_j, W_j\}_{j=1}^{l}$ is a parametrization of $\partial\Omega$.

An important quantity describing the geometry of a hypersurface $\partial\Omega$ is its associated *first fundamental form*. If $\{\Lambda_j, U_j, W_j\}_{j=1}^{l}$ is a parametrization of $\partial\Omega$, then the first fundamental form is a family of matrix valued functions given by

$$G_j : U_j \to \mathbb{R}^{(d-1)\times(d-1)}, \quad G_j(u) = \big(\langle \partial_{u_k}\Lambda_j(u), \partial_{u_l}\Lambda_j(u)\rangle\big)_{k,l=1}^{d-1}, \quad j \in \{1, \dots, l\}, \tag{2.27}$$

where $\langle\cdot,\cdot\rangle$ denotes the inner product in $\mathbb{R}^d$. The matrix G_j is always symmetric and positive definite.

In the following assume that $\Omega \subset \mathbb{R}^d$ is a Lipschitz domain in the sense of Definition 2.3.1 with parametrization $\{\Lambda_j, U_j, W_j\}_{j=1}^{l}$ as it is described above. The next goal is to introduce a suitable notion of an integral on $\partial\Omega$. Let $\{\chi_j\}_{j=1}^{l}$ be a partition of unity subordinate to $\{W_j\}_{j=1}^{l}$, that means that $\{\chi_1, \dots, \chi_l\}$ is a subset of $C_0^\infty(\mathbb{R}^d;\mathbb{K})$ such that $0 \leq \chi_j \leq 1$, $\operatorname{supp}\chi_j \subset W_j$ for $j \in \{1, \dots, l\}$ and $\sum_{j=1}^{l} \chi_j(x) = 1$ for all $x \in \partial\Omega$. Now we can define the *Hausdorff measure σ* on $\partial\Omega$ via

$$\sigma(B) := \sum_{j=1}^{l} \int_{\Lambda_j^{-1}(B)} \chi_j(\Lambda_j(u))\sqrt{\det G_j(u)}\,\mathrm{d}u$$

for any Borel set B. One can show that σ is a finite Borel measure, compare [52, Appendix C.8]. We say that a function $\varphi : \partial\Omega \to \mathbb{C}$ is integrable with respect to σ if $(\chi_j \cdot \varphi) \circ \Lambda_j \sqrt{\det G_j}$ is integrable for all $j \in \{1, \dots, l\}$. In this case, the integral of such a function is defined as

$$\int_{\partial\Omega} \varphi \mathrm{d}\sigma := \sum_{j=1}^{l} \int_{\mathbb{R}^{d-1}} (\chi_j \cdot \varphi)(\Lambda_j(u)) \sqrt{\det G_j(u)} \mathrm{d}u, \tag{2.28}$$

where $(\chi_j \cdot \varphi) \circ \Lambda_j$ is extended onto $\mathbb{R}^{d-1}$ by zero. We would like to point out that the above definitions of the integral and of the measure σ is independent of the choice of the parametrization of $\partial\Omega$.

With the Hausdorff measure on $\partial\Omega$ it is natural to define $L^2(\partial\Omega;\mathbb{K}) := L^2(\partial\Omega;\mathbb{K}, \mathrm{d}\sigma)$. Eventually, if Ω is a C^k-domain for some $k \in \mathbb{N}$, the we define for $0 \leq s \leq k$ the Sobolev space $H^s(\partial\Omega;\mathbb{K})$ on the boundary by

$$H^s(\partial\Omega;\mathbb{K}) := \left\{ \varphi \in L^2(\partial\Omega;\mathbb{K}) : (\chi_j \varphi) \circ \widetilde{\Lambda}_j \in H^s(\mathbb{R}^{d-1};\mathbb{K}) \text{ for } j \in \{1, \dots, l\} \right\}.$$

If we endow this space with the inner product

$$(\varphi, \psi)_{H^s(\partial\Omega;\mathbb{K})} := \sum_{j=1}^{l} \left((\chi_j \varphi) \circ \widetilde{\Lambda}_j, (\chi_j \psi) \circ \widetilde{\Lambda}_j \right)_{H^s(\mathbb{R}^{d-1};\mathbb{K})}, \quad \varphi, \psi \in H^s(\partial\Omega;\mathbb{K}), \tag{2.29}$$

then $H^s(\partial\Omega;\mathbb{K})$ becomes a Hilbert space. Note that different parametrizations of $\partial\Omega$ lead to different inner products in (2.29), but the induced norms are equivalent. If $s \in (0,1)$ then another equivalent norm is given by the *Sobolev-Slobodeckii* norm

$$\|\varphi\|^2_{W^s(\partial\Omega;\mathbb{K})} := \|\varphi\|^2_{\partial\Omega} + \int_{\partial\Omega} \int_{\partial\Omega} \frac{|\varphi(x) - \varphi(y)|^2}{|x-y|^{d-1+2s}} \mathrm{d}\sigma(x) \mathrm{d}\sigma(y), \quad \varphi \in H^s(\partial\Omega;\mathbb{K}). \tag{2.30}$$

For $\varphi \in H^1(\Sigma;\mathbb{K})$ we will denote sometimes by $\nabla_s \varphi$ the surface gradient or tangential derivative of φ which is given in local coordinates by

$$(\nabla_s)_n \varphi = \sum_{k=1}^{2} g^{nk} \partial_{u_k} \varphi, \quad n \in \{1, 2\},$$

where g^{nk} denote the entries of $(G_j)^{-1}$ and G_j is the first fundamental form defined by (2.27).

Finally, for $-k \leq s < 0$ we define

$$H^s(\partial\Omega;\mathbb{K}) := \left(H^{-s}(\partial\Omega;\mathbb{K}) \right)',$$

that means $H^s(\partial\Omega;\mathbb{K})$ is the dual space of $H^{-s}(\partial\Omega;\mathbb{K})$.

Clearly, by definition we have $H^s(\partial\Omega;\mathbb{K}) \subset H^t(\partial\Omega;\mathbb{K})$, if $t \leq s$. In the following proposition we state the important fact that the associated embedding is even compact:

Proposition 2.3.2. *Let $\Omega \subset \mathbb{R}^d$, $d \geq 2$, be a C^k-domain in the sense of Definition 2.3.1 for some $k \in \mathbb{N}$ and let $-k \leq t < s \leq k$. Then, the embedding $H^s(\partial\Omega;\mathbb{K}) \hookrightarrow H^t(\partial\Omega;\mathbb{K})$ is compact.*

The importance of the Sobolev spaces $H^s(\partial\Omega;\mathbb{K})$ on the boundary of a set $\Omega \subset \mathbb{R}^d$ comes from the fact that, roughly speaking, the boundary values of functions in $H^{s+1/2}(\Omega;\mathbb{K})$ belong to this space. This result is formulated precisely in the form that we need in the following theorem:

Proposition 2.3.3. *Assume that $\Omega \subset \mathbb{R}^d$, $d \geq 2$, is a C^1-domain. Then there exists a bounded and surjective operator $\tau_D : H^1(\Omega;\mathbb{K}) \to H^{1/2}(\partial\Omega;\mathbb{K})$ such that $\tau_D f = f|_{\partial\Omega}$ for all $f \in C^1(\overline{\Omega};\mathbb{K}) \cap H^1(\Omega;\mathbb{K})$. Moreover, it holds $\ker \tau_D = H_0^1(\Omega;\mathbb{K})$.*

Usually, we will write $f|_{\partial\Omega} := \tau_D f$ for $f \in H^1(\Omega;\mathbb{K})$.

Using the fact that $C^\infty(\overline{\Omega};\mathbb{K})$ is dense in $H^1(\Omega;\mathbb{K})$, see for instance [53, Theorem 3.25], it is not difficult to show the following extension of Green's first formula: if Ω is a C^1-domain with normal vector field $\nu = (\nu_1,\dots,\nu_d)^\top$, $j \in \{1,\dots,d\}$, and $f,g \in H^1(\Omega;\mathbb{K})$, then

$$\int_\Omega f \cdot (\partial_j g)\mathrm{d}x = \int_{\partial\Omega} \nu_j f|_{\partial\Omega} \cdot g|_{\partial\Omega} \mathrm{d}\sigma - \int_\Omega (\partial_j f) \cdot g \mathrm{d}x. \tag{2.31}$$

2.4 Abstract results for integral operators

In this section we provide a short overview over basic results on integral operators. As we will see in the main part of this thesis, the γ-fields and the Weyl functions associated to boundary triples suitable to define and study Dirac operators with singular interactions and Dirac operators on domains are some special integral operators. Hence, in order to apply the abstract results summarized in the previous Section 2.2 some basic knowledge on integral operators is required. The presentation in this section follows [11, Appendix A], but there is also some additional knowledge on singular integral operators added. The results are formulated such that they can be applied directly in the main part of the thesis.

Let (X,μ) and (Y,ν) be σ-finite measure spaces and let $n \in \mathbb{N}$. Roughly speaking we say that a bounded operator $T : L^2(Y,\nu;\mathbb{C}^n) \to L^2(X,\mu;\mathbb{C}^n)$ is an integral operator, if there exists a measurable function $t : X \times Y \to \mathbb{C}^{n\times n}$ such that

$$Tf(x) = \int_Y t(x,y) f(y) \mathrm{d}\nu(y), \quad x \in X,\ f \in L^2(Y,\nu;\mathbb{C}^n).$$

First, we formulate the Schur test. This is an important result to show the boundedness of integral operators acting between L^2-spaces. Its proof can be found, for instance, in [50, Example III 2.4] or [69, Satz 6.9].

Proposition 2.4.1. *Let (X,μ) and (Y,ν) be σ-finite measure spaces, let $n \in \mathbb{N}$ and let $t : X \times Y \to \mathbb{C}^{n\times n}$ be $\mu \times \nu$-measurable. Assume that there exist measurable functions $t_1, t_2 : X \times Y \to [0,\infty)$ such that $|t|^2 \le t_1 t_2$ almost everywhere and constants $\kappa_1, \kappa_2 > 0$ with*

$$\int_X t_1(x,y)\mathrm{d}\mu(x) \le \kappa_1, \quad y \in Y, \quad \textit{and} \quad \int_Y t_2(x,y)\mathrm{d}\nu(y) \le \kappa_2, \quad x \in X.$$

Then the operator $T : L^2(Y,\nu;\mathbb{C}^n) \to L^2(X,\mu;\mathbb{C}^n)$ acting as

$$Tf(x) := \int_Y t(x,y) f(y)\mathrm{d}\nu(y), \quad x \in X,\ f \in L^2(Y,\nu;\mathbb{C}^n),$$

is well-defined and bounded with $\|T\|^2 \le \kappa_1\kappa_2$. In particular, if $(X,\mu) = (Y,\nu)$ and $t_1(x,y) = t_2(y,x)$ for almost all $x,y \in X$, then $\|T\| \le \kappa_1$.

In the following we apply the Schur test in the situations that X and Y are either a subset Ω of $\mathbb{R}^d$, $d \in \{2,3\}$, with compact C^2-smooth boundary equipped with the Lebesgue measure or a C^2-smooth compact surface Σ equipped with the Hausdorff measure σ. For that we need an auxiliary result on the integrals of special functions. To prove these estimates, recall that for any $r_0 > 0$ there exists a constant $\kappa > 0$ such that

$$\sigma(\Sigma \cap B(x,r)) \le \kappa r^{d-1} \tag{2.32}$$

for all $0 < r < r_0$ and all $x \in \mathbb{R}^d$, see for instance [10, Lemma A.3].

Lemma 2.4.2. *Let $d \in \{2,3\}$ and let $\Omega \subset \mathbb{R}^d$ be a domain with compact C^2-smooth boundary $\Sigma := \partial\Omega$. Then the following assertions hold:*

(i) *Define for $\kappa, R > 0$ and $s \in (0,d)$ the function*

$$\tau(x) := \begin{cases} |x|^{-s}, & |x| < R, \\ e^{-\kappa|x|}, & |x| > R, \end{cases} \quad x \in \mathbb{R}^d \setminus \{0\}.$$

Then there exists a constant $K = K(s,\kappa) > 0$ such that

$$\int_\Omega \tau(x-y)\mathrm{d}y \le K$$

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

(ii) *Let $s \in (0,d-1)$ and $r_0 > 0$ be fixed. Then there exists a constant $K = K(s,\Sigma) > 0$ such that*

$$\int_{\Sigma\cap B(x,r)} \big(1 + |x-y|^{-s}\big)\mathrm{d}\sigma(y) \le K r^{d-1-s}$$

for all $x \in \mathbb{R}^d$ and all $r \in (0,r_0)$.

Proof. (i) Let $x \in \mathbb{R}^d$ be fixed. Using the translation invariance of the Lebesgue measure and $\tau \geq 0$, we obtain

$$\int_\Omega \tau(x-y)\mathrm{d}y \leq \int_{\mathbb{R}^d} \tau(x-y)\mathrm{d}y = \int_{\mathbb{R}^d} \tau(-y)\mathrm{d}y = \int_{B(0,R)} |y|^{-s}\mathrm{d}y + \int_{\mathbb{R}^d \setminus B(0,R)} e^{-\kappa|y|}\mathrm{d}y.$$

Since the integrals on the right hand side of the last formula are independent of x and finite for $s \in (0,d)$, the claim of assertion (i) follows.

(ii) First, in view of (2.32) it is clear that

$$\int_{\Sigma\cap B(x,r)} 1\mathrm{d}\sigma(y) = \sigma(\Sigma \cap B(x,R)) \leq Kr^{d-1} \leq Kr^{d-1-s}.$$

Hence, it remains to find an estimate for $\int_{\Sigma\cap B(x,r)} |x-y|^{-s}\mathrm{d}\sigma(y)$. Let $x \in \mathbb{R}^d$ be arbitrary, but fixed. Define for $n \in \mathbb{N}$ the sets

$$A_n := \left\{ y \in \Sigma : r2^{-n} \leq |x-y| \leq r2^{-n+1} \right\}.$$

Then $\Sigma \cap B(x,r) = \overline{\bigcup_{n=1}^\infty A_n}$ and it holds for any $y \in A_n$

$$|x-y|^{-s} \leq r^{-s}2^{sn}.$$

From this we obtain

$$\int_{\Sigma\cap B(x,r)} |x-y|^{-s}\mathrm{d}\sigma(y) = \sum_{n=1}^\infty \int_{A_n} |x-y|^{-s}\mathrm{d}\sigma(y) \leq \sum_{n=1}^\infty r^{-s}2^{sn} \int_{A_n} \mathrm{d}\sigma(y).$$

Employing (2.32) we have $\sigma(A_n) \leq \sigma(\Sigma \cap B(x, r2^{-n+1})) \leq \kappa r^{d-1}2^{-(d-1)(n-1)}$. This implies finally

$$\int_{\Sigma\cap B(x,r)} |x-y|^{-s} \leq Kr^{d-1-s} \sum_{n=1}^\infty 2^{(s-d+1)n}.$$

Since $s \in (0, d-1)$, the last sum is finite and we have the claimed result. □

Using the Schur test and the results from Lemma 2.4.2 we show now the boundedness of several families of integral operators with special integral kernels satisfying $\mathcal{O}(|x-y|^{-s})$ and we obtain estimates for their operator norms.

Proposition 2.4.3. *Let $d \in \{2,3\}$, let $\Omega \subset \mathbb{R}^d$ be a domain with compact C^2-smooth boundary, let $n \in \mathbb{N}$ and let $t : \mathbb{R}^d \to \mathbb{C}^{n\times n}$ be a measurable function. Assume that there exist constants $\kappa_1, \kappa_2, R > 0$ such that*

$$|t(x)| \leq \kappa_1 \begin{cases} |x|^{1-d}, & |x| < R, \\ e^{-\kappa_2|x|}, & |x| > R, \end{cases} \qquad x \in \mathbb{R}^d \setminus \{0\}.$$

Then the operator $T : L^2(\Omega;\mathbb{C}^n) \to L^2(\Omega;\mathbb{C}^n)$,

$$Tf(x) := \int_\Omega t(x-y)f(y)\mathrm{d}y, \quad x \in \Omega, f \in L^2(\Omega;\mathbb{C}^n),$$

is bounded and everywhere defined with $\|T\| \le \kappa_1 K$ *for some* $K = K(\kappa_2) > 0$.

Proof. Define for $x \in \mathbb{R}^d \setminus \{0\}$

$$\tau(x) := \kappa_1 \begin{cases} |x|^{1-d}, & |x| < R, \\ e^{-\kappa_2|x|}, & |x| > R, \end{cases}$$

and $t_1(x,y) = t_2(y,x) = \tau(x-y)$. Then by Lemma 2.4.2 (i) there exists a constant K such that

$$\int_\Omega t_1(x,y)\mathrm{d}x = \int_\Omega \tau(x-y)\mathrm{d}x < \kappa_1 K$$

for all $y \in \Omega$. Hence, all claimed statements follow from the Schur test (Proposition 2.4.1). □

Proposition 2.4.4. *Let* $\Omega \subset \mathbb{R}^3$ *be a domain with compact* C^2*-smooth boundary* $\partial\Omega$, *let* $n \in \mathbb{N}$ *and let* $t : \mathbb{R}^3 \to \mathbb{C}^{n\times n}$ *be a measurable function. Assume that there exist constants* $\kappa_1, \kappa_2, R > 0$ *such that*

$$|t(x)| \le \kappa_1 \begin{cases} |x|^{-2}, & |x| < R, \\ e^{-\kappa_2|x|}, & |x| > R, \end{cases} \quad x \in \mathbb{R}^3 \setminus \{0\}.$$

Then the operators $T_1 : L^2(\partial\Omega;\mathbb{C}^n) \to L^2(\Omega;\mathbb{C}^n)$,

$$T_1\varphi(x) := \int_{\partial\Omega} t(x-y)\varphi(y)\mathrm{d}\sigma(y), \quad x \in \Omega, \varphi \in L^2(\partial\Omega;\mathbb{C}^n),$$

and $T_2 : L^2(\Omega;\mathbb{C}^n) \to L^2(\partial\Omega;\mathbb{C}^n)$,

$$T_2 f(x) := \int_\Omega t(x-y)f(y)\mathrm{d}y, \quad x \in \partial\Omega, f \in L^2(\Omega;\mathbb{C}^n),$$

are bounded and everywhere defined with $\|T_1\|, \|T_2\| \le \kappa_1 K$ *for some* $K = K(\kappa_2, \partial\Omega) > 0$.

Proof. We are going to prove the claim for T_1, the statement for T_2 follows then by taking adjoints. Define for $s \in (0,1)$ and $x \in \mathbb{R}^3 \setminus \{0\}$ the functions

$$\tau_1(x) := \kappa_1 \begin{cases} |x|^{-2-s}, & |x| < R, \\ e^{-\kappa_2|x|}, & |x| > R, \end{cases}$$

and

$$\tau_2(x) := \kappa_1 \kappa_3 |x|^{-2+s}$$

where $\kappa_3 \geq 1$ is chosen such that $e^{-\kappa_2|x|} \leq \kappa_3|x|^{-2+s}$ for $|x| \geq R$. Set $t_j(x,y) := \tau_j(x-y)$, $j \in \{1,2\}$, for $x \in \Omega$ and $y \in \partial\Omega$. Then $|t(x,y)|^2 \leq t_1(x,y)t_2(x,y)$. Moreover, by Lemma 2.4.2 (i) there is a constant $K_1 = K_1(\kappa_2, s)$ such that for all $y \in \partial\Omega$

$$\int_\Omega t_1(x,y)\mathrm{d}x \leq \kappa_1 K_1.$$

Similarly, by Lemma 2.4.2 (ii) there exists $K_2 = K_2(\partial\Omega, \kappa_2, s)$ such that for all $x \in \Omega$

$$\int_{\partial\Omega} t_2(x,y)\mathrm{d}\sigma(y) \leq \kappa_1 K_2.$$

Therefore, the Schur test (Proposition 2.4.1) implies the boundedness of T_1 and the estimate for its operator norm. □

Proposition 2.4.5. *Let $\Sigma \subset \mathbb{R}^3$ be a compact and closed C^2-smooth surface, let $n \in \mathbb{N}$ and let $t : \mathbb{R}^3 \to \mathbb{C}^{n\times n}$ be a measurable function. Assume that there exists a constant $\kappa > 0$ such that*

$$|t(x)| \leq \kappa\big(1 + |x|^{-1}\big), \quad x \in \mathbb{R}^3 \setminus \{0\}.$$

Then the operator $\mathcal{T} : L^2(\Sigma;\mathbb{C}^n) \to L^2(\Sigma;\mathbb{C}^n)$,

$$\mathcal{T}\varphi(x) := \int_\Sigma t(x-y)\varphi(y)\mathrm{d}\sigma(y), \quad x \in \Sigma, \varphi \in L^2(\Sigma;\mathbb{C}^n),$$

is bounded and everywhere defined with $\|\mathcal{T}\| \leq \kappa K$ for some $K = K(\Sigma) > 0$.

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

$$\tau(x) := \kappa\big(1 + |x|^{-1}\big)$$

and $t_1(x,y) = t_2(y,x) = \tau(x-y)$. Then by Lemma 2.4.2 (ii) there exists a constant K such that

$$\int_\Sigma t_1(x,y)\mathrm{d}\sigma(x) = \int_\Sigma \tau(x-y)\mathrm{d}\sigma(x) < \kappa K$$

for all $y \in \Sigma$. Hence, all claimed statements follow from the Schur test (Proposition 2.4.1). □

Eventually, we discuss in the next proposition a special singular integral operator. With the help of Proposition 2.4.5 it will allow us to understand a boundary integral operator in Section 3.2 below that plays a crucial role in the study of Dirac operators with singular interactions and Dirac operators on domains. The result can be found for instance in [5, Lemma 3.3].

Proposition 2.4.6. *Let $j \in \{1,2,3\}$ and let $\Sigma \subset \mathbb{R}^3$ be a compact and closed C^2-smooth surface. Then the operator $\mathcal{T}_j : L^2(\Sigma;\mathbb{C}) \to L^2(\Sigma;\mathbb{C})$,*

$$\mathcal{T}_j \varphi(x) := \lim_{\varepsilon \searrow 0} \int_{\Sigma \setminus B(x,\varepsilon)} \frac{x_j - y_j}{|x-y|^3} \varphi(y) \mathrm{d}\sigma(y), \quad x \in \Sigma, \varphi \in L^2(\Sigma;\mathbb{C}),$$

is well-defined and bounded.

2.5 Multiplication operators in Sobolev spaces

In this section we state two results on operators that are associated to the multiplication with a Lipschitz continuous function. First, we have the following standard result.

Lemma 2.5.1. *Let Σ be the boundary of a bounded Lipschitz domain and let $\eta : \Sigma \to \mathbb{C}$ be Lipschitz continuous. Then for any $s \in [-1,1]$ the associated multiplication operator in $H^s(\Sigma;\mathbb{C})$ is well-defined and bounded.*

Proof. We show the claim for $s = 1$, from this the statement for $s = -1$ follows by duality. Eventually, the result for intermediate values $s \in (-1,1)$ can be shown then by a standard interpolation argument.

Since η is Lipschitz continuous, it is weakly differentiable and the weak derivatives belong to $L^\infty(\Sigma;\mathbb{C})$. Then, for $\varphi \in H^1(\Sigma;\mathbb{C})$ the surface gradient of $\eta\varphi$ is

$$\nabla_s(\eta\varphi) = (\nabla_s \eta)\varphi + \eta(\nabla_s \varphi).$$

Since $\eta, \nabla_s \eta \in L^\infty(\Sigma;\mathbb{C})$ the claim of this lemma follows. □

Next, we discuss a way how one can approximate the multiplication operator with a Lipschitz continuous function η in $H^{1/2}(\Sigma;\mathbb{C}^4)$. We are going to apply this result if η admits the value zero, in this case the zero sets of the functions η_ε defined in the proposition below are non-trivial.

Proposition 2.5.2. *Let $\Sigma \subset \mathbb{R}^3$ be the boundary of a bounded Lipschitz domain, let $\eta : \Sigma \to \mathbb{R}$ be Lipschitz continuous and define for $\varepsilon > 0$*

$$\eta_\varepsilon := (\eta - \varepsilon)_+ - (-\eta + \varepsilon)_- = \max\{\eta - \varepsilon, 0\} - \min\{-\eta + \varepsilon, 0\}.$$

Then the multiplication with η_ε gives rise to a bounded operator in $H^{1/2}(\Sigma;\mathbb{C}^4)$ and for any $t \in \left(0, \frac{1}{2}\right)$ there exists a constant $\kappa = \kappa(t) > 0$ such that

$$\|(\eta - \eta_\varepsilon)\varphi\|_{H^{1/2}(\Sigma;\mathbb{C}^4)} \leq \kappa \varepsilon^t \|\varphi\|_{H^{1/2}(\Sigma;\mathbb{C}^4)} \tag{2.33}$$

holds for all $\varphi \in H^{1/2}(\Sigma;\mathbb{C}^4)$.

Proof. In this proof κ will denote a generic constant that will have different values at different places. Let $s \in (0,1)$ be fixed. In order to prove this proposition we use the equivalent Sobolev-Slobodeckii norm from (2.30), that means we show that there exists a constant $\kappa > 0$ such that

$$\begin{aligned} \|(\eta-\eta_\varepsilon)\varphi\|_\Sigma^2 + \int_\Sigma\int_\Sigma \frac{|((\eta-\eta_\varepsilon)\varphi)(x)-((\eta-\eta_\varepsilon)\varphi)(y)|^2}{|x-y|^3} \mathrm{d}\sigma(x)\mathrm{d}\sigma(y) \\ \leq \kappa\varepsilon^{1-s}\|\varphi\|^2_{W^{1/2}(\Sigma;\mathbb{C}^4)} \end{aligned} \tag{2.34}$$

for all $\varphi \in H^{1/2}(\Sigma;\mathbb{C}^4)$, which yields then the claim.

First, since $|\eta-\eta_\varepsilon| \leq \varepsilon$ on Σ we have

$$\|(\eta-\eta_\varepsilon)\varphi\|_\Sigma \leq \varepsilon\|\varphi\|_\Sigma. \tag{2.35}$$

The estimate of the double integral in (2.34) is more delicate. We define the sets

$$\begin{aligned} \Sigma_\varepsilon^+ &:= \{x \in \Sigma : \eta(x) > \varepsilon\}, \qquad \Sigma_\varepsilon^- := \{x \in \Sigma : \eta(x) < -\varepsilon\}, \\ \Sigma_0^+ &:= \{x \in \Sigma : \eta(x) \in [0,\varepsilon]\}, \qquad \Sigma_0^- := \{x \in \Sigma : \eta(x) \in [-\varepsilon,0]\}, \end{aligned}$$

so that $\Sigma = \Sigma_\varepsilon^+ \cup \Sigma_\varepsilon^- \cup \Sigma_0^+ \cup \Sigma_0^-$. We are going to estimate the integrals over $\Sigma_\cdot^\pm \times \Sigma_\cdot^\pm$ for $\cdot \in \{0,\varepsilon\}$ separately. First, for $x \in \Sigma_\varepsilon^+$ we have $\eta(x)-\eta_\varepsilon(x) = \varepsilon$ and hence

$$\begin{aligned} \int_{\Sigma_\varepsilon^+}\int_{\Sigma_\varepsilon^+} \frac{|((\eta-\eta_\varepsilon)\varphi)(x)-((\eta-\eta_\varepsilon)\varphi)(y)|^2}{|x-y|^3} \mathrm{d}\sigma(x)\mathrm{d}\sigma(y) \\ = \varepsilon^2 \int_{\Sigma_\varepsilon^+}\int_{\Sigma_\varepsilon^+} \frac{|\varphi(x)-\varphi(y)|^2}{|x-y|^3} \mathrm{d}\sigma(x)\mathrm{d}\sigma(y) \leq \varepsilon^2\|\varphi\|^2_{W^{1/2}(\Sigma;\mathbb{C}^4)}. \end{aligned} \tag{2.36}$$

Similarly, it holds

$$\int_{\Sigma_\varepsilon^-}\int_{\Sigma_\varepsilon^-} \frac{|((\eta-\eta_\varepsilon)\varphi)(x)-((\eta-\eta_\varepsilon)\varphi)(y)|^2}{|x-y|^3} \mathrm{d}\sigma(x)\mathrm{d}\sigma(y) \leq \varepsilon^2\|\varphi\|^2_{W^{1/2}(\Sigma;\mathbb{C}^4)}. \tag{2.37}$$

Next, if $(x,y) \in \Sigma_0 \times \Sigma_0$ with $\Sigma_0 := \Sigma_0^+ \cup \Sigma_0^-$, then $\eta_\varepsilon(x) = \eta_\varepsilon(y) = 0$, $|\eta(x)|, |\eta(y)| \leq \varepsilon$, and using the Lipschitz continuity of η we find for $s \in (0,1)$

$$\begin{aligned} \big|((\eta-\eta_\varepsilon)\varphi)(x)-((\eta-\eta_\varepsilon)\varphi)(y)\big|^2 &\leq 2\big|(\eta(x)-\eta(y))\varphi(x)\big|^2 + 2\big|\eta(y)(\varphi(x)-\varphi(y))\big|^2 \\ &\leq \kappa\varepsilon^{1-s}|x-y|^{1+s}|\varphi(x)|^2 + \varepsilon^2|\varphi(x)-\varphi(y)|^2 \end{aligned}$$

and thus, employing [51, Lemma 3.2 (b)] we deduce

$$\begin{aligned} &\int_{\Sigma_0}\int_{\Sigma_0} \frac{|((\eta-\eta_\varepsilon)\varphi)(x)-((\eta-\eta_\varepsilon)\varphi)(y)|^2}{|x-y|^3} \mathrm{d}\sigma(x)\mathrm{d}\sigma(y) \\ &\quad\leq \kappa\varepsilon^{1-s}\int_{\Sigma_0}\int_{\Sigma_0}\left[\frac{|\varphi(x)|^2}{|x-y|^{2-s}} + \frac{|\varphi(x)-\varphi(y)|^2}{|x-y|^3}\right]\mathrm{d}\sigma(x)\mathrm{d}\sigma(y) \\ &\quad\leq \kappa\varepsilon^{1-s}\left(\int_{\Sigma_0}|\varphi(x)|^2\mathrm{d}\sigma(x) + \int_{\Sigma_0}\int_{\Sigma_0}\frac{|\varphi(x)-\varphi(y)|^2}{|x-y|^3}\mathrm{d}\sigma(x)\mathrm{d}\sigma(y)\right) \\ &\quad\leq \varepsilon^{1-s}\|\varphi\|^2_{W^{1/2}(\Sigma;\mathbb{C}^4)}. \end{aligned} \tag{2.38}$$

In order to estimate the integral over $\Sigma_\varepsilon^+ \times \Sigma^-$ with $\Sigma_- := \Sigma_\varepsilon^- \cup \Sigma_0^-$ we note that it holds for $(x,y) \in \Sigma_\varepsilon^+ \times \Sigma^-$ similarly as above

$$\big|((\eta-\eta_\varepsilon)\varphi)(x) - ((\eta-\eta_\varepsilon)\varphi)(y)\big| \leq \varepsilon\big|\varphi(x)\big| + \big|((\eta-\eta_\varepsilon)\varphi)(y)\big| \leq \varepsilon\big(|\varphi(x)|+|\varphi(y)|\big).$$

Moreover, using the Lipschitz continuity of η we have

$$\varepsilon \leq \eta(x) - \eta(y) \leq \kappa|x-y|,$$

which yields $|x-y|^{-1} \leq \kappa\varepsilon^{-1}$. Using again [51, Lemma 3.2 (b)] we obtain eventually

$$\begin{aligned}
&\int_{\Sigma^-}\int_{\Sigma_\varepsilon^+} \frac{|((\eta-\eta_\varepsilon)\varphi)(x) - ((\eta-\eta_\varepsilon)\varphi)(y)|^2}{|x-y|^3} \mathrm{d}\sigma(x)\mathrm{d}\sigma(y) \\
&\qquad \leq \kappa\varepsilon^{1-s}\int_{\Sigma^-}\int_{\Sigma_\varepsilon^+}\left[\frac{|\varphi(x)|^2+\varphi(y)|^2}{|x-y|^{2-s}}\right]\mathrm{d}\sigma(x)\mathrm{d}\sigma(y) \\
&\qquad \leq \kappa\varepsilon^{1-s}\left(\int_{\Sigma_\varepsilon^+}|\varphi(x)|^2\mathrm{d}\sigma(x) + \int_{\Sigma^-}|\varphi(y)|^2\mathrm{d}\sigma(y)\right) \leq \varepsilon^{1-s}\|\varphi\|^2_{W^{1/2}(\Sigma;\mathbb{C}^4)}.
\end{aligned} \tag{2.39}$$

By symmetry a similar estimate can also be shown for the integrals over $\Sigma^- \times \Sigma_\varepsilon^+$, $\Sigma^+ \times \Sigma_\varepsilon^-$, and $\Sigma_\varepsilon^- \times \Sigma^+$ with obvious notations.

Eventually, we have to estimate the integral over $\Sigma_0^+ \times \Sigma_\varepsilon^+$. For $(x,y) \in \Sigma_0^+ \times \Sigma_\varepsilon^+$ it holds

$$\begin{aligned}
\big|((\eta-\eta_\varepsilon)\varphi)(x) - ((\eta-\eta_\varepsilon)\varphi)(y)\big| &= \big|((\eta\varphi)(x) - \varepsilon\varphi(y)\big| \\
&\leq \varepsilon|\varphi(x)-\varphi(y)| + (\varepsilon - \eta(x))\cdot|\varphi(x)| \\
&\leq \varepsilon|\varphi(x)-\varphi(y)| + |\eta(y)-\eta(x)|^{1/2+s}\varepsilon^{1/2-s}|\varphi(x)|.
\end{aligned}$$

The last inequality is true as $\eta(y) > \varepsilon$ for $y \in \Sigma_\varepsilon^+$. Using the Lipschitz continuity of η we conclude from this in a similar way as in (2.38)

$$\begin{aligned}
&\int_{\Sigma_0^+}\int_{\Sigma_\varepsilon^+} \frac{|((\eta-\eta_\varepsilon)\varphi)(x) - ((\eta-\eta_\varepsilon)\varphi)(y)|^2}{|x-y|^3} \mathrm{d}\sigma(x)\mathrm{d}\sigma(y) \\
&\qquad \leq \kappa\varepsilon^{1-s}\left(\int_{\Sigma_\varepsilon^+}|\varphi(x)|^2\mathrm{d}\sigma(x) + \int_{\Sigma_0^+}\int_{\Sigma_\varepsilon^+}\frac{|\varphi(x)-\varphi(y)|^2}{|x-y|^3}\mathrm{d}\sigma(x)\mathrm{d}\sigma(y)\right) \\
&\qquad \leq \varepsilon^{1-s}\|\varphi\|^2_{W^{1/2}(\Sigma;\mathbb{C}^4)}.
\end{aligned} \tag{2.40}$$

By symmetry it is easy to see that a similar estimate is also true for the integrals over $\Sigma_\varepsilon^+ \times \Sigma_0^+$, $\Sigma_0^- \times \Sigma_\varepsilon^-$ and $\Sigma_\varepsilon^- \times \Sigma_0^-$. Combining now the estimates (2.35)–(2.40) we deduce finally that (2.34) is true and thus, the claim of this proposition is shown for $t = \frac{1}{2}(1-s)$. □

2.6 Schatten-von Neumann ideals

In this section we summarize several notions and results on Schatten-von Neumann ideals which are necessary to prove Theorem 1 (iii), Theorem 4 (iii) and some deeper results in this direction in Sections 4.2 and 5.3. The presentation of the results follows the one in [20], there one can find also further references.

Let $\mathcal{H}$ and $\mathcal{K}$ be separable Hilbert spaces. Recall that we denote the set of all bounded operators $A : \mathcal{H} \to \mathcal{K}$ by $\mathfrak{B}(\mathcal{H},\mathcal{K})$. If there is no danger of confusion, we skip the spaces and simply write $\mathfrak{B}$. In a similar manner, we use the symbol $\mathfrak{S}_\infty(\mathcal{H},\mathcal{K})$ for the space of all compact operators from $\mathcal{H}$ to $\mathcal{K}$ and $\mathfrak{S}_\infty(\mathcal{H}) := \mathfrak{S}_\infty(\mathcal{H},\mathcal{H})$. It is well known (see for instance [50, 60]) that for $K \in \mathfrak{S}_\infty(\mathcal{H},\mathcal{K})$ the operator $|K| := (K^*K)^{1/2}$ is a self-adjoint and non-negative compact operator in $\mathcal{H}$. The eigenvalues of this operator $s_k(K)$, $k \in \mathbb{N}$, ordered in a non-increasing way and taking multiplicities into account are called the singular values of K. Note that $s_k(K) = s_k(K^*)$. Making use of the singular values one can make the following further classification of $\mathfrak{S}_\infty(\mathcal{H},\mathcal{K})$:

Definition 2.6.1. *Let $\mathcal{H}$ and $\mathcal{K}$ be separable Hilbert spaces and let $p > 0$. Then the Schatten-von Neumann ideal of order p is defined by*

$$\mathfrak{S}_p(\mathcal{H},\mathcal{K}) := \left\{ K \in \mathfrak{S}_\infty(\mathcal{H},\mathcal{K}) : \sum_{k=1}^{\infty} s_k(K)^p < \infty \right\}.$$

Moreover, the weak Schatten-von Neumann ideal of order p is

$$\mathfrak{S}_{p,\infty}(\mathcal{H},\mathcal{K}) := \left\{ K \in \mathfrak{S}_\infty(\mathcal{H},\mathcal{K}) : s_k(K) = \mathcal{O}(k^{-1/p}) \right\}.$$

Assume that $0 < p < q$. Then the (weak) Schatten-von Neumann ideals are ordered as $\mathfrak{S}_p(\mathcal{H},\mathcal{K}) \subset \mathfrak{S}_q(\mathcal{H},\mathcal{K})$ and $\mathfrak{S}_{p,\infty}(\mathcal{H},\mathcal{K}) \subset \mathfrak{S}_{q,\infty}(\mathcal{H},\mathcal{K})$. Moreover, we have

$$\mathfrak{S}_p(\mathcal{H},\mathcal{K}) \subset \mathfrak{S}_{p,\infty}(\mathcal{H},\mathcal{K}) \quad \text{and} \quad \mathfrak{S}_{p,\infty}(\mathcal{H},\mathcal{K}) \subset \mathfrak{S}_q(\mathcal{H},\mathcal{K}). \tag{2.41}$$

The Schatten-von Neumann ideals are ideals in the sense that for $A \in \mathfrak{B}$ and $K \in \mathfrak{S}_p$ it holds $AK \in \mathfrak{S}_p$ and $KA \in \mathfrak{S}_p$. Similarly, it holds for $A \in \mathfrak{B}$ and $K \in \mathfrak{S}_{p,\infty}$ that $AK \in \mathfrak{S}_{p,\infty}$ and $KA \in \mathfrak{S}_{p,\infty}$. Eventually, if $p, q > 0$ and r is chosen such that $\frac{1}{r} = \frac{1}{p} + \frac{1}{q}$, then for $K_1 \in \mathfrak{S}_{p,\infty}$ and $K_2 \in \mathfrak{S}_{q,\infty}$ the product of these operators satisfies

$$K_1 K_2 \in \mathfrak{S}_{r,\infty}. \tag{2.42}$$

We would like to point out that in applications the Schatten-von Neumann ideal of order one, which is also known as trace class ideal, are of special importance. For $K \in \mathfrak{S}_1$ the trace of K is defined by

$$\operatorname{tr}(K) := \sum_{k=1}^{\infty} \lambda_k(K),$$

where $\lambda_k(K)$ are the eigenvalues of the compact operator K. Moreover, for $K_1, K_2 \in \mathfrak{B}$ with $K_1 K_2 \in \mathfrak{S}_1$ and $K_2 K_1 \in \mathfrak{S}_1$ it holds the important cyclicity property

$$\operatorname{tr}(K_1 K_2) = \operatorname{tr}(K_2 K_1). \tag{2.43}$$

Finally, let $\Sigma \subset \mathbb{R}^3$ be the boundary of a compact domain with sufficiently smooth boundary. Using a result from [2] we deduce that operators with range in the Sobolev space $H^s(\Sigma;\mathbb{C})$ belong to certain weak Schatten-von Neumann ideals. This is the main ingredient to prove Theorem 4.2.7 and Theorem 5.3.6 later. The author thanks V. Lotoreichik for showing him a proof for this proposition.

Proposition 2.6.2. *Let $k \in \mathbb{N}$, let $\Sigma \subset \mathbb{R}^3$ be the boundary of a compact C^k-smooth domain and let $l \in \{1, \dots, 2k\}$. Let $\mathcal{H}$ be a separable Hilbert space and assume that $A : \mathcal{H} \to L^2(\Sigma;\mathbb{C})$ is continuous with* $\operatorname{ran} A \subset H^{l/2}(\Sigma;\mathbb{C})$*. Then $A \in \mathfrak{S}_{4/l,\infty}\big(\mathcal{H}, L^2(\Sigma;\mathbb{C})\big)$.*

Proof. For the sake of readability we split the proof into three steps:

Step 1: We show that $A_l : \mathcal{H} \to H^{l/2}(\Sigma;\mathbb{C})$, $A_l f = Af$ is continuous. For this purpose we verify that A_l is closed. Assume that $(f_n) \subset \mathcal{H}$ such that

$$f_n \to f \text{ in } \mathcal{H} \quad \text{and} \quad A_l f_n \to g \text{ in } H^{l/2}(\Sigma;\mathbb{C}), \quad \text{as } n \to \infty.$$

Then, $f \in \mathcal{H} = \operatorname{dom} A_l$ and as $A \in \mathfrak{B}(\mathcal{H}, L^2(\Sigma;\mathbb{C}))$ we have $A_l f_n = A f_n \to Af$ in $L^2(\Sigma;\mathbb{C}^4)$ for $n \to \infty$. On the other hand, since $H^{l/2}(\Sigma;\mathbb{C})$ is embedded continuously in $L^2(\Sigma;\mathbb{C})$ we have also $A f_n = A_l f_n \to g$ in $L^2(\Sigma;\mathbb{C})$. Thus, we deduce $A_l f = Af = g$ and therefore, A_l is closed.

Step 2: Define the function

$$K(x) := \frac{1}{4\pi|x|}, \quad x \in \mathbb{R}^3 \setminus \{0\},$$

and the operator $M_0 : L^2(\Sigma;\mathbb{C}) \to L^2(\Sigma;\mathbb{C}^4)$ acting as

$$M_0 \varphi(x) := \int_\Sigma K(x-y)\varphi(y)\,\mathrm{d}\sigma(y), \quad x \in \Sigma, \varphi \in L^2(\Sigma;\mathbb{C}).$$

It is well-known, see [53, Theorem 6.8, Theorem 6.12, Theorem 7.6, and Corollary 8.13], that M_0 is well defined, self-adjoint, non-negative, and M_0 regarded as operator from $L^2(\Sigma;\mathbb{C})$ to $H^1(\Sigma,\mathbb{C})$ is bijective. Using a scaling of Hilbert spaces argument we see that also

$$M_0^{l/2} : L^2(\Sigma;\mathbb{C}) \to H^{l/2}(\Sigma;\mathbb{C}) \tag{2.44}$$

is bijective. Moreover, since K is a homogeneous function of order -1 it follows from [2, Proposition 2.3 and Proposition 2.5] that $M_0 \in \mathfrak{S}_{2,\infty}(L^2(\Sigma;\mathbb{C}))$. Thus, by the spectral theorem we have also $M_0^{l/2} \in \mathfrak{S}_{4/l,\infty}(L^2(\Sigma;\mathbb{C}))$.

Step 3: We write $A = M_0^{l/2} M_0^{-l/2} A_l$. Then using the result of *Step 1* and (2.44) we have that $M_0^{-l/2} A_l \in \mathfrak{B}(\mathcal{H}, L^2(\Sigma;\mathbb{C}))$. Since $M_0^{l/2} \in \mathfrak{S}_{4/l,\infty}(L^2(\Sigma;\mathbb{C}))$ by *Step 2* we deduce finally $A \in \mathfrak{S}_{4/l,\infty}(L^2(\Sigma;\mathbb{C}))$, which was the claimed result. □

3 THE MINIMAL, FREE, AND MAXIMAL DIRAC OPERATOR AND ASSOCIATED INTEGRAL OPERATORS

In this chapter we introduce the free Dirac operator in $\mathbb{R}^3$ and we discuss the minimal and the maximal Dirac operator acting in a bounded or unbounded domain $\Omega \subset \mathbb{R}^3$. Furthermore, we investigate several families of integral operators which are associated to the fundamental solutions of the corresponding Dirac equation. These objects will play a crucial role in Chapters 4 and 5 below to define and study the spectral properties of Dirac operators with singular interactions supported on compact surfaces $\Sigma \subset \mathbb{R}^3$ and self-adjoint Dirac operators on domains $\Omega \subset \mathbb{R}^3$.

3.1 The free, the minimal, and the maximal Dirac operator

Choose units such that $\hbar = 1$ and let m, c be positive constants denoting the mass of the particle and the speed of light. Throughout this thesis we work with the following choice of the Dirac matrices α_j and β

$$\alpha_j := \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix} \quad \text{and} \quad \beta := \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}, \tag{3.1}$$

where σ_j are the Pauli spin matrices

$$\sigma_1 := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 := \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{3.2}$$

A simple computation shows that these matrices fulfill (1.2), but we would like to note that also other choices for α_j and β satisfying (1.2) are possible, compare [68, Appendix 1.A]. Then the free Dirac operator is defined by

$$A_0 f := -ic \sum_{k=1}^{3} \alpha_k \partial_k f + mc^2 \beta f, \qquad \operatorname{dom} A_0 = H^1(\mathbb{R}^3; \mathbb{C}^4), \tag{3.3}$$

where α_k, β are the Dirac matrices given by (3.1). As in (1.5) we will often use the notation

$$A_0 f = -ic\alpha \cdot \nabla f + mc^2 \beta f.$$

Let us first summarize some of the basic properties of A_0; they can be found, for instance, in [68, Chapter 1] or [70, Chapter 20]. First, the free Dirac operator is self-adjoint. Next, using (1.2) it follows that

$$\|A_0 f\|^2_{\mathbb{R}^3} = c^2\|\nabla f\|^2_{\mathbb{R}^3} + m^2c^4\|f\|^2_{\mathbb{R}^3}. \tag{3.4}$$

In particular, the graph norm associated to A_0 is equivalent to the norm in $H^1(\mathbb{R}^3;\mathbb{C}^4)$. It is well known that the square of A_0 coincides with a shifted free Laplace operator in $\mathbb{R}^3$, that means

$$A_0^2 = (-c^2\Delta + m^2c^4)I_4, \quad \operatorname{dom} A_0^2 = H^2(\mathbb{R}^3;\mathbb{C}^4), \tag{3.5}$$

where the operator on the right hand side is understood as 4×4 diagonal operator, where each non trivial entry acts as $-c^2\Delta + m^2c^4$. Eventually, the spectrum of A_0 is

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

In the following proposition we compute the resolvent of A_0. The particular form of its integral kernel will be of great importance for our considerations in the following sections. One can find this result for instance in [68, Section 1.E], but for completeness we add a direct proof based on (3.5) here. Note that below we use the convention $\operatorname{Im}\sqrt{\mu} > 0$ for $\mu \in \mathbb{C}\setminus[0,\infty)$.

Proposition 3.1.1. *Let A_0 be the free Dirac operator from* (3.3) *and let $\lambda \in \rho(A_0) = \mathbb{C}\setminus\big((-\infty,-mc^2]\cup[mc^2,\infty)\big)$. Then, the resolvent of A_0 acts as*

$$(A_0-\lambda)^{-1}f(x) = \int_{\mathbb{R}^3} G_\lambda(x-y)f(y)\,\mathrm{d}y, \quad x\in\mathbb{R}^3,\ f\in L^2(\mathbb{R}^3;\mathbb{C}^4),$$

where the $\mathbb{C}^{4\times4}$-valued integral kernel G_λ is given by

$$G_\lambda(x) = \left(\frac{\lambda}{c^2}I_4 + m\beta + \left(1 - i\sqrt{\frac{\lambda^2}{c^2} - (mc)^2}|x|\right)\frac{i}{c|x|^2}\alpha\cdot x\right)\cdot\frac{e^{i\sqrt{\lambda^2/c^2-(mc)^2}|x|}}{4\pi|x|}. \tag{3.6}$$

Proof. The identity $(A_0-\lambda)(A_0+\lambda) = (-c^2\Delta + m^2c^4 - \lambda^2)I_4$, which follows from (3.5), implies

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

Let $f\in L^2(\mathbb{R}^3;\mathbb{C}^4)$ be fixed. It is well known that

$$\left(-\Delta + (mc)^2 - \frac{\lambda^2}{c^2}\right)^{-1} f(x) = \int_{\mathbb{R}^3} \frac{e^{i\sqrt{\lambda^2/c^2-(mc)^2}|x-y|}}{4\pi|x-y|} f(y)\,\mathrm{d}y, \tag{3.8}$$

see for instance [61, Example 1 in Section IX.7]. Since $(-\Delta+(mc)^2-\lambda^2/c^2)^{-1}f \in \operatorname{dom}(-\Delta\cdot I_4) = H^2(\mathbb{R}^3;\mathbb{C}^4)$ this function is weakly differentiable. We are going to show that its first order weak derivatives are

$$\partial_j\left(-\Delta+(mc)^2-\frac{\lambda^2}{c^2}\right)^{-1} f = T_j f, \quad j\in\{1,2,3\}, \tag{3.9}$$

where

$$T_j f(x) := \int_{\mathbb{R}^3} t_j(x-y) f(y)\mathrm{d}y, \quad x\in\mathbb{R}^3,$$

with

$$\begin{aligned} t_j(x) &:= \partial_j\left(\frac{e^{i\sqrt{\lambda^2/c^2-(mc)^2}|\cdot|}}{4\pi|\cdot|}\right)(x)\cdot I_4 \\ &= \left(i\sqrt{\frac{\lambda^2}{c^2}-(mc)^2}|x|-1\right)\frac{e^{i\sqrt{\lambda^2/c^2-(mc)^2}|x|}}{4\pi|x|^3}x_j\cdot I_4. \end{aligned}$$

Then it follows from (3.7), (3.8), and a straightforward computation that

$$\begin{aligned} (A_0-\lambda)^{-1}f(x) &= c^{-2}(A_0+\lambda)\left(-\Delta+(mc)^2-\frac{\lambda^2}{c^2}\right)^{-1} f(x) \\ &= c^{-2}(A_0+\lambda)\left(\int_{\mathbb{R}^3}\frac{e^{i\sqrt{\lambda^2/c^2-(mc)^2}|\cdot-y|}}{4\pi|\cdot-y|}f(y)\mathrm{d}y\right)(x) \\ &= \int_{\mathbb{R}^3} G_\lambda(x-y)f(y)\mathrm{d}y, \end{aligned}$$

where G_λ has the form (3.6). It remains to verify (3.9). For this purpose, we note first that there exists an $R>0$ such that for any $j\in\{1,2,3\}$ the function t_j satisfies

$$|t_j(x)| \le \kappa \begin{cases} |x|^{-2}, & |x|<R, \\ e^{-\operatorname{Im}\sqrt{\lambda^2/c^2-(mc)^2}|x|}, & |x|\ge R, \end{cases}$$

for some positive constant κ. Hence, the operator T_j is bounded and everywhere defined in $L^2(\mathbb{R}^3;\mathbb{C}^4)$; see Proposition 2.4.3. In particular, the function on the right hand side of (3.9) belongs to $L^2(\mathbb{R}^3;\mathbb{C}^4)$. For $h\in C_0^\infty(\mathbb{R}^3;\mathbb{C}^4)$ we obtain with the help of Fubini's theorem (whose application is allowed due to our previous considerations) and integration by parts that

$$\begin{aligned}
\big(T_j f, h\big)_{\mathbb{R}^3)} &= \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} t_j(x-y)f(y)\mathrm{d}y\,\overline{h(x)}\mathrm{d}x \\
&= \int_{\mathbb{R}^3} f(y)\int_{\mathbb{R}^3} t_j(x-y)\overline{h(x)}\mathrm{d}x\mathrm{d}y \\
&= -\int_{\mathbb{R}^3} f(y)\int_{\mathbb{R}^3} \frac{e^{i\sqrt{\lambda^2/c^2-(mc)^2}|x-y|}}{4\pi|x-y|}\overline{\partial_j h(x)}\mathrm{d}x\mathrm{d}y \\
&= -\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{e^{i\sqrt{\lambda^2/c^2-(mc)^2}|x-y|}}{4\pi|x-y|} f(y)\mathrm{d}y\,\overline{\partial_j h(x)}\mathrm{d}x \\
&= -\left(\left(-\Delta+(mc)^2-\frac{\lambda^2}{c^2}\right)^{-1} f, \partial_j h\right)_{\mathbb{R}^3}.
\end{aligned}$$

This shows (3.9) and completes the proof. □

Let Ω be a C^2-domain in $\mathbb{R}^3$ with compact boundary, that means Ω is either a bounded C^2-domain or the complement of such a set. In the following we study the following two operators acting in $L^2(\Omega;\mathbb{C}^4)$: The maximal Dirac operator

$$T^\Omega_{\max} f := -ic\alpha\cdot\nabla f + mc^2\beta f, \quad \operatorname{dom} T^\Omega_{\max} = \big\{f\in L^2(\Omega;\mathbb{C}^4) : \alpha\cdot\nabla f \in L^2(\Omega;\mathbb{C}^4)\big\}, \tag{3.10}$$

where the derivatives are understood in the distributional sense, and the minimal Dirac operator $T^\Omega_{\min} := T^\Omega_{\max} \upharpoonright H^1_0(\Omega;\mathbb{C}^4)$, which is represented more explicitly by

$$T^\Omega_{\min} f := -ic\alpha\cdot\nabla f + mc^2\beta f, \quad \operatorname{dom} T^\Omega_{\min} = H^1_0(\Omega;\mathbb{R}^3). \tag{3.11}$$

The basic properties of $T^\Omega_{\min}$ and $T^\Omega_{\max}$ are collected in the following lemma.

Lemma 3.1.2. *Let $\Omega \subset \mathbb{R}^3$ be a C^2-smooth domain with compact boundary and let $T^\Omega_{\max}$ and $T^\Omega_{\min}$ be defined by* (3.10) *and* (3.11)*, respectively. Then $T^\Omega_{\min}$ is a closed, simple symmetric operator in $L^2(\Omega;\mathbb{C}^4)$ and $(T^\Omega_{\min})^* = T^\Omega_{\max}$.*

Proof. First, we verify that $T^\Omega_{\min}$ is closed. For that, let $f_n \subset \operatorname{dom} T^\Omega_{\min} = H^1_0(\Omega;\mathbb{C}^4)$ such that

$$f_n \to f \quad \text{and} \quad T^\Omega_{\min} f_n \to g \quad \text{in} \quad L^2(\Omega;\mathbb{C}^4), \text{ as } n\to\infty.$$

We show $f \in \operatorname{dom} T^\Omega_{\min}$ and $T^\Omega_{\min} f = g$. Denote the extensions of f, f_n and g onto $\mathbb{R}^3$ by zero by $\widetilde{f}, \widetilde{f_n}$ and $\widetilde{g}$, respectively, that is

$$\widetilde{f} := \begin{cases} f & \text{in } \Omega, \\ 0 & \text{in } \mathbb{R}^3\setminus\Omega, \end{cases} \quad \widetilde{f_n} = \begin{cases} f_n & \text{in } \Omega, \\ 0 & \text{in } \mathbb{R}^3\setminus\Omega, \end{cases} \quad \text{and} \quad \widetilde{g} = \begin{cases} g & \text{in } \Omega, \\ 0 & \text{in } \mathbb{R}^3\setminus\Omega. \end{cases}$$

Then $\widetilde{f}_n \in H^1(\mathbb{R}^3;\mathbb{C}^4) = \operatorname{dom} A_0$, $\widetilde{f}_n \to \widetilde{f}$ and $A_0\widetilde{f}_n \to \widetilde{g}$ in $L^2(\mathbb{R}^3;\mathbb{C}^4)$, as $n \to \infty$. Since A_0 is self-adjoint and thus closed, it follows $\widetilde{f} \in \operatorname{dom} A_0$ and $A_0\widetilde{f} = \widetilde{g}$. Moreover, as the set

$$\left\{\widetilde{h} \in H^1(\mathbb{R}^3;\mathbb{C}^4) : \widetilde{h} \upharpoonright \Omega \in H^1_0(\Omega;\mathbb{C}^4)\right\}$$

is a closed subspace of $H^1(\mathbb{R}^3;\mathbb{C}^4)$ and the graph norm corresponding to A_0 is equivalent to the norm in $H^1(\mathbb{R}^3;\mathbb{C}^4)$, compare (3.4), we deduce $f = \widetilde{f} \upharpoonright \Omega \in H^1_0(\Omega;\mathbb{C}^4)$ and

$$T^\Omega_{\min} f = (A_0\widetilde{f}) \upharpoonright \Omega = \widetilde{g} \upharpoonright \Omega = g.$$

Hence $T^\Omega_{\min}$ is closed.

Next, we show that $(T^\Omega_{\min})^* = T^\Omega_{\max}$. First, we prove the inclusion $(T^\Omega_{\min})^* \subset T^\Omega_{\max}$. For this let $f \in \operatorname{dom}(T^\Omega_{\min})^*$ and let $g \in C^\infty_0(\Omega;\mathbb{C}^4) \subset \operatorname{dom} T^\Omega_{\min}$ be arbitrary, but fixed. Then it holds

$$\left((T^\Omega_{\min})^* f, g\right)_\Omega = \left(f, T^\Omega_{\min} g\right)_\Omega = \left(f, (-ic\alpha\cdot\nabla + mc^2\beta)g\right)_\Omega,$$

which is equivalent to

$$(f, \alpha\cdot\nabla g)_\Omega = \frac{1}{ic}\left((T^\Omega_{\min})^* f - mc^2\beta f, g\right)_\Omega,$$

that means by definition $\alpha\cdot\nabla f = -\frac{1}{ic}((T^\Omega_{\min})^* f - mc^2\beta f) \in L^2(\Omega;\mathbb{C}^4)$ in the distributional sense. Therefore $f \in \operatorname{dom} T^\Omega_{\max}$ and $T^\Omega_{\max} f = (T^\Omega_{\min})^* f$.

To show $T^\Omega_{\max} \subset (T^\Omega_{\min})^*$, let $f \in \operatorname{dom} T^\Omega_{\max}$ and let $g \in C^\infty_0(\Omega;\mathbb{C}^4)$ be arbitrary, but fixed. Then we have by the definition of the distributional derivative

$$(T_{\max} f, g)_\Omega = \left(f, (-ic\alpha\cdot\nabla + mc^2\beta)g\right)_\Omega = (f, T^\Omega_{\min} g)_\Omega. \tag{3.12}$$

Now, let $g \in \operatorname{dom} T^\Omega_{\min} = H^1_0(\Omega;\mathbb{C}^4)$. Then, there exists a sequence $(g_n) \subset C^\infty_0(\Omega;\mathbb{C}^4)$ such that $g_n \to g$ in $H^1(\Omega;\mathbb{C}^4)$, as $n \to \infty$. Clearly, this implies $T^\Omega_{\min} g_n \to T^\Omega_{\min} g$ in $L^2(\Omega;\mathbb{C}^4)$ for $n \to \infty$. Hence, the continuity of the scalar product implies that (3.12) holds for all $g \in \operatorname{dom} T^\Omega_{\min}$. Therefore $f \in \operatorname{dom}(T^\Omega_{\min})^*$ and $(T^\Omega_{\min})^* f = T^\Omega_{\max} f$, which shows the second inclusion as well.

It remains to prove that $T^\Omega_{\min}$ is simple. Assume that $T^\Omega_{\min} = T_1 \oplus T_2$, there T_j acts in an invariant subspace $\mathcal{H}_j \subset L^2(\Omega;\mathbb{C}^4)$ of $T^\Omega_{\min}$, $j \in \{1,2\}$, and that $T_1 = T_1^*$. We prove that T_1 must be zero. For that, note $(T^\Omega_{\min})^2 = T_1^2 \oplus T_2^2$ and $T_1^2 = (T_1^2)^*$ in $\mathcal{H}_1$ by the spectral theorem. Since T_1^2 is closed, we have $\overline{(T^\Omega_{\min})^2} = T_1^2 \oplus \overline{T_2^2}$. We want to show using (2.4) that $\overline{(T^\Omega_{\min})^2}$ is simple. For that consider the operator

$$A^\Omega f := (-ic\alpha\cdot\nabla + mc^2\beta)^2 f = (-c^2\Delta + m^2c^4)f, \quad \operatorname{dom} A^\Omega = H^2(\Omega;\mathbb{C}^4).$$

Integration by parts shows $A^\Omega \subset \big((T^\Omega_{\min})^2\big)^*$, as it holds for arbitrary $f \in \operatorname{dom} A^\Omega$ and $g \in \operatorname{dom}(T^\Omega_{\min})^2$

$$\begin{aligned}\big(A^\Omega f, g\big)_\Omega &= \big((-ic\alpha\cdot\nabla + mc^2\beta)^2 f, g\big)_\Omega = \big((-ic\alpha\cdot\nabla + mc^2\beta) f, (-ic\alpha\cdot\nabla + mc^2\beta) g\big)_\Omega \\ &= \big(f, (-ic\alpha\cdot\nabla + mc^2\beta)^2 g\big)_\Omega = \big(f, (T^\Omega_{\min})^2 g\big)_\Omega,\end{aligned}$$

as $g, (-ic\alpha\cdot\nabla + mc^2\beta) g \in H^1_0(\Omega;\mathbb{C}^4)$. It is known from [63, Proposition 4.3] (see also [24, Proposition 2.2] for unbounded Ω) that the set

$$\bigcup_{\lambda\in\mathbb{C}\setminus\mathbb{R}} \ker(A^\Omega - \lambda)$$

is dense in $L^2(\Omega;\mathbb{C}^4)$. Hence, also

$$\bigcup_{\lambda\in\mathbb{C}\setminus\mathbb{R}} \ker\Big(\big((T^\Omega_{\min})^2\big)^* - \lambda\Big) = \bigcup_{\lambda\in\mathbb{C}\setminus\mathbb{R}} \ker\Big(\big(\overline{(T^\Omega_{\min})^2}\big)^* - \lambda\Big)$$

is dense in $L^2(\Omega;\mathbb{C}^4)$. This means that $\overline{(T^\Omega_{\min})^2}$ is simple, compare (2.4). From this we obtain $T_1^2 = 0$ and hence also $T_1 = 0$. Thus $T^\Omega_{\min}$ is simple. □

Eventually, we prove that smooth functions are a core of $T^\Omega_{\max}$. The proof of this result follows ideas from [25, Lemma 2.1], see also [55, Proposition 2.12] for a similar result.

Lemma 3.1.3. *Let $\Omega \subset \mathbb{R}^3$ be a C^2-smooth domain with compact boundary and let $T^\Omega_{\max}$ be defined by* (3.10)*. Then $C^\infty(\overline{\Omega};\mathbb{C}^4)$ is dense in* $\operatorname{dom} T^\Omega_{\max}$ *equipped with its graph norm.*

Proof. We verify the claimed result when Ω is the complement of a bounded C^2-domain; the case that Ω is a bounded C^2-domain can be shown in the same way. Assume that $f \in \operatorname{dom} T^\Omega_{\max}$ fulfills

$$\begin{aligned}0 &= (f,g)_\Omega + (T^\Omega_{\max} f, T^\Omega_{\max} g)_\Omega \\ &= (f,g)_\Omega + \big((-ic\alpha\cdot\nabla + mc^2\beta) f, (-ic\alpha\cdot\nabla + mc^2\beta) g\big)_\Omega\end{aligned} \tag{3.13}$$

for all $g \in C^\infty(\overline{\Omega};\mathbb{C}^4)$. As $C_0^\infty(\Omega;\mathbb{C}^4) \subset C^\infty(\overline{\Omega};\mathbb{C}^4)$ we deduce from this that the distribution $(-ic\alpha\cdot\nabla + mc^2\beta)^2 f$ exists in $L^2(\Omega;\mathbb{C}^4)$ and is equal to $-f$.

Next, we show

$$(-ic\alpha\cdot\nabla + mc^2\beta) f \in H^1_0(\Omega;\mathbb{C}^4). \tag{3.14}$$

To see this let $h \in C_0^\infty(\mathbb{R}^3;\mathbb{C}^4)$, choose a cutoff function $\chi \in C_0^\infty(\mathbb{R}^3;\mathbb{C}^4)$ which satisfies

$$\chi(x) = \begin{cases} 1, & x \in B(0,1), \\ 0, & x \in \mathbb{R}^3 \setminus B(0,2), \end{cases}$$

and recall the definition of the free Dirac operator A_0 from (3.3). Define for $n \in \mathbb{N}$ the functions $\chi_n := \chi(\cdot/n)$ and $u_n := (\chi_n A_0^{-1} h) \upharpoonright \Omega$. Then $u_n \in C^\infty(\overline{\Omega};\mathbb{C}^4)$ and $u_n \to (A_0^{-1}h) \upharpoonright \Omega$ in $H^1(\Omega;\mathbb{C}^4)$, as $n \to \infty$. Employing (3.13) we obtain

$$\begin{aligned}\big(A_0^{-1}(-f \oplus 0), h\big)_{\mathbb{R}^3} &= -(f, (A_0^{-1}h) \upharpoonright \Omega)_\Omega = -\lim_{n\to\infty} (f, u_n)_\Omega \\ &= \lim_{n\to\infty} \big((-ic\alpha\cdot\nabla + mc^2\beta)f, (-ic\alpha\cdot\nabla + mc^2\beta)u_n\big)_\Omega \\ &= \big((-ic\alpha\cdot\nabla + mc^2\beta)f, (-ic\alpha\cdot\nabla + mc^2\beta)(A_0^{-1}h) \upharpoonright \Omega\big)_\Omega \\ &= \big((-ic\alpha\cdot\nabla + mc^2\beta)f \oplus 0, h\big)_{\mathbb{R}^3}.\end{aligned}$$

Since this is true for any $h \in C_0^\infty(\mathbb{R}^3;\mathbb{C}^4)$ we deduce

$$(-ic\alpha\cdot\nabla + mc^2\beta)f \oplus 0 = A_0^{-1}(-f \oplus 0) \in \operatorname{dom} A_0 = H^1(\mathbb{R}^3;\mathbb{C}^4).$$

As the trace of $(-ic\alpha\cdot\nabla + mc^2\beta)f \oplus 0$ at $\partial\Omega$ is zero, we get finally (3.14).

By (3.14) there exists a sequence $(h_n) \subset C_0^\infty(\Omega;\mathbb{C}^4)$ with $h_n \to (-ic\alpha\cdot\nabla + mc^2\beta)f$ in $H^1(\Omega;\mathbb{C}^4)$ for $n \to \infty$. Therefore, using the definition of the distributional derivative and $(-ic\alpha\cdot\nabla + mc^2\beta)^2 f = -f$ we conclude

$$\begin{aligned}0 &\leq \big((-ic\alpha\cdot\nabla + mc^2\beta)f, (-ic\alpha\cdot\nabla + mc^2\beta)f\big)_\Omega = \lim_{n\to\infty} \big(h_n, (-ic\alpha\cdot\nabla + mc^2\beta)f\big)_\Omega \\ &= \lim_{n\to\infty} \big((-ic\alpha\cdot\nabla + mc^2\beta)h_n, f\big)_\Omega = \big((-ic\alpha\cdot\nabla + mc^2\beta)^2 f, f\big)_\Omega \\ &= -(f,f)_\Omega \leq 0,\end{aligned}$$

that means $f = 0$. Therefore $C^\infty(\overline{\Omega};\mathbb{C}^4)$ is dense in $\operatorname{dom} T_{\max}^\Omega$. □

Finally, we construct in the case that $\Omega \subset \mathbb{R}^3$ is the complement of a bounded C^2-domain for $\lambda \in (-\infty, -mc^2] \cup [mc^2, \infty)$ a sequence $(\psi_n^\lambda) \subset \operatorname{dom} T_{\min}^\Omega$ which satisfies all properties of a singular Weyl-sequence. This will allow us to show that $(-\infty, -mc^2] \cup [mc^2, \infty)$ belongs to the essential spectrum of Dirac operators with singular interactions and of self-adjoint Dirac operators in Ω with suitable boundary conditions. Let $R > 0$ such that $\mathbb{R}^3 \setminus B(0,R) \subset \Omega$. Moreover, choose for $\lambda \in (-\infty, -mc^2] \cup [mc^2, \infty)$ a vector $\zeta \in \mathbb{C}^4$ such that $\left(\sqrt{\lambda^2 - m^2c^4}\alpha_1 + m\beta + \lambda I_4\right)\zeta \neq 0$, a cutoff-function $\chi \in C_0^\infty(\mathbb{R})$ with $\chi(r) = 1$ for $|r| < \frac{1}{2}$ and $\chi(r) = 0$ for $r > 1$ and set $x_n := (R + n^2, 0, 0)^\top$, $n \in \mathbb{N}$. Then we define the function ψ_n^λ by

$$\psi_n^\lambda(x) := \frac{1}{n^{3/2}} \chi\left(\frac{1}{n}|x - x_n|\right) e^{i\sqrt{\lambda^2/c^2 - m^2c^2}\, x\cdot e_1} \left(\sqrt{\lambda^2 - m^2c^4}\alpha_1 + mc^2\beta + \lambda I_4\right)\zeta. \quad (3.15)$$

Some useful properties of ψ_n^λ are stated in the following lemma:

Lemma 3.1.4. *Let $\Omega \subset \mathbb{R}^3$ be the complement of a bounded C^2-domain, let $T^{\Omega}_{\min}$ be given by* (3.11) *and let $\lambda \in (-\infty, -mc^2] \cup [mc^2, \infty)$. Then the functions ψ_n^λ defined by* (3.15) *have the following properties:*

(a) $\psi_n^\lambda \in \operatorname{dom} T^{\Omega}_{\min}$.

(b) $\|\psi_n^\lambda\|_\Omega = $ *const.* > 0.

(c) ψ_n^λ *converges weakly to zero, as $n \to \infty$.*

(d) $(T^{\Omega}_{\min} - \lambda)\psi_n^\lambda \to 0$ *as $n \to \infty$.*

Proof. First, by definition ψ_n^λ is smooth and $\operatorname{supp} \psi_n^\lambda \cap \partial\Omega = \emptyset$ and thus $\psi_n^\lambda \in \operatorname{dom} T^{\Omega}_{\min}$, that means item (a) is true. Moreover, it holds

$$\|\psi_n^\lambda\| = \left| \left(\sqrt{\lambda^2 - m^2c^4}\,\alpha_1 + mc^2\beta + \lambda \right) \zeta \right| \cdot \left(\int_{B(0,1)} |\chi(|y|)|^2 \mathrm{d}y \right)^{1/2} = \text{const.},$$

which is assertion (b). Furthermore, since the supports of the ψ_n^λ are pairwise disjoint, the sequence (ψ_n^λ) converges weakly to zero as $n \to \infty$. This is statement (c). Eventually, to verify (d) a straightforward computation shows

$$\begin{aligned}
(T^{\Omega}_{\min} - \lambda)\psi_n^\lambda(x) &= (-ic\alpha \cdot \nabla + mc^2\beta - \lambda)\psi_n^\lambda(x) \\
= -\frac{i}{n^{5/2}} e^{i\sqrt{\lambda^2 - m^2}x\cdot e_1} &\chi'\left(\frac{1}{n}|x - x_n|\right) \alpha \cdot \frac{x - x_n}{|x - x_n|} \left(\sqrt{\lambda^2/c^2 - m^2c^2}\,\alpha_1 + mc^2\beta + \lambda I_4 \right) \zeta \\
&+ \frac{1}{n^{3/2}} \chi\left(\frac{1}{n}|x - x_n|\right) e^{i\sqrt{\lambda^2/c^2 - m^2c^2}x\cdot e_1} \\
&\quad \cdot \left(\sqrt{\lambda^2 - m^2c^4}\,\alpha_1 + mc^2\beta - \lambda I_4 \right) \left(\sqrt{\lambda^2 - m^2c^4}\,\alpha_1 + mc^2\beta + \lambda I_4 \right) \zeta.
\end{aligned}$$

The anti-commutation relation (1.2) implies

$$\left(\sqrt{\lambda^2 - m^2c^4}\,\alpha_1 + mc^2\beta - \lambda I_4 \right) \left(\sqrt{\lambda^2 - m^2c^4}\,\alpha_1 + mc^2\beta + \lambda I_4 \right) = 0.$$

Hence, we have

$$\|(T^{\Omega}_{\min} - \lambda)\psi_n^\lambda\|_\Omega \leq \frac{C}{n} \left(\int_{B(0,1)} |\chi'(|y|)|^2 \mathrm{d}y \right)^{1/2}$$

and therefore, $(T^{\Omega}_{\min} - \lambda)\psi_n^\lambda \to 0$ as $n \to \infty$. □

3.2 Integral operators – Part I: Basic properties

In this section we introduce several families of integral operators associated to the Green's function G_λ for the resolvent of A_0 that will play an important role in the analysis of Dirac operators with singular potentials and of Dirac operators on bounded domains. In this section, we will introduce all operators as bounded operators in the corresponding L^2-spaces. Later, in Chapter 4, it will turn out that these operators are the γ-field and the Weyl function associated to a special quasi boundary triple. With this knowledge we will prove in Section 4.1.3 additional properties of these integral operators using the abstract theory of quasi boundary triples.

Throughout this section, let $\Sigma \subset \mathbb{R}^3$ be a compact and closed C^2-smooth surface that splits $\mathbb{R}^3$ into a bounded part Ω_+ and an unbounded part Ω_-. The unit normal vector field at Σ pointing inside Ω_- is denoted by ν. Recall for $\lambda \in \rho(A_0) = \mathbb{C} \setminus \big((-\infty, -mc^2] \cup [mc^2, \infty)\big)$ the definition of the function G_λ from (3.6). Then we define the operators $\Phi_\lambda : L^2(\Sigma;\mathbb{C}^4) \to L^2(\mathbb{R}^3;\mathbb{C}^4)$,

$$\Phi_\lambda \varphi(x) := \int_\Sigma G_\lambda(x-y)\varphi(y)\mathrm{d}\sigma(y), \quad x \in \mathbb{R}^3, \varphi \in L^2(\Sigma;\mathbb{C}^4), \tag{3.16}$$

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

$$\mathcal{C}_\lambda \varphi(x) := \lim_{\varepsilon \searrow 0} \int_{\Sigma \setminus B(x,\varepsilon)} G_\lambda(x-y)\varphi(y)\mathrm{d}\sigma(y), \quad x \in \Sigma, \varphi \in L^2(\Sigma;\mathbb{C}^4). \tag{3.17}$$

The basic properties of Φ_λ and $\mathcal{C}_\lambda$ are summarized in the following proposition. The proof of this result follows ideas from [5, Lemma 2.1 and Lemma 3.3].

Proposition 3.2.1. *Let for $\lambda \in \rho(A_0)$ the operators Φ_λ and $\mathcal{C}_\lambda$ be defined as in* (3.16) *and* (3.17)*, respectively. Then, the following assertions are true:*

(i) *The operator Φ_λ is bounded and everywhere defined. Its adjoint is explicitly given by $\Phi_\lambda^* : L^2(\mathbb{R}^3;\mathbb{C}^4) \to L^2(\Sigma;\mathbb{C}^4)$,*

$$\Phi_\lambda^* f(x) = \int_{\mathbb{R}^3} G_{\overline{\lambda}}(x-y) f(y)\mathrm{d}y, \quad x \in \Sigma, f \in L^2(\mathbb{R}^3;\mathbb{C}^4). \tag{3.18}$$

(ii) *The operator C_λ is bounded and everywhere defined.*

(iii) *Let $\varphi \in L^2(\Sigma;\mathbb{C}^4)$ and set $f := \Phi_\lambda \varphi$. Then, the non-tangential limits*

$$\psi_\pm(x) := \lim_{\Omega_\pm \ni y \to x \in \Sigma} f(y)$$

exist and are given by

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

(iv) $-4c^2(\mathcal{C}_\lambda \alpha\cdot\nu)^2 = -4c^2(\alpha\cdot\nu\mathcal{C}_\lambda)^2 = I_4$ *for all* $\lambda \in (-mc^2, mc^2)$.

Before we prove the preceding proposition, we note that, using the same notations as there, assertion (iii) and (1.2) imply

$$\frac{1}{2}\big(\psi_+ + \psi_-\big) = \mathcal{C}_\lambda \varphi \quad \text{and} \quad ic\alpha\cdot\nu\big(\psi_+ - \psi_-\big) = \varphi. \tag{3.19}$$

Proof of Proposition 3.2.1. (i) First, we note that there exist constants $\kappa, R > 0$ such that for $x \in \mathbb{R}^3 \setminus \{0\}$

$$|G_\lambda(x)| \le \kappa \begin{cases} |x|^{-2}, & |x| \le R, \\ e^{-\operatorname{Im}\sqrt{\lambda^2/c^2-(mc)^2}|x|}, & |x| > R. \end{cases}$$

Hence Φ_λ is bounded by Proposition 2.4.4. Next, we compute the adjoint operator $\Phi_\lambda^* : L^2(\mathbb{R}^3;\mathbb{C}^4) \to L^2(\Sigma;\mathbb{C}^4)$. Let $\varphi \in L^2(\Sigma;\mathbb{C}^4)$ and $f \in L^2(\mathbb{R}^3;\mathbb{C}^4)$ be fixed. Then, by using $\overline{G_{\overline{\lambda}}(x-y)} = G_\lambda(y-x)$ and Fubini's theorem we see

$$\begin{aligned}(\varphi, \Phi_\lambda^* f)_\Sigma = (\Phi_\lambda \varphi, f)_{\mathbb{R}^3} &= \int_{\mathbb{R}^3}\int_\Sigma G_\lambda(x-y)\varphi(y)\mathrm{d}\sigma(y)\overline{f(x)}\mathrm{d}x \\ &= \int_\Sigma \varphi(y) \int_{\mathbb{R}^3} \overline{G_{\overline{\lambda}}(y-x) f(x)}\mathrm{d}x\mathrm{d}\sigma(y).\end{aligned}$$

Since this is true for all $\varphi \in L^2(\Sigma;\mathbb{C}^4)$ the claimed representation of Φ_λ^* follows.

(ii) To show the boundedness of $\mathcal{C}_\lambda$ consider the splitting

$$\mathcal{C}_\lambda = \mathcal{T}_1^\lambda + \mathcal{T}_2^\lambda + \mathcal{T}_3^\lambda \tag{3.20}$$

with $\mathcal{T}_j^\lambda : L^2(\Sigma;\mathbb{C}^4) \to L^2(\Sigma;\mathbb{C}^4)$, $j \in \{1,2,3\}$, acting as

$$\mathcal{T}_j^\lambda \varphi(x) = \lim_{\varepsilon \searrow 0} \int_{\Sigma\setminus B(x,\varepsilon)} t_j^\lambda(x-y)\varphi(y)\mathrm{d}\sigma(y), \quad x \in \Sigma, \varphi \in L^2(\Sigma;\mathbb{C}^4), \tag{3.21}$$

and

$$t_1^\lambda(x) = \left(\frac{\lambda}{c^2} I_4 + m\beta + \sqrt{\frac{\lambda^2}{c^2} - (mc)^2}\,\frac{\alpha\cdot x}{c|x|}\right) \cdot \frac{e^{i\sqrt{\lambda^2/c^2-(mc)^2}|x|}}{4\pi|x|},$$

$$t_2^\lambda(x) = \frac{i(\alpha\cdot x)}{4\pi|x|^3}\big(e^{i\sqrt{\lambda^2/c^2-(mc)^2}|x|} - 1\big), \qquad t_3^\lambda(x) = \frac{i(\alpha\cdot x)}{4\pi|x|^3}.$$

First, there exists $\kappa_1 > 0$ such that $|t_1^\lambda(x)| \le \kappa_1\big(1 + |x|^{-1}\big)$ for all $x \in \mathbb{R}^3 \setminus \{0\}$. Hence $\mathcal{T}_1^\lambda$ is bounded by Proposition 2.4.5. Furthermore, since

$$\begin{aligned}e^{i\sqrt{\lambda^2/c^2-(mc)^2}|x|} - 1 &= \int_0^1 \frac{\mathrm{d}}{\mathrm{d}t} e^{it\sqrt{\lambda^2/c^2-(mc)^2}|x|}\mathrm{d}t \\ &= i\sqrt{\frac{\lambda^2}{c^2} - (mc)^2}|x| \int_0^1 e^{it\sqrt{\lambda^2/c^2-(mc)^2}|x|}\mathrm{d}t,\end{aligned}$$

there is a κ_2 such that $|t_2^\lambda(x)| \leq \kappa_2\big(1+|x|^{-1}\big)$ for all $x \in \mathbb{R}^3 \setminus \{0\}$. Proposition 2.4.5 shows that also $\mathcal{T}_2^\lambda$ is bounded. Finally, it follows easily from Proposition 2.4.6 that also $\mathcal{T}_3^\lambda$ is bounded. Therefore (3.20) shows that $\mathcal{C}_\lambda$ is bounded.

The proof of assertion (iii) can be found in [5, Lemma 3.3] for $\lambda = 0$. The general statement can be shown in exactly the same way. Item (iv) is shown in [6, Lemma 2.2]. □

If we have a closer look onto the proof of the boundedness of $\mathcal{C}_\lambda$, then it turns out that this family of operators is uniformly bounded for $\lambda \in (-mc^2, mc^2)$ in the operator norm. The proof of this result follows the one of [6, Lemma 3.2].

Proposition 3.2.2. *Let for $\lambda \in \rho(A_0)$ the operators $\mathcal{C}_\lambda$ be defined as in* (3.17). *Then the operators $\mathcal{C}_\lambda$ are uniformly bounded in $(-mc^2, mc^2)$, that means there exists a constant $K > 0$ such that*

$$\sup_{\lambda \in (-mc^2, mc^2)} \|\mathcal{C}_\lambda\| \leq K.$$

Proof. As in the proof of Proposition 3.2.1 (ii) we write for $\lambda \in (-mc^2, mc^2)$

$$\mathcal{C}_\lambda = \mathcal{T}_1^\lambda + \mathcal{T}_2^\lambda + \mathcal{T}_3^\lambda,$$

where $\mathcal{T}_j^\lambda$, $j \in \{1,2,3\}$, is given by (3.21). To show the claim it suffices to verify that $\mathcal{T}_1^\lambda$, $\mathcal{T}_2^\lambda$ and $\mathcal{T}_3^\lambda$ are uniformly bounded by a constant independent of λ. First, there exists a constant $\kappa_1 > 0$ such that

$$|t_1^\lambda(x)| \leq 2\left[\frac{|\lambda|}{c^2} + m + \sqrt{(mc)^2 - \frac{\lambda}{c^2}}\right]\frac{\kappa_1}{|x|}, \qquad x \in \mathbb{R}^3 \setminus \{0\},$$

and since $\lambda \in (-mc^2, mc^2)$ is uniformly bounded, we find

$$|t_1^\lambda(x)| \leq \frac{\kappa_2}{|x|}, \qquad x \in \mathbb{R}^3 \setminus \{0\},$$

with some κ_2 independent of λ. Therefore, Proposition 2.4.5 implies that $\mathcal{T}_1^\lambda$ is uniformly bounded with respect to λ.

Next, we note that

$$\begin{aligned} e^{-\sqrt{(mc)^2-\lambda^2/c^2}|x|} - 1 &= \int_0^1 \frac{\mathrm{d}}{\mathrm{d}t} e^{-t\sqrt{(mc)^2-\lambda^2/c^2}|x|}\mathrm{d}t \\ &= -\sqrt{(mc)^2 - \frac{\lambda^2}{c^2}}|x| \int_0^1 e^{-t\sqrt{(mc)^2-\lambda^2/c^2}|x|}\mathrm{d}t. \end{aligned} \tag{3.22}$$

Thus, there exists a constant κ_3 independent of λ such that

$$|t_2^\lambda(x)| \leq \frac{|\alpha \cdot x|}{4\pi c|x|^2}\sqrt{(mc)^2 - \frac{\lambda^2}{c^2}} \leq \frac{\kappa_3}{|x|}, \qquad x \in \mathbb{R}^3 \setminus \{0\}. \tag{3.23}$$

Hence, it follows from Proposition 2.4.5 that also $\mathcal{T}_2^\lambda$ is bounded by a constant independent of λ.

Eventually, we note that $\mathcal{T}_3^\lambda$ is actually independent of λ and bounded by Proposition 2.4.6. This finishes the proof of this proposition. □

In the following proposition we discuss the commutator of the singular integral operator $\mathcal{C}_\lambda$ and a Lipschitz continuous function and show that this operator increases the smoothness. This has important consequences for the analysis of self-adjoint Dirac operators on domains and with singular interactions and it will be used in the proofs of many of the main results of this thesis. The proof of the following proposition is based on a classical result of Calderón [32], but we trace our commutator back to another one treated in [55] and use a result shown there.

Proposition 3.2.3. *Let for $\lambda \in \rho(A_0) = \mathbb{C} \setminus \big((-\infty, -mc^2] \cup [mc^2, \infty)\big)$ the operator $\mathcal{C}_\lambda$ be defined by* (3.17) *and let $\tau : \Sigma \to \mathbb{R}$ be Lipschitz continuous. Then for any $s \in [0,1]$ the commutator of $\mathcal{C}_\lambda$ and τ gives rise to a bounded operator*

$$\mathcal{C}_\lambda \tau - \tau \mathcal{C}_\lambda : H^{s-1}(\Sigma;\mathbb{C}^4) \to H^s(\Sigma;\mathbb{C}^4).$$

Proof. We are going to show the claim for $s = 1$, the statement for $s = 0$ follows then by a duality argument. Finally, for $s \in (0,1)$ the claimed assertion can be shown by interpolation.

We split $\mathcal{C}_\lambda$ as

$$\mathcal{C}_\lambda = \mathcal{T}_1^\lambda + \mathcal{T}_2^\lambda,$$

where $\mathcal{T}_j^\lambda : L^2(\Sigma;\mathbb{C}^4) \to L^2(\Sigma;\mathbb{C}^4)$, $j \in \{1,2\}$, is given by

$$\mathcal{T}_j^\lambda \varphi(x) := \lim_{\varepsilon \searrow 0} \int_{\Sigma \setminus B(x,\varepsilon)} t_j^\lambda(x-y)\varphi(y)\,\mathrm{d}\sigma(y), \quad x \in \Sigma, \varphi \in L^2(\Sigma;\mathbb{C}^4),$$

with

$$\begin{aligned} t_1^\lambda(x) &:= \left[\frac{\lambda}{c^2} I_4 + m\beta + \sqrt{\frac{\lambda}{c^2} - (mc)^2}\,\frac{\alpha \cdot x}{c|x|}\right] \frac{e^{i\sqrt{\lambda^2/c^2-(mc)^2}|x|}}{4\pi|x|} \\ &\qquad + \frac{i(\alpha \cdot x)}{4\pi c|x|^3}\left(e^{i\sqrt{\lambda^2/c^2-(mc)^2}|x|} - 1\right), \\ t_2^\lambda(x) &:= \frac{i(\alpha \cdot x)}{4\pi c|x|^3}. \end{aligned}$$

We show that the commutator of τ with both operators $\mathcal{T}_1^\lambda$ and $\mathcal{T}_2^\lambda$, respectively, is bounded from $L^2(\Sigma;\mathbb{C}^4)$ to $H^1(\Sigma;\mathbb{C}^4)$.

First, we show that $\mathcal{K} := \mathcal{T}_1^\lambda \tau - \tau\mathcal{T}_1^\lambda : L^2(\Sigma;\mathbb{C}^4) \to H^1(\Sigma;\mathbb{C}^4)$ is bounded. By the closed graph theorem it is sufficient to show that $\operatorname{ran}\mathcal{K} \subset H^1(\Sigma;\mathbb{C}^4)$. Let $\varphi \in L^2(\Sigma;\mathbb{C}^4)$ be fixed. Let $\{\Lambda_j, U_j, W_j\}_{j=1}^l$ be a parametrization of Σ, let $\{\chi_j\}_{j=1}^l$ be a partition of unity subordinate to $\{W_j\}$ and define the functions $\varphi_j(v) := \varphi(\Lambda_j(v))$, $v \in U_j$, and

$$k_{ij}(u,v) := \chi_i(\Lambda_i(u))\chi_j(\Lambda_j(v))t_\lambda^1(\Lambda_i(u) - \Lambda_j(v))(\tau(\Lambda_j(v)) - \tau(\Lambda_i(u))), \quad u \in U_i, v \in U_j.$$

Moreover, we introduce for indices $i,j \in \{1,\dots,l\}$ the corresponding operators $\mathcal{K}_{ij}$: $L^2(U_j, \sqrt{\det G_j}\mathrm{d}v) \to L^2(U_i, \sqrt{\det G_i}\mathrm{d}u)$ acting as

$$\mathcal{K}_{ij}f(u) := \int_{U_j} k_{ij}(u,v)f(v)\sqrt{\det G_j(v)}\mathrm{d}v, \quad u \in U_i, f \in L^2(U_j, \sqrt{\det G_j}\mathrm{d}v).$$

Let $x \in \Sigma$ and choose for $u_i \in U_i$ with $x = \Lambda_i(u_i)$, if $x \in V_i$. Then in view of (2.28) it holds

$$\begin{aligned}\mathcal{K}\varphi(x) &= \sum_{j=1}^l \int_{U_j} t_\lambda^1(x - \Lambda_j(v))\chi_j(\Lambda_j(v))(\tau(\Lambda_j(v)) - \tau(x))\varphi(\Lambda_j(v))\sqrt{\det G_j(v)}\mathrm{d}v \\ &= \sum_{i=1}^l \sum_{j=1}^l \int_{U_j} k_{ij}(u_i,v)\varphi_j(v)\sqrt{\det G_j(v)}\mathrm{d}v = \sum_{i,j=1}^l \mathcal{K}_{ij}\varphi_j(u_i).\end{aligned}$$

Thus, it suffices to prove $\mathcal{K}_{ij}\varphi_j \in H^1(U_i)$. Using that τ is Lipschitz continuous and performing a similar calculation as in (3.22) and (3.23) we see that there exists a constant κ_1 such that for any $x,y \in \Sigma$

$$\left|t_\lambda^1(x-y)(\tau(y) - \tau(x))\right| \le \kappa_1,$$

which yields that k_{ij} is also bounded. Moreover, k_{ij} is (weakly) differentiable in u almost everywhere and it holds by the product rule

$$|\partial_{u_k} k_{ij}(u,v)| \le \frac{\kappa_2}{|u-v|}$$

for a constant κ_2. Hence, by Proposition 2.4.3 the operator $\mathcal{K}_{ij}^k : L^2(U_j, \sqrt{\det G_j}\mathrm{d}v) \to L^2(U_i, \sqrt{\det G_i}\mathrm{d}u)$ acting as

$$\mathcal{K}_{ij}^k f(u) := \int_{U_j} \partial_{u_k}(k_{ij}(u,v))f(v)\sqrt{\det G_j(v)}\mathrm{d}v, \quad u \in U_i, f \in L^2(U_j, \sqrt{\det G_j}\mathrm{d}v),$$

is bounded. Eventually, one can show in the same way as in the proof of Proposition 3.1.1 that for $f \in L^2(U_j, \sqrt{\det G_j}\mathrm{d}v)$ the function $\mathcal{K}_{ij}f$ is weakly differentiable and that its weak derivative is

$$\partial_{u_k}\mathcal{K}_{ij}f = \mathcal{K}_{ij}^k f,$$

compare (3.9). Hence, the claimed mapping properties of the commutator of $\mathcal{T}_1^\lambda$ and τ hold.

Finally, the fact that the commutator $\mathcal{T}_2^\lambda \tau - \tau \mathcal{T}_2^\lambda$ is bounded follows from [55, Proposition 2.8]. In fact, in the proof of this result it is shown that a very similar operator, which is denoted there as $K_{2,0}$ (see also the definition of the operators with kernels $c_{q,k}$ in [55]) and which is an integral operator with the same kernel as $\mathcal{T}_2^\lambda \tau - \tau \mathcal{T}_2^\lambda$ up to the multiplication with a constant matrix, is bounded as an operator from $L^2(\Sigma;\mathbb{C}^4)$ mapping to $H^1(\Sigma;\mathbb{C}^4)$. In [55] only the special case $\tau = \nu$ was considered, but the argument using a classical result from [32] applies actually for any τ which has weak derivatives in $L^\infty(\Sigma)$, in particular for all Lipschitz continuous τ. □

Finally, we provide some useful anti-commutator properties of $\mathcal{C}_\lambda$ and the Dirac matrices. These facts are also some of the main ingredients to prove later the self-adjointness of Dirac operators with singular interactions and of Dirac operators on domains.

Proposition 3.2.4. *Let for* $\lambda \in \rho(A_0) = \mathbb{C} \setminus \big((-\infty, -mc^2] \cup [mc^2, \infty)\big)$ *the operator* $\mathcal{C}_\lambda$ *be defined by* (3.17). *Then the following statements hold:*

(i) *The anti-commutator* $\mathcal{A} := \mathcal{C}_0(\alpha \cdot \nu) + (\alpha \cdot \nu)\mathcal{C}_0$ *can be extended to a bounded operator*
$$\widetilde{\mathcal{A}} : H^{-1/2}(\Sigma;\mathbb{C}^4) \to H^{1/2}(\Sigma;\mathbb{C}^4).$$

(ii) *The anti-commutator* $\mathcal{B}_\lambda := \mathcal{C}_\lambda \beta + \beta \mathcal{C}_\lambda$ *can be extended to a bounded operator*
$$\widetilde{\mathcal{B}}_\lambda : H^{-1/2}(\Sigma;\mathbb{C}^4) \to H^{1/2}(\Sigma;\mathbb{C}^4).$$

Proof. The proof of item (i) can be found in [55, Proposition 2.8]. It remains to show statement (ii). Using the anti-commutation relation (1.2) we see that $\mathcal{B}_\lambda$ is an integral operator with kernel

$$b^\lambda(x-y) := 2\left(\frac{\lambda}{c^2}\beta + mI_4\right) \frac{e^{i\sqrt{\lambda^2/c^2-(mc)^2}|x-y|}}{4\pi|x-y|}$$

and thus, $\mathcal{B}_\lambda = 2\big(\frac{\lambda}{c^2}\beta + mI_4\big)\mathrm{SL}_{\lambda^2/c^2-(mc)^2}$, where SL_μ denotes the single layer boundary integral operator for $-\Delta - \mu$. It is well known that $\mathrm{SL}_{\lambda^2/c^2-(mc)^2}$ gives rise to a bounded operator from $H^{-1/2}(\Sigma;\mathbb{C}^4)$ to $H^{1/2}(\Sigma;\mathbb{C}^4)$, see for instance [53, Theorem 6.11]. This implies the statement of item (ii). □

4 DIRAC OPERATORS WITH SINGULAR INTERACTIONS

In this chapter we investigate Dirac operators with singular interactions supported on a closed and compact surface $\Sigma \subset \mathbb{R}^3$. First, in Section 4.1.1 we introduce a quasi boundary triple $\{L^2(\Sigma;\mathbb{C}^4),\Gamma_0^\Sigma,\Gamma_1^\Sigma\}$ which is suitable to define and study these Dirac operators with singular interactions. It will turn out that the γ-field and the Weyl function associated to this quasi boundary triple coincide with the integral operators Φ_λ and $\mathcal{C}_\lambda$ introduced in Section 3.2. Moreover, we will see that the triple $\{L^2(\Sigma;\mathbb{C}^4),\Gamma_0^\Sigma,\Gamma_1^\Sigma\}$ satisfies the assumptions from Theorem 2.2.13. Hence, we can transform this quasi boundary triple to an ordinary boundary triple $\{L^2(\Sigma;\mathbb{C}^4),\Upsilon_0^\Sigma,\Upsilon_1^\Sigma\}$; cf. Theorem 4.1.5. Eventually, with the aid of the ordinary boundary triple and the abstract results from Section 2.2 we will derive more involved results on the integral operators Φ_λ and $\mathcal{C}_\lambda$ including a detailed analysis of their mapping properties in Section 4.1.3. These results will play then a crucial role in the study of Dirac operators with singular interactions.

In Section 4.2 we introduce with the help of the quasi boundary triple $\{L^2(\Sigma;\mathbb{C}^4),\Gamma_0^\Sigma,\Gamma_1^\Sigma\}$ Dirac operators with singular interactions. In the case of non-critical interaction strengths we will prove self-adjointness of the operators and provide the basic spectral properties of them.

In contrast to the non-critical interaction strengths it will turn out in Section 4.3 that for critical interaction strengths Dirac operators with singular interactions introduced in Section 4.2 with the quasi boundary triple $\{L^2(\Sigma;\mathbb{C}^4),\Gamma_0^\Sigma,\Gamma_1^\Sigma\}$ are not self-adjoint. But for constant η_e and η_s with $\eta_\mathrm{e}^2 - \eta_\mathrm{s}^2 = 4c^2$ we will be able to prove essential self-adjointness and with the help of the ordinary boundary triple $\{L^2(\Sigma;\mathbb{C}^4),\Upsilon_0^\Sigma,\Upsilon_1^\Sigma\}$ we can compute the self-adjoint realization in this case as well. Furthermore, we will be able to state some of the basic spectral properties also in the case of critical interaction strength.

Finally, in the situation of purely electrostatic and Lorentz scalar shell interactions we investigate the nonrelativistic limit. It will turn out that these Hamiltonians are the relativistic counterparts of Schrödinger operators with δ-potentials. In particular, this yields a justification for the usage of Dirac operators with singular interactions as idealized models for Dirac operators with squeezed potentials.

The results in this chapter are generalizations of [11,14] and the presentation in this section follows closely these papers.

4.1 Boundary triples for Dirac operators with singular interactions

In this section we introduce first a quasi boundary triple which allows us to introduce Dirac operators with singular interactions in a natural way via jump conditions at the surface Σ. Then, in Section 4.1.2 we will transform this quasi boundary triple with the methods described in Section 2.2 to an ordinary boundary triple, which enables us then to prove self-adjointness also in the case of critical interaction strengths.

4.1.1 A quasi boundary triple for Dirac operators with δ-shell interactions

Throughout this chapter let Ω_+ always be a bounded domain in $\mathbb{R}^3$ with C^2-smooth boundary $\Sigma := \partial\Omega_+$ and set $\Omega_- := \mathbb{R}^3 \setminus \overline{\Omega_+}$. We denote the normal vector field at Σ pointing outwards Ω_+ by ν. We will often make use of the orthogonal decomposition $L^2(\mathbb{R}^3;\mathbb{C}^4) = L^2(\Omega_+;\mathbb{C}^4) \oplus L^2(\Omega_-;\mathbb{C}^4)$ and we write for $f \in L^2(\mathbb{R}^3;\mathbb{C}^4)$, in this sense, $f = f_+ \oplus f_-$ with $f_\pm := f \upharpoonright \Omega_\pm$.

First, we define the operator T^Σ in $L^2(\mathbb{R}^3;\mathbb{C}^4)$ by

$$\begin{aligned} T^\Sigma f &:= (-ic\alpha\cdot\nabla + mc^2\beta)f_+ \oplus (-ic\alpha\cdot\nabla + mc^2\beta)f_-, \\ \operatorname{dom} T^\Sigma &:= H^1(\Omega_+;\mathbb{C}^4) \oplus H^1(\Omega_-;\mathbb{C}^4), \end{aligned} \tag{4.1}$$

and the mappings $\Gamma_0^\Sigma, \Gamma_1^\Sigma : \operatorname{dom} T^\Sigma \to L^2(\Sigma;\mathbb{C}^4)$ acting as

$$\Gamma_0^\Sigma f := ic(\alpha\cdot\nu)(f_+|_\Sigma - f_-|_\Sigma) \quad \text{and} \quad \Gamma_1^\Sigma f := \frac{1}{2}(f_+|_\Sigma + f_-|_\Sigma), \quad f \in \operatorname{dom} T^\Sigma. \tag{4.2}$$

Note that $\operatorname{ran}\Gamma_0^\Sigma, \operatorname{ran}\Gamma_1^\Sigma \subset H^{1/2}(\Sigma;\mathbb{C}^4)$, as $\operatorname{dom} T^\Sigma = H^1(\Omega_+;\mathbb{C}^4) \oplus H^1(\Omega_-;\mathbb{C}^4)$ and Σ is C^2-smooth, compare Proposition 2.3.3 and Lemma 2.5.1.

In the following theorem we show that $\{L^2(\Sigma;\mathbb{C}^4), \Gamma_0^\Sigma, \Gamma_1^\Sigma\}$ is a quasi boundary triple and that $\overline{T^\Sigma}$ coincides with the maximal Dirac operator $T_{\max}^{\Omega_+} \oplus T_{\max}^{\Omega_-}$ from (3.10).

Theorem 4.1.1. *Let A_0 be the free Dirac operator from* (3.3)*, let $T^\Sigma, \Gamma_0^\Sigma$ and Γ_1^Σ be given by* (4.1) *and* (4.2)*, respectively, and define the operator S^Σ acting in $L^2(\mathbb{R}^3;\mathbb{C}^4)$ by*

$$S^\Sigma := A_0 \upharpoonright H_0^1(\mathbb{R}^3 \setminus \Sigma;\mathbb{C}^4). \tag{4.3}$$

Then S^Σ is closed and symmetric, $(S^\Sigma)^* = \overline{T^\Sigma} = T_{\max}^{\Omega_+} \oplus T_{\max}^{\Omega_-}$ and $\{L^2(\Sigma;\mathbb{C}^4), \Gamma_0^\Sigma, \Gamma_1^\Sigma\}$ is a quasi boundary triple for $(S^\Sigma)^*$. Moreover,

$$\operatorname{ran}(\Gamma_0^\Sigma, \Gamma_1^\Sigma) = H^{1/2}(\Sigma;\mathbb{C}^4) \times H^{1/2}(\Sigma;\mathbb{C}^4) \tag{4.4}$$

and $T^\Sigma \upharpoonright \ker\Gamma_0^\Sigma$ is the free Dirac operator A_0.

Proof. First, we mention that $S^\Sigma = T^{\Omega_+}_{\min} \oplus T^{\Omega_-}_{\min}$, where $T^{\Omega_\pm}_{\min}$ is the minimal Dirac operator given by (3.11). Hence, it is clear by Lemma 3.1.2 that S^Σ is closed and symmetric and that $(S^\Sigma)^* = T^{\Omega_+}_{\max} \oplus T^{\Omega_-}_{\max}$. Moreover, Lemma 3.1.3 implies that T^Σ is dense in $T^{\Omega_+}_{\max} \oplus T^{\Omega_-}_{\max}$, as $C^\infty(\overline{\Omega_+};\mathbb{C}^4) \oplus C^\infty(\overline{\Omega_-};\mathbb{C}^4) \subset H^1(\Omega_+;\mathbb{C}^4) \oplus H^1(\Omega_-;\mathbb{C}^4) = \operatorname{dom} T^\Sigma$.

Let us prove now that the abstract Green's identity is fulfilled. Assume that $f = f_+ \oplus f_-$, $g = g_+ \oplus g_- \in \operatorname{dom} T^\Sigma = H^1(\Omega_+;\mathbb{C}^4) \oplus H^1(\Omega_-;\mathbb{C}^4)$. Then, integration by parts shows

$$\big((-ic\alpha\cdot\nabla + mc^2\beta) f_\pm, g_\pm\big)_{\Omega_\pm} - \big(f_\pm, (-ic\alpha\cdot\nabla + mc^2\beta) g_\pm\big)_{\Omega_\pm} = \mp\big(ic\alpha\cdot\nu f_\pm|_\Sigma, g_\pm|_\Sigma\big)_\Sigma,$$

as ν is pointing outwards Ω_+. By adding the above formula for Ω_+ and Ω_- we obtain

$$(T^\Sigma f, g)_{\mathbb{R}^3} - (f, T^\Sigma g)_{\mathbb{R}^3} = (\Gamma_1^\Sigma f, \Gamma_0^\Sigma g)_\Sigma - (\Gamma_0^\Sigma f, \Gamma_1^\Sigma g)_\Sigma,$$

which is Green's identity.

Next, we verify the range property (4.4). Let $\varphi, \psi \in H^{1/2}(\Sigma;\mathbb{C}^4)$ and choose functions $f_+ \in H^1(\Omega_+;\mathbb{C}^4)$ and $g \in H^1(\mathbb{R}^3;\mathbb{C}^4)$ that satisfy

$$ic\alpha\cdot\nu f_+|_\Sigma = \varphi \quad \text{and} \quad g|_\Sigma = \psi - \frac{1}{2} f_+|_\Sigma,$$

respectively. Then we have $h := (f_+ \oplus 0) + g \in \operatorname{dom} T^\Sigma$ and

$$\Gamma_0^\Sigma h = ic\alpha\cdot\nu\big(f_+|_\Sigma + g_+|_\Sigma - g_-|_\Sigma\big) = \varphi \quad \text{and} \quad \Gamma_1^\Sigma h = \frac{1}{2} f_+|_\Sigma + g|_\Sigma = \psi.$$

Therefore (4.4) is shown and, in particular, $\operatorname{ran}(\Gamma_0^\Sigma, \Gamma_1^\Sigma)$ is dense in $L^2(\Sigma;\mathbb{C}^4) \times L^2(\Sigma;\mathbb{C}^4)$.

Finally $\ker \Gamma_0^\Sigma = H^1(\mathbb{R}^3;\mathbb{C}^4)$. Hence $T^\Sigma \upharpoonright \ker \Gamma_0^\Sigma$ coincides with the self-adjoint free Dirac operator A_0. Therefore $\{L^2(\Sigma;\mathbb{C}^4), \Gamma_0^\Sigma, \Gamma_1^\Sigma\}$ is a quasi boundary triple for $(S^\Sigma)^*$ and all claims have been shown. □

Next, we compute the γ-field and the Weyl function associated to the quasi boundary triple in Theorem 4.1.1. It turns out that these operators coincide with restrictions of the integral operators Φ_λ and $\mathcal{C}_\lambda$ defined in Section 3.2.

Proposition 4.1.2. *Let $\{L^2(\Sigma;\mathbb{C}^4), \Gamma_0^\Sigma, \Gamma_1^\Sigma\}$ be given as in Theorem 4.1.1, let $\lambda \in \rho(A_0) = \mathbb{C} \setminus \big((-\infty, -mc^2] \cup [mc^2, \infty)\big)$, and let Φ_λ and $\mathcal{C}_\lambda$ be defined by* (3.16) *and* (3.17)*, respectively. Then the following holds:*

(i) *The value of the γ-field $\gamma^\Sigma(\lambda) : \operatorname{dom} \gamma^\Sigma(\lambda) \subset L^2(\Sigma;\mathbb{C}^4) \to L^2(\mathbb{R}^3;\mathbb{C}^4)$ is defined on* $\operatorname{dom} \gamma^\Sigma(\lambda) = H^{1/2}(\Sigma;\mathbb{C}^4)$ *and is explicitly given by*

$$\gamma^\Sigma(\lambda) = \Phi_\lambda \upharpoonright H^{1/2}(\Sigma;\mathbb{C}^4).$$

Each $\gamma^\Sigma(\lambda)$ is a densely defined bounded operator from $L^2(\Sigma;\mathbb{C}^4)$ to $L^2(\mathbb{R}^3;\mathbb{C}^4)$ and a bounded and everywhere defined operator from $H^{1/2}(\Sigma;\mathbb{C}^4)$ to $H^1(\Omega_+;\mathbb{C}^4) \oplus H^1(\Omega_-;\mathbb{C}^4)$. The adjoint $\gamma^\Sigma(\lambda)^* : L^2(\mathbb{R}^3;\mathbb{C}^4) \to L^2(\Sigma;\mathbb{C}^4)$ is bounded and everywhere defined and coincides with Φ_λ^*.

(ii) *The value of the Weyl function* $M^{\Sigma}(\lambda) : \operatorname{dom} M^{\Sigma}(\lambda) \subset L^2(\Sigma;\mathbb{C}^4) \to L^2(\Sigma;\mathbb{C}^4)$ *is defined on the set* $\operatorname{dom} M^{\Sigma}(\lambda) = H^{1/2}(\Sigma;\mathbb{C}^4)$ *and explicitly given by*

$$M^{\Sigma}(\lambda) = \mathcal{C}_\lambda \upharpoonright H^{1/2}(\Sigma;\mathbb{C}^4).$$

Each $M^{\Sigma}(\lambda)$ *is densely defined and bounded in* $L^2(\Sigma;\mathbb{C}^4)$ *and bounded and everywhere defined in* $H^{1/2}(\Sigma;\mathbb{C}^4)$.

Proof. First we note that $\operatorname{dom}\gamma^{\Sigma}(\lambda) = \operatorname{dom} M^{\Sigma}(\lambda) = \operatorname{ran}\Gamma_0^{\Sigma} = H^{1/2}(\Sigma;\mathbb{C}^4)$, see (4.4).

To prove item (i) we recall first that $\gamma^{\Sigma}(\lambda)^* = \Gamma_1^{\Sigma}(A_0-\overline{\lambda})^{-1}$ and this operator acts as

$$\Gamma_1^{\Sigma}(A_0-\overline{\lambda})^{-1} f(x) = \int_{\mathbb{R}^3} G_{\overline{\lambda}}(x-y) f(y) \mathrm{d}y = \Phi_{\lambda}^* f(x), \quad x \in \Sigma, f \in L^2(\mathbb{R}^3;\mathbb{C}^4),$$

see (3.18), where G_λ is the Green's function for the resolvent of A_0 from (3.6). Hence, it is clear that

$$\gamma^{\Sigma}(\lambda) = \Phi_\lambda \upharpoonright \operatorname{dom}\gamma^{\Sigma}(\lambda) = \Phi_\lambda \upharpoonright H^{1/2}(\Sigma;\mathbb{C}^4),$$

which is a bounded and densely defined operator from $L^2(\Sigma;\mathbb{C}^4)$ to $L^2(\mathbb{R}^3;\mathbb{C}^4)$, compare Proposition 3.2.1 (i). Eventually, to see that $\gamma^{\Sigma}(\lambda)$ regarded as an operator from $H^{1/2}(\Sigma;\mathbb{C}^4)$ to $H^1(\Omega_+;\mathbb{C}^4) \oplus H^1(\Omega_-;\mathbb{C}^4)$ is bounded we show that it is closed. Then the closed graph theorem implies the claim. Assume that $\varphi_n \subset \operatorname{dom}\gamma^{\Sigma}(\lambda)$ is a sequence such that

$$\varphi_n \to \varphi \text{ in } H^{1/2}(\Sigma;\mathbb{C}^4) \quad \text{and} \quad \gamma^{\Sigma}(\lambda)\varphi_n \to f \text{ in } H^1(\Omega_+;\mathbb{C}^4) \oplus H^1(\Omega_-;\mathbb{C}^4).$$

Then $\varphi \in H^{1/2}(\Sigma;\mathbb{C}^4) = \operatorname{dom}\gamma^{\Sigma}(\lambda)$ and $\gamma^{\Sigma}(\lambda)\varphi_n \to f$ in $L^2(\mathbb{R}^3;\mathbb{C}^4)$, as $H^1(\Omega_+;\mathbb{C}^4) \oplus H^1(\Omega_-;\mathbb{C}^4)$ is continuously embedded in $L^2(\mathbb{R}^3;\mathbb{C}^4)$. On the other hand, since $\gamma^{\Sigma}(\lambda)$ is continuous from $L^2(\Sigma;\mathbb{C}^4)$ to $L^2(\mathbb{R}^3;\mathbb{C}^4)$, we have also $\gamma^{\Sigma}(\lambda)\varphi_n \to \gamma^{\Sigma}(\lambda)\varphi$ in $L^2(\mathbb{R}^3;\mathbb{C}^4)$ and hence

$$f = \lim_{n\to\infty} \gamma^{\Sigma}(\lambda)\varphi_n = \gamma^{\Sigma}(\lambda)\varphi.$$

Therefore $\gamma^{\Sigma}(\lambda) : H^{1/2}(\Sigma;\mathbb{C}^4) \to H^1(\Omega_+;\mathbb{C}^4) \oplus H^1(\Omega_-;\mathbb{C}^4)$ is closed.

To show assertion (ii) we note that it holds by Definition 2.2.2, item (i), and Proposition 3.2.1 (iii) for any $\varphi \in H^{1/2}(\Sigma;\mathbb{C}^4)$

$$M^{\Sigma}(\lambda)\varphi = \Gamma_1^{\Sigma}\gamma^{\Sigma}(\lambda)\varphi = \Gamma_1^{\Sigma}\Phi_\lambda\varphi = \frac{1}{2}\big((\Phi_\lambda\varphi)_+|_\Sigma + (\Phi_\lambda\varphi)_-|_\Sigma\big) = \mathcal{C}_\lambda\varphi,$$

compare (3.19). Hence $M^{\Sigma}(\lambda) = \mathcal{C}_\lambda \upharpoonright H^{1/2}(\Sigma;\mathbb{C}^4)$. This is a densely defined and bounded operator by Proposition 3.2.1 (ii). Finally, since $\gamma^{\Sigma}(\lambda)$ is bounded from $H^{1/2}(\Sigma;\mathbb{C}^4)$ to $H^1(\Omega_+;\mathbb{C}^4) \oplus H^1(\Omega_-;\mathbb{C}^4)$ by (i), we conclude by the mapping properties of the trace operator that $M^{\Sigma}(\lambda)$ is well-defined and bounded in $H^{1/2}(\Sigma;\mathbb{C}^4)$. □

4.1.2 An ordinary boundary triple for Dirac operators with δ-shell interactions

In this section we transform and extend the quasi boundary triple $\{L^2(\Sigma;\mathbb{C}^4),\Gamma_0^\Sigma,\Gamma_1^\Sigma\}$ to an ordinary boundary triple using the techniques described in Section 2.2. Recall the definition of the sets

$$\mathscr{G}_0^\Sigma := \operatorname{ran}(\Gamma_0^\Sigma \upharpoonright \Gamma_1^\Sigma) \quad \text{and} \quad \mathscr{G}_1^\Sigma := \operatorname{ran}(\Gamma_1^\Sigma \upharpoonright \Gamma_0^\Sigma).$$

Lemma 4.1.3. *Let T^Σ be given by* (4.1), *let $(S^\Sigma)^* = T_{\max}^{\Omega_+} \oplus T_{\max}^{\Omega_-}$ and let $\{L^2(\Sigma;\mathbb{C}^4),\Gamma_0^\Sigma,\Gamma_1^\Sigma\}$ be the quasi boundary triple from Theorem 4.1.1. Then the operator $A_\infty^\Sigma := T^\Sigma \upharpoonright \ker\Gamma_1^\Sigma$ is self-adjoint in $L^2(\mathbb{R}^3;\mathbb{C}^4)$ with $\sigma(A_\infty^\Sigma) \subset \sigma(A_0)$. Moreover*

$$\mathscr{G}_0^\Sigma = \mathscr{G}_1^\Sigma = H^{1/2}(\Sigma;\mathbb{C}^4) \tag{4.5}$$

and the mappings $\Gamma_0^\Sigma,\Gamma_1^\Sigma : \operatorname{dom} T^\Sigma \to L^2(\Sigma;\mathbb{C}^4)$ have surjective extensions

$$\widetilde{\Gamma}_0^\Sigma : \operatorname{dom}(S^\Sigma)^* \to H^{-1/2}(\Sigma;\mathbb{C}^4) \quad \text{and} \quad \widetilde{\Gamma}_1^\Sigma : \operatorname{dom}(S^\Sigma)^* \to H^{-1/2}(\Sigma;\mathbb{C}^4),$$

which are bounded with respect to the graph norm induced by $(S^\Sigma)^*$.

Proof. First, we prove that A_∞^Σ is self-adjoint. Via Green's identity it is not difficult to see that A_∞^Σ is symmetric, compare (2.9). Thus, it suffices to show that A_∞^Σ is bijective. Using the Birman-Schwinger principle from Theorem 2.2.5 (i) it follows that A_∞^Σ is injective, as $M^\Sigma(0) = \mathcal{C}_0 \upharpoonright H^{1/2}(\Sigma;\mathbb{C}^4)$ is injective by Proposition 3.2.1 (iv). To show that A_∞^Σ is also surjective assume that $f \in L^2(\mathbb{R}^3;\mathbb{C}^4)$ is arbitrary, but fixed. Then $f \in \operatorname{ran} A_\infty^\Sigma$ if and only if $\gamma^\Sigma(0)^* f \in \operatorname{ran} M^\Sigma(0)$, compare Theorem 2.2.5 (ii). Because of (3.18) and the trace theorem we have $\gamma^\Sigma(0)^* f = \Phi(0)^* f = (A_0^{-1} f)|_\Sigma \in H^{1/2}(\Sigma;\mathbb{C}^4)$. Moreover, as Σ is C^2-smooth, it follows from Proposition 3.2.1 (iv) that $M^\Sigma(0) = \mathcal{C}_0 \upharpoonright H^{1/2}(\Sigma;\mathbb{C}^4)$ is bijective in $H^{1/2}(\Sigma;\mathbb{C}^4)$. Hence $\gamma^\Sigma(0)^* f \in \operatorname{ran} M^\Sigma(0)$ for any $f \in L^2(\mathbb{R}^3;\mathbb{C}^4)$, which implies that A_∞^Σ is self-adjoint. Furthermore, since $M^\Sigma(\lambda)$ is bijective in $H^{1/2}(\Sigma;\mathbb{C}^4)$ for any $\lambda \in \rho(A_0)$, see Proposition 4.1.2 and Proposition 3.2.1 (iv), it follows from Theorem 2.2.5 (i)-(ii) that $A_\infty^\Sigma - \lambda$ is bijective for any $\lambda \in \rho(A_0)$, that means $\rho(A_0) \subset \rho(A_\infty^\Sigma)$.

Next, we show that $\mathscr{G}_0^\Sigma = H^{1/2}(\Sigma;\mathbb{C}^4)$. For that let $\varphi \in H^{1/2}(\Sigma;\mathbb{C}^4)$ be arbitrary, but fixed, and choose $f_\pm \in H^1(\Omega_\pm;\mathbb{C}^4)$ such that $f_\pm|_\Sigma = \mp\frac{i}{2c}(\alpha\cdot\nu)\varphi$. Then $f := f_+ \oplus f_- \in \ker\Gamma_1^\Sigma$ and $\Gamma_0^\Sigma f = \varphi$.

To show $\mathscr{G}_1^\Sigma = H^{1/2}(\Sigma;\mathbb{C}^4)$ take for $\varphi \in H^{1/2}(\Sigma;\mathbb{C}^4)$ a function $f \in H^1(\mathbb{R}^3;\mathbb{C}^4)$ satisfying $f|_\Sigma = \varphi$. Then $f \in \ker\Gamma_0^\Sigma$ and $\Gamma_1^\Sigma f = \varphi$. Hence, also $\mathscr{G}_1^\Sigma = H^{1/2}(\Sigma;\mathbb{C}^4)$. Thus, equation (4.5) is shown.

Finally, using (4.5), the self-adjointness of A_∞^Σ, and Proposition 2.2.11 it follows immediately that Γ_0^Σ and Γ_1^Σ have surjective extensions $\widetilde{\Gamma}_0^\Sigma,\widetilde{\Gamma}_1^\Sigma : \operatorname{dom}(S^\Sigma)^* \to H^{-1/2}(\Sigma;\mathbb{C}^4)$. This finishes the proof of this lemma. □

Next, similarly as in Section 2.2 we set

$$\Lambda^\Sigma := \operatorname{Im}\overline{M^\Sigma(i)} = \frac{1}{2i}\big(\overline{M^\Sigma(i)} - \overline{M(-i)}\big) = \frac{1}{2i}(\mathcal{C}_i - \mathcal{C}_{-i}).$$

Since $\mathscr{G}_1^\Sigma = H^{1/2}(\Sigma;\mathbb{C}^4)$ is dense in $L^2(\Sigma;\mathbb{C}^4)$, compare Lemma 4.1.3, we deduce from Proposition 2.2.10 that $(\Lambda^\Sigma)^{1/2} : L^2(\Sigma;\mathbb{C}^4) \to H^{1/2}(\Sigma;\mathbb{C}^4)$ is a bijection and we define

$$\iota_+^\Sigma := (\Lambda^\Sigma)^{-1/2} : H^{1/2}(\Sigma;\mathbb{C}^4) \to L^2(\Sigma;\mathbb{C}^4) \tag{4.6}$$

and

$$\iota_-^\Sigma := \big((\Lambda^\Sigma)^{1/2}\big)' : H^{-1/2}(\Sigma;\mathbb{C}^4) \to L^2(\Sigma;\mathbb{C}^4). \tag{4.7}$$

Recall that we can express the inner product in $\mathscr{G}_1^\Sigma = H^{1/2}(\Sigma;\mathbb{C}^4)$ and the duality product in $H^{1/2}(\Sigma;\mathbb{C}^4) \times H^{-1/2}(\Sigma;\mathbb{C}^4)$ with the help of $\iota_\pm^\Sigma$, compare the useful formulae (2.15), (2.18), and (2.19). Moreover, we note that the typical scaling properties for embedding operators yield that ι_-^Σ gives rise to a bounded operator

$$\iota_-^\Sigma : H^{1/2}(\Sigma;\mathbb{C}^4) \to H^1(\Sigma;\mathbb{C}^4). \tag{4.8}$$

In the next proposition we extend with the aid of the extended boundary mappings $\widetilde{\Gamma}_0^\Sigma$ and $\widetilde{\Gamma}_1^\Sigma$ the γ-field $\gamma^\Sigma(\lambda)$ and the Weyl function $M^\Sigma(\lambda)$ from Proposition 4.1.2.

Proposition 4.1.4. *Let $\{L^2(\Sigma;\mathbb{C}^4), \Gamma_0^\Sigma, \Gamma_1^\Sigma\}$ be the quasi boundary triple for $(S^\Sigma)^*$ from Theorem 4.1.1 with corresponding γ-field γ^Σ and Weyl function M^Σ given as in Proposition 4.1.2. Then it holds for all $\lambda \in \rho(A_0) = \mathbb{C} \setminus \big((-\infty, -mc^2] \cup [mc^2, \infty)\big)$:*

(i) *The operator $\gamma^\Sigma(\lambda)$ has a continuous extension*

$$\widetilde{\gamma}^\Sigma(\lambda) = \big(\widetilde{\Gamma}_0^\Sigma \restriction \ker((S^\Sigma)^* - \lambda)\big)^{-1} : H^{-1/2}(\Sigma;\mathbb{C}^4) \to L^2(\mathbb{R}^3;\mathbb{C}^4).$$

(ii) *The operator $M^\Sigma(\lambda)$ has a continuous extension*

$$\widetilde{M}^\Sigma(\lambda) = \widetilde{\Gamma}_1^\Sigma\big(\widetilde{\Gamma}_0^\Sigma \restriction \ker((S^\Sigma)^* - \lambda)\big)^{-1} : H^{-1/2}(\Sigma;\mathbb{C}^4) \to H^{-1/2}(\mathbb{R}^3;\mathbb{C}^4).$$

Moreover, it holds for all $\varphi \in H^{-1/2}(\Sigma;\mathbb{C}^4)$ and $\psi \in H^{1/2}(\Sigma;\mathbb{C}^4)$

$$\big(\widetilde{M}^\Sigma(\lambda)\varphi, \psi\big)_{-1/2\times 1/2} = \big(\varphi, M^\Sigma(\overline{\lambda})\psi\big)_{-1/2\times 1/2}.$$

(iii) *The operator $\widetilde{M}^\Sigma(\lambda)$ is bijective in $H^{-1/2}(\Sigma;\mathbb{C}^4)$ and its inverse is given by*

$$\widetilde{M}^\Sigma(\lambda)^{-1} = -4c^2(\alpha\cdot\nu)'\widetilde{M}(\lambda)(\alpha\cdot\nu)',$$

where $(\alpha\cdot\nu)' : H^{-1/2}(\Sigma;\mathbb{C}^4) \to H^{-1/2}(\Sigma;\mathbb{C}^4)$ is the dual of the multiplication operator with $\alpha\cdot\nu$ in $H^{1/2}(\Sigma;\mathbb{C}^4)$.

(iv) *The operator*
$$\mathcal{A}_\lambda := M^\Sigma(\lambda)(\alpha\cdot\nu) + (\alpha\cdot\nu)M^\Sigma(\lambda)$$
admits a bounded extension $\widetilde{\mathcal{A}}_\lambda : H^{-1/2}(\Sigma;\mathbb{C}^4) \to H^{1/2}(\Sigma;\mathbb{C}^4)$. *In particular, the mapping* $\frac{1}{4c^2} - \big(\widetilde{M}^\Sigma(\lambda)\big)^2 : H^{-1/2}(\Sigma;\mathbb{C}^4) \to H^{1/2}(\Sigma;\mathbb{C}^4)$ *is bounded.*

Proof. Assertion (i) and the existence and the mapping properties of $\widetilde{M}^\Sigma(\lambda)$ follow immediately from Proposition 2.2.12 and Lemma 4.1.3. Moreover, employing (2.19) and Proposition 2.2.4 (iii) we observe for $\varphi \in H^{1/2}(\Sigma;\mathbb{C}^4)$ and $\psi \in H^{1/2}(\Sigma;\mathbb{C}^4)$

$$\big(\widetilde{M}^\Sigma(\lambda)\varphi,\psi\big)_{-1/2\times 1/2} = (M^\Sigma(\lambda)\varphi,\psi)_\Sigma = (\varphi, M^\Sigma(\overline{\lambda})\psi)_\Sigma = (\varphi, M^\Sigma(\overline{\lambda})\psi)_{-1/2\times 1/2}.$$

By density we obtain that the above formula can be extended for all $\varphi \in H^{-1/2}(\Sigma;\mathbb{C}^4)$. Hence, the proof of item (ii) is complete.

To verify assertion (iii) we note first that it holds $\widetilde{M}^\Sigma(\lambda) = \big(M^\Sigma(\overline{\lambda})\big)'$, when $M^\Sigma(\overline{\lambda})$ is considered as a bounded operator in $H^{1/2}(\Sigma;\mathbb{C}^4)$. Since $M^\Sigma(\overline{\lambda})$ is bijective in $H^{1/2}(\Sigma;\mathbb{C}^4)$ by Proposition 4.1.2 and Proposition 3.2.1 (iv) with

$$M^\Sigma(\overline{\lambda})^{-1} = -4c^2(\alpha\cdot\nu)M^\Sigma(\overline{\lambda})(\alpha\cdot\nu), \tag{4.9}$$

also $\widetilde{M}^\Sigma(\lambda)$ is bijective and the claimed formula for the inverse follows from (4.9) by considering the dual.

It remains to show statement (iv). For $\lambda = 0$ the claim is true by Proposition 3.2.4. Recall that it holds
$$M^\Sigma(\lambda) = M^\Sigma(0) + \lambda\gamma^\Sigma(0)^*\gamma^\Sigma(\lambda),$$
see Proposition 2.2.4 (iii). Hence, we obtain

$$\mathcal{A}_\lambda = \mathcal{A}_0 + \lambda(\alpha\cdot\nu)\gamma^\Sigma(0)^*\gamma^\Sigma(\lambda) + \lambda\gamma^\Sigma(0)^*\gamma^\Sigma(\lambda)(\alpha\cdot\nu).$$

Note that $\operatorname{ran}\gamma^\Sigma(0)^* = \operatorname{ran}\big(\Gamma_1^\Sigma A_0^{-1}\big) = H^{1/2}(\Sigma;\mathbb{C}^4)$. Hence, as $\gamma^\Sigma(0)^*$ is bounded from $L^2(\mathbb{R}^3;\mathbb{C}^4)$ to $L^2(\Sigma;\mathbb{C}^4)$ it follows from the closed graph theorem that $\gamma^\Sigma(0)^*$ acting between $L^2(\mathbb{R}^3;\mathbb{C}^4)$ and $H^{1/2}(\Sigma;\mathbb{C}^4)$ is also bounded. Therefore, the operator $\gamma^\Sigma(0)^*\gamma^\Sigma(\lambda)$ has the continuous extension

$$\gamma^\Sigma(0)^*\widetilde{\gamma}^\Sigma(\lambda) : H^{-1/2}(\Sigma;\mathbb{C}^4) \to H^{1/2}(\Sigma;\mathbb{C}^4).$$

Moreover, by duality we see that the multiplication operator $\alpha\cdot\nu$ has the bounded extension $(\alpha\cdot\nu)' : H^{-1/2}(\Sigma;\mathbb{C}^4) \to H^{-1/2}(\Sigma;\mathbb{C}^4)$. Thus, we conclude finally that $\mathcal{A}_\lambda$ has the bounded extension

$$\widetilde{\mathcal{A}}_\lambda := \widetilde{\mathcal{A}}_0 + \lambda(\alpha\cdot\nu)\gamma^\Sigma(0)^*\widetilde{\gamma}^\Sigma(\lambda) + \lambda\gamma^\Sigma(0)^*\widetilde{\gamma}^\Sigma(\lambda)(\alpha\cdot\nu)' : H^{-1/2}(\Sigma;\mathbb{C}^4) \to H^{1/2}(\Sigma;\mathbb{C}^4).$$

Eventually, using Proposition 3.2.1 (iv) we find for $\varphi \in H^{1/2}(\Sigma;\mathbb{C}^4)$

$$M^\Sigma(\lambda)(\alpha\cdot\nu)\big[(\alpha\cdot\nu)M^\Sigma(\lambda)+M^\Sigma(\lambda)(\alpha\cdot\nu)\big]\varphi = \left[(M^\Sigma(\lambda))^2 - \frac{1}{4c^2}\right]\varphi.$$

This and a density argument imply

$$\big(\widetilde{M}^\Sigma(\lambda)\big)^2 - \frac{1}{4c^2} = M^\Sigma(\lambda)(\alpha\cdot\nu)\widetilde{A}_\lambda,$$

which is a continuous mapping from $H^{-1/2}(\Sigma;\mathbb{C}^4)$ to $H^{1/2}(\Sigma;\mathbb{C}^4)$. This finishes the proof of this proposition. □

Finally, we transform the quasi boundary triple $\{L^2(\Sigma;\mathbb{C}^4),\Gamma_0^\Sigma,\Gamma_1^\Sigma\}$ from Theorem 4.1.1 into an ordinary boundary triple which is suitable to investigate Dirac operators with singular interactions. Since the boundary conditions for these operators are stated in the form $\Gamma_0^\Sigma + \vartheta\Gamma_1^\Sigma = 0$ for some linear operator ϑ acting in $L^2(\Sigma;\mathbb{C}^4)$ it is more convenient to transform the triple $\{L^2(\Sigma;\mathbb{C}^4),-\Gamma_1^\Sigma,\Gamma_0^\Sigma\}$ instead (in the proof of Theorem 4.1.5 below we will see that this is in fact a quasi boundary triple). Recall that the operator $A_\infty^\Sigma := T^\Sigma \upharpoonright \ker\Gamma_1^\Sigma$ is bijective, compare Lemma 4.1.3. This implies, in particular,

$$\operatorname{dom}(S^\Sigma)^* = \operatorname{dom}A_\infty^\Sigma \dot{+} \ker(S^\Sigma)^*.$$

Theorem 4.1.5. *Let S^Σ be defined by* (4.3) *and let $\{L^2(\Sigma;\mathbb{C}^4),\Gamma_0^\Sigma,\Gamma_1^\Sigma\}$ be the quasi boundary triple from Theorem 4.1.1. Moreover, let $\iota_\pm^\Sigma$ be defined by* (4.6) *and* (4.7)*, respectively, let $\widetilde{\Gamma}_1^\Sigma$ be the extension of Γ_1^Σ from Lemma 4.1.3 and define $\Upsilon_0^\Sigma,\Upsilon_1^\Sigma : \operatorname{dom}(S^\Sigma)^* \to L^2(\Sigma;\mathbb{C}^4)$ by*

$$\Upsilon_0^\Sigma f := -\iota_-^\Sigma\widetilde{\Gamma}_1^\Sigma f \quad \textit{and} \quad \Upsilon_1^\Sigma f := \iota_+^\Sigma\Gamma_0^\Sigma f_0$$

for $f = f_0 + g \in \operatorname{dom}A_\infty^\Sigma \dot{+} \ker(S^\Sigma)^* = \operatorname{dom}(S^\Sigma)^*$. Then $\{L^2(\Sigma;\mathbb{C}^4),\Upsilon_0^\Sigma,\Upsilon_1^\Sigma\}$ is an ordinary boundary triple for $(S^\Sigma)^*$.

Proof. First, we note that $A_\infty^\Sigma = T^\Sigma \upharpoonright \Gamma_1^\Sigma$ is self-adjoint by Lemma 4.1.3. Hence the triple $\{L^2(\Sigma;\mathbb{C}^4),-\Gamma_1^\Sigma,\Gamma_0^\Sigma\}$ fulfills all points in Definition 2.2.1, that means it is a quasi boundary triple for $(S^\Sigma)^*$. Therefore, all claims follow from Theorem 2.2.13 as $\mathscr{G}_0^\Sigma = H^{1/2}(\Sigma;\mathbb{C}^4)$ is dense in $L^2(\Sigma;\mathbb{C}^4)$ by Lemma 4.1.3. □

Note that the ordinary boundary triple $\{L^2(\Sigma;\mathbb{C}^4),\Upsilon_0^\Sigma,\Upsilon_1^\Sigma\}$ from the above theorem is not a transformation of the quasi boundary triple $\{L^2(\Sigma;\mathbb{C}^4),\Gamma_0^\Sigma,\Gamma_1^\Sigma\}$ as in Theorem 2.2.13, but of $\{L^2(\Sigma;\mathbb{C}^4),\widehat{\Gamma}_0^\Sigma,\widehat{\Gamma}_1^\Sigma\}$ with $\widehat{\Gamma}_0^\Sigma = -\Gamma_1^\Sigma$ and $\widehat{\Gamma}_1^\Sigma = \Gamma_0^\Sigma$. The Weyl function of this triple is given by

$$\widehat{M}^\Sigma(\lambda) = \widehat{\Gamma}_1^\Sigma\big(\widehat{\Gamma}_0^\Sigma \upharpoonright \ker(T^\Sigma-\lambda)\big)^{-1} = -\Gamma_0^\Sigma\big(\Gamma_1^\Sigma \upharpoonright \ker(T^\Sigma-\lambda)\big)^{-1} = -M^\Sigma(\lambda)^{-1}$$

for $\lambda \in \rho(A_\infty^\Sigma) \cap \rho(A_0)$.

In the following let B be a symmetric operator in $L^2(\Sigma;\mathbb{C}^4)$ and set

$$A_{[B]}^\Sigma = T^\Sigma \upharpoonright \ker(\Gamma_0^\Sigma + B\Gamma_1^\Sigma) = T^\Sigma \upharpoonright \ker(\widehat{\Gamma}_1^\Sigma - B\widehat{\Gamma}_0^\Sigma).$$

Then, in view of formulae (2.22) and (2.21) it holds

$$A_{[B]}^\Sigma = T^\Sigma \upharpoonright \ker(\widehat{\Gamma}_1^\Sigma - B\widehat{\Gamma}_0^\Sigma) = (S^\Sigma)^* \upharpoonright \ker(\Upsilon_1^\Sigma - \Theta^{1,\Sigma}(B)\Upsilon_0^\Sigma)$$

with

$$\begin{aligned}\Theta^{1,\Sigma}(B)\varphi &:= \iota_+^\Sigma(B + M^\Sigma(0)^{-1})(\iota_-^\Sigma)^{-1}\varphi,\\ \operatorname{dom}\Theta^{1,\Sigma}(B) &= \big\{\varphi \in L^2(\Sigma;\mathbb{C}^4) : (\iota_-^\Sigma)^{-1}\varphi \in \operatorname{dom}(B + M^\Sigma(0)^{-1}) \text{ and}\\ &\qquad (B + M^\Sigma(0)^{-1})(\iota_-^\Sigma)^{-1}\varphi \in H^{1/2}(\Sigma;\mathbb{C}^4)\big\}.\end{aligned} \tag{4.10}$$

In particular, if $\Theta^{1,\Sigma}(B)$ is self-adjoint in $L^2(\Sigma;\mathbb{C}^4)$, then $A_{[B]}^\Sigma$ is self-adjoint in $L^2(\mathbb{R}^3;\mathbb{C}^4)$.

Finally, we are interested in operators of a similar form as $\Theta^{1,\Sigma}(B)$ as above. Define for a symmetric operator B in $L^2(\Sigma;\mathbb{C}^4)$

$$\begin{aligned}\Theta^{0,\Sigma}(B)\varphi &:= \iota_+^\Sigma(B + \widetilde{M}^\Sigma(0)^{-1})(\iota_-^\Sigma)^{-1}\varphi,\\ \operatorname{dom}\Theta^{0,\Sigma}(B) &= \big\{\varphi \in L^2(\Sigma;\mathbb{C}^4) : (\iota_-^\Sigma)^{-1}\varphi \in \operatorname{dom}(B + \widetilde{M}^\Sigma(0)^{-1}) \text{ and}\\ &\qquad (B + \widetilde{M}^\Sigma(0)^{-1})(\iota_-^\Sigma)^{-1}\varphi \in H^{1/2}(\Sigma;\mathbb{C}^4)\big\}.\end{aligned}$$

Note that we have in general $\Theta^{1,\Sigma}(B) \subset \Theta^{0,\Sigma}(B)$, as in the definition of $\Theta^{0,\Sigma}(B)$ the extension $\widetilde{M}^\Sigma(0)$ appears. If the parameter $\Theta^{0,\Sigma}(B)$ is self-adjoint, then also the corresponding operator $A_{\Theta^{0,\Sigma}(B)} = (S^\Sigma)^* \upharpoonright \ker(\Upsilon_1^\Sigma - \Theta^{0,\Sigma}(B)\Upsilon_0^\Sigma)$ is self-adjoint. For such extensions the Birman Schwinger principle from Theorem 2.2.5 reads, taking the special form of the Weyl function for the triple $\{L^2(\Sigma;\mathbb{C}^4), \Upsilon_0^\Sigma, \Upsilon_1^\Sigma\}$, which is a transformation of the quasi triple $\{L^2(\Sigma;\mathbb{C}^4), \widehat{\Gamma}_0^\Sigma, \widehat{\Gamma}_1^\Sigma\}$, from (2.20) into account, that a point $\lambda \in \rho(A_\infty^\Sigma) = \rho(A_0)$ fulfills

$$\lambda \in \sigma_\mathrm{p}(A_{[B]}) \quad \text{if and only if} \quad 0 \in \sigma_\mathrm{p}\big(\iota_+(B + \widetilde{M}^\Sigma(\lambda)^{-1})\iota_-^{-1}\big). \tag{4.11}$$

Furthermore, similar statements for the discrete spectrum and the resolvent set of $A_{[B]}$ are true, compare Proposition 2.2.7.

4.1.3 Integral operators – Part II: mapping properties

In this section we collect some further knowledge on the integral operators Φ_λ and $\mathcal{C}_\lambda$ introduced in Section 3.2. As we have seen in Proposition 4.1.4 these operators are, roughly speaking, the γ-field and the Weyl function associated to the quasi boundary triple $\{L^2(\Sigma;\mathbb{C}^4), \Gamma_0^\Sigma, \Gamma_1^\Sigma\}$ from Theorem 4.1.1. Hence, we are able to deduce some further properties of these operators from the general theory of quasi boundary triples with little effort.

Proposition 4.1.6. *Let for $\lambda \in \rho(A_0) = \mathbb{C} \setminus \big((-\infty, -mc^2] \cup [mc^2, \infty)\big)$ the operators Φ_λ and $\mathcal{C}_\lambda$ be defined as in* (3.16) *and* (3.17)*, respectively, and let $s \in \big[-\frac{1}{2}, \frac{1}{2}\big]$. Then, the following holds:*

(i) *The operator Φ_λ gives rise to a bounded operator*

$$\Phi_\lambda^s : H^s(\Sigma;\mathbb{C}^4) \to H^{s+1/2}(\Omega_+;\mathbb{C}^4) \oplus H^{s+1/2}(\Omega_-;\mathbb{C}^4).$$

(ii) *The adjoint $\Phi_\lambda^* : L^2(\mathbb{R}^3;\mathbb{C}^4) \to H^{1/2}(\Sigma;\mathbb{C}^4)$ is bounded.*

(iii) *The operator $\mathcal{C}_\lambda$ gives rise to a bounded operator*

$$\mathcal{C}_\lambda^s : H^s(\Sigma;\mathbb{C}^4) \to H^s(\Sigma;\mathbb{C}^4).$$

Proof. (i) According to Proposition 4.1.2 we have that $\Phi_\lambda^{1/2} = \gamma^\Sigma(\lambda)$ and this operator is bounded from $H^{1/2}(\Sigma;\mathbb{C}^4)$ to $H^1(\Omega_+;\mathbb{C}^4) \oplus H^1(\Omega_-;\mathbb{C}^4)$. Moreover, by Proposition 4.1.4 the operator Φ_λ has the continuous extension

$$\Phi_\lambda^{-1/2} := \widetilde{\gamma}^\Sigma(\lambda) : H^{-1/2}(\Sigma;\mathbb{C}^4) \to L^2(\mathbb{R}^3;\mathbb{C}^4).$$

Hence, assertion (i) holds for $s = \pm\frac{1}{2}$. The statement for $s \in \big(-\frac{1}{2}, \frac{1}{2}\big)$ follows by interpolation.

In order to show statement (ii) we deduce first from Proposition 2.2.3 (iii) that

$$\operatorname{ran} \Phi_\lambda^* = \operatorname{ran} \big(\Gamma_1^\Sigma (A_0 - \overline{\lambda})^{-1}\big) = \Gamma_1^\Sigma(H^1(\mathbb{R}^3;\mathbb{C}^4)) = H^{1/2}(\Sigma;\mathbb{C}^4)$$

and hence Φ_λ^* regarded as an operator from $L^2(\mathbb{R}^3;\mathbb{C}^4)$ to $H^{1/2}(\Sigma;\mathbb{C}^4)$ is well-defined. We prove that this operator is closed; then the closed graph theorem implies that it is also bounded. Let $(f_n) \subset L^2(\mathbb{R}^3;\mathbb{C}^4)$ and $\varphi \in H^{1/2}(\Sigma;\mathbb{C}^4)$ such that

$$f_n \to f \text{ in } L^2(\mathbb{R}^3;\mathbb{C}^4) \quad \text{and} \quad \Phi_\lambda^* f_n \to \varphi \text{ in } H^{1/2}(\Sigma;\mathbb{C}^4).$$

Clearly $f \in L^2(\mathbb{R}^3;\mathbb{C}^4) = \operatorname{dom} \Phi_\lambda^*$ and since Φ_λ^* is bounded from $L^2(\mathbb{R}^3;\mathbb{C}^4)$ to $L^2(\Sigma;\mathbb{C}^4)$ by Proposition 3.2.1 (i) we obtain that $\Phi_\lambda^* f_n \to \Phi_\lambda^* f$ in $L^2(\Sigma;\mathbb{C}^4)$. On the other hand, since $H^{1/2}(\Sigma;\mathbb{C}^4)$ is continuously embedded in $L^2(\Sigma;\mathbb{C}^4)$ we get that $\Phi_\lambda^* f_n \to \varphi$ in $L^2(\Sigma;\mathbb{C}^4)$ as well. Thus, we have $\varphi = \Phi_\lambda^* f$ which shows that $\Phi_\lambda^* : L^2(\mathbb{R}^3;\mathbb{C}^4) \to H^{1/2}(\Sigma;\mathbb{C}^4)$ is closed and which finishes the proof of assertion (ii).

Eventually, we know from Proposition 4.1.2 that $\mathcal{C}_\lambda^{1/2} := M^\Sigma(\lambda)$ is bounded in $H^{1/2}(\Sigma;\mathbb{C}^4)$ and from Proposition 4.1.4 that $\mathcal{C}_\lambda^{-1/2} := \widetilde{M}^\Sigma(\lambda)$ is bounded in $H^{-1/2}(\Sigma;\mathbb{C}^4)$. Hence, statement (iii) is true for $s = \pm\frac{1}{2}$. Using an interpolation argument, the claim for $s \in \big(-\frac{1}{2}, \frac{1}{2}\big)$ follows as well. □

Next, we state a result on the invertibility of certain operators involving $\mathcal{C}_\lambda^s$. This result is one of the main ingredients to prove the self-adjointness of Dirac operators with singular interactions.

Proposition 4.1.7. *Let $\{L^2(\Sigma;\mathbb{C}^4),\Gamma_0^\Sigma,\Gamma_1^\Sigma\}$ be given as in Theorem 4.1.1, let $\eta_\mathrm{e},\eta_\mathrm{s}:\Sigma\to\mathbb{R}$ be Lipschitz continuous, let $\lambda\notin\sigma_\mathrm{p}\big(T^\Sigma\upharpoonright\ker\big(\Gamma_0^\Sigma\pm(\eta_\mathrm{e}I_4+\eta_\mathrm{s}\beta)\Gamma_1^\Sigma\big)\big)$, let $s\in\big[-\frac{1}{2},\frac{1}{2}\big]$, and let $\mathcal{C}_\lambda^s$ be given as in Proposition 4.1.6. Assume that $\eta_\mathrm{e}(x)^2-\eta_\mathrm{s}(x)^2\neq 4c^2$ for all $x\in\Sigma$. Then the operator*

$$I_4+(\eta_\mathrm{e}I_4+\eta_\mathrm{s}\beta)\mathcal{C}_\lambda^s$$

admits a bounded and everywhere defined inverse in $H^s(\Sigma;\mathbb{C}^4)$.

Proof. We are going to prove this statement for $s=\frac{1}{2}$, the result for $s=-\frac{1}{2}$ follows then by duality. Finally, the claim for $s\in\big(-\frac{1}{2},\frac{1}{2}\big)$ can be deduced then by interpolation.

So let us verify the claimed assertion for $s=\frac{1}{2}$. First, we note that $I_4+(\eta_\mathrm{e}I_4+\eta_\mathrm{s}\beta)\mathcal{C}_\lambda^{1/2}$ is injective, as otherwise the operator $T^\Sigma\upharpoonright\ker\big(\Gamma_0^\Sigma+(\eta_\mathrm{e}I_4+\eta_\mathrm{s}\beta)\Gamma_1^\Sigma\big)$ has the eigenvalue λ by Theorem 2.2.6 (i). To show that $I_4+(\eta_\mathrm{e}I_4+\eta_\mathrm{s}\beta)\mathcal{C}_\lambda^{1/2}$ is also surjective we note first

$$\operatorname{ran}\,(I_4+(\eta_\mathrm{e}I_4+\eta_\mathrm{s}\beta)\mathcal{C}_\lambda^{1/2})\supset\operatorname{ran}\big[(I_4+(\eta_\mathrm{e}I_4+\eta_\mathrm{s}\beta)\mathcal{C}_\lambda^{1/2})(I_4-(\eta_\mathrm{e}I_4+\eta_\mathrm{s}\beta)\mathcal{C}_\lambda^{1/2})\big].$$

Observe that

$$I_4-(\eta_\mathrm{e}I_4+\eta_\mathrm{s}\beta)\mathcal{C}_\lambda^{1/2}=I_4-\mathcal{C}_\lambda^{1/2}(\eta_\mathrm{e}-\eta_\mathrm{s}\beta)+\mathcal{K}_{1,\lambda}$$

with

$$\begin{aligned}\mathcal{K}_{1,\lambda}:&=\mathcal{C}_\lambda^{1/2}(\eta_\mathrm{e}-\eta_\mathrm{s}\beta)-(\eta_\mathrm{e}I_4+\eta_\mathrm{s}\beta)\mathcal{C}_\lambda^{1/2}\\&=(\mathcal{C}_\lambda^{1/2}\eta_\mathrm{e}-\eta_\mathrm{e}\mathcal{C}_\lambda^{1/2})-\eta_\mathrm{s}(\mathcal{C}_\lambda^{1/2}\beta+\beta\mathcal{C}_\lambda^{1/2})+(\eta_\mathrm{s}\mathcal{C}_\lambda^{1/2}-\mathcal{C}_\lambda^{1/2}\eta_\mathrm{s})\beta.\end{aligned}$$

Since η_e and η_s are Lipschitz continuous it follows from Proposition 3.2.3 and Proposition 3.2.4 (ii) that $\mathcal{K}_{1,\lambda}$ is a compact operator in $H^{1/2}(\Sigma;\mathbb{C}^4)$. Hence, also

$$\mathcal{K}_{2,\lambda}:=(I_4+(\eta_\mathrm{e}I_4+\eta_\mathrm{s}\beta)\mathcal{C}_\lambda^{1/2})\mathcal{K}_{1,\lambda}$$

is compact in $H^{1/2}(\Sigma;\mathbb{C}^4)$. Thus, we have

$$\begin{aligned}&(I_4+(\eta_\mathrm{e}I_4+\eta_\mathrm{s}\beta)\mathcal{C}_\lambda^{1/2})(I_4-(\eta_\mathrm{e}I_4+\eta_\mathrm{s}\beta)\mathcal{C}_\lambda^{1/2})\\&\qquad=(I_4+(\eta_\mathrm{e}I_4+\eta_\mathrm{s}\beta)\mathcal{C}_\lambda^{1/2})(I_4-\mathcal{C}_\lambda^{1/2}(\eta_\mathrm{e}-\eta_\mathrm{s}\beta))+\mathcal{K}_{2,\lambda}\\&\qquad=I_4-(\eta_\mathrm{e}I_4+\eta_\mathrm{s}\beta)(\mathcal{C}_\lambda^{1/2})^2(\eta_\mathrm{e}-\eta_\mathrm{s}\beta)+(\eta_\mathrm{e}\mathcal{C}_\lambda^{1/2}-\mathcal{C}_\lambda^{1/2}\eta_\mathrm{e})\\&\qquad\qquad+\eta_\mathrm{s}(\beta\mathcal{C}_\lambda^{1/2}+\mathcal{C}_\lambda^{1/2}\beta)+(\mathcal{C}_\lambda^{1/2}\eta_\mathrm{s}-\eta_\mathrm{s}\mathcal{C}_\lambda^{1/2})\beta+\mathcal{K}_{2,\lambda}\\&\qquad=I_4-\frac{1}{4c^2}(\eta_\mathrm{e}^2-\eta_\mathrm{s}^2)+\mathcal{K}_{3,\lambda}\end{aligned}$$

with

$$\mathcal{K}_{3,\lambda} := (\eta_e I_4 + \eta_s \beta)\left(\frac{1}{4c^2} - (\mathcal{C}_\lambda^{1/2})^2\right)(\eta_e - \eta_s \beta) + (\eta_e \mathcal{C}_\lambda^{1/2} - \mathcal{C}_\lambda^{1/2}\eta_e) \\ + \eta_s(\beta \mathcal{C}_\lambda^{1/2} + \mathcal{C}_\lambda^{1/2}\beta) + (\mathcal{C}_\lambda^{1/2}\eta_s - \eta_s \mathcal{C}_\lambda^{1/2})\beta + \mathcal{K}_{2,\lambda}.$$

Making again use of Proposition 3.2.3 and Proposition 3.2.4 (ii) and employing Proposition 4.1.4 (iv) we deduce that $\mathcal{K}_{3,\lambda}$ is compact in $H^{1/2}(\Sigma;\mathbb{C}^4)$. Since $\eta_e^2 - \eta_s^2 \neq 4c^2$ by assumption, the multiplication operator $I_4 - \frac{1}{4c^2}(\eta_e^2 - \eta_s^2)$ is bijective in $H^{1/2}(\Sigma;\mathbb{C}^4)$. Hence, we have found

$$\big(I_4 + (\eta_e I_4 + \eta_s \beta)\mathcal{C}_\lambda^{1/2}\big)\big(I_4 - (\eta_e I_4 + \eta_s \beta)\mathcal{C}_\lambda^{1/2}\big) \\ = \frac{4c^2 - \eta_e^2 + \eta_s^2}{4c^2}\left(I_4 + \frac{4c^2}{4c^2 - \eta_e^2 + \eta_s^2}\mathcal{K}_{3,\lambda}\right).$$

The operator on the left hand side is injective, as $I_4 + (\eta_e I_4 + \eta_s \beta)\mathcal{C}_\lambda^{1/2}$ and $I_4 - (\eta_e I_4 + \eta_s \beta)\mathcal{C}_\lambda^{1/2}$ are injective; otherwise, one of the operators $T^\Sigma \restriction \ker\big(\Gamma_0^\Sigma \pm (\eta_e I_4 + \eta_s \beta)\Gamma_1^\Sigma\big)$ would have the eigenvalue λ, compare Theorem 2.2.6 (i), which is not the case by assumption. Hence, we obtain from Fredholm's alternative that

$$(I_4 + (\eta_e I_4 + \eta_s \beta)\mathcal{C}_\lambda^{1/2})(I_4 - (\eta_e I_4 + \eta_s \beta)\mathcal{C}_\lambda^{1/2})$$

is bijective in $H^{1/2}(\Sigma;\mathbb{C}^4)$. Therefore, we deduce finally

$$\operatorname{ran}(I_4 + (\eta_e I_4 + \eta_s \beta)\mathcal{C}_\lambda^{1/2}) \supset \operatorname{ran}\big[(I_4 + (\eta_e I_4 + \eta_s \beta)\mathcal{C}_\lambda^{1/2})(I_4 - (\eta_e I_4 + \eta_s \beta)\mathcal{C}_\lambda^{1/2})\big] \\ = H^{1/2}(\Sigma;\mathbb{C}^4),$$

that means $I_4 + (\eta_e I_4 + \eta_s \beta)\mathcal{C}_\lambda^{1/2}$ is also surjective. This finishes the proof of this proposition. □

In the next proposition we state that Φ_λ and $\mathcal{C}_\lambda$ are holomorphic and that their derivatives belong to certain (weak) Schatten-von Neumann classes. For the proof we make use of Proposition 2.6.2, which allows us to extend a similar result in [11, Lemma 4.5] that was only shown for C^∞-smooth surfaces. To make notations short, we use the shortcut $\mathfrak{S}_{p,\infty}$ for the weak Schatten-von Neumann ideals and omit the spaces; this will not cause any confusion.

Proposition 4.1.8. *Let $n \in \mathbb{N}$ and let $\Sigma \subset \mathbb{R}^3$ be the boundary of a compact C^n-smooth domain. Moreover, let for $\lambda \in \rho(A_0) = \mathbb{C} \setminus \big((-\infty, -mc^2] \cup [mc^2, \infty)\big)$ the operators Φ_λ and $\mathcal{C}_\lambda$ be defined as in* (3.16) *and* (3.17)*, respectively. Then, the following holds:*

(i) *The operator-valued functions* $\lambda \mapsto \Phi_\lambda$ *and* $\lambda \mapsto \Phi^*_{\overline{\lambda}}$ *are holomorphic and it holds for any* $k \in \{0,1,\dots,n-1\}$

$$\frac{\mathrm{d}^k}{\mathrm{d}\lambda^k}\Phi_\lambda \in \mathfrak{S}_{4/(2k+1),\infty} \quad \text{and} \quad \frac{\mathrm{d}^k}{\mathrm{d}\lambda^k}\Phi^*_{\overline{\lambda}} \in \mathfrak{S}_{4/(2k+1),\infty}.$$

In particular, Φ_λ *and* Φ^*_λ *are compact.*

(ii) *The operator-valued function* $\lambda \mapsto \mathcal{C}_\lambda$ *is holomorphic and it holds for any number* $k \in \{1,\dots,n-1\}$

$$\frac{\mathrm{d}^k}{\mathrm{d}\lambda^k}\mathcal{C}_\lambda \in \mathfrak{S}_{2/k,\infty}.$$

Moreover, the mapping $(-mc^2, mc^2) \ni \lambda \to \mathcal{C}_\lambda$ *is monotonously increasing.*

Proof. (i) We use that $\Phi^*_{\overline{\lambda}} = \gamma^\Sigma(\overline{\lambda})^* = \Gamma_1^\Sigma(A_0-\lambda)^{-1}$ which implies that $\Phi^*_{\overline{\lambda}}$ is holomorphic and

$$\frac{\mathrm{d}^k}{\mathrm{d}\lambda^k}\Phi^*_{\overline{\lambda}} = k!\Gamma_1^\Sigma(A_0-\lambda)^{-k-1},$$

see Proposition 2.2.3 (iii). Since $(-\Delta)^l(H^s(\mathbb{R}^3;\mathbb{C})) = H^{2l+s}(\mathbb{R}^3;\mathbb{C})$ for $s \geq 0$ it follows from (3.5) that $\operatorname{dom} A_0^{k+1} = H^{k+1}(\mathbb{R}^3;\mathbb{C}^4)$ and hence

$$\operatorname{ran}\frac{\mathrm{d}^k}{\mathrm{d}\lambda^k}\Phi^*_{\overline{\lambda}} = k!\operatorname{ran}\left[\Gamma_1^\Sigma(A_0-\lambda)^{-k-1}\right] = H^{k+1/2}(\Sigma;\mathbb{C}^4).$$

Therefore Proposition 2.6.2 yields

$$\frac{\mathrm{d}^k}{\mathrm{d}\lambda^k}\Phi^*_{\overline{\lambda}} = k!\Gamma_1^\Sigma(A_0-\lambda)^{-k-1} \in \mathfrak{S}_{4/(2k+1),\infty}.$$

From this, the statements on the differentiability of Φ_λ follow by taking adjoint.

To show item (ii) we recall that it holds by Proposition 2.2.4 (iv) for $\varphi \in H^{1/2}(\Sigma;\mathbb{C}^4)$

$$\frac{\mathrm{d}^k}{\mathrm{d}\lambda^k}\mathcal{C}_\lambda\varphi = \frac{\mathrm{d}^k}{\mathrm{d}\lambda^k}M^\Sigma(\lambda)\varphi = k!\Gamma_1^\Sigma(A_0-\lambda)^{-k}\gamma^\Sigma(\lambda)\varphi = k!\Gamma_1^\Sigma(A_0-\lambda)^{-k}\Phi_\lambda\varphi.$$

Taking closure this yields

$$\frac{\mathrm{d}^k}{\mathrm{d}\lambda^k}\mathcal{C}_\lambda = k!\Gamma_1^\Sigma(A_0-\lambda)^{-k}\Phi_\lambda = k\left(\frac{\mathrm{d}^{k-1}}{\mathrm{d}\lambda^{k-1}}\Phi^*_{\overline{\lambda}}\right)\Phi_\lambda.$$

Thus, item (i) and (2.42) show

$$\frac{\mathrm{d}^k}{\mathrm{d}\lambda^k}\mathcal{C}_\lambda \in \mathfrak{S}_{2/k,\infty}.$$

Finally, $\mathcal{C}_\lambda$ is monotonously increasing by Proposition 2.2.4 (iv) and a density argument. □

4.2 Dirac operators with singular interactions – definition and basic spectral properties for non-critical interaction strengths

In this section we define Dirac operators with electrostatic and Lorentz scalar δ-shell interactions supported on a compact C^2-smooth surface $\Sigma \subset \mathbb{R}^3$ via the quasi boundary triple $\{L^2(\Sigma;\mathbb{C}^4), \Gamma_0^\Sigma, \Gamma_1^\Sigma\}$ from Theorem 4.1.1. These Dirac operators are formally given by

$$A^\Sigma_{\eta_e,\eta_s} := -ic\alpha\cdot\nabla + mc^2\beta + \eta_e I_4 \delta_\Sigma + \eta_s \beta\delta_\Sigma,$$

where $\eta_e, \eta_s : \Sigma \to \mathbb{R}$ are Lipschitz continuous functions. First, we are going to show for non-critical interaction strengths, that means if $\eta_e(x)^2 - \eta_s(x)^2 \neq 4c^2$ for all $x \in \Sigma$, the self-adjointness of these operators and provide their basic spectral properties. In particular, in the physically interesting cases of purely electrostatic interactions, that means η_e is disjoint from $\pm 2c$ and $\eta_s = 0$, and of Dirac operators with purely scalar interactions, that means η_s is arbitrary and $\eta_e = 0$, we can give a more detailed picture in Corollary 4.2.5 and Corollary 4.2.6, respectively, below. The critical case is then treated in Section 4.3.

Let us start with the rigorous mathematical definition of $A^\Sigma_{\eta_e,\eta_s}$:

Definition 4.2.1. *Let $\{L^2(\Sigma;\mathbb{C}^4), \Gamma_0^\Sigma, \Gamma_1^\Sigma\}$ be the quasi boundary triple from Theorem 4.1.1 and let $\eta_e, \eta_s : \Sigma \to \mathbb{R}$ be Lipschitz continuous functions. Then we define the operator $A^\Sigma_{\eta_e,\eta_s} := T^\Sigma \upharpoonright \ker(\Gamma_0^\Sigma + (\eta_e I_4 + \eta_s\beta)\Gamma_1^\Sigma)$. This operator is given in a more explicit way by*

$$\begin{aligned} A^\Sigma_{\eta_e,\eta_s} f &:= (-ic\alpha\cdot\nabla + mc^2\beta) f_+ \oplus (-ic\alpha\cdot\nabla + mc^2\beta) f_-, \\ \mathrm{dom}\, A^\Sigma_{\eta_e,\eta_s} &:= \Big\{ f = f_+ \oplus f_- \in H^1(\Omega_+;\mathbb{C}^4) \oplus H^1(\Omega_-;\mathbb{C}^4) : \\ &\qquad ic(\alpha\cdot\nu)(f_+|_\Sigma - f_-|_\Sigma) = -\frac{1}{2}(\eta_e I_4 + \eta_s\beta)(f_+|_\Sigma + f_-|_\Sigma) \Big\}. \end{aligned} \tag{4.12}$$

Let us state an remark on the transmission condition which models the δ-shell interaction:

Remark 4.2.2. Another way to write $\big(\Gamma_0^\Sigma + (\eta_e I_4 + \eta_s\beta)\Gamma_1^\Sigma\big) f = 0$ is

$$\left(ic(\alpha\cdot\nu) + \frac{1}{2}(\eta_e I_4 + \eta_s\beta) \right) f_+|_\Sigma + \left(-ic(\alpha\cdot\nu) + \frac{1}{2}(\eta_e I_4 + \eta_s\beta) \right) f_-|_\Sigma = 0. \tag{4.13}$$

If $\eta_e(x)^2 - \eta_s(x)^2 \neq -4c^2$ for all $x \in \Sigma$, then the matrices $\pm ic(\alpha\cdot\nu) + \frac{1}{2}(\eta_e I_4 + \eta_s\beta)$ are invertible and

$$\left(\pm ic(\alpha\cdot\nu) + \frac{1}{2}(\eta_e I_4 + \eta_s\beta) \right)^{-1} = -\frac{4}{4c^2 + \eta_e^2 - \eta_s^2} \left(\pm ic(\alpha\cdot\nu) - \frac{1}{2}(\eta_e I_4 - \eta_s\beta) \right).$$

Setting

$$R^{\pm}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}} := -\left(\pm ic(\alpha\cdot\nu)+\frac{1}{2}(\eta_{\mathrm{e}}I_4+\eta_{\mathrm{s}}\beta)\right)^{-1}\left(\mp ic(\alpha\cdot\nu)+\frac{1}{2}(\eta_{\mathrm{e}}I_4+\eta_{\mathrm{s}}\beta)\right),$$

we see that in this case the transmission condition (4.13) can be rewritten as

$$f_{\pm}|_{\Sigma} = R^{\pm}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}} f_{\mp}|_{\Sigma}.$$

On the other hand, if $\eta_{\mathrm{e}}(x)^2-\eta_{\mathrm{s}}(x)^2=-4c^2$ for all $x\in\Sigma$, then (4.13) is equivalent to

$$\big(2cI_4 - i(\alpha\cdot\nu)(\eta_{\mathrm{e}}I_4+\eta_{\mathrm{s}}\beta)\big)f_+|_{\Sigma}=0, \quad \big(2cI_4 + i(\alpha\cdot\nu)(\eta_{\mathrm{e}}I_4+\eta_{\mathrm{s}}\beta)\big)f_-|_{\Sigma}=0, \quad (4.14)$$

that means that $A^{\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}}$ is decoupled to Dirac operators in $\Omega_{\pm}$ with the boundary conditions (4.14). This phenomenon is known as confinement, as a particle, which is initially located in $\Omega_{\pm}$ will stay in $\Omega_{\pm}$, and it is investigated in a more detailed way for constant η_{e} and η_{s} in [6, Section 5].

It follows immediately from Green's abstract identity that $A^{\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}}$ is symmetric for all real-valued Lipschitz continuous interaction strengths $\eta_{\mathrm{e}},\eta_{\mathrm{s}}$, compare (2.9). For non-critical interaction strengths, that means $\eta_{\mathrm{e}}^2-\eta_{\mathrm{s}}^2\neq 4c^2$, we prove in the following theorem self-adjointness, a Krein type resolvent formula and some basic spectral properties. The main tool to prove the self-adjointness is Proposition 4.1.7 which is only true, if $\eta_{\mathrm{e}}^2-\eta_{\mathrm{s}}^2\neq 4c^2$ everywhere on Σ. In fact, we will see in Proposition 4.3.1 that otherwise, for critical interaction strengths, the operator $A^{\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}}$ is not self-adjoint. I would like to thank Konstantin Pankrashkin for showing me an efficient way to prove item (iv) of the following theorem; a similar argument is used for instance in [48, Proposition 3.6].

Theorem 4.2.3. *Let $\eta_{\mathrm{e}},\eta_{\mathrm{s}}:\Sigma\to\mathbb{R}$ be Lipschitz continuous such that $\eta_{\mathrm{e}}(x)^2-\eta_{\mathrm{s}}(x)^2\neq 4c^2$ for all $x\in\Sigma$ and let $A^{\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}}$ be defined by* (4.12)*. Moreover, let A_0 be the free Dirac operator defined by* (3.3)*, let Φ_λ and $\mathcal{C}_\lambda$ be given by* (3.16) *and* (3.17)*, respectively, and let γ^{Σ} and M^{Σ} be as in Proposition 4.1.2. Then $A^{\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}}$ is self-adjoint and the following assertions hold:*

(i) *For $\lambda\in\mathbb{C}\setminus\mathbb{R}$ the resolvent of $A^{\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}}$ is given by*

$$\begin{aligned}(A^{\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}}-\lambda)^{-1} &= (A_0-\lambda)^{-1}-\Phi_\lambda\big(I_4+(\eta_{\mathrm{e}}I_4+\eta_{\mathrm{s}}\beta)\mathcal{C}_\lambda\big)^{-1}(\eta_{\mathrm{e}}I_4+\eta_{\mathrm{s}}\beta)\Phi^*_{\overline{\lambda}}\\ &= (A_0-\lambda)^{-1}-\gamma^{\Sigma}(\lambda)\big(I_4+(\eta_{\mathrm{e}}I_4+\eta_{\mathrm{s}}\beta)M^{\Sigma}(\lambda)\big)^{-1}(\eta_{\mathrm{e}}I_4+\eta_{\mathrm{s}}\beta)\gamma^{\Sigma}(\overline{\lambda})^*.\end{aligned}$$

(ii) $\sigma_{\mathrm{ess}}(A^{\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}})=(-\infty,-mc^2]\cup[mc^2,\infty)$.

(iii) $\lambda\in\sigma_{\mathrm{p}}(A^{\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}})$ *if and only if* $-1\in\sigma_{\mathrm{p}}((\eta_{\mathrm{e}}I_4+\eta_{\mathrm{s}}\beta)M^{\Sigma}(\lambda))$.

(iv) $\sigma_{\mathrm{p}}(A^{\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}})$ *is finite.*

(v) *There exists a constant* $K > 0$ *such that* $\sigma_\mathrm{p}(A^\Sigma_{\eta_\mathrm{e},\eta_\mathrm{s}}) = \emptyset$, *if* $|\eta_\mathrm{e}(x)I_4 + \eta_\mathrm{s}(x)\beta| < K$ *for all* $x \in \Sigma$.

Proof. First we prove the self-adjointness of $A^\Sigma_{\eta_\mathrm{e},\eta_\mathrm{s}}$. Due to Green's identity it is clear that $A^\Sigma_{\eta_\mathrm{e},\eta_\mathrm{s}}$ is symmetric, compare (2.9). Thus, it suffices to prove $\operatorname{ran}(A^\Sigma_{\eta_\mathrm{e},\eta_\mathrm{s}} - \lambda) = L^2(\mathbb{R}^3;\mathbb{C}^4)$ for $\lambda \in \mathbb{C}\setminus\mathbb{R}$.

Let $f \in L^2(\mathbb{R}^3;\mathbb{C}^4)$ and $\lambda \in \mathbb{C}\setminus\mathbb{R}$ be fixed. Then, by Theorem 2.2.6 (ii) we have $f \in \operatorname{ran}(A^\Sigma_{\eta_\mathrm{e},\eta_\mathrm{s}} - \lambda)$ if and only if $(\eta_\mathrm{e}I_4 + \eta_\mathrm{s}\beta)\gamma^\Sigma(\overline{\lambda})^* f \in \operatorname{ran}(I_4 - (\eta_\mathrm{e}I_4 + \eta_\mathrm{s}\beta)M^\Sigma(\lambda))$. Since $\gamma^\Sigma(\overline{\lambda})^* = \Gamma^\Sigma_1(A_0 - \lambda)^{-1}$, see Proposition 2.2.3 (iii), and $\operatorname{dom} A_0 = H^1(\mathbb{R}^3;\mathbb{C}^4)$ we deduce from Lemma 2.5.1 that $\operatorname{ran}\big((\eta_\mathrm{e}I_4 + \eta_\mathrm{s}\beta)\gamma^\Sigma(\overline{\lambda})^*\big) \subset H^{1/2}(\Sigma;\mathbb{C}^4)$. On the other hand by Proposition 4.1.7 the operator

$$I_4 + (\eta_\mathrm{e}I_4 + \eta_\mathrm{s}\beta)M^\Sigma(\lambda) = I_4 + (\eta_\mathrm{e}I_4 + \eta_\mathrm{s}\beta)\mathcal{C}^{1/2}_\lambda$$

is bijective in $H^{1/2}(\Sigma;\mathbb{C}^4)$. Thus, we get that $f \in \operatorname{ran}(A^\Sigma_{\eta_\mathrm{e},\eta_\mathrm{s}} - \lambda)$. Since $f \in L^2(\mathbb{R}^3;\mathbb{C}^4)$ was arbitrary, it follows that $A^\Sigma_{\eta_\mathrm{e},\eta_\mathrm{s}} - \lambda$ is bijective and hence, that $A^\Sigma_{\eta_\mathrm{e},\eta_\mathrm{s}}$ is self-adjoint.

Next, the Krein-type resolvent formula follows directly from Theorem 2.2.6 and Proposition 4.1.2.

In order to show item (ii) we note that for $\lambda \in \mathbb{C}\setminus\mathbb{R}$ all operators Φ_λ, $\eta_\mathrm{e}I_4 + \eta_\mathrm{s}\beta$, $\Phi^*_{\overline{\lambda}}$, and $\big(I_4 + (\eta_\mathrm{e}I_4 + \eta_\mathrm{s}\beta)\mathcal{C}_\lambda\big)^{-1}$ are bounded in the respective L^2-spaces by Proposition 3.2.1, Lemma 2.5.1 and Proposition 4.1.7. Moreover, Φ_λ is compact by Proposition 4.1.8. This and assertion (i) show now that

$$(A^\Sigma_{\eta_\mathrm{e},\eta_\mathrm{s}} - \lambda)^{-1} - (A_0 - \lambda)^{-1} = -\Phi_\lambda\big(I_4 + (\eta_\mathrm{e}I_4 + \eta_\mathrm{s}\beta)\mathcal{C}_\lambda\big)^{-1}(\eta_\mathrm{e}I_4 + \eta_\mathrm{s}\beta)\Phi^*_{\overline{\lambda}}$$

is compact. Therefore $\sigma_\mathrm{ess}(A^\Sigma_{\eta_\mathrm{e},\eta_\mathrm{s}}) = \sigma_\mathrm{ess}(A_0) = (-\infty, -mc^2] \cup [mc^2, \infty)$.

Assertion (iii) is just an application of Theorem 2.2.6 (i).

In order to verify statement (iv) we note first that the number of discrete eigenvalues of $A^\Sigma_{\eta_\mathrm{e},\eta_\mathrm{s}}$ in the gap $(-mc^2, mc^2)$ is equal to the number of eigenvalues of $(A^\Sigma_{\eta_\mathrm{e},\eta_\mathrm{s}})^2$ below the threshold of its essential spectrum $(mc^2)^2$. Let us denote the quadratic form associated to $(A^\Sigma_{\eta_\mathrm{e},\eta_\mathrm{s}})^2$ by $\mathfrak{a}$. Then it holds for any $f = f_+ \oplus f_- \in \operatorname{dom} A^\Sigma_{\eta_\mathrm{e},\eta_\mathrm{s}} = \operatorname{dom}\mathfrak{a}$

$$\begin{aligned}
\mathfrak{a}[f] = \|A^\Sigma_{\eta_\mathrm{e},\eta_\mathrm{s}} f\|^2_{\mathbb{R}^3} &= \big\|(-ic\alpha\cdot\nabla + mc^2\beta)f_+\big\|^2_{\Omega_+} + \big\|(-ic\alpha\cdot\nabla + mc^2\beta)f_-\big\|^2_{\Omega_-} \\
&= \|c(\alpha\cdot\nabla)f_+\|^2_{\Omega_+} + \|c(\alpha\cdot\nabla)f_-\|^2_{\Omega_-} + (mc^2)^2\|f\|^2_{\mathbb{R}^3} \\
&\quad + (-ic\alpha\cdot\nabla f_+, mc^2\beta f_+)_{\Omega_+} + (mc^2\beta f_+, -ic\alpha\cdot\nabla f_+)_{\Omega_+} \\
&\quad + (-ic\alpha\cdot\nabla f_-, mc^2\beta f_-)_{\Omega_-} + (mc^2\beta f_-, -ic\alpha\cdot\nabla f_-)_{\Omega_-}.
\end{aligned}$$

Employing integration by parts we see that

$$(-ic\alpha\cdot\nabla f_\pm, mc^2\beta f_\pm)_{\Omega_\pm} + (mc^2\beta f_\pm, -ic\alpha\cdot\nabla f_\pm)_{\Omega_\pm} = \mp(ic\alpha\cdot\nu f_\pm|_\Sigma, mc^2\beta f_\pm|_\Sigma)_\Sigma,$$

which yields then

$$\begin{aligned}\mathfrak{a}[f] &= \|c(\alpha\cdot\nabla)f\|^2_{\Omega_+\cup\Omega_-} + (mc^2)^2\|f\|^2_{\mathbb{R}^3}\\ &\quad - (ic\alpha\cdot\nu f_+|_\Sigma, mc^2\beta f_+|_\Sigma)_\Sigma + (ic\alpha\cdot\nu f_-|_\Sigma, mc^2\beta f_-|_\Sigma)_\Sigma.\end{aligned}\tag{4.15}$$

Choose $R>0$ such that $\Sigma\subset B(0,R)$. Then, we see that the quadratic form associated to $(A^\Sigma_{\eta_e,\eta_s})^2$ is minorated by the closed quadratic form $\mathfrak{b} := \mathfrak{b}_{\text{int}}\oplus\mathfrak{b}_{\text{ext}}$, where

$$\begin{aligned}\mathfrak{b}_{\text{int}}[f] &:= \|c(\alpha\cdot\nabla)f\|^2_{\Omega_+\cup(\Omega_-\cap B(0,R))} + (mc^2)^2\|f\|^2_{B(0,R)}\\ &\qquad - (ic\alpha\cdot\nu f_+|_\Sigma, mc^2\beta f_+|_\Sigma)_\Sigma + (ic\alpha\cdot\nu f_-|_\Sigma, mc^2\beta f_-|_\Sigma)_\Sigma,\\ \operatorname{dom}\mathfrak{b}_{\text{int}} &:= \Big\{ f = f_+\oplus f_- \in H^1(\Omega_+;\mathbb{C}^4)\oplus H^1(\Omega_-\cap B(0,R);\mathbb{C}^4):\\ &\qquad ic(\alpha\cdot\nu)(f_+|_\Sigma - f_-|_\Sigma) = -\frac{1}{2}(\eta_e I_4 + \eta_s\beta)(f_+|_\Sigma - f_-|_\Sigma)\Big\},\end{aligned}$$

and

$$\begin{aligned}\mathfrak{b}_{\text{ext}}[f] &:= \|c(\alpha\cdot\nabla)f\|^2_{\mathbb{R}^3\setminus B(0,R)} + (mc^2)^2\|f\|^2_{\mathbb{R}^3\setminus B(0,R)},\\ \operatorname{dom}\mathfrak{b}_{\text{ext}} &:= H^1(\mathbb{R}^3\setminus B(0,R);\mathbb{C}^4).\end{aligned}$$

Then it holds $\mathfrak{b}\le\mathfrak{a}$ in the sense of quadratic forms. In particular, if the operator associated to $\mathfrak{b}$ has finitely many eigenvalues below $(mc^2)^2$, then $(A^\Sigma_{\eta_e,\eta_s})^2$ has only finitely many eigenvalues below $(mc^2)^2$.

Clearly, the operator B_{ext} associated to $\mathfrak{b}_{\text{ext}}$ is a shifted Neumann Laplacian and hence $B_{\text{ext}}\ge(mc^2)^2$. Thus, the number of eigenvalues of $(A^\Sigma_{\eta_e,\eta_s})^2$ below $(mc^2)^2$ is equal to the number of eigenvalues of the operator B_{int} associated to the semibounded and closed form $\mathfrak{b}_{\text{int}}$, compare for instance [62, Section XIII.15] for a similar argument. Moreover, as $\operatorname{dom}\mathfrak{b}_{\text{int}}\subset H^1(\Omega_+;\mathbb{C}^4)\oplus H^1(B(0,R)\cap\Omega_-;\mathbb{C}^4)$ is compactly embedded in $L^2(B(0,R);\mathbb{C}^4)$ it follows that the resolvent of B_{int} is compact. Therefore, the spectrum of B_{int} is purely discrete and consists of eigenvalues that accumulate only at ∞, as B_{int} is bounded from below. Thus B_{int} has only finitely many eigenvalues below $(mc^2)^2$. Hence, also the operator associated to $\mathfrak{b}$ has only finitely many eigenvalues below $(mc^2)^2$. This shows finally that $(A^\Sigma_{\eta_e,\eta_s})^2$ has only finitely many eigenvalues below $(mc^2)^2$ which finishes the proof of assertion (iv).

Finally, item (v) is just a simple consequence of the Birman-Schwinger principle in (iii) and Proposition 3.2.2. □

In the following corollary we state several consequences of the Birman-Schwinger principle from Theorem 4.2.3 (iii).

Corollary 4.2.4. *Let* $\eta_e, \eta_s : \Sigma \to \mathbb{R}$ *be Lipschitz continuous such that* $\eta_e(x)^2 - \eta_s(x)^2 \notin \{0, 4c^2\}$ *for all* $x \in \Sigma$ *and let* $A^\Sigma_{\eta_e,\eta_s}$ *be defined by* (4.12). *Then the following is true:*

(i) $\lambda \in \sigma_p(A^\Sigma_{\eta_e,\eta_s})$ *if and only if* $\lambda \in \sigma_p\big(A^\Sigma_{-4c^2\eta_e/(\eta_e^2-\eta_s^2),-4c^2\eta_s/(\eta_e^2-\eta_s^2)}\big)$*;*

(ii) *There exists some* $K > 4c^2$ *such that* $\sigma_p(A^\Sigma_{\eta_e,\eta_s}) = \emptyset$*, if* $|\eta_e(x) \pm \eta_s(x)| \geq K$ *for all* $x \in \Sigma$*.*

Proof. According to Theorem 4.2.3 (iii) a number λ is an eigenvalue of $A^\Sigma_{\eta_e,\eta_s}$ if and only if -1 is an eigenvalue of $(\eta_e I_4 + \eta_s\beta)M^\Sigma(\lambda)$, that means if and only if there exists a function $0 \neq \varphi \in \operatorname{dom} M^\Sigma(\lambda) = H^{1/2}(\Sigma;\mathbb{C}^4)$ such that

$$0 = (I_4 + (\eta_e I_4 + \eta_s\beta)M^\Sigma(\lambda))\varphi = (I_4 + (\eta_e I_4 + \eta_s\beta)\mathcal{C}_\lambda)\varphi.$$

Multiplying this equation with $(\eta_e I_4 + \eta_s\beta)^{-1} = \frac{1}{\eta_e^2-\eta_s^2}(\eta_e I_4 - \eta_s\beta)$, which is a bounded operator in $H^{1/2}(\Sigma;\mathbb{C}^4)$ due to the assumptions of this corollary, yields

$$0 = \left(\frac{1}{\eta_e^2-\eta_s^2}(\eta_e I_4 - \eta_s\beta) + \mathcal{C}_\lambda\right)\varphi.$$

Using $-4c^2(\alpha\cdot\nu\mathcal{C}_\lambda)^2 = I_4$, see Proposition 3.2.1, and the anti-commutation relation (1.2) we see that the last equation can be rewritten as

$$\begin{aligned} 0 &= \left(-4c^2\frac{1}{\eta_e^2-\eta_s^2}(\eta_e I_4 - \eta_s\beta)(\alpha\cdot\nu\mathcal{C}_\lambda)^2 + (\alpha\cdot\nu)^2\mathcal{C}_\lambda\right)\varphi \\ &= \left(-4c^2\frac{1}{\eta_e^2-\eta_s^2}(\eta_e I_4 - \eta_s\beta)(\alpha\cdot\nu)\mathcal{C}_\lambda + \alpha\cdot\nu\right)(\alpha\cdot\nu)\mathcal{C}_\lambda\varphi \\ &= (\alpha\cdot\nu)\left(-4c^2\frac{1}{\eta_e^2-\eta_s^2}(\eta_e I_4 + \eta_s\beta)\mathcal{C}_\lambda + I_4\right)(\alpha\cdot\nu)\mathcal{C}_\lambda\varphi. \end{aligned}$$

Because of the mapping properties of $\mathcal{C}_\lambda$ from Proposition 4.1.6 and the regularity of Σ we see that $0 \neq (\alpha\cdot\nu)\mathcal{C}_\lambda\varphi \in H^{1/2}(\Sigma;\mathbb{C}^4)$. By the Birman-Schwinger principle this can only be true if and only if $\lambda \in \sigma_p\big(A^\Sigma_{-4c^2\eta_e/(\eta_e^2-\eta_s^2),-4c^2\eta_s/(\eta_e^2-\eta_s^2)}\big)$.

Item (ii) follows now directly from assertion (i) and Theorem 4.2.3 (v). □

In the cases of purely electrostatic and purely scalar interactions one can give a more detailed picture of the spectral properties of the associated Dirac operators and many of the previously shown results simplify significantly. First we reformulate these statements for Dirac operators with purely electrostatic δ-shell interactions, that means we assume $\eta_s \equiv 0$. Then the corollary below follows immediately from Theorem 4.2.3 and Corollary 4.2.4:

Corollary 4.2.5. *Let $\eta_e : \Sigma \to \mathbb{R}$ be Lipschitz continuous such that $\eta_e(x) \neq \pm 2c$ for all $x \in \Sigma$ and let the self-adjoint operator $A^\Sigma_{\eta_e,0}$ be defined by* (4.12). *Moreover, let A_0 be the free Dirac operator defined by* (3.3)*, let Φ_λ and $\mathcal{C}_\lambda$ be given by* (3.16) *and* (3.17)*, respectively, and let γ^Σ and M^Σ be given as in Proposition 4.1.2. Then the following assertions hold:*

(i) *For $\lambda \in \mathbb{C} \setminus \mathbb{R}$ the resolvent of $A^\Sigma_{\eta_e,0}$ is given by*

$$\begin{aligned}(A^\Sigma_{\eta_e,0} - \lambda)^{-1} &= (A_0 - \lambda)^{-1} - \gamma^\Sigma(\lambda)\big(I_4 + \eta_e M^\Sigma(\lambda)\big)^{-1}\eta_e \gamma^\Sigma(\overline{\lambda})^* \\ &= (A_0 - \lambda)^{-1} - \Phi_\lambda\big(I_4 + \eta_e \mathcal{C}_\lambda\big)^{-1}\eta_e \Phi^*_{\overline{\lambda}}.\end{aligned}$$

(ii) $\sigma_{\mathrm{ess}}(A^\Sigma_{\eta_e,0}) = (-\infty, -mc^2] \cup [mc^2, \infty)$.

(iii) $\lambda \in \sigma_{\mathrm{p}}(A^\Sigma_{\eta_e,0})$ *if and only if* $-1 \in \sigma_{\mathrm{p}}(\eta_e M^\Sigma(\lambda))$.

(iv) *If $|\eta_e(x)| > 0$ for all $x \in \Sigma$, then $\lambda \in \sigma_{\mathrm{p}}(A^\Sigma_{\eta_e,0})$ if and only if $\lambda \in \sigma_{\mathrm{p}}\big(A^\Sigma_{-4c^2/\eta_e,0}\big)$.*

(v) $\sigma_{\mathrm{p}}(A^\Sigma_{\eta_e,0})$ *is finite.*

(vi) *There exists a constant $K > 0$ such that $\sigma_{\mathrm{p}}(A^\Sigma_{\eta_e,0}) = \emptyset$, if either $|\eta_e(x)| < K$ or $|\eta_e(x)| \geq \frac{4c^2}{K}$ for all $x \in \Sigma$.*

Next, let us discuss Dirac operators with purely Lorentz scalar δ-shell interactions, that means we assume $\eta_e \equiv 0$. Note that in this case there is no critical interaction strength, as $\eta_s^2 \neq -4c^2$ always in this case. On the other hand we have for $\eta_s \equiv \pm 2c$ confinement, compare Remark 4.2.2. For purely scalar interactions many of the spectral properties of $A^\Sigma_{\eta_e,\eta_s}$ from Theorem 4.2.3 simplify and we have some additional interesting symmetry relations in the spectrum. Most of the results are also formulated in [48, Theorem 2.3].

Corollary 4.2.6. *Let $\eta_s : \Sigma \to \mathbb{R}$ be Lipschitz continuous and let the self-adjoint operator A^Σ_{0,η_s} be defined by* (4.12)*. Moreover, let A_0 be the free Dirac operator defined by* (3.3)*, let Φ_λ and $\mathcal{C}_\lambda$ be given by* (3.16) *and* (3.17)*, respectively, and let γ^Σ and M^Σ be given as in Proposition 4.1.2. Then the following assertions hold:*

(i) *For $\lambda \in \mathbb{C} \setminus \mathbb{R}$ the resolvent of A^Σ_{0,η_s} is given by*

$$\begin{aligned}(A^\Sigma_{0,\eta_s} - \lambda)^{-1} &= (A_0 - \lambda)^{-1} - \gamma^\Sigma(\lambda)\big(I_4 + \eta_s \beta M^\Sigma(\lambda)\big)^{-1}\eta_s \beta \gamma^\Sigma(\overline{\lambda})^* \\ &= (A_0 - \lambda)^{-1} - \Phi_\lambda\big(I_4 + \eta_s \beta \mathcal{C}_\lambda\big)^{-1}\eta_s \beta \Phi^*_{\overline{\lambda}}.\end{aligned}$$

(ii) $\sigma_{\mathrm{ess}}(A^\Sigma_{0,\eta_s}) = (-\infty, -mc^2] \cup [mc^2, \infty)$*;*

(iii) $\sigma_{\mathrm{p}}(A^\Sigma_{0,\eta_s})$ *is finite.*

(iv) $\lambda \in \sigma(A^{\Sigma}_{0,\eta_s})$ *if and only if* $-\lambda \in \sigma(A^{\Sigma}_{0,\eta_s})$.

(v) *Discrete eigenvalues of* A^{Σ}_{0,η_s} *have always even multiplicity.*

(vi) *If* $\eta_s(x) \geq 0$ *for all* $x \in \Sigma$*, then* $\sigma_p(A^{\Sigma}_{0,\eta_s}) = \emptyset$.

(vii) $\lambda \in \sigma_p(A^{\Sigma}_{0,\eta_s})$ *if and only if* $-1 \in \sigma_p(\eta_s \beta M^{\Sigma}(\lambda))$.

(viii) *If* $|\eta_s(x)| > 0$ *for all* $x \in \Sigma$*, then* $\lambda \in \sigma_p(A^{\Sigma}_{0,\eta_s})$ *if and only if* $\lambda \in \sigma_p\big(A^{\Sigma}_{0,4c^2/\eta_s}\big)$.

(ix) *There exists a constant* $K > 0$ *such that* $\sigma_p(A^{\Sigma}_{0,\eta_s}) = \emptyset$*, if* $|\eta_s(x)| < K$ *or* $|\eta_s(x)| \geq \frac{4c^2}{K}$ *for all* $x \in \Sigma$.

Proof. The results in items (i)–(iii) and (vii)–(ix) are special cases of Theorem 4.2.3 and Corollary 4.2.4 for $\eta_e \equiv 0$. It remains to show assertion (iv)–(vi).

First, to prove statement (iv) it is sufficient to verify the symmetry of the discrete spectrum, as $\sigma_{ess}(A^{\Sigma}_{0,\eta_s}) = (-\infty, -mc^2] \cup [mc^2, \infty)$ by (ii). Define the (nonlinear) charge conjugation operator

$$Cf := i\beta\alpha_2\overline{f}, \qquad f \in L^2(\mathbb{R}^3;\mathbb{C}^4).$$

A simple calculation using $\overline{\alpha_2} = -\alpha_2$ (where the complex conjugate is understood component wise) shows $C^2 f = f$. Moreover, it is not difficult to see that $f \in \operatorname{dom} A^{\Sigma}_{0,\eta_s}$ if and only if $Cf \in \operatorname{dom} A^{\Sigma}_{0,\eta_s}$. Eventually, employing (1.2) we get

$$\begin{aligned}(-ic\alpha\cdot\nabla + mc^2\beta)Cf &= (-ic\alpha\cdot\nabla + mc^2\beta)i\beta\alpha_2\overline{f} \\ &= i\beta\alpha_2(-ic\overline{\alpha}\cdot\nabla - mc^2\beta)\overline{f} = -C\big((-ic\alpha\cdot\nabla + mc^2\beta)f\big).\end{aligned} \tag{4.16}$$

Hence, we deduce $A^{\Sigma}_{0,\eta_s}C = -CA^{\Sigma}_{0,\eta_s}$. This yields then the claim of item (iv).

For the proof of statement (v) we employ a similar idea and define the (nonlinear) time reversal operator

$$Tf := -i\gamma_5\alpha_2\overline{f}, \qquad f \in L^2(\mathbb{R}^3;\mathbb{C}^4), \quad \gamma_5 := \begin{pmatrix} 0 & I_2 \\ I_2 & 0 \end{pmatrix}.$$

Note that we have $\beta\gamma_5 = -\gamma_5\beta$ and $(\alpha\cdot x)\gamma_5 = \gamma_5(\alpha\cdot x)$ for any $x \in \mathbb{R}^3$. Similarly as above we have $f \in \operatorname{dom} A^{\Sigma}_{0,\eta_s}$ if and only if $Tf \in \operatorname{dom} A^{\Sigma}_{0,\eta_s}$ and $T^2 = -I_4$. Furthermore, a similar calculation as in (4.16) shows

$$(-ic\alpha\cdot\nabla + mc^2\beta)Tf = T(-ic\alpha\cdot\nabla + mc^2\beta)f,$$

which yields $A^{\Sigma}_{0,\eta_s}T = TA^{\Sigma}_{0,\eta_s}$. Another calculation gives $\langle -i\gamma_5\alpha_2\overline{f}, f\rangle_{\mathbb{C}^4} = \overline{\langle f, i\gamma_5\alpha_2\overline{f}\rangle_{\mathbb{C}^4}}$ which implies

$$(Tf,f)_{\mathbb{R}^3} = \int_{\mathbb{R}^3} Tf(x)\cdot\overline{f(x)}\mathrm{d}x = 0.$$

Hence, if f is an eigenfunction of A^{Σ}_{0,η_s}, then also Tf is a linearly independent and non-trivial eigenfunction of A^{Σ}_{0,η_s}. Therefore, also assertion (v) is proven.

Finally, to show item (vi) we note first that we have for any $f = f_+ \oplus f_- \in \operatorname{dom} A^{\Sigma}_{0,\eta_s}$ by (4.15)

$$\begin{aligned}
\|A^{\Sigma}_{0,\eta_s} f\|^2_{\mathbb{R}^3} &= \|c(\alpha\cdot\nabla)f_+\|^2_{\Omega_+\cup\Omega_-} + (mc^2)^2\|f\|^2_{\mathbb{R}^3} \\
&\qquad - (ic\alpha\cdot\nu f_+|_\Sigma, mc^2\beta f_+|_\Sigma)_\Sigma + (ic\alpha\cdot\nu f_-|_\Sigma, mc^2\beta f_-|_\Sigma)_\Sigma \\
&= \|c(\alpha\cdot\nabla)f_+\|^2_{\Omega_+\cup\Omega_-} + (mc^2)^2\|f\|^2_{\mathbb{R}^3} \\
&\qquad - \big(ic\alpha\cdot\nu(f_+|_\Sigma - f_-|_\Sigma), mc^2\beta(f_+|_\Sigma + f_-|_\Sigma)\big)_\Sigma \\
&\qquad + (ic\alpha\cdot\nu f_+|_\Sigma, mc^2\beta f_-|_\Sigma)_\Sigma - (ic\alpha\cdot\nu f_-|_\Sigma, mc^2\beta f_+|_\Sigma)_\Sigma.
\end{aligned}$$

Using the transmission condition $-ic\alpha\cdot\nu(f_+|_\Sigma - f_-|_\Sigma) = \frac{\eta_s}{2}(f_+|_\Sigma + f_-|_\Sigma)$ and (1.2), we see

$$-\big(ic\alpha\cdot\nu(f_+|_\Sigma - f_-|_\Sigma), mc^2\beta(f_+|_\Sigma + f_-|_\Sigma)\big)_\Sigma = \frac{1}{2}\big(\eta_s(f_+|_\Sigma + f_-|_\Sigma), mc^2(f_+|_\Sigma + f_-|_\Sigma)\big)_\Sigma.$$

In particular, due to the assumption $\eta_s \geq 0$ this is a non-negative real number. Moreover, employing again (1.2) we get

$$(ic\alpha\cdot\nu f_+|_\Sigma, mc^2\beta f_-|_\Sigma)_\Sigma - (ic\alpha\cdot\nu f_-|_\Sigma, mc^2\beta f_+|_\Sigma)_\Sigma = 2i\operatorname{Im}(ic\alpha\cdot\nu f_+|_\Sigma, mc^2\beta f_-|_\Sigma)_\Sigma.$$

This leads to

$$\begin{aligned}
\|A^{\Sigma}_{0,\eta_s} f\|^2_{\mathbb{R}^3} &= \|c(\alpha\cdot\nabla)f_+\|^2_{\Omega_+\cup\Omega_-} + (mc^2)^2\|f\|^2_{\mathbb{R}^3} \\
&\qquad + \frac{1}{2}\big(\eta_s(f_+|_\Sigma + f_-|_\Sigma), mc^2\beta(f_+|_\Sigma + f_-|_\Sigma)\big)_\Sigma + 2i\operatorname{Im}(ic\alpha\cdot\nu f_+|_\Sigma, mc^2\beta f_-|_\Sigma)_\Sigma.
\end{aligned}$$

As all other terms in the last equation are real, we conclude $i\operatorname{Im}(ic\alpha\cdot\nu f_+|_\Sigma, mc^2\beta f_-|_\Sigma)_\Sigma = 0$ and thus, using $\eta_s \geq 0$

$$\begin{aligned}
\|A^{\Sigma}_{0,\eta_s} f\|^2_{\mathbb{R}^3} &= \|c(\alpha\cdot\nabla)f_+\|^2_{\Omega_+\cup\Omega_-} + (mc^2)^2\|f\|^2_{\mathbb{R}^3} \\
&\qquad + \frac{1}{2}\big(\eta_s(f_+|_\Sigma + f_-|_\Sigma), mc^2\beta(f_+|_\Sigma + f_-|_\Sigma)\big)_\Sigma \\
&\geq (mc^2)^2\|f\|^2_{\mathbb{R}^3}.
\end{aligned}$$

Therefore A^{Σ}_{0,η_s} can not have eigenvalues in $(-mc^2, mc^2)$. □

Next, we prove that the difference of the l-th power of the resolvent of the free Dirac operator and of $A^{\Sigma}_{\eta_e,\eta_s}$ belongs to a certain weak Schatten-von Neumann ideal. The proof of the following theorem is based on Proposition 4.1.8. Hence, we have to assume some additional smoothness of Σ.

Theorem 4.2.7. *Let $l \in \mathbb{N}$ be fixed and assume here additionally that Σ is C^l-smooth. Let $\eta_e, \eta_s : \Sigma \to \mathbb{R}$ be Lipschitz continuous such that $\eta_e(x)^2 - \eta_s(x)^2 \neq 4c^2$ for all $x \in \Sigma$ and let $A^\Sigma_{\eta_e,\eta_s}$ be defined by* (4.12). *Moreover, let A_0 be the free Dirac operator given by* (3.3). *Then it holds for any $\lambda \in \mathbb{C} \setminus \mathbb{R}$*

$$(A^\Sigma_{\eta_e,\eta_s} - \lambda)^{-l} - (A_0 - \lambda)^{-l} \in \mathfrak{S}_{2/l,\infty}.$$

Proof. Let $l \in \mathbb{N}$ and $\lambda \in \mathbb{C} \setminus \mathbb{R}$ be fixed. For convenience we set $\eta := \eta_e I_4 + \eta_s \beta$. Using the resolvent formula from Theorem 4.2.3 (i) and (2.1) we get

$$\begin{aligned}(A^\Sigma_{\eta_e,\eta_s} - \lambda)^{-l} - (A_0 - \lambda)^{-l} &= \frac{1}{(l-1)!}\frac{\mathrm{d}^{l-1}}{\mathrm{d}\lambda^{l-1}}\big((A^\Sigma_{\eta_e,\eta_s} - \lambda)^{-1} - (A_0 - \lambda)^{-1}\big) \\ &= -\frac{1}{(l-1)!}\frac{\mathrm{d}^{l-1}}{\mathrm{d}\lambda^{l-1}}\big(\Phi_\lambda \big(I_4 + \eta \mathcal{C}_\lambda\big)^{-1} \eta \Phi^*_{\bar\lambda}\big) \\ &= -\sum_{p+q+r=l-1} \frac{1}{p!q!r!}\frac{\mathrm{d}^p}{\mathrm{d}\lambda^p}\Phi_\lambda \frac{\mathrm{d}^q}{\mathrm{d}\lambda^q}\big(I_4 + \eta \mathcal{C}_\lambda\big)^{-1} \eta \frac{\mathrm{d}^r}{\mathrm{d}\lambda^r}\Phi^*_{\bar\lambda}.\end{aligned} \tag{4.17}$$

We know from Proposition 4.1.8 that

$$\frac{\mathrm{d}^p}{\mathrm{d}\lambda^p}\Phi_\lambda \in \mathfrak{S}_{4/(2p+1),\infty} \quad \text{and} \quad \frac{\mathrm{d}^r}{\mathrm{d}\lambda^r}\Phi^*_{\bar\lambda} \in \mathfrak{S}_{4/(2r+1),\infty}. \tag{4.18}$$

Furthermore, Proposition 4.1.7 yields $\big(I_4 + \eta \mathcal{C}_\lambda\big)^{-1} \in \mathcal{B}$. Eventually, we claim for $q \in \{1, \dots, l-1\}$

$$\frac{\mathrm{d}^q}{\mathrm{d}\lambda^q}\big(I_4 + \eta \mathcal{C}_\lambda\big)^{-1} \in \mathfrak{S}_{2/q,\infty}. \tag{4.19}$$

This claim will be shown by induction.

Employing identity (2.2), Proposition 2.2.4 (iv), and (2.42) we get for $q = 1$

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}\lambda}(I_4 + \eta \mathcal{C}_\lambda)^{-1} &= -(I_4 + \eta \mathcal{C}_\lambda)^{-1} \eta \frac{\mathrm{d}}{\mathrm{d}\lambda}\mathcal{C}_\lambda (I_4 + \eta \mathcal{C}_\lambda)^{-1} \\ &= -(I_4 + \eta \mathcal{C}_\lambda)^{-1} \eta \Phi^*_{\bar\lambda}\Phi_\lambda (I_4 + \eta \mathcal{C}_\lambda)^{-1} \in \mathfrak{S}_{2,\infty}.\end{aligned}$$

So let us assume now that the statement is true for $k = 1, \dots, q$. With the aid of (2.1) we get

$$\begin{aligned}\frac{\mathrm{d}^{q+1}}{\mathrm{d}\lambda^{q+1}}(1 + \eta \mathcal{C}_\lambda)^{-1} &= \frac{\mathrm{d}^q}{\mathrm{d}\lambda^q}\left[\frac{\mathrm{d}}{\mathrm{d}\lambda}(I_4 + \eta \mathcal{C}_\lambda)^{-1}\right] \\ &= -\frac{\mathrm{d}^q}{\mathrm{d}\lambda^q}\left[(I_4 + \eta \mathcal{C}_\lambda)^{-1} \eta \Phi^*_{\bar\lambda}\Phi_\lambda (I_4 + \eta \mathcal{C}_\lambda)^{-1}\right] \\ &= -\sum_{k+m+n=q} \frac{q!}{k!m!n!}\frac{\mathrm{d}^k}{\mathrm{d}\lambda^k}(1 + \eta \mathcal{C}_\lambda)^{-1} \eta \frac{\mathrm{d}^m}{\mathrm{d}\lambda^m}\big(\Phi^*_{\bar\lambda}\Phi_\lambda\big)\frac{\mathrm{d}^n}{\mathrm{d}\lambda^n}(I_4 + \eta \mathcal{C}_\lambda)^{-1}.\end{aligned}$$

From (2.1) (with $C(\lambda) = I_4$) and Proposition 4.1.8 (i) we deduce

$$\frac{\mathrm{d}^m}{\mathrm{d}\lambda^m}\big(\Phi_{\bar{\lambda}}^*\Phi_\lambda\big) = \sum_{s+t=m} \frac{m!}{s!t!}\frac{\mathrm{d}^s}{\mathrm{d}\lambda^s}\Phi_{\bar{\lambda}}^*\frac{\mathrm{d}^t}{\mathrm{d}\lambda^t}\Phi_\lambda \in \mathfrak{S}_{2/(m+1),\infty}.$$

This and the assumption of the induction imply eventually that

$$\begin{aligned}\frac{\mathrm{d}^{q+1}}{\mathrm{d}\lambda^{q+1}}&(1+\eta\mathcal{C}_\lambda)^{-1}\\ &= -\sum_{k+m+n=q}\frac{q!}{k!l!m!}\frac{\mathrm{d}^k}{\mathrm{d}\lambda^k}(1+\eta\mathcal{C}_\lambda)^{-1}\eta\frac{\mathrm{d}^m}{\mathrm{d}\lambda^m}\big(\Phi_{\bar{\lambda}}^*\Phi_\lambda\big)\frac{\mathrm{d}^n}{\mathrm{d}\lambda^n}(1+\eta\mathcal{C}_\lambda)^{-1}\end{aligned}$$

belongs to $\mathfrak{S}_{2/(q+1),\infty}$.

Making use of (4.17), (4.18), (4.19), and (2.42) we deduce finally that

$$\begin{aligned}(A^\Sigma_{\eta_e,\eta_s}&-\lambda)^{-l}-(A_0-\lambda)^{-l}\\ &= -\sum_{p+q+r=l-1}\frac{1}{p!q!r!}\frac{\mathrm{d}^p}{\mathrm{d}\lambda^p}\Phi_\lambda\frac{\mathrm{d}^q}{\mathrm{d}\lambda^q}(I_4+\eta\mathcal{C}_\lambda)^{-1}\eta\frac{\mathrm{d}^r}{\mathrm{d}\lambda^r}\Phi_{\bar{\lambda}}^* \in \mathfrak{S}_{2/l,\infty}.\end{aligned}$$

This was the claimed result of this theorem. □

In the following corollary we state that the difference of the third powers of the resolvents of $A^\Sigma_{\eta_e,\eta_s}$ and A_0 is a trace class operator. This is an important result for mathematical scattering theory, as it ensures the existence and completeness of the wave operators for the scattering system $\{A^\Sigma_{\eta_e,\eta_s}, A_0\}$ and that the absolute continuous parts of $A^\Sigma_{\eta_e,\eta_s}$ and A_0 are unitarily equivalent. Furthermore, we provide an explicit formula for the trace of $(A^\Sigma_{\eta_e,\eta_s} - \lambda)^{-3} - (A_0-\lambda)^{-3}$ in terms of the singular integral operator $\mathcal{C}_\lambda$. Note that the trace in the left-hand side of (4.20) is taken in $L^2(\mathbb{R}^3;\mathbb{C}^4)$, whereas the trace on the right-hand side is taken in $L^2(\Sigma;\mathbb{C}^4)$.

Corollary 4.2.8. *Let $\Sigma \subset \mathbb{R}^3$ be the boundary of a C^3-smooth compact domain and let all assumptions of Theorem 4.2.7 be fulfilled. Then for any $\lambda \in \mathbb{C}\setminus\mathbb{R}$ the operator*

$$(A^\Sigma_{\eta_e,\eta_s}-\lambda)^{-3}-(A_0-\lambda)^{-3}$$

belongs to the trace class ideal and

$$\begin{aligned}\mathrm{tr}\big[(A^\Sigma_{\eta_e,\eta_s}&-\lambda)^{-3}-(A_0-\lambda)^{-3}\big]\\ &= -\frac{1}{2}\mathrm{tr}\left[\frac{d^2}{d\lambda^2}\left(\big(I_4+(\eta_e I_4+\eta_s\beta)\mathcal{C}_\lambda\big)^{-1}(\eta_e I_4+\eta_s\beta)\frac{d}{d\lambda}\mathcal{C}_\lambda\right)\right].\end{aligned} \tag{4.20}$$

In particular, the wave operators for the scattering system $\{A^\Sigma_{\eta_e,\eta_s}, A_0\}$ exist and are complete, and the absolute continuous parts of $A^\Sigma_{\eta_e,\eta_s}$ and A_0 are unitarily equivalent.

Proof. The first statement follows immediately from Theorem 4.2.7 for the special choice $l = 3$ and the fact that $\mathfrak{S}_{2/3,\infty}$ is contained in the trace class ideal, compare (2.41). Moreover, the last assertion is a standard result in scattering theory, see for instance [71, Chapter 0, Theorem 8.2] and the standard definition of the existence and completeness of wave operators.

So it remains to prove the trace formula (4.20). We use the abbreviation $\eta := \eta_{\mathrm{e}} I_4 + \eta_{\mathrm{s}}\beta$. Employing the resolvent formula from Theorem 4.2.3 (i), Proposition 2.2.4 (iv) and the cyclicity of the trace (2.43) we get

$$\begin{aligned}
\operatorname{tr}\big[(A^{\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}} - \lambda)^{-3} - (A_0 - \lambda)^{-3}\big] &= \frac{1}{2}\operatorname{tr}\left[\frac{\mathrm{d}^2}{\mathrm{d}\lambda^2}\big((A^{\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}} - \lambda)^{-1} - (A_0 - \lambda)^{-1}\big)\right]\\
&= -\frac{1}{2}\operatorname{tr}\left[\frac{\mathrm{d}^2}{\mathrm{d}\lambda^2}\big(\Phi_\lambda (I_4 + \eta\mathcal{C}_\lambda)^{-1}\eta\Phi^*_{\overline{\lambda}}\big)\right]\\
&= -\sum_{p+q+r=2}\frac{1}{p!q!r!}\operatorname{tr}\left[\frac{\mathrm{d}^p}{\mathrm{d}\lambda^p}\Phi_\lambda\frac{\mathrm{d}^q}{\mathrm{d}\lambda^q}(I_4 + \eta\mathcal{C}_\lambda)^{-1}\eta\frac{\mathrm{d}^r}{\mathrm{d}\lambda^r}\Phi^*_{\overline{\lambda}}\right]\\
&= -\sum_{p+q+r=2}\frac{1}{p!q!r!}\operatorname{tr}\left[\frac{\mathrm{d}^q}{\mathrm{d}\lambda^q}(I_4 + \eta\mathcal{C}_\lambda)^{-1}\eta\frac{\mathrm{d}^r}{\mathrm{d}\lambda^r}\Phi^*_{\overline{\lambda}}\frac{\mathrm{d}^p}{\mathrm{d}\lambda^p}\Phi_\lambda\right]\\
&= -\frac{1}{2}\operatorname{tr}\left[\frac{\mathrm{d}^2}{\mathrm{d}\lambda^2}(I_4 + \eta\mathcal{C}_\lambda)^{-1}\eta\Phi^*_{\overline{\lambda}}\Phi_\lambda\right]\\
&= -\frac{1}{2}\operatorname{tr}\left[\frac{\mathrm{d}^2}{\mathrm{d}\lambda^2}(I_4 + \eta\mathcal{C}_\lambda)^{-1}\eta\frac{\mathrm{d}}{\mathrm{d}\lambda}\mathcal{C}_\lambda\right].
\end{aligned}$$

This is the claimed formula. □

4.3 Dirac operators with δ-shell interactions of critical strength – self-adjointness and basic spectral properties

In this section we study Dirac operators with a singular interaction of the form $\eta_{\mathrm{e}} I_4 + \eta_{\mathrm{s}}\beta$ in the critical case, that means when $\eta_{\mathrm{e}}(x)^2 - \eta_{\mathrm{s}}(x)^2 = 4c^2$ for some $x \in \Sigma$. We will see that under these assumptions $A^{\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}}$ defined by (4.12) is not self-adjoint. But using the ordinary boundary triple $\{L^2(\Sigma;\mathbb{C}^4), \Upsilon^{\Sigma}_0, \Upsilon^{\Sigma}_1\}$ from Theorem 4.1.5 it turns out for constant η_{e} and η_{s} that these operators are essentially self-adjoint and we can characterize and study the self-adjoint realizations. First, we have the following result:

Proposition 4.3.1. *Assume that $\eta_{\mathrm{e}}, \eta_{\mathrm{s}} : \Sigma \to \mathbb{R}$ are Lipschitz continuous functions such that $\eta_{\mathrm{e}}(x)^2 - \eta_{\mathrm{s}}(x)^2 = 4c^2$ for some $x \in \Sigma$. Then $A^{\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}}$ defined by* (4.12) *is symmetric, but not self-adjoint.*

Proof. The fact that $A^{\Sigma}_{\eta_e,\eta_s}$ is symmetric follows immediately from Green's identity, compare (2.9). The claim that $A^{\Sigma}_{\eta_e,\eta_s}$ is not self-adjoint will be shown in an indirect way.

Assume that $A^{\Sigma}_{\eta_e,\eta_s}$ is self-adjoint. Then $\operatorname{ran}(A^{\Sigma}_{\eta_e,\eta_s} - \lambda) = L^2(\mathbb{R}^3;\mathbb{C}^4)$ for all $\lambda \in \mathbb{C}\setminus\mathbb{R}$. Since $A^{\Sigma}_{\infty} := T^{\Sigma} \upharpoonright \ker \Gamma_1^{\Sigma}$ is self-adjoint by Lemma 4.1.3 it follows that $\{L^2(\Sigma;\mathbb{C}^4), \widehat{\Gamma}_0^{\Sigma}, \widehat{\Gamma}_1^{\Sigma}\}$ with $\widehat{\Gamma}_0^{\Sigma} = \Gamma_1^{\Sigma}$ and $\widehat{\Gamma}_1^{\Sigma} := -\Gamma_0^{\Sigma}$ is also a quasi boundary triple with Weyl function $\widehat{M}^{\Sigma}(\lambda) = -M^{\Sigma}(\lambda)^{-1}$, compare the considerations after Theorem 4.1.5. Hence we deduce from Theorem 2.2.5 that

$$\operatorname{ran}\big(\widehat{\Gamma}_1(A^{\Sigma}_{\infty} - \lambda)^{-1}\big) = \operatorname{ran}\big(\Gamma_0^{\Sigma} \upharpoonright \ker\Gamma_1^{\Sigma}\big) \subset \operatorname{ran}\big(\eta_e I_4 + \eta_s\beta + (M^{\Sigma}(\lambda))^{-1}\big).$$

By Lemma 4.1.3 it holds $\operatorname{ran}\big(\Gamma_0^{\Sigma} \upharpoonright \ker\Gamma_1^{\Sigma}\big) = H^{1/2}(\Sigma;\mathbb{C}^4)$ and thus the last condition is equivalent to the fact that $\eta_e I_4 + \eta_s\beta + (M^{\Sigma}(\lambda))^{-1}$ is bijective in $H^{1/2}(\Sigma;\mathbb{C}^4)$.

Next, recall that $M^{\Sigma}(\lambda) = \mathcal{C}_{\lambda}^{1/2}$ and $(\mathcal{C}_{\lambda}^{1/2})^{-1} = -4c^2(\alpha\cdot\nu)\mathcal{C}_{\lambda}^{1/2}(\alpha\cdot\nu)$, compare Proposition 4.1.2 and Proposition 3.2.1. Since Σ is C^2-smooth and $\alpha\cdot\nu$ is pointwise unitary the multiplication with $\alpha\cdot\nu$ yields a bijective operator in $H^{1/2}(\Sigma;\mathbb{C}^4)$. Thus, using (1.2) we see that

$$\eta_e I_4 - \eta_s\beta - 4c^2\mathcal{C}_{\lambda}^{1/2} = (\alpha\cdot\nu)\big(\eta_e I_4 + \eta_s\beta + (\mathcal{C}_{\lambda}^{1/2})^{-1}\big)(\alpha\cdot\nu)$$

is bijective. Moreover, since $\mathcal{C}_{\lambda}^{1/2}$ is bijective in $H^{1/2}(\Sigma;\mathbb{C}^4)$ we obtain that also the operator $I_4 + (\eta_e I_4 + \eta_s\beta)\mathcal{C}_{\lambda}^{1/2}$ is bijective in $H^{1/2}(\Sigma;\mathbb{C}^4)$. Therefore, also the product

$$\begin{aligned}&\big(\eta_e I_4 - \eta_s\beta - 4c^2\mathcal{C}_{\lambda}^{1/2}\big)\big(I_4 + (\eta_e I_4 + \eta_s\beta)\mathcal{C}_{\lambda}^{1/2}\big)\\ &\qquad = \eta_e I_4 - \eta_s\beta - 4c^2\mathcal{C}_{\lambda}^{1/2}(\eta_e I_4 + \eta_s\beta)\mathcal{C}_{\lambda}^{1/2} + (\eta_e^2 - \eta_s^2 - 4c^2)\mathcal{C}_{\lambda}^{1/2}\end{aligned}$$

is bijective. We set

$$C := \big\|\big(\eta_e I_4 - \eta_s\beta - 4c^2\mathcal{C}_{\lambda}^{1/2}(\eta_e I_4 + \eta_s\beta)\mathcal{C}_{\lambda}^{1/2} + (\eta_e^2 - \eta_s^2 - 4c^2)\mathcal{C}_{\lambda}^{1/2}\big)^{-1}\big\| < \infty. \tag{4.21}$$

Next, choose a function η such that

$$\Sigma_0 := \Sigma \setminus \operatorname{supp}\eta \neq \emptyset \quad \text{and} \quad C\big\|\big((\eta_e^2 - \eta_s^2 - 4c^2) - \eta\big)\mathcal{C}_{\lambda}^{1/2}\big\| < 1,$$

where C is the same constant as in (4.21) and the norm is the one in $\mathfrak{B}(H^{1/2}(\Sigma;\mathbb{C}^4))$. Such a choice is possible by Proposition 2.5.2; the fact that $\Sigma_0 \neq \emptyset$ follows from the assumption that there exist some $x \in \Sigma$ such that $\eta_e(x)^2 - \eta_s(x)^2 - 4c^2 = 0$. Then

$$\begin{aligned}C\big\|&\big(\eta_e I_4 - \eta_s\beta - 4c^2\mathcal{C}_{\lambda}^{1/2}(\eta_e I_4 + \eta_s\beta)\mathcal{C}_{\lambda}^{1/2} + (\eta_e^2 - \eta_s^2 - 4c^2)\mathcal{C}_{\lambda}^{1/2}\big)\\ &\qquad - \big(\eta_e I_4 - \eta_s\beta - 4c^2\mathcal{C}_{\lambda}^{1/2}(\eta_e I_4 + \eta_s\beta)\mathcal{C}_{\lambda}^{1/2} + \eta\,\mathcal{C}_{\lambda}^{1/2}\big)\big\|\\ &= C\big\|\big((\eta_e^2 - \eta_s^2 - 4c^2) - \eta\big)\mathcal{C}_{\lambda}^{1/2}\big\| < 1\end{aligned}$$

and thus [50, Theorem IV 1.16] yields that $\eta_e I_4 - \eta_s\beta - 4c^2\mathcal{C}_\lambda^{1/2}(\eta_e I_4 + \eta_s\beta)\mathcal{C}_\lambda^{1/2} + \eta\,\mathcal{C}_\lambda^{1/2}$ is bijective in $H^{1/2}(\Sigma;\mathbb{C}^4)$.

Next, denote by $\mathcal{P} : H^{1/2}(\Sigma;\mathbb{C}^4) \to H^{1/2}(\Sigma_0;\mathbb{C}^4)$ the restriction operator acting as $\mathcal{P}\varphi = \varphi \upharpoonright \Sigma_0$. Then since $\operatorname{supp}\eta = \Sigma \setminus \Sigma_0$ we obtain

$$\begin{aligned} H^{1/2}(\Sigma_0;\mathbb{C}^4) &\subset \operatorname{ran}\mathcal{P}\left(\eta_e I_4 - \eta_s\beta - 4c^2\mathcal{C}_\lambda^{1/2}(\eta_e I_4 + \eta_s\beta)\mathcal{C}_\lambda^{1/2} + \eta\,\mathcal{C}_\lambda^{1/2}\right) \\ &= \operatorname{ran}\mathcal{P}\left(\eta_e I_4 - \eta_s\beta - 4c^2\mathcal{C}_\lambda^{1/2}(\eta_e I_4 + \eta_s\beta)\mathcal{C}_\lambda^{1/2}\right). \end{aligned} \tag{4.22}$$

Finally, we claim that $\eta_e I_4 - \eta_s\beta - 4c^2\mathcal{C}_\lambda^{1/2}(\eta_e I_4 + \eta_s\beta)\mathcal{C}_\lambda^{1/2}$ is compact in $H^{1/2}(\Sigma;\mathbb{C}^4)$. This gives then a contradiction to (4.22). To verify the last claim we write

$$\mathcal{C}_\lambda^{1/2}(\eta_e I_4 + \eta_s\beta) = (\eta_e I_4 - \eta_s\beta)\mathcal{C}_\lambda^{1/2} + \mathcal{K}_{1,\lambda}$$

with

$$\mathcal{K}_{1,\lambda} := \big(\mathcal{C}_\lambda^{1/2}\eta_e - \eta_e\mathcal{C}_\lambda^{1/2}\big) + \big(\mathcal{C}_\lambda^{1/2}\eta_s - \eta_s\mathcal{C}_\lambda^{1/2}\big)\beta + \eta_s\big(\mathcal{C}_\lambda^{1/2}\beta + \beta\mathcal{C}_\lambda^{1/2}\big).$$

Using Propositions 3.2.3 and 3.2.4 we conclude that $\mathcal{K}_{1,\lambda}$ is compact in $H^{1/2}(\Sigma;\mathbb{C}^4)$. Moreover, recall that $(\mathcal{C}_\lambda^{1/2})^2 = \frac{1}{4c^2} + \mathcal{K}_{2,\lambda}$, where $\mathcal{K}_{2,\lambda}$ is compact in $H^{1/2}(\Sigma;\mathbb{C}^4)$, compare Proposition 4.1.4 (iv). Thus, we get eventually that

$$\begin{aligned} \eta_e I_4 - \eta_s\beta - 4c^2\mathcal{C}_\lambda^{1/2}(\eta_e I_4 + \eta_s\beta)\mathcal{C}_\lambda^{1/2} &= \big(\eta_e I_4 - \eta_s\beta\big)\big(I_4 - 4c^2(\mathcal{C}_\lambda^{1/2})^2\big) + \mathcal{K}_{1,\lambda}\mathcal{C}_\lambda^{1/2} \\ &= -4c^2(\eta_e I_4 - \eta_s\beta)\mathcal{K}_{2,\lambda} + \mathcal{K}_{1,\lambda}\mathcal{C}_\lambda^{1/2}, \end{aligned}$$

which is compact in $H^{1/2}(\Sigma;\mathbb{C}^4)$. This finishes the proof of this proposition. □

In the following let $\eta_e, \eta_s \in \mathbb{R}$ with $\eta_e^2 - \eta_s^2 = 4c^2$. We are going to show that $A^\Sigma_{\eta_e,\eta_s}$ is in this case essentially self-adjoint and compute the closure of this operator, which is then the self-adjoint realization of the Dirac operator with a δ-shell interaction of strength $\eta_e I_4 + \eta_s\beta$. For that purpose we use the ordinary boundary triple $\{L^2(\Sigma;\mathbb{C}^4), \Upsilon_0^\Sigma, \Upsilon_1^\Sigma\}$ from Theorem 4.1.5. Recall that

$$A^\Sigma_{\eta_e,\eta_s} = T^\Sigma \upharpoonright \ker\big(\Gamma_0^\Sigma + (\eta_e I_4 + \eta_s\beta)\Gamma_1^\Sigma\big) = (S^\Sigma)^* \upharpoonright \big(\Upsilon_1^\Sigma - \Theta^{1,\Sigma}_{\eta_e,\eta_s}\Upsilon_0^\Sigma\big),$$

where $\Theta^{1,\Sigma}_{\eta_e,\eta_s} = \iota_+^\Sigma\big(\eta_e I_4 + \eta_s\beta + (\mathcal{C}_0^{1/2})^{-1}\big)(\iota_-^\Sigma)^{-1}$, $\iota_\pm^\Sigma$ is defined by (4.6) and (4.7), and $\mathcal{C}_0^{1/2}$ is the restriction of $\mathcal{C}_0$ onto $H^{1/2}(\Sigma;\mathbb{C}^4)$ from Proposition 4.1.6, compare (4.10). The operator $\Theta^{1,\Sigma}_{\eta_e,\eta_s}$ is explicitly given by

$$\begin{aligned} \Theta^{1,\Sigma}_{\eta_e,\eta_s}\varphi &:= \iota_+^\Sigma\big(\eta_e I_4 + \eta_s\beta + (\mathcal{C}_0^{1/2})^{-1}\big)(\iota_-^\Sigma)^{-1}\varphi, \\ \operatorname{dom}\Theta^{1,\Sigma}_{\eta_e,\eta_s} &:= H^1(\Sigma;\mathbb{C}^4). \end{aligned} \tag{4.23}$$

Due to the mapping properties of $\mathcal{C}_0^{1/2}$ from Proposition 4.1.6 we see that $\Theta^{1,\Sigma}_{\eta_e,\eta_s}$ is well-defined. Moreover, using Propositions 4.1.6 and 4.1.2 it is not difficult to see that $\Theta^{1,\Sigma}_{\eta_e,\eta_s}$ is symmetric in $L^2(\Sigma;\mathbb{C}^4)$. Our goal is to show that $\Theta^{1,\Sigma}_{\eta_e,\eta_s}$ is essentially self-adjoint and that its closure coincides with the maximal parameter

$$\begin{aligned}\Theta^{0,\Sigma}_{\eta_e,\eta_s}\varphi &:= \iota_+^\Sigma\big(\eta_e I_4 + \eta_s\beta + (\mathcal{C}_0^{-1/2})^{-1}\big)(\iota_-^\Sigma)^{-1}\varphi,\\ \operatorname{dom}\Theta^{0,\Sigma}_{\eta_e,\eta_s} &:= \Big\{\varphi\in L^2(\Sigma;\mathbb{C}^4) : \big(\eta_e I_4 + \eta_s\beta + (\mathcal{C}_0^{-1/2})^{-1}\big)(\iota_-^\Sigma)^{-1}\varphi \in H^{1/2}(\Sigma;\mathbb{C}^4)\Big\}.\end{aligned} \tag{4.24}$$

Here $\mathcal{C}_0^{-1/2}$ is the extension of $\mathcal{C}_0$ onto $H^{-1/2}(\Sigma;\mathbb{C}^4)$. A density argument and Proposition 3.2.1 show that $(\mathcal{C}_0^{-1/2})^{-1} = -4c^2(\alpha\cdot\nu)'\mathcal{C}_0^{-1/2}(\alpha\cdot\nu)'$, where $(\alpha\cdot\nu)'$ is the dual of the multiplication operator with $\alpha\cdot\nu$ in $H^{1/2}(\Sigma;\mathbb{C}^4)$.

Proposition 4.3.2. *Let $\eta_e,\eta_s\in\mathbb{R}$ such that $\eta_e^2-\eta_s^2=4c^2$. Moreover, let $\Theta^{1,\Sigma}_{\eta_e,\eta_s}$ and $\Theta^{0,\Sigma}_{\eta_e,\eta_s}$ be given by* (4.23) *and* (4.24)*, respectively. Then $\Theta^{1,\Sigma}_{\eta_e,\eta_s}$ is essentially self-adjoint in $L^2(\Sigma;\mathbb{C}^4)$ and the closure of $\Theta^{1,\Sigma}_{\eta_e,\eta_s}$ is $\Theta^{0,\Sigma}_{\eta_e,\eta_s}$. In particular $\Theta^{0,\Sigma}_{\eta_e,\eta_s}$ is self-adjoint.*

Proof. The proof of this proposition consists of three steps. First, we verify that $\Theta^{0,\Sigma}_{\eta_e,\eta_s}$ is closed, then in *Step 2* we prove that $(\Theta^{1,\Sigma}_{\eta_e,\eta_s})^*\subset\Theta^{0,\Sigma}_{\eta_e,\eta_s}$. Finally, in *Step 3* we show $\Theta^{0,\Sigma}_{\eta_e,\eta_s}\subset\overline{\Theta^{1,\Sigma}_{\eta_e,\eta_s}}$ which yields then together with the results from *Step 1* and *Step 2* the claim of this proposition.

Step 1: We prove that $\Theta^{0,\Sigma}_{\eta_e,\eta_s}$ is closed. For that choose a sequence $\varphi_n\subset\operatorname{dom}\Theta^{0,\Sigma}_{\eta_e,\eta_s}$ such that

$$\varphi_n\to\varphi \quad\text{and}\quad \Theta^{0,\Sigma}_{\eta_e,\eta_s}\varphi_n\to\psi,\quad n\to\infty,$$

in $L^2(\Sigma;\mathbb{C}^4)$ for some $\varphi,\psi\in L^2(\Sigma;\mathbb{C}^4)$. Since $\iota_+^\Sigma : H^{1/2}(\Sigma;\mathbb{C}^4)\to L^2(\Sigma;\mathbb{C}^4)$ is bijective, compare (4.6), it follows that

$$\big(\eta_e I_4+\eta_s\beta+(\mathcal{C}_0^{-1/2})^{-1}\big)(\iota_-^\Sigma)^{-1}\varphi_n\to(\iota_+^\Sigma)^{-1}\psi \quad\text{in } H^{1/2}(\Sigma;\mathbb{C}^4),\ n\to\infty.$$

On the other hand, since $\iota_-^\Sigma : H^{-1/2}(\Sigma;\mathbb{C}^4)\to L^2(\Sigma;\mathbb{C}^4)$ is bijective and $\eta_e I_4+\eta_s\beta-(\mathcal{C}_0^{-1/2})^{-1}$ is continuous in $H^{-1/2}(\Sigma;\mathbb{C}^4)$ we see that also

$$\big(\eta_e I_4+\eta_s\beta+(\mathcal{C}_0^{-1/2})^{-1}\big)(\iota_-^\Sigma)^{-1}\varphi_n\to\big(\eta_e I_4+\eta_s\beta+(\mathcal{C}_0^{-1/2})^{-1}\big)(\iota_-^\Sigma)^{-1}\varphi$$

in $H^{-1/2}(\Sigma;\mathbb{C}^4)$, as $n\to\infty$. Hence, we conclude

$$\big(\eta_e I_4+\eta_s\beta+(\mathcal{C}_0^{-1/2})^{-1}\big)(\iota_-^\Sigma)^{-1}\varphi=(\iota_+^\Sigma)^{-1}\psi\in H^{1/2}(\Sigma;\mathbb{C}^4).$$

This shows that $\varphi\in\operatorname{dom}\Theta^{0,\Sigma}_{\eta_e,\eta_s}$ and $\Theta^{0,\Sigma}_{\eta_e,\eta_s}\varphi=\psi$, that means $\Theta^{0,\Sigma}_{\eta_e,\eta_s}$ is closed.

Step 2: We verify that $(\Theta^{1,\Sigma}_{\eta_e,\eta_s})^* \subset \Theta^{0,\Sigma}_{\eta_e,\eta_s}$. For that fix some $\varphi \in \operatorname{dom}(\Theta^{1,\Sigma}_{\eta_e,\eta_s})^*$ and let $\psi \in \operatorname{dom}\Theta^{1,\Sigma}_{\eta_e,\eta_s} = H^1(\Sigma;\mathbb{C}^4)$ be arbitrary, but fixed. Then using the definition of $\Theta^{1,\Sigma}_{\eta_e,\eta_s}$, equation (2.18), Proposition 4.1.4 (ii) and $(\mathcal{C}_0^{1/2})^{-1} = -4c^2(\alpha\cdot\nu)\mathcal{C}_0^{1/2}(\alpha\cdot\nu)$ we get

$$\begin{aligned}
\big((\Theta^{1,\Sigma}_{\eta_e,\eta_s})^*\varphi,\psi\big)_\Sigma &= \big(\varphi,\Theta^{1,\Sigma}_{\eta_e,\eta_s}\psi\big)_\Sigma = \big(\varphi,\iota_+^\Sigma\big(\eta_e I_4+\eta_s\beta+(\mathcal{C}_0^{1/2})^{-1}\big)(\iota_-^\Sigma)^{-1}\psi\big)_\Sigma\\
&= \big((\iota_-^\Sigma)^{-1}\varphi,\big(\eta_e I_4+\eta_s\beta+(\mathcal{C}_0^{1/2})^{-1}\big)(\iota_-^\Sigma)^{-1}\psi\big)_{-1/2\times 1/2}\\
&= \big((\iota_-^\Sigma)^{-1}\varphi,\big(\eta_e I_4+\eta_s\beta-4c^2(\alpha\cdot\nu)\mathcal{C}_0^{1/2}(\alpha\cdot\nu)\big)\iota_+^\Sigma\psi\big)_{-1/2\times 1/2}\\
&= \big(\big(\eta_e I_4+\eta_s\beta-4c^2(\alpha\cdot\nu)'\mathcal{C}_0^{-1/2}(\alpha\cdot\nu)'\big)(\iota_-^\Sigma)^{-1}\varphi,\iota_+^\Sigma\psi\big)_{-1/2\times 1/2}\\
&= \big(\iota_-^\Sigma\big(\eta_e I_4+\eta_s\beta-4c^2(\alpha\cdot\nu)'\mathcal{C}_0^{-1/2}(\alpha\cdot\nu)'\big)(\iota_-^\Sigma)^{-1}\varphi,(\iota_+^\Sigma)^2\psi\big)_\Sigma.
\end{aligned}$$

Since this is true for all $\psi \in H^1(\Sigma;\mathbb{C}^4) = \operatorname{dom}(\iota_+^\Sigma)^2$ and as $(\iota_+^\Sigma)^2$ regarded as an unbounded operator in $L^2(\Sigma;\mathbb{C}^4)$ is self-adjoint we conclude that

$$\iota_-^\Sigma\big(\eta_e I_4+\eta_s\beta-4c^2(\alpha\cdot\nu)'\mathcal{C}_0^{-1/2}(\alpha\cdot\nu)'\big)(\iota_-^\Sigma)^{-1}\varphi \in \operatorname{dom}(\iota_+^\Sigma)^2 = H^1(\Sigma;\mathbb{C}^4)$$

and

$$\begin{aligned}
(\Theta^{1,\Sigma}_{\eta_e,\eta_s})^*\varphi &= (\iota_+^\Sigma)^2\iota_-^\Sigma\big(\eta_e I_4+\eta_s\beta-4c^2(\alpha\cdot\nu)'\mathcal{C}_0^{-1/2}(\alpha\cdot\nu)'\big)(\iota_-^\Sigma)^{-1}\varphi\\
&= \iota_+^\Sigma\big(\eta_e I_4+\eta_s\beta-4c^2(\alpha\cdot\nu)'\mathcal{C}_0^{-1/2}(\alpha\cdot\nu)'\big)(\iota_-^\Sigma)^{-1}\varphi.
\end{aligned}$$

Thus $\varphi \in \operatorname{dom}\Theta^{0,\Sigma}_{\eta_e,\eta_s}$ and $(\Theta^{1,\Sigma}_{\eta_e,\eta_s})^*\varphi = \Theta^{0,\Sigma}_{\eta_e,\eta_s}\varphi$, that means $(\Theta^{1,\Sigma}_{\eta_e,\eta_s})^* \subset \Theta^{0,\Sigma}_{\eta_e,\eta_s}$.

Step 3: We show that $\Theta^{0,\Sigma}_{\eta_e,\eta_s} \subset \overline{\Theta^{1,\Sigma}_{\eta_e,\eta_s}}$. Let $\varphi \in \operatorname{dom}\Theta^{0,\Sigma}_{\eta_e,\eta_s}$ be fixed and choose a sequence $(\psi_n) \subset H^1(\Sigma;\mathbb{C}^4)$ such that $(\iota_-^\Sigma)^{-1}\psi_n \to (\iota_-^\Sigma)^{-1}\varphi$ in $H^{-1/2}(\Sigma;\mathbb{C}^4)$. We define

$$\varphi_n := \varphi + \frac{1}{2}\iota_-^\Sigma\left(I_4-(\eta_e I_4-\eta_s\beta)\mathcal{C}_0^{-1/2}\right)(\iota_-^\Sigma)^{-1}(\psi_n-\varphi).$$

Note that

$$\begin{aligned}
\varphi_n &= \frac{1}{2}\iota_-^\Sigma\left(I_4-(\eta_e I_4-\eta_s\beta)\mathcal{C}_0^{-1/2}\right)(\iota_-^\Sigma)^{-1}\psi_n + \frac{1}{2}\iota_-^\Sigma\left(I_4+(\eta_e I_4-\eta_s\beta)\mathcal{C}_0^{-1/2}\right)(\iota_-^\Sigma)^{-1}\varphi\\
&= \frac{1}{2}\iota_-^\Sigma\left(I_4-(\eta_e I_4-\eta_s\beta)\mathcal{C}_0^{1/2}\right)(\iota_-^\Sigma)^{-1}\psi_n - \frac{\eta_s}{2}\iota_-^\Sigma\big(\beta\mathcal{C}_0^{-1/2}+\mathcal{C}_0^{-1/2}\beta\big)(\iota_-^\Sigma)^{-1}\varphi\\
&\qquad + \frac{1}{2}\iota_-^\Sigma\left(I_4+\mathcal{C}_0^{-1/2}(\eta_e I_4+\eta_s\beta)\right)(\iota_-^\Sigma)^{-1}\varphi.
\end{aligned}$$

Since ι_-^Σ gives rise to a bounded operator from $H^{1/2}(\Sigma;\mathbb{C}^4)$ onto $H^1(\Sigma;\mathbb{C}^4)$ by (4.8), we deduce from the mapping properties of $\mathcal{C}_0^{1/2}$ from Proposition 4.1.6 that

$$\frac{1}{2}\iota_-^\Sigma\left(I_4-(\eta_e I_4-\eta_s\beta)\mathcal{C}_0^{1/2}\right)(\iota_-^\Sigma)^{-1}\psi_n \in H^1(\Sigma;\mathbb{C}^4).$$

Next, since $\varphi \in \operatorname{dom}\Theta^{0,\Sigma}_{\eta_e,\eta_s}$ we have that

$$\frac{1}{2}\iota_-^\Sigma\Big(I_4+\mathcal{C}_0^{-1/2}(\eta_e I_4+\eta_s\beta)\Big)(\iota_-^\Sigma)^{-1}\varphi=\frac{1}{2}\iota_-^\Sigma\mathcal{C}_0^{1/2}\Big((\mathcal{C}_0^{-1/2})^{-1}+\eta_e I_4+\eta_s\beta\Big)(\iota_-^\Sigma)^{-1}\varphi$$

belongs to $H^1(\Sigma;\mathbb{C}^4)$. Eventually, by Proposition 3.2.4 we deduce that

$$\frac{\eta_s}{2}\iota_-^\Sigma\big(\beta\mathcal{C}_0^{-1/2}+\mathcal{C}_0^{-1/2}\beta\big)(\iota_-^\Sigma)^{-1}\varphi\in H^1(\Sigma;\mathbb{C}^4).$$

Therefore, we conclude $\varphi_n \in H^1(\Sigma;\mathbb{C}^4)$. Next, as $I_4-(\eta_e I_4-\eta_s\beta)\mathcal{C}_0^{-1/2}$ is continuous in $H^{-1/2}(\Sigma;\mathbb{C}^4)$ by Proposition 4.1.6 we get that

$$\varphi_n-\varphi=\frac{1}{2}\iota_-^\Sigma\Big(I_4-(\eta_e I_4-\eta_s\beta)\mathcal{C}_0^{-1/2}\Big)(\iota_-^\Sigma)^{-1}(\psi_n-\varphi)\to 0$$

in $L^2(\Sigma;\mathbb{C}^4)$, as $n\to\infty$. Finally, using $\eta_s^2-\eta_e^2=4c^2$ we obtain that

$$\begin{aligned}
&\Theta^{0,\Sigma}_{\eta_e,\eta_s}(\varphi_n-\varphi)\\
&\quad=\frac{1}{2}\iota_+^\Sigma\Big(\eta_e I_4+\eta_s\beta+(\mathcal{C}_0^{-1/2})^{-1}\Big)\Big(I_4-(\eta_e I_4-\eta_s\beta)\mathcal{C}_0^{-1/2}\Big)(\iota_-^\Sigma)^{-1}(\psi_n-\varphi)\\
&\quad=\frac{1}{2}\iota_+^\Sigma\Big(\eta_e I_4+\eta_s\beta+(\mathcal{C}_0^{-1/2})^{-1}\Big)\Big((\mathcal{C}_0^{-1/2})^{-1}-(\eta_e I_4-\eta_s\beta)\Big)\mathcal{C}_0^{-1/2}(\iota_-^\Sigma)^{-1}(\psi_n-\varphi)\\
&\quad=\frac{1}{2}\iota_+^\Sigma\Big(-4c^2I_4+(\mathcal{C}_0^{-1/2})^{-2}+\eta_s\big(\beta(\mathcal{C}_0^{-1/2})^{-1}+(\mathcal{C}_0^{-1/2})^{-1}\beta\big)\Big)\mathcal{C}_0^{-1/2}(\iota_-^\Sigma)^{-1}(\psi_n-\varphi).
\end{aligned}$$

Using $(\mathcal{C}_0^{-1/2})^{-1}=-4c^2(\alpha\cdot\nu)'\mathcal{C}_0^{-1/2}(\alpha\cdot\nu)'$ and Proposition 3.2.1 (iv) we deduce

$$\begin{aligned}
\big(\mathcal{C}_0^{-1/2}\big)^{-2}&=16c^4(\alpha\cdot\nu)'(\mathcal{C}_0^{-1/2})^2(\alpha\cdot\nu)'\\
&=16c^4(\alpha\cdot\nu)\mathcal{C}_0^{1/2}(\alpha\cdot\nu)\big[(\alpha\cdot\nu)'(\mathcal{C}_0^{-1/2})+(\mathcal{C}_0^{-1/2})(\alpha\cdot\nu)'\big](\alpha\cdot\nu)'\\
&\qquad-16c^4((\alpha\cdot\nu)'\mathcal{C}_0^{-1/2})^2=\mathcal{K}_1+4c^2I_4,
\end{aligned}$$

where $\mathcal{K}_1: H^{-1/2}(\Sigma;\mathbb{C}^4)\to H^{1/2}(\Sigma;\mathbb{C}^4)$ is bounded, see Proposition 4.1.4 (iv). Hence

$$\Theta^{0,\Sigma}_{\eta_e,\eta_s}(\varphi_n-\varphi)=\frac{1}{2}\iota_+^\Sigma\Big(\mathcal{K}_1+\eta_s\big(\beta(\mathcal{C}_0^{-1/2})^{-1}+(\mathcal{C}_0^{-1/2})^{-1}\beta\big)\Big)\mathcal{C}_0^{-1/2}(\iota_-^\Sigma)^{-1}(\psi_n-\varphi)$$

and as $\psi_n\to\varphi$ in $H^{-1/2}(\Sigma;\mathbb{C}^4)$, as $n\to\infty$, we conclude with Proposition 3.2.4 (ii) finally that $\Theta^{0,\Sigma}_{\eta_e,\eta_s}(\varphi_n-\varphi)\to 0$ in $L^2(\Sigma;\mathbb{C}^4)$, as $n\to\infty$. This shows now $\Theta^{0,\Sigma}_{\eta_e,\eta_s}\subset\overline{\Theta^{1,\Sigma}_{\eta_e,\eta_s}}$, which completes the proof of this proposition. □

With the aid of Proposition 4.3.2 we are now able to show that the operator $A^\Sigma_{\eta_e,\eta_s}$ defined by (4.12) is essentially self-adjoint in the critical case and we can describe its self-adjoint closure explicitly. To formulate the corresponding theorem recall the definitions of the maximal operator $(S^\Sigma)^*=T^{\Omega_+}_{\max}\oplus T^{\Omega_-}_{\max}$ with $T^{\Omega_\pm}_{\max}$ given by (3.10), the extended boundary mappings $\widetilde{\Gamma}_0^\Sigma,\widetilde{\Gamma}_1^\Sigma$ from Lemma 4.1.3, and the ordinary boundary triple $\{L^2(\Sigma;\mathbb{C}^4),\Upsilon_0^\Sigma,\Upsilon_1^\Sigma\}$ from Theorem 4.1.5.

Theorem 4.3.3. *Let $\eta_{\mathrm{e}}, \eta_{\mathrm{s}} \in \mathbb{R}$ such that $\eta_{\mathrm{e}}^2 - \eta_{\mathrm{s}}^2 = 4c^2$ and let $A^{\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}}$ be defined by* (4.12). *Then $A^{\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}}$ is essentially self-adjoint in $L^2(\mathbb{R}^3;\mathbb{C}^4)$. Its self-adjoint closure is given by*

$$\overline{A^{\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}}} = (S^{\Sigma})^* \upharpoonright \ker\big(\Upsilon_1^{\Sigma} - \Theta^{0,\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}}\Upsilon_0^{\Sigma}\big) = (S^{\Sigma})^* \upharpoonright \ker\big(\widetilde{\Gamma}_0^{\Sigma} + (\eta_{\mathrm{e}} I_4 + \eta_{\mathrm{s}}\beta)\widetilde{\Gamma}_1^{\Sigma}\big). \tag{4.25}$$

Moreover, $A^{\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}} \subsetneq \overline{A^{\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}}}$ and $\operatorname{dom}\overline{A^{\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}}} \not\subset H^1(\Omega_+;\mathbb{C}^4) \oplus H^1(\Omega_-;\mathbb{C}^4)$.

Proof. By Proposition 4.3.2 the operator $\Theta^{1,\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}}$ is essentially self-adjoint. Thus Proposition 2.2.7 implies that

$$A^{\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}} = T^{\Sigma} \upharpoonright \ker\big(\Gamma_0^{\Sigma} + (\eta_{\mathrm{e}} I_4 + \eta_{\mathrm{s}}\beta)\Gamma_1^{\Sigma}\big) = (S^{\Sigma})^* \upharpoonright \big(\Upsilon_1^{\Sigma} - \Theta^{1,\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}}\Upsilon_0^{\Sigma}\big)$$

is essentially self-adjoint. Furthermore, since $\{L^2(\Sigma;\mathbb{C}^4), \Upsilon_0^{\Sigma}, \Upsilon_1^{\Sigma}\}$ is an ordinary boundary triple the closure $\overline{A^{\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}}}$ of $A^{\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}}$ corresponds to the closure of the parameter $\Theta^{1,\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}}$; by Proposition 4.3.2 this is $\Theta^{0,\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}}$. Employing [22, Corollary 3.14] we deduce then (4.25). The last statement of this theorem is a direct consequence of Proposition 4.3.1. □

Remark 4.3.4. According to [55, Proposition 2.1] functions $f_{\pm} \in \operatorname{dom} T^{\Omega_{\pm}}_{\max}$ have traces in $H^{-1/2}(\Sigma;\mathbb{C}^4)$. Hence, the boundary condition $\widetilde{\Gamma}_0^{\Sigma} + (\eta_{\mathrm{e}} I_4 + \eta_{\mathrm{s}}\beta)\widetilde{\Gamma}_1^{\Sigma} = 0$ is equivalent to

$$-ic(\alpha\cdot\nu)'(f_+|_{\Sigma} - f_-|_{\Sigma}) = \frac{1}{2}(\eta_{\mathrm{e}} I_4 + \eta_{\mathrm{s}}\beta)(f_+|_{\Sigma} + f_-|_{\Sigma}) \quad \text{in } H^{-1/2}(\Sigma;\mathbb{C}^4).$$

This is in accordance to the jump condition in Definition 4.2.1.

In the next proposition we summarize some of the basic spectral properties of the self-adjoint realization $\overline{A^{\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}}}$ in the case of critical interaction strengths. These results complement those from Theorem 4.2.3.

Proposition 4.3.5. *Let $\eta_{\mathrm{e}}, \eta_{\mathrm{s}} \in \mathbb{R}$ such that $\eta_{\mathrm{e}}^2 - \eta_{\mathrm{s}}^2 = 4c^2$ and let $\overline{A^{\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}}}$ be defined by* (4.25). *Moreover, let A_0 be the free Dirac operator given by* (3.3) *and let for $\lambda \in \mathbb{C}\setminus\mathbb{R}$ the operators $\Phi_{\lambda}^{-1/2}$ and $\mathcal{C}_{\lambda}^{-1/2}$ be as in Proposition 4.1.6. Then the following assertions are true:*

(i) $(-\infty, -mc^2] \cup [mc^2, \infty) \subset \sigma_{\mathrm{ess}}(\overline{A^{\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}}})$.

(ii) $\lambda \in (-mc^2, mc^2) \cap \sigma_{\mathrm{p}}(\overline{A^{\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}}})$ *if and only if* $0 \in \sigma_{\mathrm{p}}\big(\eta_{\mathrm{e}} I_4 + \eta_{\mathrm{s}}\beta + (\mathcal{C}_0^{-1/2})^{-1}\big)$.

(iii) *The discrete and the essential spectra of the operators $\overline{A^{\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}}}$ and $\overline{A^{\Sigma}_{-\eta_{\mathrm{e}},-\eta_{\mathrm{s}}}}$ coincide.*

(iv) *For $\lambda \in \mathbb{C}\setminus\mathbb{R}$ it holds*

$$(\overline{A^{\Sigma}_{\eta_{\mathrm{e}},\eta_{\mathrm{s}}}} - \lambda)^{-1} = (A_0 - \lambda)^{-1} - \Phi_{\lambda}^{-1/2}\big(I_4 + (\eta_{\mathrm{e}} I_4 + \eta_{\mathrm{s}}\beta)\mathcal{C}_{\lambda}^{-1/2}\big)^{-1}(\eta_{\mathrm{e}} I_4 + \eta_{\mathrm{s}}\beta)\Phi_{\bar{\lambda}}^{*}.$$

Proof. (i) Let $\lambda \in (-\infty, -mc^2] \cup [mc^2, \infty)$ and set $\varphi_n^\lambda := 0 \oplus \psi_n^\lambda$, $n \in \mathbb{N}$, with ψ_n^λ defined by (3.15). Then it holds $\varphi_n^\lambda \in \operatorname{dom} S^\Sigma \subset \operatorname{dom} A_{\eta_e,\eta_s}^\Sigma$. Furthermore, by Lemma 3.1.4 we see that φ_n^λ converges weakly to zero,

$$\|\varphi_n^\lambda\|_{\mathbb{R}^3} = \|\psi_n^\lambda\|_{\Omega_-} = \text{const.} > 0, \text{ and } (\overline{A_{\eta_e,\eta_s}^\Sigma} - \lambda)\varphi_n^\lambda = 0 \oplus (T_{\min}^{\Omega_-} - \lambda)\psi_n^\lambda \to 0,\ n \to \infty.$$

Thus (φ_n^λ) is a singular sequence for $\overline{A_{\eta_e,\eta_s}^\Sigma}$ and λ which shows $\lambda \in \sigma_{\text{ess}}(\overline{A_{\eta_e,\eta_s}^\Sigma})$.

Assertions (ii) and (iv) are direct consequences of Proposition 2.2.7 and Theorem 2.2.5 (iii) taking the special form of the γ-field and the Weyl function for the ordinary boundary triple $\{L^2(\Sigma;\mathbb{C}^4), \Upsilon_0^\Sigma, \Upsilon_1^\Sigma\}$ from (2.20) into account, compare also (4.11).

Therefore, it remains to verify statement (iii). First, using that $\iota_\pm^\Sigma$ are bijections, the formula $(\mathcal{C}_\lambda^{-1/2})^{-1} = -4c^2(\alpha\cdot\nu)'\mathcal{C}_\lambda^{-1/2}(\alpha\cdot\nu)'$, and the Birman Schwinger principle for the discrete spectrum, compare Proposition 2.2.7 and (4.11) the proof of the statement $\sigma_{\text{disc}}(\overline{A_{\eta_e,\eta_s}^\Sigma}) = \sigma_{\text{disc}}(\overline{A_{-\eta_e,-\eta_s}^\Sigma})$ follows word by word the proof of Corollary 4.2.4. Eventually, we prove

$$\rho(\overline{A_{\eta_e,\eta_s}^\Sigma}) \cap (-mc^2, mc^2) = \rho(\overline{A_{-\eta_e,-\eta_s}^\Sigma}) \cap (-mc^2, mc^2).$$

This and the previously shown facts imply then $\sigma_{\text{ess}}(\overline{A_{\eta_e,\eta_s}^\Sigma}) = \sigma_{\text{ess}}(\overline{A_{-\eta_e,-\eta_s}^\Sigma})$. Due to symmetry reasons it suffices to verify $\rho(\overline{A_{\eta_e,\eta_s}^\Sigma}) \cap (-mc^2, mc^2) \subset \rho(\overline{A_{-\eta_e,-\eta_s}^\Sigma}) \cap (-mc^2, mc^2)$.

Let $\lambda \in \rho(\overline{A_{\eta_e,\eta_s}^\Sigma}) \cap (-mc^2, mc^2)$. Then, by Proposition 2.2.7 we have that $0 \in \rho(\Theta_{\eta_e,\eta_s}^{0,\Sigma} - \mathcal{M}^\Sigma(\lambda))$, where $\mathcal{M}^\Sigma(\lambda)$ is the Weyl function associated to $\{L^2(\Sigma;\mathbb{C}^4), \Upsilon_0^\Sigma, \Upsilon_1^\Sigma\}$. Taking the special form of $\mathcal{M}^\Sigma(\lambda)$ from (2.20) and $\Theta_{\eta_e,\eta_s}^{0,\Sigma}$ into account this yields that the operator $\eta_e I_4 + \eta_s\beta + (\mathcal{C}_\lambda^{-1/2})^{-1}$ is injective and that $H^{1/2}(\Sigma;\mathbb{C}^4)$ belongs to its range. Employing $(\eta_e I_4 + \eta_s\beta)^{-1} = \frac{1}{4c^2}(\eta_e I_4 - \eta_s\beta)$, equation (1.2), Proposition 3.2.1 (iv), and a density argument we find

$$\begin{aligned} &-\eta_e I_4 - \eta_s\beta + (\mathcal{C}_\lambda^{-1/2})^{-1} \\ &\qquad = -(\alpha\cdot\nu)'(\eta_e I_4 - \eta_s\beta)\left[\eta_e I_4 + \eta_s\beta + (\mathcal{C}_\lambda^{-1/2})^{-1}\right]\mathcal{C}_\lambda^{-1/2}(\alpha\cdot\nu)'. \end{aligned}$$

Since $(\alpha\cdot\nu)'$ and $\eta_e I_4 - \eta_s\beta$ are invertible and $\mathcal{C}_\lambda^{-1/2}$ is bijective in $H^{-1/2}(\Sigma;\mathbb{C}^4)$, also $-\eta_e I_4 - \eta_s\beta + (\mathcal{C}_\lambda^{-1/2})^{-1}$ is injective and $H^{1/2}(\Sigma;\mathbb{C}^4)$ belongs to the range of this operator. This yields, using again Proposition 2.2.7, that $\lambda \in \rho(\overline{A_{\tau_e,\tau_s}^\Sigma})$. □

Finally, we prove that in the case of critical interaction strengths under certain assumptions there might be essential spectrum of $\overline{A_{\eta_e,\eta_s}^\Sigma}$ also in the gap of $\sigma(A_0)$. To be more precise, we show that if there is some flat part contained in Σ and the interaction is purely electrostatic, then the point zero belongs to $\sigma_{\mathrm{ess}}(\overline{A^\Sigma_{\pm 2c,0}})$. This result shows that in the case of critical interaction strengths the spectral properties can be of a completely different nature as in the non-critical case. The proof of this theorem follows closely the one of [14, Theorem 5.9].

Theorem 4.3.6. *Let $\Sigma \subset \mathbb{R}^3$ be a bounded C^2-smooth surface such that there exists an open set $\Sigma_0 \subset \Sigma$ that is contained in a plane. Moreover, let $\eta_\mathrm{e} \in \{\pm 2c\}$ and $\eta_\mathrm{s} = 0$ be constant and let $A^\Sigma_{\pm 2c,0}$ be defined by* (4.12). *Then $0 \in \sigma_{\mathrm{ess}}(\overline{A^\Sigma_{\pm 2c,0}})$.*

Proof. The proof is indirect and for a simpler readability it is split into four steps. We are going to show the claim for $\eta_\mathrm{e} = 2c$, the proof for $\eta_\mathrm{e} = -2c$ follows the same lines. Assume that

$$0 \in \rho(\overline{A^\Sigma_{2c,0}}) \cup \sigma_{\mathrm{disc}}(\overline{A^\Sigma_{2c,0}}). \tag{4.26}$$

In our considerations the operator $\Xi^\Sigma : L^2(\Sigma;\mathbb{C}^4) \to L^2(\Sigma;\mathbb{C}^4)$ acting on $\varphi \in L^2(\Sigma;\mathbb{C}^4)$ as

$$\Xi^\Sigma \varphi := -\iota^\Sigma_+ (\alpha \cdot \nu)\big(2cI_4 - 4c^2 \mathcal{C}_0^{-1/2}\big)\big(2cI_4 + 4c^2 \mathcal{C}_0^{-1/2}\big)(\alpha \cdot \nu)'(\iota^\Sigma_-)^{-1}\varphi \tag{4.27}$$

will play an important role.

Step 1. We claim that Ξ^Σ is bounded and self-adjoint in $L^2(\Sigma;\mathbb{C}^4)$. First, we find for $\varphi \in L^2(\Sigma;\mathbb{C}^4)$

$$\Xi^\Sigma \varphi = -4c^2 \iota^\Sigma_+ (\alpha \cdot \nu)\big(I_4 - 4c^2 (\mathcal{C}_0^{-1/2})^2\big)(\alpha \cdot \nu)'(\iota^\Sigma_-)^{-1}\varphi.$$

Since $\iota^\Sigma_\pm : H^{\pm 1/2}(\Sigma;\mathbb{C}^4) \to L^2(\Sigma;\mathbb{C}^4)$ are bounded and bijective, it follows from Proposition 4.1.6 (iv) that also Ξ^Σ is well-defined and bounded. Next, using (1.2) we note that Ξ^Σ acts on $\varphi \in H^1(\Sigma;\mathbb{C}^4)$ as

$$\Xi^\Sigma \varphi = -4c^2 \iota^\Sigma_+ (\alpha \cdot \nu)\big(I_4 - 4c^2 (\mathcal{C}_0^{1/2})^2\big)(\alpha \cdot \nu)(\iota^\Sigma_-)^{-1}\varphi.$$

Since the operators $\alpha \cdot \nu$, $\mathcal{C}_0^{1/2}$, and $\iota^\Sigma_- \upharpoonright H^{1/2}(\Sigma;\mathbb{C}^4) = (\iota^\Sigma_+)^{-1}$ are symmetric this yields for $\varphi \in H^1(\Sigma;\mathbb{C}^4)$

$$\big(\Xi^\Sigma \varphi, \varphi\big)_\Sigma = -4c^2 \big(\big(I_4 - 4c^2 (\mathcal{C}_0^{1/2})^2\big)(\alpha \cdot \nu)\iota^\Sigma_+ \varphi, (\alpha \cdot \nu)\iota^\Sigma_+ \varphi\big)_\Sigma \in \mathbb{R}.$$

By a density argument this extends to all $\varphi \in L^2(\Sigma;\mathbb{C}^4)$ and hence Ξ^Σ is self-adjoint in $L^2(\Sigma;\mathbb{C}^4)$.

Step 2. We show that the direct sum decomposition

$$\ker \Xi^\Sigma = \ker \Theta^{0,\Sigma}_{2c,0} \dot{+} \ker \Theta^{0,\Sigma}_{-2c,0} \tag{4.28}$$

holds. Together with a similar consideration for the discrete spectrum as in (4.11) for $\lambda = 0$, Proposition 4.3.5 (iii) and assumption (4.26) this yields that $\dim \ker \Xi^\Sigma < \infty$. Clearly

$\ker(2cI_4 + 4c^2\mathcal{C}_0^{-1/2}) \cap \ker(2cI_4 - 4c^2\mathcal{C}_0^{-1/2}) = \{0\}$. Hence, in view of the definition of $\Theta^{0,\Sigma}_{\pm 2c,0}$ it follows that the sum in (4.28) is direct. Next, using (1.2) we see

$$\begin{aligned}
\Xi^\Sigma &= \Theta^{0,\Sigma}_{-2c,0}\iota^\Sigma_-(\iota^\Sigma_+)^{-1}\Theta^{0,\Sigma}_{2c,0} \\
&= -\iota^\Sigma_+(\alpha\cdot\nu)\left(2cI_4 + 4c^2\mathcal{C}_0^{-1/2}\right)\left(2cI_4 - 4c^2\mathcal{C}_0^{-1/2}\right)(\alpha\cdot\nu)'(\iota^\Sigma_-)^{-1} \\
&= -\iota^\Sigma_+(\alpha\cdot\nu)\left(2cI_4 - 4c^2\mathcal{C}_0^{-1/2}\right)\left(2cI_4 + 4c^2\mathcal{C}_0^{-1/2}\right)(\alpha\cdot\nu)'(\iota^\Sigma_-)^{-1} \\
&= \Theta^{0,\Sigma}_{2c,0}\iota^\Sigma_-(\iota^\Sigma_+)^{-1}\Theta^{0,\Sigma}_{-2c,0}
\end{aligned} \tag{4.29}$$

and get the inclusion

$$\ker\Theta^{0,\Sigma}_{2c,0} \dot{+} \ker\Theta^{0,\Sigma}_{-2c,0} \subset \ker\Xi^\Sigma. \tag{4.30}$$

To get the other inclusion let us denote by $\ker\Xi^\Sigma \ominus \ker\Theta^{0,\Sigma}_{-2c,0}$ the orthogonal complement of $\ker\Theta^{0,\Sigma}_{-2c,0}$ in the subspace $\ker\Xi^\Sigma$ of $L^2(\Sigma;\mathbb{C}^4)$. Then (4.29) yields

$$\left(2cI_4 + 4c^2\mathcal{C}_0^{-1/2}\right)(\alpha\cdot\nu)'(\iota^\Sigma_-)^{-1}\left(\ker\Xi^\Sigma \ominus \ker\Theta^{0,\Sigma}_{-2c,0}\right) \subset \ker\left(2cI_4 - 4c^2\mathcal{C}_0^{-1/2}\right).$$

Since

$$\left(2cI_4 + 4c^2\mathcal{C}_0^{-1/2}\right)(\alpha\cdot\nu)'(\iota^\Sigma_-)^{-1}\left(\ker\Xi^\Sigma \ominus \ker\Theta^{0,\Sigma}_{-2c,0}\right)$$

is injective and $\alpha\cdot\nu$ and $\iota^\Sigma_\pm$ are bijective we conclude

$$\begin{aligned}
\dim\ker\Xi^\Sigma &\le \dim\ker\left(2cI_4 + 4c^2\mathcal{C}_0^{-1/2}\right) + \dim\ker\left(2cI_4 - 4c^2\mathcal{C}_0^{-1/2}\right) \\
&= \dim\ker\Theta^{0,\Sigma}_{-2c,0} + \dim\ker\Theta^{0,\Sigma}_{2c,0},
\end{aligned}$$

which together with (4.30) implies finally (4.28).

Step 3. We define $\mathscr{H} := (\ker\Xi^\Sigma)^\perp$ and claim that assumption (4.26) implies that Ξ^Σ, which is clearly injective in the invariant subspace $\mathscr{H}$, is boundedly invertible in $\mathscr{H}$. In other words, this means that $\Xi \upharpoonright \mathscr{H}$ is a bounded, self-adjoint and bijective operator in $\mathscr{H}$.

Let $P^\Sigma_\pm$ be the orthogonal projectors onto $\ker\Theta^{0,\Sigma}_{\pm 2c,0}$. Making use of (4.26), Proposition 4.3.5 (iii) and a similar consideration as in (4.11) we see that the self-adjoint operators

$$\Theta^{0,\Sigma}_{\pm 2c,0} \upharpoonright (1 - P^\Sigma_\pm)L^2(\Sigma;\mathbb{C}^4)$$

are boundedly invertible in $(1 - P^\Sigma_\pm)L^2(\Sigma;\mathbb{C}^4)$. Let us these restrictions by $\Theta^\Sigma_\pm$. Now, let $\varphi \in \operatorname{ran}\Xi^\Sigma \subset \mathscr{H}$ and choose $\psi \in \mathscr{H}$ with $\varphi = \Xi^\Sigma\psi$. If we define

$$\psi_\pm := \iota^\Sigma_-\left(\mp 2cI_4 - 4c^2(\alpha\cdot\nu)'\mathcal{C}_0^{-1/2}(\alpha\cdot\nu)'\right)(\iota^\Sigma_-)^{-1}\psi \in \operatorname{dom}\Theta^{0,\Sigma}_{\pm 2c,0},$$

then $\varphi = \Xi^{\Sigma}\psi = \Theta^{0,\Sigma}_{\pm 2c,0}\psi_{\pm}$. Hence, we get $\psi_{\pm} = (\Theta^{\Sigma}_{\pm})^{-1}\varphi + P^{\Sigma}_{\pm}\psi_{\pm}$ and therefore

$$4c(\Xi^{\Sigma} \upharpoonright \mathscr{H})^{-1}\varphi = 4c\psi = \psi_- - \psi_+ = (\Theta^{\Sigma}_{-})^{-1}\varphi - (\Theta^{\Sigma}_{+})^{-1}\varphi + P^{\Sigma}_{-}\psi_- - P^{\Sigma}_{+}\psi_+.$$

Since $P^{\Sigma}_{-}\psi_- - P^{\Sigma}_{+}\psi_+ \in \ker \Xi^{\Sigma} = \mathscr{H}^{\perp}$ by (4.28) we deduce

$$\begin{aligned}\left\|4c(\Xi^{\Sigma} \upharpoonright \mathscr{H})^{-1}\varphi\right\|^2_{\Sigma} &\leq \left\|4c(\Xi^{\Sigma} \upharpoonright \mathscr{H})^{-1}\varphi\right\|^2_{\Sigma} + \left\|P^{\Sigma}_{+}\psi_+ - P^{\Sigma}_{-}\psi_-\right\|^2_{\Sigma} \\ &= \left\|4c(\Xi^{\Sigma} \upharpoonright \mathscr{H})^{-1}\varphi + (P^{\Sigma}_{+}\psi_+ - P^{\Sigma}_{-}\psi_-)\right\|^2_{\Sigma} \\ &= \left\|(\Theta^{\Sigma}_{-})^{-1}\varphi - (\Theta^{\Sigma}_{+})^{-1}\varphi\right\|^2_{\Sigma}.\end{aligned}$$

Since $(\Theta^{\Sigma}_{\pm})^{-1}$ are bounded we conclude that also $(\Xi^{\Sigma} \upharpoonright \mathscr{H})^{-1}$ is bounded in $\mathscr{H}$. As $(\Xi^{\Sigma} \upharpoonright \mathscr{H})^{-1}$ is self-adjoint in $\mathscr{H}$ it is clear that it is everywhere defined on $\mathscr{H}$.

Step 4. Finally, we prove that the assumption that a flat part Σ_0 is contained in Σ yields that there are infinitely many linearly independent functions not belonging to $\operatorname{ran}\Xi^{\Sigma}$. This is then a contradiction to the previous findings in this proof, which shows that the assumption (4.26) can not be true.

We consider the linear operator

$$\mathcal{A} := \mathcal{C}_0^{-1/2}(\alpha \cdot \nu)' + (\alpha \cdot \nu)'\mathcal{C}_0^{-1/2}.$$

Then by Proposition 3.2.4 the operator $\mathcal{A} : H^{-1/2}(\Sigma;\mathbb{C}^4) \to H^{1/2}(\Sigma;\mathbb{C}^4)$ is a well-defined and bounded and by Proposition 3.2.1 (iv) and a density argument we obtain

$$\Xi^{\Sigma} = 16c^4 \iota^{\Sigma}_{+}(\alpha \cdot \nu)'\mathcal{C}_0^{-1/2}\mathcal{A}(\iota^{\Sigma}_{-})^{-1}.$$

Since $\iota^{\Sigma}_{\pm}$, $(\alpha \cdot \nu)'$, and $\mathcal{C}_0^{-1/2}$ are isomorphisms, we see by comparing with (4.27) that infinitely many linearly independent functions do not belong to $\operatorname{ran}\Xi^{\Sigma}$ if and only if infinitely many linearly independent functions do not belong to $\operatorname{ran}\mathcal{A}$. We are going to verify the last claim.

Employing the anti-commutation relation (1.2) one sees that $\mathcal{A}$ acts on $\varphi \in L^2(\Sigma;\mathbb{C}^4)$ as

$$\mathcal{A}\varphi(x) = \int_{\Sigma} a(x,y)\varphi(y)\mathrm{d}\sigma(y) \tag{4.31}$$

with integral kernel

$$a(x,y) = G_0(x-z)\alpha \cdot (\nu(y) - \nu(x)) + \frac{ie^{-mc|x-y|}}{2\pi|x-y|^3}(1 + mc|x-y|)\,\nu(x)\cdot(x-y),$$

where G_0 is the Green's function for the resolvent of the free Dirac operator A_0 given by (3.6). Note that the integral operator in (4.31) is not singular, as $|a(x,y)| \leq C|x-y|^{-1}$, compare for instance [5, equation (22) and Lemma 3.5] and [45, Proposition 3.11]. Choose a subset $\Sigma_1 \subset \Sigma$ with $\overline{\Sigma_1} \subset \Sigma_0$. Note that $a(x,y) = 0$ for $x, y \in \Sigma_0$. Let $U_1 \subset \mathbb{R}^2$ and $\phi : U_1 \to \mathbb{R}^3$ be a linear affine function which parametrizes Σ_1, that means $\operatorname{ran}\phi = \Sigma_1$, and let $\varphi \in L^2(\Sigma;\mathbb{C}^4)$ be arbitrary, but fixed. Since ν is constant on Σ_0 and $\overline{\Sigma_1} \subset \Sigma_0$, we see that the mapping $U_1 \ni u \mapsto a(\phi(u),y)$ is C^∞-smooth for any $y \in \Sigma$ and the function $\Sigma \ni y \mapsto a(\phi(u),y)$ is C^1-smooth for any $u \in U_1$. From this, it is easy to deduce that $(\mathcal{A}\varphi)\circ\phi$ is differentiable on U_1 and

$$\partial_{u_j}(\mathcal{A}\varphi)(\phi(u)) = \int_\Sigma \partial_{u_j} a(\phi(u),y)\varphi(y)\mathrm{d}\sigma(y), \qquad j \in \{1,2\}.$$

Let us denote the elements of the 4×4-matrix $a(x,y)$ by $a_{lk}(x,y)$ and those of $\varphi(x) \in \mathbb{C}^4$ by $\varphi_k(x)$, $l,k \in \{1,2,3,4\}$. Then the last observation implies, in particular, that

$$\begin{aligned}
\|\partial_{u_j}\mathcal{A}\varphi\|^2_{L^2(\Sigma_1;\mathbb{C}^4)} &= C_1 \int_{U_1} \left|\partial_{u_j}\mathcal{A}\varphi(\phi(u))\right|^2 \mathrm{d}u \\
&= C_1 \int_{U_1} \left| \int_\Sigma \partial_{u_j} a(\phi(u),y)\varphi(y)\mathrm{d}\sigma(y)\right|^2 \mathrm{d}u \\
&= C_1 \int_{U_1} \sum_{k,l=1}^4 \left| \left(\partial_{u_j} a_{lk}(\phi(u),\cdot), \overline{\varphi_k}\right)_{1/2\times -1/2}\right|^2 \mathrm{d}u \\
&\leq C_1 \int_{U_1} \sum_{l=1}^4 \|\partial_{u_j} a_{l\cdot}(\phi(u),\cdot)\|^2_{H^{1/2}(\Sigma;\mathbb{C}^4)} \|\varphi\|_{H^{-1/2}(\Sigma;\mathbb{C}^4)} \mathrm{d}u \\
&= C_2 \|\varphi\|_{H^{-1/2}(\Sigma;\mathbb{C}^4)}.
\end{aligned}$$

Continuity and density yield that $\mathcal{A}\varphi|_{\Sigma_1} \in H^1(\Sigma_1;\mathbb{C}^4)$ for all $\varphi \in H^{-1/2}(\Sigma;\mathbb{C}^4)$. Thus, any function $\psi \in H^{1/2}(\Sigma;\mathbb{C}^4)$ with $\psi|_{\Sigma_1} \notin H^1(\Sigma_1;\mathbb{C}^4)$ is not contained in $\operatorname{ran}\mathcal{A}$. Hence, there are infinitely many linearly independent functions in $H^{1/2}(\Sigma;\mathbb{C}^4)$ that are not contained in $\operatorname{ran}\mathcal{A}$. This completes the proof of this Theorem. □

Theorem 4.3.6 has also some interesting consequences for the domain of the operator $\overline{A^\Sigma_{\eta_e,\eta_s}}$, namely that it is not contained in any Sobolev space of positive order. This extends the finding from Proposition 4.3.1 and complements one of the main results from Theorem 4.2.3, namely that functions in $\operatorname{dom} A^\Sigma_{\eta_e,\eta_s}$ have in the non-critical case H^1-smoothness.

Corollary 4.3.7. *Let $\Sigma \subset \mathbb{R}^3$ be the boundary of a bounded C^2-smooth domain such that there exists an open set $\Sigma_0 \subset \Sigma$ which is contained in a plane. Moreover, let $\eta_e \in \{\pm 2c\}$ be constant. Then $\operatorname{dom}\overline{A^\Sigma_{\eta_e,0}} \not\subset H^s(\mathbb{R}^3\setminus\Sigma;\mathbb{C}^4)$ for all $s > 0$.*

Proof. We are going to show the claim for $\eta_e = 2c$, the proof for $\eta_e = -2c$ is similar. This corollary will be shown in an indirect way. Namely, we prove that the difference

$(\overline{A^{\Sigma}_{2c,0}} - \lambda)^{-1} - (A_0 - \lambda)^{-1}$ is compact for $\lambda \in \mathbb{C} \setminus \mathbb{R}$, if $\mathrm{dom}\,\overline{A_{2c,0}} \subset H^s(\mathbb{R}^3 \setminus \Sigma; \mathbb{C}^4)$ for some $s > 0$. But this is not possible, as $\sigma_{\mathrm{ess}}(A_0) = (-\infty, -mc^2] \cup [mc^2, \infty) \neq \sigma_{\mathrm{ess}}(\overline{A^{\Sigma}_{2c,0}})$ by Theorem 4.3.6.

The proof of the claim requires some preliminaries. For $s \in [0,1]$ define the Hilbert spaces

$$\mathcal{H}^s := H^s(\mathbb{R}^3 \setminus \Sigma; \mathbb{C}^4) \cap \mathrm{dom}\,(S^{\Sigma})^*$$

equipped with the norms

$$\|f\|^2_{\mathcal{H}^s} := \|f\|^2_{H^s(\mathbb{R}^3\setminus\Sigma;\mathbb{C}^4)} + \|(S^{\Sigma})^* f\|^2_{L^2(\mathbb{R}^3;\mathbb{C}^4)}, \quad f \in \mathcal{H}^s.$$

Then $\Gamma^{\Sigma}_{j,1} := \Gamma^{\Sigma}_j : H^1(\mathbb{R}^3 \setminus \Sigma; \mathbb{C}^4) = \mathcal{H}^1 \to H^{1/2}(\Sigma; \mathbb{C}^4)$ and $\Gamma^{\Sigma}_{j,0} := \widetilde{\Gamma}^{\Sigma}_j : \mathrm{dom}\,(S^{\Sigma})^* = \mathcal{H}^0 \to H^{-1/2}(\Sigma; \mathbb{C}^4)$ are continuous for $j \in \{0,1\}$. By interpolation we get that also

$$\Gamma^{\Sigma}_{j,s} := \widetilde{\Gamma}^{\Sigma}_j \upharpoonright \mathcal{H}^s : \mathcal{H}^s \to H^{s-1/2}(\Sigma; \mathbb{C}^4)$$

is continuous for any $s \in [0,1]$.

Let us assume now that $\mathrm{dom}\,\overline{A^{\Sigma}_{2c,0}} = \ker\big(\Upsilon^{\Sigma}_1 - \Theta^{0,\Sigma}_{2c,0}\Upsilon^{\Sigma}_0\big) \subset \mathcal{H}^s$ for some $s > 0$. Then it holds $\mathrm{dom}\,\Theta^{0,\Sigma}_{2c,0} \subset H^s(\Sigma; \mathbb{C}^4)$ as $\Upsilon^{\Sigma}_0 = -\iota^{\Sigma}_{-}\widetilde{\Gamma}^{\Sigma}_1$. Let β^{Σ} and $\mathcal{M}^{\Sigma}$ be the γ-field and Weyl function corresponding to the ordinary boundary triple $\{L^2(\Sigma; \mathbb{C}^4), \Upsilon^{\Sigma}_0, \Upsilon^{\Sigma}_1\}$, see (2.20). For $\lambda \in \mathbb{C} \setminus \mathbb{R}$ we have

$$\mathrm{ran}\,\big(\Theta^{0,\Sigma}_{2c,0} - \mathcal{M}^{\Sigma}(\lambda)\big)^{-1} = \mathrm{dom}\,\big(\Theta^{0,\Sigma}_{2c,0} - \mathcal{M}^{\Sigma}(\lambda)\big) \subset H^s(\Sigma; \mathbb{C}^4).$$

Moreover, by Proposition 2.2.7 the operator $\big(\Theta^{0,\Sigma}_{2c,0} - \mathcal{M}(\lambda)\big)^{-1}$ is continuous in $L^2(\Sigma; \mathbb{C}^4)$. It follows that

$$\big(\Theta^{0,\Sigma}_{2c,0} - \mathcal{M}^{\Sigma}(\lambda)\big)^{-1} : L^2(\Sigma; \mathbb{C}^4) \to H^s(\Sigma; \mathbb{C}^4)$$

is closed and hence continuous. As the embedding from $H^s(\Sigma; \mathbb{C}^4)$ to $L^2(\Sigma; \mathbb{C}^4)$ is compact, compare Proposition 2.3.2, we conclude that $(\Theta^{0,\Sigma}_{2c,0} - \mathcal{M}^{\Sigma}(\lambda))^{-1}$ is a compact operator in $L^2(\Sigma; \mathbb{C}^4)$. Finally, Krein's resolvent formula from Theorem 2.2.5 shows that

$$(\overline{A^{\Sigma}_{2c,0}} - \lambda)^{-1} - (A_0 - \lambda)^{-1} = \beta^{\Sigma}(\lambda)\big(\Theta^{0,\Sigma}_{2c,0} - \mathcal{M}^{\Sigma}(\lambda)\big)^{-1}\beta^{\Sigma}(\overline{\lambda})^*, \quad \lambda \in \mathbb{C} \setminus \mathbb{R},$$

is a compact operator in $L^2(\mathbb{R}^3; \mathbb{C}^4)$. This yields the desired contradiction. □

4.3.1 Dirac operators with δ-shell interactions of variable critical strength

Finally, we would like to state several remarks on the operator $A^{\Sigma}_{\eta_e,\eta_s}$, if the interaction strengths $\eta_e, \eta_s : \Sigma \to \mathbb{R}$ are Lipschitz continuous functions in the critical case, that means if there are some $x \in \Sigma$ such that $\eta_e(x)^2 - \eta_s(x)^2 = 4c^2$. We have seen already in Proposition 4.3.1 that $A^\Sigma_{\eta_e,\eta_s}$ is symmetric, but not self-adjoint. We will sketch here that, if η_e and η_s fulfill some suitable assumptions, then one can still show similarly as in Section 4.3 that $A^\Sigma_{\eta_e,\eta_s}$ is essentially self-adjoint, compute the self-adjoint realization and provide some spectral properties of this operator like in Theorem 4.3.3 and Proposition 4.3.5.

The crucial result in Section 4.3 is Proposition 4.3.2 – the following main results are based on this. *Step 1* and *Step 2* of its proof could be done for any Lipschitz continuous and real valued functions η_e and η_s without any difference, the critical point is *Step 3*. But with some assumptions on η_e and η_s one can modify this also for more general interaction strengths. This consideration is based on the fact that any $\varphi \in \operatorname{dom} \Theta^{0,\Sigma}_{\eta_e,\eta_s}$ fulfills

$$(\eta_e^2 - \eta_s^2 - 4c^2)\varphi \in H^{1/2}(\Sigma;\mathbb{C}^4). \tag{4.32}$$

Hence, if we assume that η_e and η_s are such that for all $\varphi \in H^{-1/2}(\Sigma;\mathbb{C}^4)$ which satisfy (4.32) there is a sequence $(\varphi_n) \subset H^{1/2}(\Sigma;\mathbb{C}^4)$ with

$$\begin{aligned} \varphi_n \to \varphi \text{ in } H^{-1/2}(\Sigma;\mathbb{C}^4) \quad \text{and} \\ (\eta_e^2 - \eta_s^2 - 4c^2)\varphi_n \to (\eta_e^2 - \eta_s^2 - 4c^2)\varphi \text{ in } H^{1/2}(\Sigma;\mathbb{C}^4), \end{aligned} \tag{4.33}$$

as $n \to \infty$, then one could also adapt *Step 3* in the proof of Proposition 4.3.2 with just little modifications such that its claim is still true. One only must be careful that non-constant functions η_e and η_s do not commute with $\mathcal{C}_0^{-1/2}$. But due to Proposition 3.2.3 the commutator of $\mathcal{C}_0^{-1/2}$ with any Lipschitz continuous function is a bounded operator from $H^{-1/2}(\Sigma;\mathbb{C}^4)$ to $H^{1/2}(\Sigma;\mathbb{C}^4)$, which allows to prove the desired claim. Note that the above assumptions are clearly fulfilled, if $\eta_e(x)^2 - \eta_s(x)^2 = 4c^2$ everywhere on Σ.

Having Proposition 4.3.2 one can then proceed as for constant interaction strengths: in the same way as in Theorem 4.3.3 it follows that $A^\Sigma_{\eta_e,\eta_s}$ is essentially self-adjoint and that the self-adjoint closure is given by

$$\begin{aligned} \overline{A^\Sigma_{\eta_e,\eta_s}} f &:= (-ic\alpha\cdot\nabla + mc^2\beta)f_+ \oplus (-ic\alpha\cdot\nabla + mc^2\beta)f_-, \\ \operatorname{dom}\overline{A^\Sigma_{\eta_e,\eta_s}} &:= \left\{ f = f_+ \oplus f_- \in \operatorname{dom}(S^\Sigma)^* : (\widetilde{\Gamma}^\Sigma_0 + (\eta_e I_4 + \eta_s\beta)\widetilde{\Gamma}^\Sigma_1) f = 0 \right\}. \end{aligned}$$

Moreover, if for all $\varphi \in H^{-1/2}(\Sigma;\mathbb{C}^4)$ satisfying (4.32) it holds (4.33), then the spectral properties of $\overline{A^\Sigma_{\eta_e,\eta_s}}$ can be deduced in a similar way as in Proposition 4.3.5 and we get that:

(i) $(-\infty, -mc^2] \cup [mc^2, \infty) \subset \sigma_{\mathrm{ess}}(\overline{A^\Sigma_{\eta_e,\eta_s}})$.

(ii) $\lambda \in (-mc^2, mc^2) \cap \sigma_{\mathrm{p}}(\overline{A^\Sigma_{\eta_e,\eta_s}})$ if and only if $0 \in \sigma_{\mathrm{p}}\big(\eta_e I_4 + \eta_s\beta + (\mathcal{C}_0^{-1/2})^{-1}\big)$.

(iii) For $\lambda \in \mathbb{C}\setminus\mathbb{R}$ it holds

$$(\overline{A^\Sigma_{\eta_e,\eta_s}} - \lambda)^{-1} = (A_0 - \lambda)^{-1} - \Phi_\lambda^{-1/2}\big(I_4 + (\eta_e I_4 + \eta_s\beta)\mathcal{C}_\lambda^{-1/2}\big)^{-1}(\eta_e I_4 + \eta_s\beta)\Phi^*_{\bar\lambda}.$$

Moreover, if $\eta_e^2 \neq \eta_s^2$ on Σ, then one can show with similar arguments as in the proof of Proposition 4.3.5 (iii) that the discrete and the essential spectra and hence also the resolvent sets of the operators $\overline{A^{\Sigma}_{\eta_e,\eta_s}}$ and $\overline{A^{\Sigma}_{-4c^2\eta_e/(\eta_e^2-\eta_s^2),-4c^2\eta_s/(\eta_e^2-\eta_s^2)}}$ coincide.

4.4 Convergence in the nonrelativistic limit of Dirac operators with electrostatic and Lorentz scalar δ-shell interactions

In this section we study the nonrelativistic limit of Dirac operators with purely electrostatic or purely Lorentz scalar δ-shell interactions, that means we study this limit of $A^{\Sigma}_{\eta_e,\eta_s}$ in the case that either $\eta_s \equiv 0$ or $\eta_e \equiv 0$. In the nonrelativistic limit one subtracts/adds the energy of the mass of the particle mc^2 from the total energy and and computes the limit of the resolvent as $c \to \infty$. The expected result is the resolvent a nonrelativistic Schrödinger operator which describes the same physical problem with the same parameters times a projection onto the upper/lower components of the Dirac wave function. In our case we will see that the Dirac operator with an electrostatic or a scalar δ-shell interaction converges in the nonrelativistic limit to a Schrödinger operator with a δ-potential of the same strength. This gives a justification for the usage of the operator $A^{\Sigma}_{\eta_e,0}$ and A^{Σ}_{0,η_s} as a Dirac operator with a singular δ-interaction supported on Σ. The presentation in this section follows closely [11, Section 5].

First, let us recall the definition of Schrödinger operators with δ-potentials and some of their properties that are needed for our purposes here. As usual let $\Sigma \subset \mathbb{R}^3$ be the boundary of a compact C^2-domain and let $\eta : \Sigma \to \mathbb{R}$ be a Lipschitz continuous function. We define the sesquilinear form

$$\mathfrak{a}_\eta[f,g] := \frac{1}{2m}(\nabla f, \nabla g)_{\mathbb{R}^3} + (\eta f|_\Sigma, g|_\Sigma)_\Sigma, \quad f,g \in \operatorname{dom} \mathfrak{a}_\eta := H^1(\mathbb{R}^3;\mathbb{C}). \tag{4.34}$$

It is not difficult to show that $\mathfrak{a}_\eta$ is symmetric, semibounded from below and closed, see for instance [28, Section 4] or [19]. The associated self-adjoint operator $-\Delta_\eta$ is the Schrödinger operator with a δ-potential of strength η supported on Σ. In what follows we want to find a suitable resolvent formula for $-\Delta_\eta$. For that we define for $\lambda \in \mathbb{C} \setminus \mathbb{R}$ the function

$$K_\lambda(x) := 2m \frac{e^{i\sqrt{2m\lambda}|x|}}{4\pi|x|}, \qquad x \in \mathbb{R}^3 \setminus \{0\}, \tag{4.35}$$

and recall that

$$\left(-\frac{1}{2m}\Delta - \lambda\right)^{-1} f(x) = \int_{\mathbb{R}^3} K_\lambda(x-y) f(y) \mathrm{d}y, \qquad x \in \mathbb{R}^3, f \in L^2(\mathbb{R}^3;\mathbb{C}), \tag{4.36}$$

see for instance [67, Chapter 7.4]. Moreover, we introduce the bounded integral operators $\Psi_\lambda : L^2(\Sigma;\mathbb{C}) \to L^2(\mathbb{R}^3;\mathbb{C})$ acting as

$$\Psi_\lambda \varphi(x) := \int_\Sigma K_\lambda(x-y)\varphi(y)\mathrm{d}\sigma(y), \qquad x \in \mathbb{R}^3, \varphi \in L^2(\Sigma;\mathbb{C}^4), \tag{4.37}$$

and $\mathcal{D}_\lambda : L^2(\Sigma;\mathbb{C}) \to L^2(\Sigma;\mathbb{C})$,

$$\mathcal{D}_\lambda \varphi(x) := \int_\Sigma K_\lambda(x-y)\varphi(y)\mathrm{d}\sigma(y), \qquad x \in \Sigma, \varphi \in L^2(\Sigma;\mathbb{C}^4). \tag{4.38}$$

It is not difficult to see that Ψ_λ and $\mathcal{D}_\lambda$ are bounded, compare Propositions 2.4.4 and 2.4.5. Moreover, a simple calculation shows that the adjoint $\Psi_\lambda^* : L^2(\mathbb{R}^3;\mathbb{C}) \to L^2(\Sigma;\mathbb{C})$ is

$$\psi_\lambda^* f(x) = \int_{\mathbb{R}^3} K_{\overline{\lambda}}(x-y) f(y)\mathrm{d}y, \qquad x \in \Sigma, f \in L^2(\mathbb{R}^3;\mathbb{C}).$$

With these notations in hand we can state now an explicit resolvent formula for $-\Delta_\eta$; for a proof of this result see for instance [19, Theorem 3.5] or [28, Lemma 2.3].

Proposition 4.4.1. *Let $\eta : \Sigma \to \mathbb{R}$ be a Lipschitz continuous function and let $-\Delta_\eta$ be the self-adjoint operator associated to the quadratic form* (4.34). *Then for all $\lambda \in \mathbb{C} \setminus \mathbb{R}$ the operator $I_1 + \eta\mathcal{D}_\lambda$ is boundedly invertible and*

$$(-\Delta_\eta - \lambda)^{-1} = \left(-\frac{1}{2m}\Delta - \lambda\right)^{-1} - \Psi_\lambda (I_1 + \eta\mathcal{D}_\lambda)^{-1}\Psi_{\overline{\lambda}}^*.$$

In the rest of this section we are going to prove that the Dirac operators $A_{\eta,0}^\Sigma$ with a purely electrostatic δ-shell potential and $A_{0,\eta}^\Sigma$ with a purely scalar interaction given by (4.12) converge in the nonrelativistic limit to a Schrödinger operator $-\Delta_\eta$ with a δ-potential of strength η. That means that we are going to show

$$\lim_{c\to\infty} (A_{\eta,0}^\Sigma - (\lambda + mc^2))^{-1} = (-\Delta_\eta - \lambda)^{-1} P_+$$

and

$$\lim_{c\to\infty} (A_{0,\eta}^\Sigma - (\lambda \pm mc^2))^{-1} = (\pm(-\Delta_\eta) - \lambda)^{-1} P_\pm,$$

where

$$P_+ := \begin{pmatrix} I_2 & 0 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad P_- := \begin{pmatrix} 0 & 0 \\ 0 & I_2 \end{pmatrix}.$$

This shows then that $A_{\eta,0}^\Sigma$ and $A_{0,\eta}^\Sigma$ are the relativistic counterparts of $-\Delta_\eta$ with electrostatic and scalar interactions, respectively.

Note that for a fixed parameter η there is no critical interaction strength for sufficiently large c, as $4c^2 > \eta(x)^2$ for all $x \in \Sigma$ in this case. Furthermore, the operators $(A_{\eta,0}^\Sigma - (\lambda + mc^2))^{-1}$ and $(A_{0,\eta}^\Sigma - (\lambda \pm mc^2))^{-1}$ can be expressed by Theorem 4.2.3 in terms of $(A_0 - (\lambda \pm mc^2))^{-1}$, $\Phi_{\lambda \pm mc^2}$, $\mathcal{C}_{\lambda \pm mc^2}$ and $\Phi_{\overline{\lambda} \pm mc^2}$. The convergence of these operators is analyzed in the following lemma:

Lemma 4.4.2. *Let $\lambda \in \mathbb{C}\setminus\mathbb{R}$, let A_0 be the free Dirac operator defined by* (3.3)*, and let Φ_λ and $\mathcal{C}_\lambda$ be given by* (3.16) *and* (3.17)*, respectively. Moreover, let $-\Delta$ be the free Laplace operator in $L^2(\mathbb{R}^3;\mathbb{C})$ and let Ψ_λ and $\mathcal{D}_\lambda$ be given by* (4.37) *and* (4.38)*, respectively. Then, there exists a constant $K > 0$ independent of c such that the following estimates are true for all sufficiently large c:*

$$\left\| (A_0 - (\lambda \pm mc^2))^{-1} - \left(\mp\frac{1}{2m}\Delta - \lambda \right)^{-1} P_\pm \right\| \leq \frac{K}{c}; \tag{4.39a}$$

$$\|\Phi_{\lambda\pm mc^2} \mp \Psi_{\pm\lambda} P_\pm\| \leq \frac{K}{c}; \tag{4.39b}$$

$$\|\Phi^*_{\lambda\pm mc^2} \mp \Psi^*_{\pm\lambda} P_\pm\| \leq \frac{K}{c}; \tag{4.39c}$$

$$\|\mathcal{C}_{\lambda\pm mc^2} \mp \mathcal{D}_{\pm\lambda} P_\pm\| \leq \frac{K}{c}. \tag{4.39d}$$

Proof. We only prove the claims on $(A_0 - (\lambda + mc^2))^{-1}$, $\Phi_{\lambda+mc^2}$, $\Phi^*_{\lambda+mc^2}$, and $\mathcal{C}_{\lambda+mc^2}$ here, the convergence of $(A_0 - (\lambda - mc^2))^{-1}$, $\Phi_{\lambda-mc^2}$, $\Phi^*_{\lambda-mc^2}$, and $\mathcal{C}_{\lambda-mc^2}$ can be studied in exactly the same way.

Note first that all differences that shall be estimated in (4.39) are integral operators with the integral kernel $G_{\lambda+mc^2} - K_\lambda P_+$. Thus, we have first a closer look onto this function. Recall the definition of K_λ from (4.35) and note that

$$G_{\lambda+mc^2}(x) = \left(\frac{\lambda}{c^2} I_4 + 2mP_+ + \left(1 - i\sqrt{\frac{\lambda^2}{c^2} + 2m\lambda}\,|x| \right) \frac{i(\alpha\cdot x)}{c|x|^2} \right) \frac{e^{i\sqrt{\lambda^2/c^2+2m\lambda}|x|}}{4\pi|x|}.$$

We make the decomposition

$$G_{\lambda+mc^2}(x) - K_\lambda(x)P_+ = t_1(x) + t_2(x), \tag{4.40}$$

where the functions t_1 and t_2 are defined by

$$\begin{aligned} t_1(x) &= \left(\frac{\lambda}{c^2} I_4 + \left(1 - i\sqrt{\frac{\lambda^2}{c^2} + 2m\lambda}\,|x| \right) \frac{i(\alpha\cdot x)}{c|x|^2} \right) \frac{e^{i\sqrt{\lambda^2/c^2+2m\lambda}|x|}}{4\pi|x|}; \\ t_2(x) &= \left(e^{i\sqrt{\lambda^2/c^2+2m\lambda}|x|} - e^{i\sqrt{2m\lambda}|x|} \right) \frac{2m}{4\pi|x|} P_+. \end{aligned} \tag{4.41}$$

It is easy to see that there exist positive constants $\kappa_1 = \kappa_1(m,\lambda)$ and $\kappa_2 = \kappa_2(m,\lambda)$ depending on λ and m and independent of c and an $R > 0$ such that

$$|t_1(x)| \leq \frac{\kappa_1(m,\lambda)}{c} \begin{cases} |x|^{-2}, & |x| < R, \\ e^{-\kappa_2(m,\lambda)|x|}, & |x| \geq R. \end{cases} \tag{4.42}$$

In order to estimate t_2 we compute first

$$\begin{aligned}\left|e^{i\sqrt{\lambda^2/c^2+2m\lambda}|x|}-e^{i\sqrt{2m\lambda}|x|}\right| &= \left|\int_0^1 \frac{\mathrm{d}}{\mathrm{d}t} e^{i\sqrt{t\lambda^2/c^2+2m\lambda}|x|}\mathrm{d}t\right| \\ &\leq \frac{|x|}{c}\int_0^1 \left| e^{i\sqrt{t\lambda^2/c^2+2m\lambda}|x|}\frac{i\lambda^2}{2c\sqrt{t\lambda^2/c^2+2m\lambda}}\right|\mathrm{d}t.\end{aligned}$$

Since $\lambda \in \mathbb{C}\setminus\mathbb{R}$ there exist constants $\kappa_3(m,\lambda), \kappa_4(m,\lambda) > 0$ which are again independent of the speed of light such that for all sufficiently large c

$$\left|\frac{i\lambda^2}{2c\sqrt{t\lambda^2/c^2+2m\lambda}}\right| \leq \kappa_3(m,\lambda) \quad \text{and} \quad \mathrm{Re}\left(i\sqrt{t\lambda^2/c^2+2m\lambda}\right) \leq -\kappa_4(m,\lambda)$$

hold for all $t \in [0,1]$. This implies

$$\begin{aligned}|t_2(x)| &= \left|\frac{2m}{4\pi|x|}\left(e^{i\sqrt{\lambda^2/c^2+2m\lambda}|x|}-e^{i\sqrt{2m\lambda}|x|}\right)P_+\right| \\ &\leq \kappa_3(m,\lambda)\frac{m}{2\pi c}e^{-\kappa_4(m,\lambda)|x|}.\end{aligned} \tag{4.43}$$

Eventually, by (4.40), (4.42) and (4.43) there exist constants $\kappa_5(m,\lambda), \kappa_6(m,\lambda) > 0$ such that

$$\begin{aligned}|G_{\lambda+mc^2}(x) - K_\lambda(x)P_+| &\leq |t_1(x)| + |t_2(x)| \\ &\leq \frac{\kappa_5(m,\lambda)}{c}\begin{cases}|x|^{-2}, & |x| < R, \\ e^{-\kappa_6(m,\lambda)|x|}, & |x| \geq R.\end{cases}\end{aligned} \tag{4.44}$$

Now, we are prepared to prove (4.39a)–(4.39c). By Proposition 3.1.1 and (4.36) we have

$$\begin{aligned}&\left(\left(A_0 - (\lambda + mc^2)\right)^{-1} - \left(-\frac{1}{2m}\Delta - \lambda\right)^{-1} P_+\right) f(x) \\ &\qquad = \int_{\mathbb{R}^3}\left(G_{\lambda+mc^2}(x-y) - K_\lambda(x-y)P_+\right) f(y)\mathrm{d}y\end{aligned}$$

for $x \in \mathbb{R}^3$ and $f \in L^2(\mathbb{R}^3;\mathbb{C}^4)$. With (4.44) and Proposition 2.4.3 we get

$$\left\|\left(A_0 - (\lambda + mc^2)\right)^{-1} - \left(-\frac{1}{2m}\Delta - \lambda\right)^{-1} P_+\right\| \leq \frac{\kappa_7(m,\lambda)}{c}$$

for some constant $\kappa_7(m,\lambda)$ and hence (4.39a) holds. Next we prove (4.39b). By Proposition 4.1.2 (i) and (4.37) we have

$$\left(\Phi_{\lambda+mc^2} - \Psi_\lambda P_+\right)\varphi(x) = \int_\Sigma \left(G_{\lambda+mc^2}(x-y) - K_\lambda(x-y)P_+\right)\varphi(y)\mathrm{d}\sigma(y)$$

for $x \in \mathbb{R}^3$ and $\varphi \in L^2(\Sigma;\mathbb{C}^4)$. Here, the asymptotics in (4.44) and Proposition 2.4.4 yield

$$\|\Phi_{\lambda+mc^2} - \Psi_\lambda P_+\| \leq \frac{\kappa_8(m,\lambda)}{c},$$

which is already the claimed estimate. Moreover, the relation (4.39c) follows by taking adjoints.

Finally, we verify $\mathcal{C}_{\lambda+mc^2} \to \mathcal{D}_\lambda P_+$. For that, we use the decomposition

$$\begin{aligned}\big(\mathcal{C}_{\lambda+mc^2} - \mathcal{D}_\lambda P_+\big)\varphi(x) &= \lim_{\varepsilon\searrow 0}\int_{|x-y|>\varepsilon} \big(G_{\lambda+mc^2}(x-y) - K_\lambda(x-y)P_+\big)\varphi(y)\mathrm{d}\sigma(y)\\ &= (\mathcal{S}_1+\mathcal{S}_2+\mathcal{S}_3+\mathcal{S}_4)\varphi(x), \quad x\in\Sigma,\ \varphi\in L^2(\Sigma;\mathbb{C}^4),\end{aligned}$$

where for $j \in \{1,2,3,4\}$ the integral operators $\mathcal{S}_j : L^2(\Sigma;\mathbb{C}^4) \to L^2(\Sigma;\mathbb{C}^4)$ are given by

$$\mathcal{S}_j\varphi(x) := \lim_{\varepsilon\searrow 0}\int_{|x-y|>\varepsilon} s_j(x-y)\varphi(y)\mathrm{d}\sigma(y), \quad x\in\Sigma,\ \varphi\in L^2(\Sigma;\mathbb{C}^4),$$

with

$$\begin{aligned} s_1(x) &:= \left(\frac{\lambda}{c^2}I_4 + \frac{\alpha\cdot x}{c|x|}\sqrt{\frac{\lambda^2}{c^2}+2m\lambda}\right)\frac{e^{i\sqrt{\lambda^2/c^2+2m\lambda}|x|}}{4\pi|x|}, & s_2(x) &:= t_2(x),\\ s_3(x) &:= \frac{i(\alpha\cdot x)}{4c\pi|x|^3}\left(e^{i\sqrt{\lambda^2/c^2+2m\lambda}|x|}-1\right), & s_4(x) &:= \frac{i(\alpha\cdot x)}{4c\pi|x|^3},\end{aligned}$$

with t_2 as in (4.41). We remark that $s_1+s_3+s_4 = t_1$ with t_1 given by (4.41). It is easy to see that $|s_1(x)| \leq \frac{\kappa_9(m,\lambda)}{c|x|}$ for some constant $\kappa_9(m,\lambda)$ depending only on m and λ and all $x\in\mathbb{R}^3\setminus\{0\}$. Furthermore, $|s_2(x)| \leq \kappa_3(m,\lambda)\frac{m}{2\pi c}$ for all $x\in\mathbb{R}^3$ by (4.43). Next, because of

$$\begin{aligned}\left|e^{i\sqrt{\lambda^2/c^2+2m\lambda}|x|}-1\right| &= \left|\int_0^1 \frac{\mathrm{d}}{\mathrm{d}t}e^{it\sqrt{\lambda^2/c^2+2m\lambda}|x|}\mathrm{d}t\right|\\ &\leq |x|\int_0^1\left|e^{it\sqrt{\lambda^2/c^2+2m\lambda}|x|}\cdot i\sqrt{\frac{\lambda^2}{c^2}+2m\lambda}\right|\mathrm{d}t,\end{aligned}$$

we deduce that there exists $\kappa_{10}(m,\lambda)$ such that $|s_3(x)| \leq \frac{\kappa_{10}(m,\lambda)}{c|x|}$ for all $x\in\mathbb{R}^3\setminus\{0\}$. Therefore, we can apply Proposition 2.4.5 and obtain

$$\|\mathcal{S}_j\| \leq \frac{\kappa_{11}(m,\lambda)}{c}, \quad j\in\{1,2,3\},$$

for some constant $\kappa_{11}(m,\lambda)$ depending only on m and λ. Eventually, we note that $\mathcal{S}_4 = \frac{1}{c}\mathcal{T}$, where $\mathcal{T}$ is the integral operator with integral kernel $cs_4(x-y) = \frac{i(\alpha\cdot(x-y))}{4\pi|x-y|^3}$; this operator is independent of c, everywhere defined and bounded, see Proposition 2.4.6. Therefore, $\|\mathcal{S}_4\| \leq \frac{\kappa_{12}}{c}$. This yields finally that

$$\left\|\mathcal{C}_{\lambda+mc^2} - \mathcal{D}_\lambda P_+\right\| \leq \|\mathcal{S}_1\| + \|\mathcal{S}_2\| + \|\mathcal{S}_3\| + \|\mathcal{S}_4\| \leq \frac{\kappa_{13}(m,\lambda)}{c}$$

and completes the proof of (4.39d). □

Now we are prepared to compute the nonrelativistic limit of Dirac operators with electrostatic and scalar δ-shell interactions. The proofs of these results are based on the resolvent formulae from Theorem 4.2.3 and Proposition 4.4.1 and on Lemma 4.4.2.

Theorem 4.4.3. *Assume that $\eta : \Sigma \to \mathbb{R}$ is a Lipschitz continuous function and let the operators $A_{\eta,0}^\Sigma$ and $-\Delta_\eta$ be defined by* (4.12) *and* (4.34)*, respectively. Then for any $\lambda \in \mathbb{C} \setminus \mathbb{R}$ there exists a constant $K > 0$ such that for all sufficiently large c*

$$\left\|\left(A_{\eta,0}^\Sigma - (\lambda + mc^2)\right)^{-1} - (-\Delta_\eta - \lambda)^{-1} P_+\right\| \leq \frac{K}{c}.$$

Proof. According to Theorem 4.2.3 the resolvent of $A_{\eta,0}^\Sigma$ is given by

$$\left(A_{\eta,0}^\Sigma - (\lambda + mc^2)\right)^{-1} = \left(A_0 - (\lambda + mc^2)\right)^{-1} - \Phi_{\lambda+mc^2}\left(I_4 + \eta\,\mathcal{C}_{\lambda+mc^2}\right)^{-1}\eta\,\Phi_{\overline{\lambda}+mc^2}^*.$$

From Lemma 4.4.2 we know that there exists a constant $\kappa_1 > 0$ such that for all sufficiently large c it holds

$$\left\|\left(A_0 - (\lambda + mc^2)\right)^{-1} - \left(-\frac{1}{2m}\Delta - \lambda\right)^{-1} P_+\right\| \leq \frac{\kappa_1}{c}, \qquad \|\Phi_{\lambda+mc^2} - \Psi_\lambda P_+\| \leq \frac{\kappa_1}{c},$$

$$\|\mathcal{C}_{\lambda+mc^2} - \mathcal{D}_\lambda P_+\| \leq \frac{\kappa_1}{c}, \quad \text{and} \quad \|\Phi_{\overline{\lambda}+mc^2}^* - \Psi_{\overline{\lambda}}^* P_+\| \leq \frac{\kappa_1}{c}.$$

Using that $I_4 + \eta\,\mathcal{C}_{\lambda+mc^2}$ and $I_4 + \eta\,\mathcal{D}_\lambda P_+$ are boundedly invertible for $\lambda \in \mathbb{C} \setminus \mathbb{R}$, see Proposition 4.1.7 and Proposition 4.4.1, we conclude from [50, Theorem IV 1.16] that also

$$\left\|\left(I_4 + \eta\,\mathcal{C}_{\lambda+mc^2}\right)^{-1} - \left(I_4 + \eta\,\mathcal{D}_\lambda P_+\right)^{-1}\right\| \leq \frac{\kappa_2}{c}$$

for some $\kappa_2 > 0$. This implies

$$\begin{aligned}
\lim_{c\to\infty}\left(A_{\eta,0}^\Sigma - (\lambda + mc^2)\right)^{-1} &= \lim_{c\to\infty}\Big[\left(A_0 - (\lambda + mc^2)\right)^{-1} \\
&\qquad\qquad - \Phi_{\lambda+mc^2}\left(I_4 + \eta\,\mathcal{C}_{\lambda+mc^2}\right)^{-1}\eta\,\Phi_{\overline{\lambda}+mc^2}^*\Big] \\
&= \left(-\frac{1}{2m}\Delta - \lambda\right)^{-1} P_+ - \Psi_\lambda P_+\left(I_4 + \eta\,\mathcal{D}_\lambda P_+\right)^{-1}\Psi_{\overline{\lambda}}^* P_+ \\
&= (-\Delta_\eta - \lambda)^{-1} P_+,
\end{aligned}$$

compare Proposition 4.4.1, and that the order of convergence is $\frac{1}{c}$. This is the claimed result. □

Eventually, we prove that the Dirac operator with a Lorentz scalar δ-shell interaction converges in the nonrelativistic limit also to a Schrödinger operator $-\Delta_\eta$ with a δ-potential supported on Σ. This theorem is very similar as Theorem 4.4.3, but we would like to point out that we have a slightly stronger statement for scalar as for electrostatic interactions: for scalar δ-shell interactions we also have convergence of the negative part of the operator (that means of $A^\Sigma_{0,\eta}+mc^2$) to $-(-\Delta_\eta)$.

Theorem 4.4.4. *Assume that $\eta:\Sigma\to\mathbb{R}$ is a Lipschitz continuous function and let the operators $A^\Sigma_{0,\eta}$ and $-\Delta_\eta$ be defined by* (4.12) *and* (4.34)*, respectively. Then for any $\lambda\in\mathbb{C}\setminus\mathbb{R}$ there exists a constant $K>0$ such that for all sufficiently large c*

$$\left\|\big(A^\Sigma_{0,\eta}-(\lambda\pm mc^2)\big)^{-1}-\big(\pm(-\Delta_\eta)-\lambda\big)^{-1}P_\pm\right\|\leq\frac{K}{c}.$$

Proof. The convergence of $A^\Sigma_{0,\eta}-mc^2$ can be analyzed with exactly the same arguments as the one of $A^\Sigma_{\eta,0}-mc^2$ in Theorem 4.4.3; hence, we omit the treatment of this case here and study only $A^\Sigma_{0,\eta}+mc^2$. According to Theorem 4.2.3 the resolvent of $A^\Sigma_{0,\eta}$ is given by

$$\big(A^\Sigma_{0,\eta}-(\lambda-mc^2)\big)^{-1}=\big(A_0-(\lambda-mc^2)\big)^{-1}-\Phi_{\lambda-mc^2}\big(I_4+\eta\beta\mathcal{C}_{\lambda-mc^2}\big)^{-1}\eta\beta\Phi^*_{\overline{\lambda}-mc^2}.$$

From Lemma 4.4.2 we know that there exists a constant $\kappa_1>0$ such that for all sufficiently large c

$$\left\|(A_0-(\lambda-mc^2))^{-1}+\left(-\frac{1}{2m}\Delta+\lambda\right)^{-1}P_-\right\|\leq\frac{\kappa_1}{c},\qquad\|\Phi_{\lambda-mc^2}+\Psi_{-\lambda}P_-\|\leq\frac{\kappa_1}{c},$$

$$\|\mathcal{C}_{\lambda-mc^2}+\mathcal{D}_{-\lambda}P_-\|\leq\frac{\kappa_1}{c},\quad\text{and}\quad\|\Phi^*_{\overline{\lambda}-mc^2}+\Psi^*_{-\overline{\lambda}}P_-\|\leq\frac{\kappa_1}{c}.$$

Using that $I_4+\eta\beta\mathcal{C}_{\lambda-mc^2}$ and $I_4+\eta\mathcal{D}_\lambda P_-=I_4-\eta\beta\mathcal{D}_\lambda P_-$ are boundedly invertible for $\lambda\in\mathbb{C}\setminus\mathbb{R}$, see Proposition 4.1.7 and Proposition 4.4.1, we conclude from [50, Theorem IV 1.16] that also

$$\left\|\big(I_4+\eta\beta\mathcal{C}_{\lambda-mc^2}\big)^{-1}-\big(I_4-\eta\beta\mathcal{D}_\lambda P_-\big)^{-1}\right\|\leq\frac{\kappa_2}{c}$$

for some $\kappa_2>0$. Note that $\beta P_-=-P_-$. Hence, we obtain finally

$$\begin{aligned}\lim_{c\to\infty}\big(A^\Sigma_{0,\eta}-(\lambda-mc^2)\big)^{-1}&=\lim_{c\to\infty}\Big[\big(A_0-(\lambda-mc^2)\big)^{-1}\\&\qquad-\Phi_{\lambda-mc^2}\big(I_4+\eta\beta\mathcal{C}_{\lambda-mc^2}\big)^{-1}\eta\beta\Phi^*_{\overline{\lambda}-mc^2}\Big]\\&=-\left(-\frac{1}{2m}\Delta+\lambda\right)^{-1}P_--\Psi_{-\lambda}P_-\big(I_4-\eta\beta\mathcal{D}_{-\lambda}P_-\big)^{-1}\eta\beta\Psi^*_{-\overline{\lambda}}P_-\\&=-\left(-\frac{1}{2m}\Delta+\lambda\right)^{-1}P_-+\Psi_{-\lambda}\big(I_4+\eta\mathcal{D}_{-\lambda}\big)^{-1}\eta\Psi^*_{-\overline{\lambda}}P_-\\&=-(-\Delta_\eta+\lambda)^{-1}P_-=\big(-(-\Delta_\eta)-\lambda\big)^{-1}P_-,\end{aligned}$$

compare Proposition 4.4.1, and that the order of convergence is $\frac{1}{c}$. This is the claimed result. □

Finally, we show that for large c and constant $\eta < 0$ sufficiently large the number of eigenvalues of $A^{\Sigma}_{\eta,0}$ in the gap $(-mc^2, mc^2)$ of $\sigma_{\text{ess}}(A^{\Sigma}_{\eta,0})$ becomes large. The proof is based on Theorem 4.4.3 and a result from [42] on the spectrum of $-\Delta_\eta$. In a similar way, one can derive also other results on the spectrum of $A_{\eta,0}$ from the well-known properties of $-\Delta_\eta$. A similar result can also be shown for $A^{\Sigma}_{0,\eta}$ with exactly the same arguments.

Proposition 4.4.5. *For any fixed $j \in \mathbb{N}$ there exists a constant $\eta < 0$ depending on j such that the number of discrete eigenvalues of $A^{\Sigma}_{\eta,0}$ taking multiplicities into account is at least j for all sufficiently large c.*

Proof. First, we show that for a suitable $\eta < 0$ the operator $-\Delta_\eta P_+$ has the desired properties; then via a continuity argument the claim follows also for A_η. It is easy to see that $\sigma_{\text{ess}}(-\Delta_\eta P_+) = \sigma_{\text{ess}}(-\Delta_\eta) \cup \{0\} = [0, \infty)$. Moreover, we know from [19, Theorem 3.14] that $\sigma_{\text{disc}}(-\Delta_\eta P_+) = \sigma_{\text{disc}}(-\Delta_\eta)$ is finite and from [42, Theorem 2.1] that for some fixed $j \in \mathbb{N}$ there exists an $\eta < 0$ such that $-\Delta_\eta P_+$ has at least j discrete eigenvalues. Let this η be fixed and choose $a < b < 0$ with $\sigma_{\text{disc}}(-\Delta_\eta) \subset (a,b)$ and denote the spectral projections of $-\Delta_\eta P_+$ and $A_\eta - mc^2$ for the interval (a,b) by $E_{-\Delta_\eta P_+}((a,b))$ and $E_{A^{\Sigma}_{\eta,0} - mc^2}((a,b))$, respectively.

According to Theorem 4.4.3 the operators $(A^{\Sigma}_{\eta,0} - (\lambda + mc^2))^{-1}$ converge to $(-\Delta_\eta - \lambda)^{-1} P_+$ for $c \to \infty$ and $\lambda \in \mathbb{C} \setminus \mathbb{R}$. The latter operator is the resolvent of a self-adjoint relation (multivalued operator) and hence one can show in the same way as in [69, Satz 9.24 b)] together with [69, Satz 2.58 a)] that for all sufficiently large c the dimensions of the ranges of $E_{-\Delta_\eta P_+}((a,b))$ and $E_{A^{\Sigma}_{\eta,0} - mc^2}((a,b))$ coincide, that means

$$\dim \operatorname{ran} E_{A^{\Sigma}_{\eta,0} - mc^2}((a,b)) = \dim \operatorname{ran} E_{-\Delta_\eta P_+}((a,b)) \geq j.$$

Thus, the operator $A^{\Sigma}_{\eta,0}$ has at least j eigenvalues (counted with multiplicities) in the interval $(a + mc^2, b + mc^2) \subset (-mc^2, mc^2)$ for sufficiently large c. □

5 DIRAC OPERATORS ON DOMAINS

In this chapter we investigate self-adjoint Dirac operators on a domain $\Omega \subset \mathbb{R}^3$ which is either a bounded C^2-domain or the complement of a bounded C^2-domain. The self-adjointness is achieved in this case by requiring suitable boundary conditions on $\partial\Omega$. First, in Section 5.1 we investigate the so called MIT bag model. This is a Dirac operator with special boundary conditions which is known to be self-adjoint and, as the free Dirac operator on the whole Euclidean space $\mathbb{R}^3$, the MIT bag operator will serve as a reference operator. Moreover, we will study several properties of this operator.

Then, in Section 5.2.1 we introduce a quasi boundary triple $\{\mathcal{G}_\Omega, \Gamma_0^\Omega, \Gamma_1^\Omega\}$ which is suitable to define and study self-adjoint Dirac operators on domains. Here $\mathcal{G}_\Omega = P_+\big(L^2(\Sigma;\mathbb{C}^4)\big)$ and $P_+ = \frac{1}{2}\big(I_4 + i\beta\alpha\cdot\nu\big)$ is a projection which turns out to have some very convenient properties. Again the γ-field and the Weyl function associated to this quasi boundary triple are closely related to the integral operators Φ_λ and $\mathcal{C}_\lambda$ introduced in Section 3.2. Moreover, we will see that the triple $\{\mathcal{G}_\Omega, \Gamma_0^\Omega, \Gamma_1^\Omega\}$ satisfies the assumptions from Theorem 2.2.13. Hence, we can transform this quasi boundary triple to an ordinary boundary triple $\{\mathcal{G}_\Omega, \Upsilon_0^\Omega, \Upsilon_1^\Omega\}$; compare Theorem 5.2.6.

Next, in Section 5.3 we introduce with the help of the quasi boundary triple $\{\mathcal{G}_\Omega, \Gamma_0^\Omega, \Gamma_1^\Omega\}$ Dirac operators acting in Ω. In the case of non-critical boundary values we prove self-adjointness of the operators and provide the basic spectral properties of them. Furthermore, we will see that there is a close relation of Dirac operators on domains and Dirac operators with singular interactions in the confinement case, compare Remark 4.2.2.

Similarly as for Dirac operators with singular interactions there exist also some critical boundary values for which self-adjointness can not be shown with the aid of the quasi boundary triple $\{\mathcal{G}_\Omega, \Gamma_0^\Omega, \Gamma_1^\Omega\}$. Following the strategy from Section 4.3 we compute the self-adjoint realization for constant critical τ. Moreover, making use of the ordinary boundary triple $\{\mathcal{G}_\Omega, \Upsilon_0^\Omega, \Upsilon_1^\Omega\}$ we will then deduce some further spectral properties of the self-adjoint realization.

The material presented in this chapter is part of the paper in preparation [15].

5.1 The MIT bag operator

Let $\Omega \subset \mathbb{R}^3$ be a domain with a compact C^2-boundary $\partial\Omega$ with outer unit normal vector field ν. In this first preliminary section we discuss the MIT-bag Dirac operator in Ω which will often play the role of a self-adjoint reference operator in this chapter. It is defined as follows:

Definition 5.1.1. *The MIT-bag operator $T^{\Omega}_{\mathrm{MIT}}$ is given by*

$$\begin{aligned} T^{\Omega}_{\mathrm{MIT}} f &:= (-ic\alpha\cdot\nabla + mc^2\beta)f, \\ \operatorname{dom} T^{\Omega}_{\mathrm{MIT}} &= \{f \in H^1(\Omega;\mathbb{C}^4) : f|_{\partial\Omega} = -i\beta(\alpha\cdot\nu)f|_{\partial\Omega}\}. \end{aligned} \tag{5.1}$$

In the following proposition we summarize the basic properties of $T^{\Omega}_{\mathrm{MIT}}$. The proof is rather simple due to the fact that $T^{\Omega}_{\mathrm{MIT}} \oplus T^{\Omega^c}_{\mathrm{MIT}} = A^{\partial\Omega}_{0,2c}$ with $A^{\partial\Omega}_{0,2c}$ given by (4.12), compare (4.14). In order to formulate the results, we define the orthogonal projections

$$P_\Omega : L^2(\mathbb{R}^3;\mathbb{C}^4) \to L^2(\Omega;\mathbb{C}^4), \quad P_\Omega f = f \upharpoonright \Omega, \tag{5.2}$$

and

$$P^*_\Omega : L^2(\Omega;\mathbb{C}^4) \to L^2(\mathbb{R}^3;\mathbb{C}^4), \quad P_\Omega g = \begin{cases} g & \text{in } \Omega, \\ 0 & \text{in } \Omega^c. \end{cases}$$

Note that assertions (iii) and (iv) of the proposition below are shown in [4] with similar ideas.

Proposition 5.1.2. *Let $T^{\Omega}_{\mathrm{MIT}}$ be defined by* (5.1) *and let for $\lambda \in \mathbb{C}\setminus\mathbb{R}$ the operators Φ_λ and $\mathcal{C}_\lambda$ be defined by* (3.16) *and* (3.17)*, respectively. Then $T^{\Omega}_{\mathrm{MIT}}$ is self-adjoint and the following assertions are true:*

(i) *For $\lambda \in \mathbb{C}\setminus\mathbb{R}$ the resolvent of $T^{\Omega}_{\mathrm{MIT}}$ is given by*

$$(T^{\Omega}_{\mathrm{MIT}} - \lambda)^{-1} = P_\Omega(A_0 - \lambda)^{-1}P^*_\Omega - P_\Omega\Phi_\lambda\big(I_4 + 2c\beta\mathcal{C}_\lambda\big)^{-1}2c\beta\Phi^*_{\overline{\lambda}}P^*_\Omega.$$

(ii) $(-mc^2, mc^2) \subset \rho(T^{\Omega}_{\mathrm{MIT}})$.

(iii) $\lambda \in \sigma(T^{\Omega}_{\mathrm{MIT}})$ *if and only if* $-\lambda \in \sigma(T^{\Omega}_{\mathrm{MIT}})$.

(iv) *Discrete eigenvalues of $T^{\Omega}_{\mathrm{MIT}}$ have always even multiplicity.*

Proof. First, since $T^{\Omega}_{\mathrm{MIT}} \oplus T^{\Omega^c}_{\mathrm{MIT}} = A^{\partial\Omega}_{0,2c}$ is self-adjoint in $L^2(\mathbb{R}^3;\mathbb{C}^4)$ by Theorem 4.2.3 it follows immediately that $T^{\Omega}_{\mathrm{MIT}} = P_\Omega A^{\partial\Omega}_{0,2c} P^*_\Omega$ is self-adjoint in $L^2(\Omega;\mathbb{C}^4)$; compare also Remark 4.2.2. Moreover, this block structure and Theorem 4.2.3 (i) imply the claimed resolvent formula.

Next, assertion (ii) is a direct consequence of Corollary 4.2.6 (vii). Finally, items (iii) and (iv) can be shown in exactly the same way as Corollary 4.2.6 (iv) and (v); we omit the proof here. □

In the following lemma we give a more detailed picture of the spectral properties of T^{Ω}_{MIT}. The properties are entirely different depending on whether Ω is bounded or not.

Lemma 5.1.3. *Let T^{Ω}_{MIT} be defined by* (5.1)*. Then the following assertions are true:*

(i) *If Ω is bounded, then $\sigma(T^{\Omega}_{\text{MIT}}) = \sigma_{\text{disc}}(T^{\Omega}_{\text{MIT}})$.*

(ii) *If Ω is unbounded, then $\sigma(T^{\Omega}_{\text{MIT}}) = \sigma_{\text{ess}}(T^{\Omega}_{\text{MIT}}) = (-\infty, -mc^2] \cup [mc^2, \infty)$.*

Proof. (i) Since Ω is a bounded C^2-domain $\operatorname{dom} T^{\Omega}_{\text{MIT}} \subset H^1(\Omega;\mathbb{C}^4)$ is compactly embedded in $L^2(\Omega;\mathbb{C}^4)$. Hence $\sigma(T^{\Omega}_{\text{MIT}})$ is purely discrete.

(ii) First, we know from Proposition 5.1.2 that $\sigma(T^{\Omega}_{\text{MIT}}) \subset (-\infty, -mc^2] \cup [mc^2, \infty)$. To prove the other inclusion, fix some $\lambda \in (-\infty, -mc^2] \cup [mc^2, \infty)$. Then, since Ω is unbounded, the functions ψ^{λ}_n from Lemma 3.1.4 belong to $\operatorname{dom} T^{\Omega}_{\min} \subset \operatorname{dom} T^{\Omega}_{\text{MIT}}$. Furthermore ψ^{λ}_n converge weakly to zero and

$$\|\psi^{\lambda}_n\|_{\Omega} = \text{const.} > 0 \quad \text{and} \quad (T^{\Omega}_{\text{MIT}} - \lambda)\psi^{\lambda}_n = (T^{\Omega}_{\min} - \lambda)\psi^{\lambda}_n \to 0, \quad \text{as } n \to \infty.$$

Thus (ψ^{λ}_n) is a singular sequence for T^{Ω}_{MIT} and λ which shows $\lambda \in \sigma_{\text{ess}}(T^{\Omega}_{\text{MIT}})$. This finishes the proof of this lemma. □

Finally, we state in a similar fashion as for the MIT bag model the basic spectral properties of another distinguished self-adjoint realization of the Dirac operator on Ω. This operator has similar boundary conditions as T^{Ω}_{MIT}, but with opposite sign, and it is given by

$$\begin{aligned} T^{\Omega}_{-\text{MIT}} f &:= (-ic\alpha \cdot \nabla + mc^2\beta) f, \\ \operatorname{dom} T^{\Omega}_{-\text{MIT}} &= \{ f \in H^1(\Omega;\mathbb{C}^4) : f|_{\partial\Omega} = i\beta(\alpha \cdot \nu) f|_{\partial\Omega} \}. \end{aligned} \tag{5.3}$$

Lemma 5.1.4. *The operator $T^{\Omega}_{-\text{MIT}}$ is self-adjoint. Moreover, $\sigma(T^{\Omega}_{-\text{MIT}}) \cap (-mc^2, mc^2)$ consists of at most finitely many discrete eigenvalues.*

Proof. First, it holds $T^{\Omega}_{-\text{MIT}} \oplus T^{\Omega^c}_{-\text{MIT}} = A^{\partial\Omega}_{0,-2c}$ and this operator is self-adjoint in $L^2(\mathbb{R}^3;\mathbb{C}^4)$ by Theorem 4.2.3. This implies with P_Ω given by (5.2) that $T^{\Omega}_{-\text{MIT}} = P_\Omega A^{\partial\Omega}_{0,-2c} P^*_\Omega$ is self-adjoint in $L^2(\Omega;\mathbb{C}^4)$.

Finally, since we have $T^{\Omega}_{-\text{MIT}} \oplus T^{\Omega^c}_{-\text{MIT}} = A^{\partial\Omega}_{0,-2c}$ it follows immediately from Corollary 4.2.6 that $\sigma(T^{\Omega}_{-\text{MIT}}) \cap (-mc^2, mc^2)$ consists only of at most finitely many discrete eigenvalues. This finishes the proof of this proposition. □

5.2 Boundary triples for Dirac operators on domains

In this section we introduce first a quasi boundary triple which allows us to define self-adjoint Dirac operators on domains via suitable boundary conditions on $\partial\Omega$. Then in Section 5.2.2 we will transform this quasi boundary triple with the methods described in Section 2.2 to an ordinary boundary triple, which enables us then to prove self-adjointness also in the case of critical boundary conditions.

5.2.1 A quasi boundary triple for Dirac operators on domains

Throughout this chapter let Ω be either a bounded domain in $\mathbb{R}^3$ with C^2-smooth boundary or the complement of a bounded C^2-domain. We denote the normal vector field at $\partial\Omega$ pointing outwards of Ω by ν. Furthermore, we define

$$P_\pm := \frac{1}{2}\big(I_4 \pm i\beta(\alpha\cdot\nu)\big). \tag{5.4}$$

Using the anti-commutation relation (1.2) it is easy to see that $P_\pm$ is an orthogonal projection. Furthermore, it is clear that $P_- = I_4 - P_+$. This implies, in particular, that $P_+P_- = P_-P_+ = 0$. Eventually, we set for $s \in [0,1]$

$$\mathcal{G}_\Omega^s := P_+(H^s(\partial\Omega;\mathbb{C}^4)). \tag{5.5}$$

For convenience we set $\mathcal{G}_\Omega := \mathcal{G}_\Omega^0$. Since P_+ is an orthogonal projection in $L^2(\partial\Omega;\mathbb{C}^4)$ the space $\mathcal{G}_\Omega$ is a Hilbert space. Moreover, as $\partial\Omega$ is C^2-smooth $\mathcal{G}_\Omega^s \subset H^s(\partial\Omega;\mathbb{C}^4)$ for any $s \in [0,1]$ and $\mathcal{G}_\Omega^s$ is a closed subspace of $H^s(\partial\Omega;\mathbb{C}^4)$.

Next, we define the operator T^Ω in $L^2(\Omega;\mathbb{C}^4)$ by

$$T^\Omega f := (-ic\alpha\cdot\nabla + mc^2\beta)f, \qquad \operatorname{dom} T^\Omega := H^1(\Omega;\mathbb{C}^4), \tag{5.6}$$

and the mappings $\Gamma_0^\Omega, \Gamma_1^\Omega : \operatorname{dom} T^\Omega \to \mathcal{G}_\Omega$ acting as

$$\Gamma_0^\Omega f := \sqrt{c}P_+ f|_{\partial\Omega} \quad \text{and} \quad \Gamma_1^\Omega f := \sqrt{c}P_+\beta f|_{\partial\Omega}, \quad f \in \operatorname{dom} T^\Omega. \tag{5.7}$$

Note that the trace theorem and Lemma 2.5.1 imply that $\operatorname{ran}\Gamma_0^\Omega, \operatorname{ran}\Gamma_1^\Omega \subset \mathcal{G}_\Omega^{1/2}$, as $\partial\Omega$ is C^2-smooth and $\operatorname{dom} T^\Omega = H^1(\Omega;\mathbb{C}^4)$.

In the following theorem we show that $\{\mathcal{G}_\Omega, \Gamma_0^\Omega, \Gamma_1^\Omega\}$ is a quasi boundary triple and that $\overline{T^\Omega}$ coincides with the maximal Dirac operator $T_{\max}^\Omega$ from (3.10). Moreover, it turns out that the reference operator $T \restriction \ker\Gamma_0^\Omega$ is the MIT bag operator T_{MIT}^Ω studied in Section 5.1.

Theorem 5.2.1. *Let $S^\Omega := T^\Omega_{\min}$ be the minimal Dirac operator from* (3.11)*, let $\mathcal{G}_\Omega$ be given by* (5.5) *and let $T^\Omega, \Gamma_0^\Omega$ and Γ_1^Ω be given by* (5.6) *and* (5.7)*, respectively. Then S^Ω is closed and symmetric, $(S^\Omega)^* = \overline{T^\Omega} = T^\Omega_{\max}$ and $\{\mathcal{G}_\Omega, \Gamma_0^\Omega, \Gamma_1^\Omega\}$ is a quasi boundary triple for $(S^\Omega)^*$. Moreover, $T^\Omega \upharpoonright \ker \Gamma_0^\Omega$ is the Dirac operator T^Ω_{MIT} with MIT bag boundary conditions and*

$$\operatorname{ran}(\Gamma_0^\Omega \upharpoonright \ker \Gamma_1^\Omega) = \operatorname{ran}(\Gamma_1^\Omega \upharpoonright \ker \Gamma_0^\Omega) = \mathcal{G}_\Omega^{1/2}. \tag{5.8}$$

In particular, it holds $\operatorname{ran}(\Gamma_0^\Omega, \Gamma_1^\Omega) = \mathcal{G}_\Omega^{1/2} \times \mathcal{G}_\Omega^{1/2}$.

Proof. First, it is clear by Lemma 3.1.2 that $S^\Omega = T^\Omega_{\min}$ is closed and symmetric and that $(S^\Omega)^* = T^\Omega_{\max}$. Moreover, Lemma 3.1.3 implies that T^Ω is dense in $T^\Omega_{\max}$, as $C^\infty(\overline{\Omega};\mathbb{C}^4) \subset H^1(\Omega;\mathbb{C}^4) = \operatorname{dom} T^\Omega$.

Next, we prove that Green's identity is fulfilled. Let $f, g \in \operatorname{dom} T^\Omega = H^1(\Omega;\mathbb{C}^4)$. Then, integration by parts (2.31) and the self-adjointness of $\alpha \cdot \nu$ yield

$$\begin{aligned}(Tf,g)_\Omega - (f,Tg)_\Omega &= \big((-ic\alpha\cdot\nabla + mc^2\beta)f, g\big)_\Omega - \big(f, (-ic\alpha\cdot\nabla + mc^2\beta)g\big)_\Omega \\ &= \big(-ic\alpha\cdot\nu f|_{\partial\Omega}, g|_{\partial\Omega}\big)_{\partial\Omega} \\ &= \frac{1}{2}\big(-i\sqrt{c}\alpha\cdot\nu f|_{\partial\Omega}, \sqrt{c} g|_{\partial\Omega}\big)_{\partial\Omega} - \frac{1}{2}\big(\sqrt{c} f|_{\partial\Omega}, -i\sqrt{c}\alpha\cdot\nu g|_{\partial\Omega}\big)_{\partial\Omega}.\end{aligned}$$

Using that β is unitary and self-adjoint and the anti-commutation relation (1.2) we see that the last expression is equal to

$$\begin{aligned}&\frac{1}{2}\big(-i\sqrt{c}\beta\alpha\cdot\nu f|_{\partial\Omega}, \sqrt{c}\beta g|_{\partial\Omega}\big)_{\partial\Omega} - \frac{1}{2}\big(\sqrt{c}\beta f|_{\partial\Omega}, -i\sqrt{c}\beta\alpha\cdot\nu g|_{\partial\Omega}\big)_{\partial\Omega} \\ &\qquad = \frac{1}{2}\big(\sqrt{c}\beta f|_{\partial\Omega}, \sqrt{c}(g|_{\partial\Omega} + i\beta\alpha\cdot\nu g|_{\partial\Omega})\big)_{\partial\Omega} \\ &\qquad\quad - \frac{1}{2}\big(\sqrt{c}(f|_{\partial\Omega} + i\beta\alpha\cdot\nu f|_{\partial\Omega}), \sqrt{c}\beta g|_{\partial\Omega}\big)_{\partial\Omega} \\ &\qquad = (\sqrt{c}\beta f|_{\partial\Omega}, \sqrt{c}P_+ g|_{\partial\Omega})_{\partial\Omega} - (\sqrt{c}P_+ f|_{\partial\Omega}, \sqrt{c}\beta g|_{\partial\Omega})_{\partial\Omega}.\end{aligned}$$

Since P_+ is a orthogonal projection we have $P_+ = (P_+)^2 = (P_+)^*$, which implies eventually

$$\begin{aligned}(Tf,g)_\Omega - (f,Tg)_\Omega &= (\sqrt{c}P_+\beta f|_{\partial\Omega}, \sqrt{c}P_+ g|_{\partial\Omega})_{\partial\Omega} - (\sqrt{c}P_+ f|_{\partial\Omega}, \sqrt{c}P_+\beta g|_{\partial\Omega})_{\partial\Omega} \\ &= (\Gamma_1^\Omega f, \Gamma_0^\Omega g)_{\partial\Omega} - (\Gamma_0^\Omega f, \Gamma_1^\Omega g)_{\partial\Omega},\end{aligned}$$

which is Green's identity (2.5).

Next, we verify the range property (5.8). Clearly, by the definition of Γ_0^Ω and Γ_1^Ω and $\operatorname{dom}\Gamma_0^\Omega = \operatorname{dom}\Gamma_1^\Omega = H^1(\Omega;\mathbb{C}^4)$ it holds

$$\operatorname{ran}(\Gamma_0^\Omega \upharpoonright \ker\Gamma_1^\Omega), \operatorname{ran}(\Gamma_1^\Omega \upharpoonright \ker\Gamma_0^\Omega) \subset \mathcal{G}_\Omega^{1/2}.$$

On the other hand, let $\varphi \in \mathcal{G}_\Omega^{1/2}$ and choose a function $f \in H^1(\Omega;\mathbb{C}^4)$ with $f|_{\partial\Omega} = \frac{1}{\sqrt{c}}\varphi$. Since $\varphi \in \mathcal{G}_\Omega^{1/2}$ it holds $\varphi = P_+\varphi$ and hence we deduce

$$\Gamma_0^\Omega f = \sqrt{c} P_+ f|_{\partial\Omega} = P_+\varphi = \varphi.$$

Moreover, the relation (1.2) implies $\beta P_+ = P_- \beta$. Hence, we have

$$\Gamma_1^\Omega f = \sqrt{c} P_+ \beta f|_{\partial\Omega} = P_+\beta\varphi = P_+\beta P_+\varphi = P_+ P_- \beta\varphi = 0,$$

that means $f \in \ker \Gamma_1^\Omega$. Thus, $\varphi \in \operatorname{ran}(\Gamma_0^\Omega \upharpoonright \ker \Gamma_1^\Omega)$.

To prove $\mathcal{G}_\Omega^{1/2} \subset \operatorname{ran}(\Gamma_1^\Omega \upharpoonright \ker \Gamma_0^\Omega)$ let $\psi \in \mathcal{G}_\Omega^{1/2}$ and choose $g \in H^1(\Omega;\mathbb{C}^4)$ satisfying $g|_{\partial\Omega} = \frac{1}{\sqrt{c}}\beta\psi$. Then it holds

$$\Gamma_0^\Omega g = P_+\beta\psi = \beta P_-\psi = 0,$$

as $\psi \in \mathcal{G}_\Omega$, and

$$\Gamma_1^\Omega g = \sqrt{c} P_+ \beta g|_{\partial\Omega} = P_+\beta^2\psi = \psi,$$

that means $\psi \in \operatorname{ran}(\Gamma_1^\Omega \upharpoonright \ker \Gamma_0^\Omega)$. Hence, equation (5.8) has been shown.

Finally,

$$\ker \Gamma_0^\Omega = \{ f \in H^1(\Omega;\mathbb{C}^4) : f|_{\partial\Omega} = -i\beta(\alpha\cdot\nu) f|_{\partial\Omega} \} = \operatorname{dom} T_{\mathrm{MIT}}^\Omega.$$

Hence $T^\Omega \upharpoonright \ker \Gamma_0^\Omega$ coincides with the MIT bag Dirac operator T_{MIT}^Ω which is known to be self-adjoint, see Proposition 5.1.2. Therefore $\{\mathcal{G}_\Omega, \Gamma_0^\Omega, \Gamma_1^\Omega\}$ is a quasi boundary triple for $(S^\Omega)^*$ and all claims have been shown. □

Next, we compute the γ-field and the Weyl function associated to the quasi boundary triple in Theorem 5.2.1. It turns out that these operators are closely related with restrictions of the integral operators Φ_λ and $\mathcal{C}_\lambda$ defined in Section 3.2. In order to formulate the result recall that $\frac{1}{2c}\beta + \mathcal{C}_\lambda^{1/2}$ admits a bounded and everywhere defined inverse in $H^{1/2}(\Sigma;\mathbb{C}^4)$ for $\lambda \in \mathbb{C} \setminus \big((-\infty, -mc^2] \cup [mc^2, \infty)\big)$, see Proposition 4.1.7.

Proposition 5.2.2. *Let* $\{\mathcal{G}_\Omega, \Gamma_0^\Omega, \Gamma_1^\Omega\}$ *be the quasi boundary triple from Theorem 5.2.1, let* $\lambda \in \mathbb{C} \setminus \big((-\infty, -mc^2] \cup [mc^2, \infty)\big) \subset \rho(T_{\mathrm{MIT}}^\Omega)$*, let* P_Ω *be given by* (5.2)*, and let* Φ_λ *and* $\mathcal{C}_\lambda$ *be defined by* (3.16) *and* (3.17)*, respectively. Then the following holds:*

(i) *The value of the γ-field* $\gamma^\Omega(\lambda) : \operatorname{dom}\gamma^\Omega(\lambda) \subset \mathcal{G}_\Omega \to L^2(\Omega;\mathbb{C}^4)$ *is defined on the set* $\operatorname{dom}\gamma^\Omega(\lambda) = \mathcal{G}_\Omega^{1/2}$ *and is explicitly given by*

$$\gamma^\Omega(\lambda) = \frac{1}{\sqrt{c}} P_\Omega \Phi_\lambda^{1/2} \left(\frac{1}{2c}\beta + \mathcal{C}_\lambda^{1/2} \right)^{-1}.$$

Each $\gamma^\Omega(\lambda)$ *is a densely defined bounded operator from* $\mathcal{G}_\Omega$ *to* $L^2(\Omega;\mathbb{C}^4)$ *and a bounded and everywhere defined operator from* $\mathcal{G}_\Omega^{1/2}$ *to* $H^1(\Omega;\mathbb{C}^4)$*.*

(ii) *The value of the Weyl function* $M^\Omega(\lambda) : \operatorname{dom} M^\Omega(\lambda) \subset \mathcal{G}_\Omega \to \mathcal{G}_\Omega$ *is defined on the set* $\operatorname{dom} M^\Omega(\lambda) = \mathcal{G}_\Omega^{1/2}$ *and explicitly given by*

$$M^\Omega(\lambda) = -\frac{1}{c} P_+ \left(\frac{1}{2c}\beta + \mathcal{C}_\lambda^{1/2} \right)^{-1} P_+.$$

Each $M^\Omega(\lambda)$ *is densely defined and bounded in* $\mathcal{G}_\Omega$ *and bounded and everywhere defined in* $\mathcal{G}_\Omega^{1/2}$.

Proof. Let $\lambda \in \mathbb{C} \setminus \big((-\infty, -mc^2] \cup [mc^2, \infty) \big)$ be fixed. First we note that $\operatorname{dom} \gamma^\Omega(\lambda) = \operatorname{dom} M^\Omega(\lambda) = \operatorname{ran} \Gamma_0^\Omega = \mathcal{G}_\Omega^{1/2}$, see (5.8).

For the proof of item (i) let $\varphi \in \operatorname{ran} \Gamma_0^\Omega$ be fixed and recall that $\gamma^\Omega(\lambda)\varphi$ is the unique solution of the boundary value problem

$$(T^\Omega - \lambda) f = 0 \quad \text{and} \quad \Gamma_0^\Omega f = \varphi, \tag{5.9}$$

compare (2.7). We set

$$f_\lambda := \frac{1}{\sqrt{c}} P_\Omega \Phi_\lambda^{1/2} \left(\frac{1}{2c}\beta + \mathcal{C}_\lambda^{1/2} \right)^{-1} \varphi.$$

Then, due to the mapping properties of $\Phi_\lambda^{1/2}$ and $\big(\frac{1}{2c}\beta + \mathcal{C}_\lambda^{1/2} \big)^{-1}$, see Proposition 4.1.6 and Proposition 4.1.7, we have $f_\lambda \in H^1(\Omega; \mathbb{C}^4) = \operatorname{dom} T^\Omega$. We are going to show that f_λ solves the boundary value problem (5.9).

First, by Proposition 4.1.2 it is clear that $(T^\Omega - \lambda) f_\lambda = 0$, as $\Phi_\lambda \upharpoonright H^{1/2}(\Sigma; \mathbb{C}^4)$ is the γ-field for the quasi boundary triple $\{L^2(\partial\Omega; \mathbb{C}^4), \Gamma_0^{\partial\Omega}, \Gamma_1^{\partial\Omega}\}$. Moreover, employing Proposition 3.2.1 (iii) we get

$$\begin{aligned}
\Gamma_0^\Omega f_\lambda = \sqrt{c} P_+ f_\lambda|_{\partial\Omega} &= P_+ \left(-\frac{i}{2c} \alpha \cdot \nu + \mathcal{C}_\lambda \right) \left(\frac{1}{2c}\beta + \mathcal{C}_\lambda^{1/2} \right)^{-1} \varphi \\
&= P_+ \left(-\frac{i}{2c} \alpha \cdot \nu - \frac{1}{2c}\beta + \frac{1}{2c}\beta + \mathcal{C}_\lambda \right) \left(\frac{1}{2c}\beta + \mathcal{C}_\lambda^{1/2} \right)^{-1} \varphi \\
&= P_+ \left(-\frac{i}{2c} (\alpha \cdot \nu)\beta - \frac{1}{2c} I_4 \right) \beta \left(\frac{1}{2c}\beta + \mathcal{C}_\lambda^{1/2} \right)^{-1} \varphi + P_+ \varphi.
\end{aligned}$$

Using that $\varphi \in \mathcal{G}_\Omega$, $P_+^2 = P_+$ and the anti-commutation relation (1.2) we deduce

$$\begin{aligned}
\Gamma_0^\Omega f_\lambda &= P_+ \left(\frac{i}{2c} \beta (\alpha \cdot \nu) - \frac{1}{2c} I_4 \right) \beta \left(\frac{1}{2c}\beta + \mathcal{C}_\lambda^{1/2} \right)^{-1} \varphi + \varphi \\
&= -\frac{1}{c} P_+ P_- \beta \left(\frac{1}{2c}\beta + \mathcal{C}_\lambda^{1/2} \right)^{-1} \varphi + \varphi = \varphi.
\end{aligned}$$

Hence, f_λ is a solution of the boundary value problem (5.9), that means that $\gamma^\Omega(\lambda)\varphi = f_\lambda$. This is the claimed representation of $\gamma^\Omega(\lambda)$.

Next, by the definition of the γ-field it is clear that $\gamma^\Omega(\lambda)$ is a densely defined bounded operator from $\mathcal{G}_\Omega$ to $L^2(\Omega;\mathbb{C}^4)$. Moreover, using Propositions 4.1.7 and 4.1.6 we deduce that $\gamma^\Omega(\lambda)$ regarded as an operator from $\mathcal{G}_\Omega^{1/2}$ to $H^1(\Omega;\mathbb{C}^4)$ is continuous.

To show assertion (ii) we note that it holds by Definition 2.2.2, item (i) and Proposition 3.2.1 (iii) for any $\varphi \in \mathcal{G}_\Omega^{1/2}$

$$\begin{aligned} M^\Omega(\lambda)\varphi = \Gamma_1^\Omega \gamma^\Omega(\lambda)\varphi &= P_+\beta \left(P_\Omega \Phi_\lambda^{1/2} \left(\frac{1}{2c}\beta + \mathcal{C}_\lambda^{1/2} \right)^{-1} \varphi \right)\bigg|_{\partial\Omega} \\ &= P_+\beta \left(-\frac{i}{2c}\alpha\cdot\nu - \frac{1}{2c}\beta + \frac{1}{2c}\beta + \mathcal{C}_\lambda \right) \left(\frac{1}{2c}\beta + \mathcal{C}_\lambda^{1/2} \right)^{-1} \varphi \\ &= P_+ \left(-\frac{i}{2c}\beta(\alpha\cdot\nu) - \frac{1}{2c} \right) \left(\frac{1}{2c}\beta + \mathcal{C}_\lambda^{1/2} \right)^{-1} \varphi + P_+\beta\varphi. \end{aligned}$$

Using that $\varphi \in \mathcal{G}_\Omega$, $P_+^2 = P_+$, and the anti-commutation relation (1.2) we deduce

$$M^\Omega(\lambda)\varphi = -\frac{1}{c}P_+^2 \left(\frac{1}{2c}\beta + \mathcal{C}_\lambda^{1/2} \right)^{-1} \varphi + \beta P_-\varphi = -\frac{1}{c}P_+ \left(\frac{1}{2c}\beta + \mathcal{C}_\lambda^{1/2} \right)^{-1} P_+\varphi,$$

which is the claimed representation of the Weyl function. Due to the mapping properties of $\left(\frac{1}{2c}\beta + \mathcal{C}_\lambda^{1/2}\right)^{-1}$ from Proposition 4.1.7 we obtain finally that $M^\Omega(\lambda)$ is bounded and densely defined in $\mathcal{G}_\Omega$ and bounded and everywhere defined in $\mathcal{G}_\Omega^{1/2}$. □

Eventually, we state an explicit formula for the inverse of $M^\Omega(\lambda)$. This will be one of the main ingredients to prove the self-adjointness of Dirac operators on Ω with suitable boundary conditions. Recall that the operator $-\frac{1}{2c}\beta + \mathcal{C}_\lambda^{1/2}$ admits a bounded and everywhere defined inverse in $H^{1/2}(\partial\Omega;\mathbb{C}^4)$; see Proposition 4.1.7.

Proposition 5.2.3. *Let $T_{-\mathrm{MIT}}^\Omega$ be defined by* (5.3)*, assume that $\lambda \in \mathbb{C} \setminus \big((-\infty, -mc^2] \cup \sigma(T_{-\mathrm{MIT}}) \cup [mc^2, \infty)\big)$, let $\mathcal{C}_\lambda^{1/2}$ be given as in Proposition 4.1.6, and let $M^\Omega(\lambda)$ be as in Proposition 5.2.2. Then $M^\Omega(\lambda)$ admits a bounded and everywhere defined inverse in $\mathcal{G}_\Omega^{1/2}$ which acts as*

$$(M^\Omega(\lambda))^{-1} = \frac{1}{c}P_+\beta \left(-\frac{1}{2c}\beta + \mathcal{C}_\lambda^{1/2} \right)^{-1} \beta P_+.$$

Proof. First, we note that functions f in the domain of $T^\Omega \upharpoonright \ker \Gamma_1^\Omega$ satisfy

$$\Gamma_1^\Omega f = 0 \quad \Leftrightarrow \quad f|_{\partial\Omega} = i\beta(\alpha\cdot\nu) f|_{\partial\Omega},$$

which means that this operator coincides with the self-adjoint operator $T^{\Omega}_{-\mathrm{MIT}}$. Therefore, the triple $\{\mathcal{G}_\Omega, \widehat{\Gamma}^{\Omega}_0, \widehat{\Gamma}^{\Omega}_1\}$ with

$$\widehat{\Gamma}^{\Omega}_0 := \Gamma^{\Omega}_1 \quad \text{and} \quad \widehat{\Gamma}^{\Omega}_1 := -\Gamma^{\Omega}_0$$

is a quasi boundary triple for $(S^{\Omega})^*$ with Weyl function

$$\widehat{M}^{\Omega}(\lambda) = \widehat{\Gamma}^{\Omega}_1 \big(\widehat{\Gamma}^{\Omega}_0 \restriction \ker(T^{\Omega} - \lambda)\big)^{-1} = -(M^{\Omega}(\lambda))^{-1}, \qquad \lambda \in \rho(T^{\Omega}_{\mathrm{MIT}}) \cap \rho(T^{\Omega}_{-\mathrm{MIT}}).$$

So in order to compute $(M^{\Omega}(\lambda))^{-1}$ we calculate the Weyl function associated to the triple $\{\mathcal{G}_\Omega, \widehat{\Gamma}^{\Omega}_0, \widehat{\Gamma}^{\Omega}_1\}$. For that we derive first an explicit formula for the γ-field $\widehat{\gamma}^{\Omega}(\lambda)$. Let $\lambda \in \mathbb{C} \setminus \big((-\infty, -mc^2] \cup \sigma(T^{\Omega}_{-\mathrm{MIT}}) \cup [mc^2, \infty)\big)$, let $\varphi \in \operatorname{dom} \widehat{\gamma}^{\Omega}(\lambda) = \operatorname{ran} \widehat{\Gamma}^{\Omega}_0 = \operatorname{ran} \Gamma^{\Omega}_1 = \mathcal{G}^{1/2}_{\Omega}$ be fixed and set

$$f_\lambda := \frac{1}{\sqrt{c}} P_\Omega \Phi^{1/2}_{\lambda} \left(-\frac{1}{2c}\beta + \mathcal{C}^{1/2}_{\lambda}\right)^{-1} \beta\varphi,$$

where $\Phi^{1/2}_{\lambda}$ is given as in Proposition 4.1.6. We prove that f_λ is a solution of the boundary value problem

$$(T^{\Omega} - \lambda) = 0 \quad \text{and} \quad \widehat{\Gamma}^{\Omega}_0 f_\lambda = \varphi.$$

This shows then $\widehat{\gamma}^{\Omega}(\lambda)\varphi = f_\lambda$, compare (2.7).

First, due to the mapping properties of $\big(-\frac{1}{2c}\beta + \mathcal{C}^{1/2}_{\lambda}\big)^{-1}$ and $\Phi^{1/2}_{\lambda}$ from Proposition 4.1.7 and Proposition 4.1.6 we get $f_\lambda \in H^1(\Omega;\mathbb{C}^4) = \operatorname{dom} T^{\Omega}$. Moreover, we easily deduce $(T^{\Omega} - \lambda) f_\lambda = 0$ because of Proposition 4.1.2. Eventually, employing Proposition 3.2.1 (iii) we have

$$\begin{aligned}
\widehat{\Gamma}^{\Omega}_0 f_\lambda = \Gamma^{\Omega}_1 f_\lambda &= P_+\beta \left(P_\Omega \Phi^{1/2}_{\lambda} \left(-\frac{1}{2c}\beta + \mathcal{C}^{1/2}_{\lambda}\right)^{-1} \beta\varphi \right)\bigg|_{\partial\Omega} \\
&= P_+\beta \left(-\frac{i}{2c}\alpha\cdot\nu + \frac{1}{2c}\beta - \frac{1}{2c}\beta + \mathcal{C}_\lambda\right)\left(-\frac{1}{2c}\beta + \mathcal{C}^{1/2}_{\lambda}\right)^{-1} \beta\varphi \\
&= \frac{1}{c} P_+\beta^2 P_- \left(-\frac{1}{2c}\beta + \mathcal{C}^{1/2}_{\lambda}\right)^{-1} \beta\varphi + P_+\beta^2\varphi.
\end{aligned}$$

Since $\beta^2 = I_4$, $P_+P_- = 0$ and $\varphi \in \mathcal{G}_\Omega$, we deduce $\widehat{\Gamma}^{\Omega}_0 f_\lambda = \varphi$, which was the claim.

Eventually, we compute $\widehat{M}^{\Omega}(\lambda)\varphi = \widehat{\Gamma}^{\Omega}_1 \widehat{\gamma}^{\Omega}(\lambda)\varphi$. Using again Proposition 3.2.1 (iii) we obtain

$$\begin{aligned}
\widehat{M}^\Omega(\lambda)\varphi &= \widehat{\Gamma}_1^\Omega \widehat{\gamma}^\Omega(\lambda)\varphi = -\Gamma_0^\Omega \widehat{\gamma}^\Omega(\lambda)\varphi \\
&= -P_+ \left(P_\Omega \Phi_\lambda^{1/2} \left(-\frac{1}{2c}\beta + \mathcal{C}_\lambda^{1/2} \right)^{-1} \beta\varphi \right) \Bigg|_{\partial\Omega} \\
&= -P_+ \left(-\frac{i}{2c}\alpha\cdot\nu + \frac{1}{2c}\beta - \frac{1}{2c}\beta + \mathcal{C}_\lambda \right) \left(-\frac{1}{2c}\beta + \mathcal{C}_\lambda^{1/2} \right)^{-1} \beta\varphi \\
&= -\frac{1}{c} P_+ \beta P_- \left(-\frac{1}{2c}\beta + \mathcal{C}_\lambda^{1/2} \right)^{-1} \beta\varphi - P_+\beta\varphi.
\end{aligned}$$

Using the anti-commutation relation (1.2) we deduce $\beta P_- = P_+\beta$. Thus, as $\varphi \in \mathcal{G}_\Omega$ we conclude finally

$$\begin{aligned}
-(M^\Omega(\lambda))^{-1} = \widehat{M}^\Omega(\lambda)\varphi &= -\frac{1}{c} P_+\beta \left(-\frac{1}{2c}\beta + \mathcal{C}_\lambda^{1/2} \right)^{-1} \beta P_+\varphi - \beta P_- P_+\varphi \\
&= -\frac{1}{c} P_+\beta \left(-\frac{1}{2c}\beta + \mathcal{C}_\lambda^{1/2} \right)^{-1} \beta P_+\varphi,
\end{aligned}$$

which is the claimed result. □

5.2.2 An ordinary boundary triple for Dirac operators on domains

In this section we transform and extend the quasi boundary triple $\{\mathcal{G}_\Omega, \Gamma_0^\Omega, \Gamma_1^\Omega\}$ from Theorem 5.2.1 to an ordinary boundary triple using the techniques described in Section 2.2. Recall that we have by (5.8)

$$\mathscr{G}_0^\Omega := \operatorname{ran}(\Gamma_0^\Omega \upharpoonright \ker\Gamma_1^\Omega) = \mathcal{G}_\Omega^{1/2} \quad \text{and} \quad \mathscr{G}_1^\Omega := \operatorname{ran}(\Gamma_1^\Omega \upharpoonright \ker\Gamma_0^\Omega) = \mathcal{G}_\Omega^{1/2}.$$

Following the procedure described in Section 2.2 we see that

$$\Lambda^\Omega := \operatorname{Im}\overline{M^\Omega(i)} = \frac{1}{2i}\big(\overline{M^\Omega(i)} - \overline{M^\Omega(-i)}\big)$$

is a non-negative self-adjoint operator and we define the bijections

$$\iota_+^\Omega := (\Lambda^\Omega)^{-1/2} : \mathcal{G}_\Omega^{1/2} \to \mathcal{G}_\Omega \tag{5.10}$$

and

$$\iota_-^\Omega := \big((\Lambda^\Omega)^{1/2}\big)' : \mathcal{G}_\Omega^{-1/2} \to \mathcal{G}_\Omega, \tag{5.11}$$

where

$$\mathcal{G}_\Omega^{-1/2} := \big(\mathcal{G}_\Omega^{1/2}\big)'$$

is the dual space of $\mathcal{G}_\Omega^{1/2}$. Recall that we can express with the aid of the embeddings $\iota_\pm^\Omega$ the inner product in $\mathcal{G}_\Omega^{\pm 1/2}$ and the duality product in $\mathcal{G}_\Omega^{-1/2} \times \mathcal{G}_\Omega^{1/2}$ by (2.15), (2.18), and (2.19). Eventually, we note that the typical scaling properties for embedding operators yield that ι_-^Ω gives rise to a bounded operator

$$\iota_-^\Omega : \mathcal{G}_\Omega^{1/2} \to \mathcal{G}_\Omega^1. \tag{5.12}$$

Now, we have all tools and notations in hand to introduce the extensions of the boundary mappings Γ_0^Ω and Γ_1^Ω. This result can be shown using that $A_\infty^\Omega := T^\Omega \upharpoonright \ker \Gamma_1^\Omega = T_{-\mathrm{MIT}}^\Omega$ is self-adjoint, which was shown in the proof of Lemma 5.1.4, equation (5.8), and Proposition 2.2.11.

Lemma 5.2.4. *Let $(S^\Omega)^* = T_{\max}^\Omega$ and let $\{\mathcal{G}_\Omega, \Gamma_0^\Omega, \Gamma_1^\Omega\}$ be the quasi boundary triple from Theorem 5.2.1. Then, the operator $A_\infty^\Omega := T^\Omega \upharpoonright \ker \Gamma_1^\Omega$ is self-adjoint in $L^2(\Omega;\mathbb{C}^4)$. Moreover, the mappings $\Gamma_0^\Omega, \Gamma_1^\Omega : \mathrm{dom}\, T^\Omega \to \mathcal{G}_\Omega$ have surjective extensions*

$$\widetilde{\Gamma}_0^\Omega : \mathrm{dom}\,(S^\Omega)^* \to \mathcal{G}_\Omega^{-1/2} \quad \textit{and} \quad \widetilde{\Gamma}_1^\Omega : \mathrm{dom}\,(S^\Omega)^* \to \mathcal{G}_\Omega^{-1/2},$$

which are bounded with respect to the graph norm of $(S^\Omega)^*$.

With the aid of the extended boundary mappings $\widetilde{\Gamma}_0^\Omega$ and $\widetilde{\Gamma}_1^\Omega$ we are able to extend the γ-field $\gamma^\Omega(\lambda)$ and the Weyl function $M^\Omega(\lambda)$ from Proposition 5.2.2.

Proposition 5.2.5. *Let $\{\mathcal{G}_\Omega, \Gamma_0^\Omega, \Gamma_1^\Omega\}$ be the quasi boundary triple for $(S^\Omega)^*$ from Theorem 5.2.1 with corresponding γ-field γ^Ω and Weyl function M^Ω given as in Proposition 5.2.2. Moreover, let $T_{-\mathrm{MIT}}^\Omega$ be given by* (5.3) *and let $\lambda \in \mathbb{C} \setminus \big((-\infty, -mc^2] \cup [mc^2, \infty)\big)$. Then it holds:*

(i) *The operator $\gamma^\Omega(\lambda)$ has a continuous extension*

$$\widetilde{\gamma}^\Omega(\lambda) = \big(\widetilde{\Gamma}_0^\Omega \upharpoonright \ker((S^\Omega)^* - \lambda)\big)^{-1} : \mathcal{G}_\Omega^{-1/2} \to \mathcal{G}_\Omega.$$

(ii) *The operator $M^\Omega(\lambda)$ has a continuous extension*

$$\widetilde{M}^\Omega(\lambda) = \widetilde{\Gamma}_1^\Omega \big(\widetilde{\Gamma}_0^\Omega \upharpoonright \ker((S^\Omega)^* - \lambda)\big)^{-1} : \mathcal{G}_\Omega^{-1/2} \to \mathcal{G}_\Omega^{-1/2}.$$

Moreover, it holds for all $\varphi \in \mathcal{G}_\Omega^{-1/2}$ and $\psi \in \mathcal{G}_\Omega^{1/2}$

$$\big\langle \widetilde{M}^\Omega(\lambda)\varphi, \psi \big\rangle_{-1/2 \times 1/2} = \big\langle \varphi, M^\Omega(\overline{\lambda})\psi \big\rangle_{-1/2 \times 1/2}.$$

(iii) *For $\lambda \in \mathbb{C} \setminus \big((-\infty, -mc^2] \cup \sigma(T_{-\mathrm{MIT}}^\Omega) \cup [mc^2 \infty)\big)$ the operator $(M^\Omega(\lambda))^{-1}$ has a continuous extension*

$$\big(\widetilde{M}^\Omega(\lambda)\big)^{-1} = \widetilde{\Gamma}_0^\Omega \big(\widetilde{\Gamma}_1^\Omega \upharpoonright \ker((S^\Omega)^* - \lambda)\big)^{-1} : \mathcal{G}_\Omega^{-1/2} \to \mathcal{G}_\Omega^{-1/2}.$$

(iv) *For* $\lambda \in \mathbb{C} \setminus \big((-\infty, -mc^2] \cup \sigma(T^\Omega_{-\mathrm{MIT}}) \cup [mc^2\infty)\big)$ *the operator*

$$\widetilde{M}^\Omega(\lambda) - \big(\widetilde{M}^\Omega(\lambda)\big)^{-1} : \mathcal{G}_\Omega^{-1/2} \to \mathcal{G}_\Omega^{1/2}$$

is bounded and everywhere defined.

Proof. Assertion (i) and the existence and the mapping properties of $\widetilde{M}^\Omega(\lambda)$ follow immediately from Proposition 2.2.12. Also item (iii) is a consequence of Proposition 2.2.12, as $-(M^\Omega(\lambda))^{-1}$ is the Weyl function for the quasi boundary triple $\{\mathcal{G}_\Omega, \Gamma_1^\Omega, -\Gamma_0^\Omega\}$, compare the proof of Proposition 5.2.3, and this triple fulfills also the assumptions of Proposition 2.2.12. Moreover, employing (2.18) and Proposition 2.2.4 (iii) we observe for $\varphi \in \mathcal{G}_\Omega^{1/2}$ and $\psi \in \mathcal{G}_\Omega^{1/2}$

$$\big\langle \widetilde{M}^\Omega(\lambda)\varphi, \psi\big\rangle_{-1/2\times 1/2} = (M^\Omega(\lambda)\varphi, \psi)_{\partial\Omega} = (\varphi, M^\Omega(\overline{\lambda})\psi)_{\partial\Omega} = \langle \varphi, M^\Omega(\overline{\lambda})\psi\rangle_{-1/2\times 1/2}.$$

By density we obtain that the above formula can be extended for all $\varphi \in \mathcal{G}_\Omega^{-1/2}$. Hence, also item (ii) is completely proved.

It remains to show statement (iv). We are going to prove that $M^\Omega(\lambda) - (M^\Omega(\lambda))^{-1}$ can be extended to a bounded operator from $\mathcal{G}_\Omega^{-1/2}$ to $\mathcal{G}_\Omega^{1/2}$. By Proposition 5.2.2 and Proposition 5.2.3 it holds

$$M^\Omega(\lambda) - (M^\Omega(\lambda))^{-1} = -\frac{1}{c}P_+\left(\frac{1}{2c}\beta + \mathcal{C}_\lambda^{1/2}\right)^{-1} P_+ - \frac{1}{c}P_+\beta\left(-\frac{1}{2c}\beta + \mathcal{C}_\lambda^{1/2}\right)^{-1}\beta P_+.$$

Using that β is an invertible matrix and that all involved operators are bounded and everywhere defined this implies

$$\begin{aligned} M^\Omega(\lambda) - (M^\Omega(\lambda))^{-1} &= -\frac{1}{c}P_+\left(\frac{1}{2c}\beta + \mathcal{C}_\lambda^{1/2}\right)^{-1} P_+ - \frac{1}{c}P_+\left(-\frac{1}{2c}\beta + \beta\mathcal{C}_\lambda^{1/2}\beta\right)^{-1} P_+ \\ &= -\frac{1}{c}P_+\left(-\frac{1}{2c}\beta + \beta\mathcal{C}_\lambda^{1/2}\beta\right)^{-1}\left(\beta\mathcal{C}_\lambda^{1/2} + \mathcal{C}_\lambda^{1/2}\beta\right)\beta\left(\frac{1}{2c}\beta + \mathcal{C}_\lambda^{1/2}\right)^{-1} P_+. \end{aligned}$$

Since $\left(\frac{1}{2c}\beta + \mathcal{C}_\lambda^{1/2}\right)^{-1}$ has a bounded extension in $H^{-1/2}(\partial\Omega;\mathbb{C}^4)$, see Proposition 4.1.7, and $\beta\mathcal{C}_\lambda^{1/2} + \mathcal{C}_\lambda^{1/2}\beta$ has a bounded extension from $H^{-1/2}(\partial\Omega;\mathbb{C}^4)$ to $H^{1/2}(\partial\Omega;\mathbb{C}^4)$ by Proposition 3.2.4, the claim of item (iv) follows. □

Eventually, since $\mathscr{G}_1^\Omega = \mathcal{G}_\Omega^{1/2}$ is dense in $\mathcal{G}_\Omega$ we are able to apply the construction described in Section 2.2 to transform the quasi boundary triple from Theorem 5.2.1 to an ordinary boundary triple. Here we fix some $\mu \in \rho(T^\Omega_{-\mathrm{MIT}}) \cap (-mc^2, mc^2) \subset \rho(T^\Omega_{\mathrm{MIT}})$. Note that such a μ exists by Lemma 5.1.4. This implies, in particular, that

$$\mathrm{dom}\,(S^\Omega)^* = \mathrm{dom} A_0^\Omega \dot{+} \ker\big((S^\Omega)^* - \mu\big).$$

see (2.6).

Theorem 5.2.6. *Let* $S^\Omega = T^\Omega_{\min}$ *be given by* (3.11) *and let* $\{\mathcal{G}_\Omega, \Gamma_0^\Omega, \Gamma_1^\Omega\}$ *be the quasi boundary triple from Theorem 5.2.1. Moreover, let* $\iota_\pm^\Omega$ *be defined by* (5.10) *and* (5.11)*, respectively, let* $\widetilde{\Gamma}_0^\Omega$ *be the extension of* Γ_0^Ω *from Lemma 5.2.4 and define* $\Upsilon_0^\Omega, \Upsilon_1^\Omega : \mathrm{dom}\,(S^\Omega)^* \to \mathcal{G}_\Omega$ *by*

$$\Upsilon_0^\Omega f := \iota_-^\Omega \widetilde{\Gamma}_0^\Omega f \quad \text{and} \quad \Upsilon_1^\Omega f := \iota_+^\Omega \Gamma_1^\Omega f_0$$

for $f = f_0 + g \in \mathrm{dom} A_0^\Omega \dotplus \ker\big((S^\Omega)^* - \mu\big) = \mathrm{dom}\,(S^\Omega)^*$. *Then* $\{\mathcal{G}_\Omega, \Upsilon_0^\Omega, \Upsilon_1^\Omega\}$ *is an ordinary boundary triple for* $(S^\Omega)^*$ *and* $(S^\Omega)^* \upharpoonright \ker \Upsilon_0^\Omega = T^\Omega \upharpoonright \ker \Gamma_0^\Omega = T^\Omega_{\mathrm{MIT}}$.

5.3 Dirac operators on domains – definition and basic spectral properties in the case of non-critical boundary values

In this section we define self-adjoint Dirac operators in a domain $\Omega \subset \mathbb{R}^3$, which has a compact C^2-smooth boundary, with suitable boundary conditions via the quasi boundary triple $\{\mathcal{G}_\Omega, \Gamma_0^\Omega, \Gamma_1^\Omega\}$ from Theorem 5.2.1. To be more precise, we are going to study Dirac operators with the boundary conditions

$$\tau P_+ f|_{\partial\Omega} = P_+ \beta f|_{\partial\Omega},$$

where the function $\tau : \partial\Omega \to \mathbb{R}$ is Lipschitz continuous and the matrix P_+ is given by (5.4). In the case of non-critical boundary values, that means if $\tau(x) \neq \pm 1$ for all $x \in \partial\Omega$, we are going to prove self-adjointness and basic spectral properties. The critical case is then treated in Section 5.4.

Definition 5.3.1. *Let* $\{\mathcal{G}_\Omega, \Gamma_0^\Omega, \gamma_1^\Omega\}$ *be the quasi boundary triple from Theorem 5.2.1 and let* $\tau : \partial\Omega \to \mathbb{R}$ *be Lipschitz continuous. Then we define* $A_\tau^\Omega := T^\Omega \upharpoonright \ker(\Gamma_1^\Omega - \tau\Gamma_0^\Omega)$. *This operator is given in a more explicit way by*

$$\begin{aligned} A_\tau^\Omega f &:= (-ic\alpha\cdot\nabla + mc^2\beta) f, \\ \mathrm{dom} A_\tau^\Omega &:= \{ f \in H^1(\Omega;\mathbb{C}^4) : \tau P_+ f|_{\partial\Omega} = P_+\beta f|_{\partial\Omega} \}. \end{aligned} \tag{5.13}$$

First, we show that A_τ^Ω is unitarily equivalent to $-A_{-\tau}^\Omega$. This technical property will be useful in the study of A_τ^Ω later. In the proof of this result we use the matrix

$$\gamma_5 := \begin{pmatrix} 0 & I_2 \\ I_2 & 0 \end{pmatrix}.$$

Lemma 5.3.2. *Let* $\tau : \partial\Omega \to \mathbb{R}$ *be a Lipschitz continuous function, let* A_τ^Ω *be defined by* (5.13) *and define the unitary matrix* $\mathcal{B} := \beta\gamma_5$ *with* γ_5 *given as above. Then it holds* $A_\tau^\Omega = -\mathcal{B}^* A_{-\tau}^\Omega \mathcal{B}$. *In particular,* A_τ^Ω *is self-adjoint if and only if* $A_{-\tau}^\Omega$ *is self-adjoint.*

Proof. First, we show that $\mathcal{B}(\mathrm{dom} A_\tau^\Omega) = \mathrm{dom} A_{-\tau}^\Omega$. In fact, the anti-commutation relation (1.2), $(\alpha\cdot\nu)\gamma_5 = \gamma_5(\alpha\cdot\nu)$, and $\beta\gamma_5 = -\gamma_5\beta$ imply for $f \in \mathrm{dom} A_\tau^\Omega$

$$\begin{aligned}\Gamma_1^\Omega \mathcal{B} f &= P_+\beta^2\gamma_5 f|_{\partial\Omega} = \gamma_5 P_-\beta^2 f|_{\partial\Omega} = \gamma_5\beta P_+\beta f|_{\partial\Omega} \\ &= \gamma_5\beta\tau P_+ f|_{\partial\Omega} = \tau P_+\gamma_5\beta f|_{\partial\Omega} = -\tau P_+\mathcal{B} f|_{\partial\Omega},\end{aligned}$$

that means $\mathcal{B}f \in \mathrm{dom} A_{-\tau}^\Omega$. By a similar argument we see that $f \in \mathrm{dom} A_{-\tau}^\Omega$ yields $\mathcal{B}f \in \mathrm{dom} A_\tau^\Omega$ which shows $\mathcal{B}(\mathrm{dom} A_\tau^\Omega) = \mathrm{dom} A_{-\tau}^\Omega$. Eventually, employing again (1.2) we get for any $f \in H^1(\Omega;\mathbb{C}^4)$

$$\begin{aligned}(-ic\alpha\cdot\nabla + mc^2\beta)\mathcal{B}f &= (-ic\alpha\cdot\nabla + mc^2\beta)\beta\gamma_5 f = \beta(ic\alpha\cdot\nabla + mc^2\beta)\gamma_5 f \\ &= \beta\gamma_5(ic\alpha\cdot\nabla - mc^2\beta)f = -\mathcal{B}(-ic\alpha\cdot\nabla + mc^2\beta)f.\end{aligned}$$

This finishes the proof of this lemma. □

It follows immediately from Green's abstract identity that A_τ^Ω is symmetric for any Lipschitz continuous and real valued function τ, see (2.9). In order to prove self-adjointness, we employ Theorem 2.2.5; this gives us also a Krein type resolvent formula. Note that this resolvent formula below is explicit as we know from Proposition 5.1.2 the resolvent $\big(T_{\mathrm{MIT}}^\Omega - \lambda\big)^{-1}$ explicitly.

Theorem 5.3.3. *Let $\tau : \partial\Omega \to \mathbb{R}$ be a Lipschitz continuous function satisfying $|\tau(x)| \neq 1$ for all $x \in \partial\Omega$ and let A_τ^Ω be defined by* (5.13)*. Moreover, let γ^Ω and M^Ω be given as in Proposition 5.2.2. Then A_τ^Ω is self-adjoint and it holds for all $\lambda \in \mathbb{C}\setminus\mathbb{R}$*

$$(A_\tau^\Omega - \lambda)^{-1} = \big(T_{\mathrm{MIT}}^\Omega - \lambda\big)^{-1} + \gamma^\Omega(\lambda)\big(\tau - M^\Omega(\lambda)\big)^{-1}\gamma^\Omega(\overline{\lambda})^*.$$

Proof. Due to Green's identity it is clear that A_τ^Ω is symmetric, compare (2.9). Thus, it suffices to prove $\mathrm{ran}\,(A_\tau^\Omega - \lambda) = L^2(\Omega;\mathbb{C}^4)$ for $\lambda \in \mathbb{C}\setminus\mathbb{R}$.

Let $f \in L^2(\Omega;\mathbb{C}^4)$ and $\lambda \in \mathbb{C}\setminus\mathbb{R}$ be arbitrary, but fixed. Then by Theorem 2.2.5 (ii) we have $f \in \mathrm{ran}\,(A_\tau^\Omega - \lambda)$ if and only if $\gamma^\Omega(\overline{\lambda})^* f \in \mathrm{ran}\,(\tau - M^\Omega(\lambda))$. Since $\gamma^\Omega(\overline{\lambda})^* = \Gamma_1^\Omega\big(T_{\mathrm{MIT}}^\Omega - \lambda\big)^{-1}$, see Proposition 2.2.3 (iii), and $\mathrm{dom}\, T_{\mathrm{MIT}}^\Omega \subset H^1(\Omega;\mathbb{C}^4)$ we deduce that $\gamma^\Omega(\overline{\lambda})^* f \in \mathcal{G}_\Omega^{1/2}$. We prove that $\tau - M^\Omega(\lambda)$ is surjective in $\mathcal{G}_\Omega^{1/2}$. Clearly we have

$$\begin{aligned}\mathrm{ran}\,(\tau - M^\Omega(\lambda)) &\supset \mathrm{ran}\,\big[(\tau - M^\Omega(\lambda))\big(\tau + (M^\Omega(\lambda))^{-1}\big)\big] \\ &= \mathrm{ran}\,\big[\tau^2 - 1 + \tau(M^\Omega(\lambda))^{-1} - M^\Omega(\lambda)\tau\big].\end{aligned}$$

Making use of the explicit form of $M^\Omega(\lambda)$ from Proposition 5.2.2 we deduce from Proposition 3.2.3 that

$$\tau M^\Omega(\lambda) - M^\Omega(\lambda)\tau = \frac{1}{c}P_+\left(\frac{1}{2c}\beta + \mathcal{C}_\lambda^{1/2}\right)^{-1}\left(\tau\mathcal{C}_\lambda^{1/2} - \mathcal{C}_\lambda^{1/2}\tau\right)\left(\frac{1}{2c}\beta + \mathcal{C}_\lambda^{1/2}\right)^{-1}P_+$$

is compact in $\mathcal{G}_\Omega^{1/2}$, as τ is Lipschitz continuous. Moreover, by Proposition 5.2.5 (iv) also $(M^\Omega(\lambda))^{-1} - M^\Omega(\lambda)$ is compact in $\mathcal{G}_\Omega^{1/2}$. Thus, the operator

$$\mathcal{K}_\lambda := \tau(M^\Omega(\lambda))^{-1} - M^\Omega(\lambda)\tau = \tau\big[(M^\Omega(\lambda))^{-1} - M^\Omega(\lambda)\big] + \tau M^\Omega(\lambda) - M^\Omega(\lambda)\tau$$

is compact in $\mathcal{G}_\Omega^{1/2}$. Note that both operators $\tau - M^\Omega(\lambda)$ and $\tau + (M^\Omega(\lambda))^{-1}$ are injective, as otherwise one of the symmetric operators A_τ^Ω or $T^\Omega \upharpoonright \ker(\Gamma_0^\Omega + \tau\Gamma_1^\Omega)$ would have the non-real eigenvalue λ, see Theorem 2.2.5 (recall that $-(M^\Omega(\lambda))^{-1}$ is the Weyl function for the quasi boundary triple $\{\mathcal{G}_\Omega, \Gamma_1^\Omega, -\Gamma_0^\Omega\}$, compare the proof of Proposition 5.2.3). Thus, Fredholm's alternative implies that

$$(\tau - M^\Omega(\lambda))\big(\tau + (M^\Omega(\lambda))^{-1}\big) = (\tau^2 - 1)\left[1 + \frac{1}{\tau^2 - 1}\mathcal{K}_\lambda\right]$$

is bijective in $\mathcal{G}_\Omega^{1/2}$. Therefore $\mathcal{G}_\Omega^{1/2} \subset \operatorname{ran}(\tau - M^\Omega(\lambda))$, which yields $f \in \operatorname{ran}(A_\tau^\Omega - \lambda)$. Since f was arbitrary we get eventually $\operatorname{ran}(A_\tau^\Omega - \lambda) = L^2(\Omega;\mathbb{C}^4)$ and that A_τ^Ω is self-adjoint.

Finally, the stated resolvent formula follows from Theorem 2.2.5. □

In the following we discuss the basic spectral properties of A_τ^Ω. Since these are of a very different nature whether Ω is bounded or Ω is the complement of a bounded domain, we discuss these two cases separately. First, we treat the simpler case, when Ω is the complement of a bounded C^2-domain. Then the essential spectrum of A_τ^Ω is $(-\infty, -mc^2] \cup [mc^2, \infty)$ and the discrete eigenvalues in the gap of the essential spectrum can be computed with the aid of the Birman-Schwinger principle.

Proposition 5.3.4. *Let Ω be the complement of a bounded C^2-domain, let $\tau : \partial\Omega \to \mathbb{R}$ be a Lipschitz continuous function satisfying $|\tau(x)| \neq 1$ for all $x \in \partial\Omega$ and let A_τ^Ω be defined by* (5.13). *Then the following is true:*

(i) $\sigma_{\text{ess}}(A_\tau^\Omega) = (-\infty, -mc^2] \cup [mc^2, \infty)$.

(ii) *The number of discrete eigenvalues is finite.*

(iii) $\lambda \in \sigma(A_\tau^\Omega)$ *if and only if* $0 \in \sigma(\tau - M^\Omega(\lambda))$.

Proof. (i) Note first that due to Theorem 5.3.3 we have for $\lambda \in \mathbb{C} \setminus \mathbb{R}$

$$\begin{aligned}(A_\tau - \lambda)^{-1} - \big(T_{\text{MIT}}^\Omega - \lambda\big)^{-1} &= \gamma^\Omega(\lambda)\big(\tau - M^\Omega(\lambda)\big)^{-1}\gamma^\Omega(\overline{\lambda})^* \\ &= \overline{\gamma^\Omega(\lambda)}\big(\tau - M^\Omega(\lambda)\big)^{-1}\gamma^\Omega(\overline{\lambda})^*.\end{aligned} \tag{5.14}$$

The operator $\gamma^\Omega(\overline{\lambda})^*$ is bounded from $L^2(\Omega;\mathbb{C}^4)$ to $\mathcal{G}_\Omega^{1/2}$, because by Proposition 2.2.3 (iii) and (5.8) we have $\operatorname{ran}\gamma^\Omega(\overline{\lambda})^* = \operatorname{ran}\big[\Gamma_1^\Omega(T_{\text{MIT}}^\Omega)^{-1}\big] = \mathcal{G}_\Omega^{1/2}$ and the closed graph theorem.

Moreover $\big(\tau - M^\Omega(\lambda)\big)^{-1}$ is bijective in $\mathcal{G}_\Omega^{1/2}$, as it is shown in the proof of Theorem 5.3.3. Hence, we deduce that

$$\big(\tau - M^\Omega(\lambda)\big)^{-1}\gamma^\Omega(\overline{\lambda})^* : L^2(\Omega;\mathbb{C}^4) \to \mathcal{G}_\Omega^{1/2}$$

is bounded. Since $\mathcal{G}_\Omega^{1/2}$ is compactly embedded into $\mathcal{G}_\Omega$ this operator is compact from $L^2(\Omega;\mathbb{C}^4)$ to $\mathcal{G}_\Omega$. Moreover, $\gamma^\Omega(\lambda)$ can always be extended to a bounded and everywhere defined operator from $\mathcal{G}_\Omega$ to $L^2(\Omega;\mathbb{C}^4)$, compare Proposition 2.2.3. Thus, we deduce that the left hand side of (5.14) is compact in $L^2(\Omega;\mathbb{C}^4)$, which yields

$$\sigma_{\mathrm{ess}}(A_\tau^\Omega) = \sigma_{\mathrm{ess}}(T_{\mathrm{MIT}}^\Omega) = (-\infty, -mc^2] \cup [mc^2, \infty).$$

Assertion (ii) can be shown in exactly the same way as Theorem 4.2.3 (iv). Finally, item (iii) is an immediate consequence of Theorem 2.2.5 (i). □

If Ω is a bounded C^2-domain, then it is more difficult to describe the spectrum of A_τ^Ω in terms of the Weyl function M^Ω. Since $\mathrm{dom} A_\tau^\Omega \subset H^1(\Omega;\mathbb{C}^4)$ is compactly embedded in $L^2(\Omega;\mathbb{C}^4)$ in this case, the spectrum of A_τ^Ω is purely discrete. On the other hand, we have only an expression for the value of the Weyl function $M^\Omega(\lambda)$ in Proposition 5.2.2 for $\lambda \in \mathbb{C} \setminus \big((-\infty, -mc^2] \cup [mc^2, \infty)\big)$. Hence, we can not use the Birman Schwinger principle from Theorem 2.2.5 directly to detect discrete eigenvalues in $(-\infty, -mc^2] \cup [mc^2, \infty)$. But since the symmetry $S^\Omega = T_{\min}^\Omega$ is simple by Lemma 3.1.2, we can apply Proposition 2.2.8 and obtain immediately the following result.

Proposition 5.3.5. *Let Ω be a bounded C^2-smooth domain, let $\tau : \partial\Omega \to \mathbb{R}$ be a Lipschitz continuous function satisfying $|\tau(x)| \neq 1$ for all $x \in \partial\Omega$ and let A_τ^Ω be defined by* (5.13). *Then $\sigma(A_\tau^\Omega) = \sigma_{\mathrm{disc}}(A_\tau^\Omega)$ and λ is an eigenvalue of A_τ^Ω if and only if there exists a $\varphi \in \mathcal{G}_\Omega^{1/2}$ such that*

$$\lim_{\varepsilon \searrow 0} i\varepsilon \big(M^\Omega(\lambda + i\varepsilon) - \tau\big)^{-1}\varphi \neq 0.$$

Next, we state the analogue of Theorem 4.2.7 for Dirac operators on domains. In this case we compare the differences of powers of the resolvents of A_τ^Ω and T_{MIT}^Ω. The results are very similar to those of Theorem 4.2.7. Hence, we also give just a sketch of the proof. Again, we have to assume here some additional smoothness of $\partial\Omega$.

Theorem 5.3.6. *Let $l \in \mathbb{N}$ be fixed and assume that Ω is has a C^l-smooth boundary. Let $\tau : \partial\Omega \to \mathbb{R}$ be Lipschitz continuous such that $|\tau(x)| \neq 1$ for all $x \in \partial\Omega$ and let A_τ^Ω be defined by* (5.13). *Moreover, let T_{MIT}^Ω be the MIT-bag operator defined by* (5.1). *Then it holds for all $\lambda \in \mathbb{C} \setminus \mathbb{R}$*

$$(A_\tau^\Omega - \lambda)^{-l} - (T_{\mathrm{MIT}}^\Omega - \lambda)^{-l} \in \mathfrak{S}_{2/l,\infty}.$$

In particular, for $l = 3$ the operator $(A^\Omega_\tau - \lambda)^{-3} - (T^\Omega_{\mathrm{MIT}} - \lambda)^{-3}$ belongs to the trace class ideal and

$$tr\big[(A^\Omega_\tau - \lambda)^{-3} - (T^\Omega_{\mathrm{MIT}} - \lambda)^{-3}\big] = -\frac{1}{2} tr\left[\frac{\mathrm{d}^2}{\mathrm{d}\lambda^2}\left(\big(\tau - M^\Omega(\lambda)\big)^{-1}\frac{\mathrm{d}}{\mathrm{d}\lambda}M^\Omega(\lambda)\right)\right]. \quad (5.15)$$

Moreover, the wave operators for the scattering system $\{A^\Omega_\tau, T^\Omega_{\mathrm{MIT}}\}$ exist and are complete and the absolute continuous parts of A^Ω_τ and T^Ω_{MIT} are unitarily equivalent.

Proof. The proof of this theorem follows the one of Theorem 4.2.7. Thus, we give here just a sketch and point out the differences to the proof of Theorem 4.2.7. Let $\lambda \in \mathbb{C}\setminus\mathbb{R}$ be fixed and denote by $P_\Omega : L^2(\mathbb{R}^3;\mathbb{C}^4) \to L^2(\Omega;\mathbb{C}^4)$ the restriction operator which acts as $P_\Omega f = f \upharpoonright \Omega$, $f \in L^2(\mathbb{R}^3;\mathbb{C}^4)$. Then it holds by Proposition 5.2.2

$$\gamma^\Omega(\lambda) = \frac{1}{\sqrt{c}} P_\Omega \Phi_\lambda^{1/2}\left(\frac{1}{2c}\beta + \mathcal{C}_\lambda^{1/2}\right)^{-1}$$

with the operators $\Phi_\lambda^{1/2}$ and $\mathcal{C}_\lambda^{1/2}$ defined as in Proposition 4.1.6. Hence, we have

$$\overline{\gamma^\Omega(\lambda)} = \frac{1}{\sqrt{c}} P_\Omega \Phi_\lambda\left(\frac{1}{2c}\beta + \mathcal{C}_\lambda\right)^{-1}.$$

In a similar way one gets

$$\overline{M^\Omega(\lambda)} = -\frac{1}{c} P_+\left(\frac{1}{2c}\beta + \mathcal{C}_\lambda\right)^{-1} P_+.$$

In the proof of Theorem 4.2.7 it was shown that

$$\frac{\mathrm{d}^k}{\mathrm{d}\lambda^k}(I_4 + 2c\beta\mathcal{C}_\lambda)^{-1} \in \mathfrak{S}_{2/k,\infty},$$

see (4.19). Hence, it follows

$$\frac{\mathrm{d}^k}{\mathrm{d}\lambda^k}\overline{M^\Omega(\lambda)} \in \mathfrak{S}_{2/k,\infty} \quad (5.16)$$

and using (2.42), Proposition 4.1.8 and (2.1)

$$\frac{\mathrm{d}^k}{\mathrm{d}\lambda^k}\overline{\gamma^\Omega(\lambda)} = P_\Omega \sum_{s+t=k}\frac{k!}{s!t!}\frac{\mathrm{d}^s}{\mathrm{d}\lambda^s}\Phi_\lambda \frac{\mathrm{d}^t}{\mathrm{d}\lambda^t}\left(\frac{1}{2c}\beta + \mathcal{C}_\lambda\right)^{-1} \in \mathfrak{S}_{4/(2k+1),\infty}.$$

By taking adjoints this implies that also $\frac{\mathrm{d}^k}{\mathrm{d}\lambda^k}\gamma^\Omega(\overline{\lambda})^* \in \mathfrak{S}_{4/(2k+1),\infty}$. Note that (5.16) yields

$$\frac{\mathrm{d}^k}{\mathrm{d}\lambda^k}\big(\tau - \overline{M^\Omega(\lambda)}\big)^{-1} \in \mathfrak{S}_{2/k,\infty};$$

this can be shown in exactly the same way as (4.19). Thus, using the resolvent formula from Theorem 5.3.3 we get finally in a similar way as in (4.17) that

$$(A_\tau^\Omega-\lambda)^{-l}-(T_{\mathrm{MIT}}^\Omega-\lambda)^{-l}=\sum_{p+q+r=l-1}\frac{1}{p!q!r!}\frac{\mathrm{d}^p}{\mathrm{d}\lambda^p}\overline{\gamma(\lambda)}\frac{\mathrm{d}^q}{\mathrm{d}\lambda^q}\big(\tau-\overline{M^\Omega(\lambda)}\big)^{-1}\frac{\mathrm{d}^r}{\mathrm{d}\lambda^r}\gamma(\overline{\lambda})^*$$

belongs to $\mathfrak{S}_{2/l,\infty}$.

Finally, the trace formula (5.15) can be shown in exactly the same way as Corollary 4.2.8.

□

5.3.1 A remark on A_τ^Ω and $A_{\eta_\mathrm{e},\eta_\mathrm{s}}^\Sigma$ in the confinement case

Let $\Omega_+\subset\mathbb{R}^3$ be a bounded C^2-domain, set $\Sigma:=\partial\Omega_+$ and $\Omega_-:=\mathbb{R}^3\setminus\overline{\Omega_+}$ and denote the unit normal vector pointing outwards of $\Omega_\pm$ by $\nu_\pm$. Moreover, let $\eta_\mathrm{e},\eta_\mathrm{s}:\Sigma\to\mathbb{R}$ be Lipschitz continuous. If $\eta_\mathrm{e}(x)^2-\eta_\mathrm{s}(x)^2=-4c^2$ for all $x\in\Sigma$, then the operator $A_{\eta_\mathrm{e},\eta_\mathrm{s}}^\Sigma$ given by (4.12) is self-adjoint and it decouples into

$$A_{\eta_\mathrm{e},\eta_\mathrm{s}}^\Sigma=\widetilde{A}_{\eta_\mathrm{e},\eta_\mathrm{s}}^{\Omega_+}\oplus\widetilde{A}_{\eta_\mathrm{e},\eta_\mathrm{s}}^{\Omega_-},$$

where $\widetilde{A}_{\eta_\mathrm{e},\eta_\mathrm{s}}^{\Omega_\pm}$ is a Dirac operator in $L^2(\Omega_\pm;\mathbb{C}^4)$ with boundary conditions

$$\big(2cI_4-i(\alpha\cdot\nu_\pm)(\eta_\mathrm{e}+\eta_\mathrm{s}\beta)\big)f_\pm|_\Sigma=0\quad\text{for}\quad f_\pm\in\operatorname{dom}\widetilde{A}_{\eta_\mathrm{e},\eta_\mathrm{s}}^{\Omega_\pm},\tag{5.17}$$

compare Remark 4.2.2 and Theorem 4.2.3. We will show that the operators $\widetilde{A}_{\eta_\mathrm{e},\eta_\mathrm{s}}^{\Omega_\pm}$ are of the form $A_\tau^{\Omega_\pm}$ and, on the other hand, for every Lipschitz continuous τ in the non-critical case, that means $\tau(x)\neq\pm1$ for all $x\in\Sigma$, the operator $A_\tau^{\Omega_\pm}$ is the compression of some $A_{\eta_\mathrm{e},\eta_\mathrm{s}}^\Sigma$ in the confinement case. This allows, in particular, to deduce some properties of $A_\tau^{\Omega_\pm}$ of those of $A_{\eta_\mathrm{e},\eta_\mathrm{s}}^\Sigma$ from Chapter 4 with very small effort.

Proposition 5.3.7. *Let for some Lipschitz continuous functions $\eta_\mathrm{e},\eta_\mathrm{s},\tau:\Sigma\to\mathbb{R}$ the operators $A_{\eta_\mathrm{e},\eta_\mathrm{s}}^\Sigma$ and $A_\tau^{\Omega_\pm}$ be defined as in* (4.12) *and* (5.13)*, respectively.*

(i) *Assume that $\eta_\mathrm{e}(x)^2-\eta_\mathrm{s}(x)^2=-4c^2$ for all $x\in\Sigma$. If $\tau:=\frac{\eta_\mathrm{e}}{2c-\eta_\mathrm{s}}$, then $\tau\neq\pm1$ everywhere on Σ and $A_{\eta_\mathrm{e},\eta_\mathrm{s}}^\Sigma=A_\tau^{\Omega_+}\oplus A_\tau^{\Omega_-}$.*

(ii) *Conversely, let τ be such that $\tau(x)\neq\pm1$ for all $x\in\Sigma$. If*

$$\eta_\mathrm{e}:=\frac{4c\tau}{1-\tau^2}\quad\textit{and}\quad\eta_\mathrm{s}:=\frac{2c(1+\tau^2)}{\tau^2-1},$$

then $\eta_\mathrm{e}^2-\eta_\mathrm{s}^2=-4c^2$ on Σ and $A_{\eta_\mathrm{e},\eta_\mathrm{s}}^\Sigma=A_\tau^{\Omega_+}\oplus A_\tau^{\Omega_-}$.

Proof. Let us start with some general observations. Using the anti-commutation relation (1.2) and $\beta^2 = I_4$ we see that

$$I_4 = P_+ + P_- = P_+ + \beta P_+ \beta.$$

Thus, the boundary condition (5.17) is equivalent to

$$\big(2cI_4 - i(\alpha \cdot \nu_\pm)(\eta_\mathrm{e} + \eta_\mathrm{s}\beta)\big)P_+ f_\pm|_\Sigma = -\big(2cI_4 - i(\alpha \cdot \nu_\pm)(\eta_\mathrm{e} + \eta_\mathrm{s}\beta)\big)\beta P_+ \beta f_\pm|_\Sigma.$$

Multiplying both sides with β, using again (1.2) and $i\beta(\alpha \cdot \nu_\pm)P_+ = P_+$ we deduce that the last line can be rewritten as

$$\big((2c+\eta_s)\beta - \eta_\mathrm{e} I_4\big)P_+ f_\pm|_\Sigma = -\big((2c-\eta_\mathrm{s})I_4 + \eta_\mathrm{e}\beta\big)P_+ \beta f_\pm|_\Sigma. \tag{5.18}$$

To prove now assertion (i) we use first $\eta_\mathrm{e}^2 - \eta_\mathrm{s}^2 = -4c^2$ to see

$$\big((2c-\eta_\mathrm{s})I_4 - \eta_\mathrm{e}\beta\big)\big((2c+\eta_\mathrm{s})\beta - \eta_\mathrm{e} I_4\big) = -4c\eta_\mathrm{e}$$

and

$$\big((2c-\eta_\mathrm{s})I_4 - \eta_\mathrm{e}\beta\big)\big((2c-\eta_\mathrm{s})I_4 + \eta_\mathrm{e}\beta\big) = 8c^2 - 4c\eta_\mathrm{s}.$$

Thus, multiplying (5.18) with the invertible matrix $\big((2c-\eta_\mathrm{s})I_4 - \eta_\mathrm{e}\beta\big)$ we see that it is equivalent to

$$\frac{\eta_\mathrm{e}}{2c-\eta_\mathrm{s}}\Gamma_0^{\Omega_\pm} f_\pm = \Gamma_1^{\Omega_\pm} f_\pm. \tag{5.19}$$

This implies the claim of item (i).

In order to verify item (ii) define η_e and η_s as in the proposition. Then a simple calculation shows that $\eta_\mathrm{e}^2 - \eta_\mathrm{s}^2 = -4c^2$ and that this choice fulfills $\tau = \frac{\eta_\mathrm{e}}{2c-\eta_\mathrm{s}}$. Since (5.19) is equivalent to (5.17) for $\eta_\mathrm{e}, \eta_\mathrm{s}$ satisfying $\eta_\mathrm{e}^2 - \eta_\mathrm{s}^2 = -4c^2$ everywhere on Σ, we deduce that $A^\Sigma_{\eta_\mathrm{e},\eta_\mathrm{s}} = A^{\Omega_+}_\tau \oplus A^{\Omega_-}_\tau$. This finishes the proof of this proposition. □

Proposition 5.3.7 shows us that there is a one-to-one correspondence between the operators A^Ω_τ for non-critical boundary values and $A^\Sigma_{\eta_\mathrm{e},\eta_\mathrm{s}}$ in the confinement case. Using this result and the findings of Section 4.2 we are able to state and reformulate some properties of A^Ω_τ. For instance, using the previous proposition and Theorem 4.2.3 one can show with very little effort the following resolvent identity:

Corollary 5.3.8. *Let $\Omega \subset \mathbb{R}^3$ be a C^2-domain with compact boundary, let $\tau : \partial\Omega \to \mathbb{R}$ be Lipschitz continuous such that $\tau(x) \neq \pm 1$ for all $x \in \partial\Omega$. Moreover, set*

$$\eta_\mathrm{e} := \frac{4c\tau}{1-\tau^2} \quad \textit{and} \quad \eta_\mathrm{s} := \frac{2c(1+\tau^2)}{\tau^2 - 1}$$

and let P_Ω be the projection defined by (5.2)*. Eventually, let A_0 be the free Dirac operator and let Φ_λ and $\mathcal{C}_\lambda$ be defined by* (3.16) *and* (3.17)*, respectively. Then it holds for all $\lambda \in \mathbb{C}\setminus\mathbb{R}$*

$$(A_\tau^\Omega - \lambda)^{-1} = P_\Omega(A_0-\lambda)^{-1}P_\Omega^* - P_\Omega\Phi_\lambda\big(I_4+(\eta_e I_4+\eta_s\beta)\mathcal{C}_\lambda\big)^{-1}(\eta_e I_4+\eta_s\beta)\Phi_{\overline{\lambda}}^* P_\Omega^*.$$

In a similar way as in Corollary 5.3.8 one can deduce almost immediately other properties of A_τ^Ω. For instance Theorem 5.3.6 follows from Theorem 4.2.7. Furthermore, the fact that for unbounded Ω it holds $\sigma_{\mathrm{ess}}(A_\tau^{\Omega_\pm}) = (-\infty,-mc^2]\cup[mc^2,\infty)$ and that the number of discrete eigenvalues in $(-mc^2,mc^2)$ is finite is a simple consequence of Theorem 4.2.3.

A translation of the Birman Schwinger principle is a little bit more delicate: if for some $\lambda \in (-mc^2,mc^2)$ it holds $-1\in\sigma_{\mathrm{p}}((\eta_e I_4+\eta_s\beta)\mathcal{C}_\lambda)$, then $\lambda\in\sigma_{\mathrm{p}}(A^\Sigma_{\eta_e,\eta_s}) = \sigma_{\mathrm{p}}(A_\tau^{\Omega_+}\oplus A_\tau^{\Omega_-})$, but it is not clear whether λ is an eigenvalue of $A_\tau^{\Omega_+}$ or of $A_\tau^{\Omega_-}$. If Ω_- is connected, then one can say more on eigenvalues of $A_\tau^{\Omega_+}$ in $(-\infty,-mc^2]\cup[mc^2,\infty)$, as $A_\tau^{\Omega_-}$ does not have embedded eigenvalues there in this case (see [6, Theorem 3.7] and the discussion after this result). This means that

$$\sigma_{\mathrm{p}}(A_\tau^\Omega)\cap(-\infty,-mc^2]\cup[mc^2,\infty) = \sigma_{\mathrm{p}}(A^\Sigma_{\eta_e,\eta_s})\cap(-\infty,-mc^2]\cup[mc^2,\infty).$$

Since $S^\Sigma = T_{\min}^{\Omega_+}\oplus T_{\min}^{\Omega_-}$ is simple by Lemma 3.1.2 we can detect the eigenvalues of $A^\Sigma_{\eta_e,\eta_s}$ in $(-\infty,-mc^2]\cup[mc^2,\infty)$ with the aid of Proposition 2.2.8 and get for $\lambda\in(-\infty,-mc^2]\cup[mc^2,\infty)$ that

$$\lambda\in\sigma(A_\tau^{\Omega_+}) \Leftrightarrow \exists\varphi\in H^{1/2}(\Sigma;\mathbb{C}^4): \lim_{\varepsilon\searrow 0} i\varepsilon\big(I_4+(\eta_e I_4+\eta_s\beta)\mathcal{C}_{\lambda+i\varepsilon}\big)^{-1}\varphi\neq 0.$$

It seems that the approach presented in this subsection has many advantages compared to the direct one discussed in Section 5.3. But it has one big drawback (in the opinion of the author of this thesis): there is no chance here to study $A_\tau^{\Omega_\pm}$ in the case of critical boundary values to obtain similar results as below in Section 5.4 with the techniques available from the direct approach.

5.4 Dirac operators on domains with critical boundary values – self-adjointness and basic spectral properties

In this section we study Dirac operators on a domain $\Omega\subset\mathbb{R}^3$ with the boundary condition $\tau P_+ f|_{\partial\Omega} = P_+\beta f|_{\partial\Omega}$ in the critical case, that means if there are $x\in\partial\Omega$ with $|\tau(x)|=1$. Under this assumption A_τ^Ω defined by (5.13) is not self-adjoint. With a similar strategy as in Section 4.3 we will show then for constant boundary value $\tau\in\{\pm1\}$ that A_τ^Ω is essentially self-adjoint and with the aid of the ordinary boundary triple $\{\mathcal{G}_\Omega, \Upsilon_0^\Omega, \Upsilon_1^\Omega\}$ from Theorem 5.2.6 we can compute the self-adjoint closure of this operator and deduce some of its spectral properties.

First, we show that A_τ^Ω defined by (5.13) is symmetric, but not self-adjoint. The proof of this result relies on Lemma 5.3.2 and similar arguments as in Proposition 4.3.1.

Proposition 5.4.1. *Assume that $\tau : \partial\Omega \to \mathbb{R}$ is a Lipschitz continuous function such that $|\tau(x)| = 1$ for some $x \in \partial\Omega$. Then A_τ^Ω defined by* (5.13) *is symmetric, but not self-adjoint.*

Proof. The proof is very similar to the one of Proposition 4.3.1 and hence, we provide just a sketch here. The fact that A_τ^Ω is symmetric follows immediately from Green's identity, see (2.9). The claim that A_τ^Ω is not self-adjoint will be shown in an indirect way.

Assume that A_τ^Ω is self-adjoint. Then $\operatorname{ran}(A_\tau^\Omega - \lambda) = L^2(\Omega;\mathbb{C}^4)$ for all $\lambda \in \mathbb{C}\setminus\mathbb{R}$. According to Theorems 2.2.5 and 5.2.1 this is equivalent to

$$\operatorname{ran}\gamma^\Omega(\overline{\lambda})^* = \operatorname{ran}\big(\Gamma_1^\Omega(T_{\mathrm{MIT}}^\Omega - \lambda)^{-1}\big) \subset \operatorname{ran}(\tau - M^\Omega(\lambda)).$$

By (5.8) it holds $\operatorname{ran}\big(\Gamma_1^\Omega(T_{\mathrm{MIT}}^\Omega - \lambda)^{-1}\big) = \operatorname{ran}\big(\Gamma_1^\Omega \upharpoonright \ker\Gamma_0^\Omega\big) = \mathcal{G}_\Omega^{1/2}$ and thus the last condition is equivalent to the fact that $\tau - M^\Omega(\lambda)$ is bijective in $\mathcal{G}_\Omega^{1/2}$.

Next, Lemma 5.3.2 and the assumption $A_\tau^\Omega = (A_\tau^\Omega)^*$ imply that also $A_{-\tau}^\Omega$ is self-adjoint and hence, with a similar argument as above we see that $\tau + M^\Omega(\lambda)$ is bijective in $\mathcal{G}_\Omega^{1/2}$. We claim that this implies that also $\tau + (M^\Omega(\lambda))^{-1}$ is bijective. Clearly, this operator is injective, as otherwise the symmetric operator $T^\Omega \upharpoonright \ker(\Gamma_0^\Omega + \tau\Gamma_1^\Omega)$ would have the non-real eigenvalue λ by Theorem 2.2.6 (i). Moreover, we have

$$\begin{aligned}\tau + (M^\Omega(\lambda))^{-1} &= \tau + M^\Omega(\lambda) - M^\Omega(\lambda) + (M^\Omega(\lambda))^{-1} \\ &= (\tau + M^\Omega(\lambda))\big(I_4 - (\tau + M^\Omega(\lambda))^{-1}(M^\Omega(\lambda) - (M^\Omega(\lambda))^{-1})\big).\end{aligned}$$

Since $M^\Omega(\lambda) - (M^\Omega(\lambda))^{-1}$ is compact in $\mathcal{G}_\Omega^{1/2}$ by Proposition 5.2.5 it follows from Fredholm's alternative that $\tau + (M^\Omega(\lambda))^{-1}$ must be bijective.

Since $\tau - M^\Omega(\lambda)$ and $\tau + (M^\Omega(\lambda))^{-1}$ are bijective, also the product

$$(\tau - M^\Omega(\lambda))\big(\tau + (M^\Omega(\lambda))^{-1}\big) = (\tau^2 - 1)I_4 + \tau(M^\Omega(\lambda))^{-1} - M^\Omega(\lambda)\tau$$

is bijective. We set

$$C := \big\|\big((\tau^2 - 1)I_4 + \tau(M^\Omega(\lambda))^{-1} - M^\Omega(\lambda)\tau\big)^{-1}\big\|. \tag{5.20}$$

Next, by assumption there exist some $x \in \partial\Omega$ such that $\tau(x)^2 = 1$. Thus, there is a function $\widetilde{\tau}$ such that

$$\Sigma_0 := \partial\Omega \setminus \operatorname{supp}\widetilde{\tau} \neq \emptyset \quad \text{and} \quad C\big\|(\tau^2 - 1) - \widetilde{\tau}\big\| < 1$$

with C chosen as in (5.20) and the norm is the operator norm in $\mathfrak{B}(\mathcal{G}_\Omega^{1/2})$. Note that such a choice is possible by Proposition 2.5.2. This and (5.20) imply then

$$C\big\|\big(\widetilde{\tau}I_4+\tau(M^\Omega(\lambda))^{-1}-M^\Omega(\lambda)\tau\big)-\big((\tau^2-1)I_4+\tau(M^\Omega(\lambda))^{-1}-M^\Omega(\lambda)\tau\big)\big\| \\ = C\big\|(\tau^2-1)-\widetilde{\tau}\big\|<1.$$

Therefore, also the operator $\widetilde{\tau}I_4+\tau(M^\Omega(\lambda))^{-1}-M^\Omega(\lambda)\tau$ is bijective in $\mathcal{G}_\Omega^{1/2}$ by [50, Theorem IV 1.16].

Eventually, let $\mathcal{P}: H^{1/2}(\partial\Omega;\mathbb{C}^4)\to H^{1/2}(\Sigma_0;\mathbb{C}^4)$ be the restriction operator acting as $\mathcal{P}\varphi=\varphi\upharpoonright\Sigma_0$. Using $\operatorname{supp}\widetilde{\tau}=\partial\Omega\setminus\Sigma_0$ this yields that

$$\begin{aligned}\big\{\varphi\upharpoonright\Sigma_0:\varphi\in\mathcal{G}_\Omega^{1/2}\big\}&\subset\operatorname{ran}\mathcal{P}\left(\widetilde{\tau}I_4+\tau(M^\Omega(\lambda))^{-1}-M^\Omega(\lambda)\tau\right)\\&=\operatorname{ran}\mathcal{P}\left(\tau(M^\Omega(\lambda))^{-1}-M^\Omega(\lambda)\tau\right).\end{aligned}\tag{5.21}$$

One can show in exactly the same way as in the proof of Theorem 5.3.3 that $\tau(M^\Omega(\lambda))^{-1}-M^\Omega(\lambda)\tau$ is compact in $\mathcal{G}_\Omega^{1/2}$. This gives then a contradiction to (5.21) and finishes the proof of this proposition. □

In the following assume that $\tau\in\{\pm1\}$ is constant. In the rest of this section we show that $A_{\pm1}^\Omega$ is essentially self-adjoint and using the ordinary boundary triple $\{\mathcal{G}_\Omega,\Upsilon_0^\Omega,\Upsilon_1^\Omega\}$ from Theorem 5.2.6 we are going to compute its self-adjoint closure and some of its spectral properties. Choose the same $\mu\in\rho(T_{-\mathrm{MIT}}^\Omega)\cap(-mc^2,mc^2)$ as in the definition of $\{\mathcal{G}_\Omega,\Upsilon_0^\Omega,\Upsilon_1^\Omega\}$. Then

$$A_\tau^\Omega=T^\Omega\upharpoonright\ker\big(\Gamma_1^\Omega-\tau\Gamma_0^\Omega\big)=(S^\Omega)^*\upharpoonright\big(\Upsilon_1^\Omega-\Theta_\tau^{1,\Omega}\Upsilon_1^\Omega\big),$$

where $\Theta_\tau^{1,\Omega}=\iota_+^\Omega\big(\tau-M^\Omega(\mu)\big)(\iota_-^\Omega)^{-1}$ and $M^\Omega(\mu)$ is the value of the Weyl function given as in Proposition 5.2.2, compare (2.22). The operator $\Theta_\tau^{1,\Omega}$ is explicitly given by

$$\Theta_\tau^{1,\Omega}\varphi:=\iota_+^\Omega\big(\tau-M^\Omega(\mu)\big)(\iota_-^\Omega)^{-1}\varphi,\quad\operatorname{dom}\Theta_\tau^{1,\Omega}:=\mathcal{G}_\Omega^1.\tag{5.22}$$

Due to the mapping properties of $M^\Omega(\mu)$ from Proposition 5.2.2 we see that $\Theta_\tau^{1,\Omega}$ is well-defined. Our goal is to show that $\Theta_\tau^{1,\Omega}$ is essentially self-adjoint and that its closure coincides with the maximal parameter

$$\begin{aligned}\Theta_\tau^{0,\Omega}\varphi&:=\iota_+^\Omega\big(\tau-\widetilde{M}^\Omega(\mu)\big)(\iota_-^\Omega)^{-1}\varphi,\\ \operatorname{dom}\Theta_\tau^{0,\Omega}&:=\left\{\varphi\in\mathcal{G}_\Omega:\big(\tau-\widetilde{M}^\Omega(\mu)\big)(\iota_-^\Omega)^{-1}\varphi\in\mathcal{G}_\Omega^{1/2}\right\},\end{aligned}\tag{5.23}$$

where $\widetilde{M}^\Omega(\mu)$ is the extension of $M^\Omega(\mu)$ onto $\mathcal{G}_\Omega^{-1/2}$ from Proposition 5.2.5. The (essential) self-adjointness of $\Theta_\tau^{1,\Omega}$ and $\Theta_\tau^{0,\Omega}$ is studied in the following proposition; the proof of this result follows closely the one of Proposition 4.3.2 and hence we give just a sketch here.

Proposition 5.4.2. *Let $\tau \in \{\pm 1\}$ and let $\Theta_\tau^{1,\Omega}$ and $\Theta_\tau^{0,\Omega}$ be given by* (5.22) *and* (5.23)*, respectively. Then $\Theta_\tau^{1,\Omega}$ is essentially self-adjoint in $\mathcal{G}_\Omega$ and the closure of $\Theta_\tau^{1,\Omega}$ is $\Theta_\tau^{0,\Omega}$. In particular $\Theta_\tau^{0,\Omega}$ is self-adjoint.*

Proof. The proof of this proposition is very similar as the one of Proposition 4.3.2. First, one can verify that $\Theta_\tau^{0,\Omega}$ is a closed operator in $\mathcal{G}_\Omega$. This can be done with exactly the same arguments as in *Step 1* of the proof of Proposition 4.3.2 and hence, we omit it. Then one can check that $\Theta_\tau^{0,\Omega} \subset \overline{\Theta_\tau^{1,\Omega}}$, which implies that $\Theta_\tau^{0,\Omega}$ is also symmetric, and $(\Theta_\tau^{1,\Omega})^* \subset \Theta_\tau^{0,\Omega}$, which yields finally that $\Theta_\tau^{0,\Omega}$ is self-adjoint. It remains to verify the inclusions $\Theta_\tau^{0,\Omega} \subset \overline{\Theta_\tau^{1,\Omega}}$ and $(\Theta_\tau^{1,\Omega})^* \subset \Theta_\tau^{0,\Omega}$. This will be done in the following.

First, to show $\Theta_\tau^{0,\Omega} \subset \overline{\Theta_\tau^{1,\Omega}}$ fix some $\varphi \in \operatorname{dom} \Theta_\tau^{0,\Omega}$ and choose a sequence $(\psi_n) \subset \mathcal{G}_\Omega^1$ such that $(\iota_-^\Omega)^{-1}\psi_n \to (\iota_-^\Omega)^{-1}\varphi$ in $\mathcal{G}_\Omega^{-1/2}$. We define

$$\varphi_n := \varphi + \frac{1}{2}\iota_-^\Omega \left(I_4 + (\widetilde{M}^\Omega(\mu))^{-1}\tau \right) (\iota_-^\Omega)^{-1}(\psi_n - \varphi).$$

Note that

$$\varphi_n = \frac{1}{2}\iota_-^\Omega \left(I_4 + (M^\Omega(\mu))^{-1}\tau \right) (\iota_-^\Omega)^{-1}\psi_n + \frac{1}{2}\iota_-^\Omega (M^\Omega(\mu))^{-1} \left(\widetilde{M}(\mu) - \tau \right) (\iota_-^\Omega)^{-1}\varphi. \tag{5.24}$$

Since $(M^\Omega(\mu))^{-1}$ is bounded in $\mathcal{G}_\Omega^{1/2}$ by Proposition 5.2.3 and ι_-^Ω gives rise to a bounded operator from $\mathcal{G}_\Omega^{1/2}$ onto $\mathcal{G}_\Omega^1$ by (5.12) we deduce

$$\frac{1}{2}\iota_-^\Omega \left(I_4 + (M^\Omega(\mu))^{-1}\tau \right) (\iota_-^\Omega)^{-1}\psi_n \in \mathcal{G}_\Omega^1.$$

Because of the same reasons and $\varphi \in \operatorname{dom} \Theta_\tau^{0,\Omega}$ we have

$$\frac{1}{2}\iota_-^\Omega (M^\Omega(\mu))^{-1} \left(\widetilde{M}(\mu) - \tau \right) (\iota_-^\Omega)^{-1}\varphi \in \mathcal{G}_\Omega^1.$$

Hence, we conclude from (5.24) that $\varphi_n \in \mathcal{G}_\Omega^1$. Next, as $I_4 + (\widetilde{M}^\Omega(\mu))^{-1}\tau$ is continuous in $\mathcal{G}_\Omega^{-1/2}$ by Proposition 5.2.5 (iii) and $\iota_-^\Omega : \mathcal{G}_\Omega^{-1/2} \to \mathcal{G}_\Omega$ by construction we find

$$\varphi_n - \varphi = \frac{1}{2}\iota_-^\Omega \left(I_4 + (\widetilde{M}^\Omega(\mu))^{-1}\tau \right) (\iota_-^\Omega)^{-1}(\psi_n - \varphi) \to 0 \quad \text{in } \mathcal{G}_\Omega.$$

Finally, using $\tau^2 = 1$ we obtain that

$$\begin{aligned} \Theta_\tau^{0,\Omega}(\varphi_n - \varphi) &= \frac{1}{2}\iota_+^\Omega \Big(\tau - \widetilde{M}(\mu) \Big) \left(I_4 + (\widetilde{M}^\Omega(\mu))^{-1}\tau \right) (\iota_-^\Omega)^{-1}(\psi_n - \varphi) \\ &= \frac{1}{2}\iota_+^\Omega \big((\widetilde{M}(\mu))^{-1} - \widetilde{M}(\mu) \big) (\iota_-^\Sigma)^{-1}(\psi_n - \varphi). \end{aligned} \tag{5.25}$$

Since $(\widetilde{M}(\mu))^{-1} - \widetilde{M}(\mu) : \mathcal{G}_\Omega^{-1/2} \to \mathcal{G}_\Omega^{1/2}$ is continuous by Proposition 5.2.5 (iv) we deduce eventually from (5.25) that $\Theta_\tau^{0,\Omega}(\varphi_n - \varphi) \to 0$ in $\mathcal{G}_\Omega$. This finishes the proof of the statement that $\Theta_\tau^{0,\Omega} \subset \overline{\Theta_\tau^{1,\Omega}}$.

It remains to prove that $(\Theta_\tau^{1,\Omega})^* \subset \Theta_\tau^{0,\Omega}$. But this can be done in exactly the same way as in *Step 2* in the proof of Proposition 4.3.2. One just has to use Proposition 5.2.5 (ii) instead of Proposition 4.1.4 (ii). This finishes the proof of this proposition. □

With the aid of Proposition 5.4.2 we are now able to show that the operator $A_{\pm 1}^\Omega$ defined by (5.13) is essentially self-adjoint and we can describe its self-adjoint closure $\overline{A_{\pm 1}^\Omega}$ in terms of the boundary triple $\{\mathcal{G}_\Omega, \Upsilon_0^\Omega, \Upsilon_1^\Omega\}$ from Theorem 5.2.6, which allows us further to state some of the spectral properties of $\overline{A_\tau^\Omega}$. Recall the definitions of the maximal operator $(S^\Omega)^* = T_{\max}^\Omega$ given by (3.10) and the extended boundary mappings $\widetilde{\Gamma}_0^\Omega, \widetilde{\Gamma}_1^\Omega$ from Lemma 5.2.4.

Theorem 5.4.3. *Let $\tau \in \{\pm 1\}$ and let A_τ^Ω be defined by* (5.13)*. Moreover, let $T_{\max}^\Omega$ be given by* (3.10) *and let $\widetilde{\gamma}^\Omega$ and $\widetilde{M}^\Omega$ be given as in Proposition 5.2.5. Then A_τ^Ω is essentially self-adjoint in $L^2(\Omega;\mathbb{C}^4)$ and its self-adjoint closure is given by*

$$\overline{A_\tau^\Omega} = T_{\max}^\Omega \upharpoonright \ker\big(\Upsilon_1^\Omega - \Theta_\tau^{0,\Omega}\Upsilon_0^\Omega\big) = T_{\max}^\Omega \upharpoonright \ker\big(\widetilde{\Gamma}_1^\Omega - \tau\widetilde{\Gamma}_0^\Sigma\big). \tag{5.26}$$

Furthermore $A_\tau^\Omega \subsetneq \overline{A_\tau^\Omega}$, $\operatorname{dom}\overline{A_\tau^\Omega} \not\subset H^1(\Omega;\mathbb{C}^4)$*, and the following assertions are true:*

(i) *For $\lambda \in \mathbb{C}\setminus\mathbb{R}$ it holds*

$$(\overline{A_\tau^\Omega} - \lambda)^{-1} = (T_{\mathrm{MIT}}^\Omega - \lambda)^{-1} + \widetilde{\gamma}^\Omega(\lambda)\big(\tau - \widetilde{M}^\Omega(\lambda)\big)^{-1}\gamma^\Omega(\overline{\lambda})^*.$$

(ii) *If Ω is unbounded, then $(-\infty, -mc^2] \cup [mc^2, \infty) \subset \sigma_{\mathrm{ess}}(A_\tau^\Omega)$ and $\lambda \in (-mc^2, mc^2) \cap \sigma_{\mathrm{p}}(\overline{A_\tau^\Omega})$ if and only if $0 \in \sigma_{\mathrm{p}}(\tau - \widetilde{M}^\Omega(\lambda))$.*

(iii) *If Ω is bounded, then λ is an eigenvalue of $\overline{A_\tau^\Omega}$ if and only if there exists a $\varphi \in \mathcal{G}_\Omega$ such that*

$$\lim_{\varepsilon \searrow 0} i\varepsilon\big[\iota_+^\Omega(\widetilde{M}^\Omega(\lambda + i\varepsilon) - \tau)(\iota_-^\Omega)^{-1}\big]^{-1}\varphi \neq 0.$$

Proof. First, by Proposition 5.4.2 the operator $\Theta_\tau^{1,\Omega}$ is essentially self-adjoint. Thus Proposition 2.2.7 implies that

$$A_\tau^\Omega = T^\Omega \upharpoonright \ker\big(\Gamma_1^\Omega - \tau\Gamma_0^\Omega\big) = T_{\max}^\Omega \upharpoonright \big(\Upsilon_1^\Omega - \Theta_\tau^{1,\Omega}\Upsilon_0^\Omega\big)$$

is essentially self-adjoint. Furthermore, since $\{\mathcal{G}_\Omega, \Upsilon_0^\Omega, \Upsilon_1^\Omega\}$ is an ordinary boundary triple the closure $\overline{A_\tau^\Omega}$ of A_τ^Ω corresponds to the closure of the parameter $\Theta_\tau^{1,\Omega}$; by Proposition 5.4.2

this is $\Theta_\tau^{0,\Omega}$. Employing (2.22) and [22, Corollary 3.14] we deduce then (5.26). Eventually, it follows immediately from Proposition 5.4.1 that $A_\tau^\Omega \subsetneq \overline{A_\tau^\Omega}$.

The Krein type resolvent formula in item (i) is an immediate consequence of Theorem 2.2.5 taking the special form of the γ-field and the Weyl function for the triple $\{\mathcal{G}_\Omega, \Upsilon_0^\Omega, \Upsilon_1^\Omega\}$ from (2.20) into account.

Next, we prove statement (ii). First, let $\lambda \in (-\infty, -mc^2] \cup [mc^2, \infty)$ and define the function ψ_n^λ as in Lemma 3.1.4. Then $\psi_n^\lambda \in \operatorname{dom} T_{\min}^\Omega \subset \operatorname{dom} \overline{A_\tau^\Omega}$ for any $n \in \mathbb{N}$ and this sequence has all properties of a singular Weyl sequence for λ and $\overline{A_\tau^\Omega}$. Hence $\lambda \in \sigma_{\text{ess}}(\overline{A_\tau^\Omega})$. Since $\lambda \in (-\infty, -mc^2] \cup [mc^2, \infty)$ was arbitrary, we deduce $(-\infty, -mc^2] \cup [mc^2, \infty) \subset \sigma_{\text{ess}}(\overline{A_\tau^\Omega})$. Furthermore, the Birman-Schwinger principle in (ii) is a direct consequence of Theorem 2.2.5 (i) due to the special form of the Weyl function corresponding to the triple $\{\mathcal{G}_\Omega, \Upsilon_0^\Omega, \Upsilon_1^\Omega\}$, compare (2.20).

Finally, since $S^\Omega = T_{\min}^\Omega$ is simple by Lemma 3.1.2, statement (iii) is a consequence of Proposition 2.2.9 and (2.20). □

Remark 5.4.4. According to [55, Proposition 2.1] functions $f \in \operatorname{dom} T_{\max}^\Omega$ have traces in $H^{-1/2}(\partial\Omega; \mathbb{C}^4)$. Hence, the boundary condition $\tau\widetilde{\Gamma}_0^\Omega = \widetilde{\Gamma}_1^\Omega$ is equivalent to

$$\tau P_+ f|_{\partial\Omega} = P_+ \beta f|_{\partial\Omega} \quad \text{in} \quad H^{-1/2}(\Sigma; \mathbb{C}^4)$$

and hence, it is formally the same as for non-critical boundary values in Definition 5.3.1.

Finally, we provide a result which shows that the spectral properties of A_τ^Ω can be significantly different in the case of critical boundary values. This can be seen as the analogue of Theorem 4.3.6 for Dirac operators on domains. But a more careful look shows that the principle behind this effect is a completely different one as in Theorem 4.3.6. Using super symmetry, we prove that $\pm mc^2$ is an eigenvalue of infinite multiplicity of $\overline{A_{\pm 1}^\Omega}$. This implies that for bounded Ω the essential spectrum of A_τ^Ω can be non-empty in the critical case. The proof of this result follows closely the one of [64, Proposition 2] in the 2D-case; I would like to thank K.M. Schmidt for providing me a copy of [64] which was very helpful. We would like to remark that, differently from Theorem 4.3.6, we do not have to make a restriction on the geometry of Ω here.

Theorem 5.4.5. *Assume that $\tau \in \{\pm 1\}$ is constant let $\overline{A_{\pm 1}^\Omega}$ be defined by* (5.26)*. Then $\pm mc^2$ is an eigenvalue of infinite multiplicity of $\overline{A_{\pm 1}^\Omega}$.*

Remark 5.4.6. If Ω is bounded, then one can deduce similarly as in Corollary 4.3.7 that $\operatorname{dom} \overline{A_{\pm 1}^\Omega}$ is not contained in $H^s(\Omega; \mathbb{C}^4)$ for any $s > 0$.

Proof of Theorem 5.4.5. We are going to prove the claim of the theorem for $\tau = 1$, the statement for $\tau = -1$ can be shown with the same arguments. For a simpler readability we split the proof into three steps. First, we introduce a new operator $\mathcal{A}_m^\Omega$ and show via a super symmetry argument that $\mathcal{A}_m^\Omega$ is self-adjoint. Then we verify that $\mathcal{A}_m^\Omega$ is an extension of A_1^Ω. Since this operator is essentially self-adjoint we conclude $\mathcal{A}_m^\Omega = \overline{A_1^\Omega}$. Finally, using the special structure of $\mathcal{A}_m^\Omega$ we show that this operator has the eigenvalue mc^2 with infinite multiplicity.

Step 1: We use for $f \in L^2(\Omega;\mathbb{C}^4)$ the splitting $f = (f_1, f_2)$ with $f_1, f_2 \in L^2(\Omega;\mathbb{C}^4)$, that means f_1 and f_2 are the upper and lower two components of the Dirac spinor, respectively. We define the operator

$$\mathcal{A}_m^\Omega := T_{\max}^\Omega \restriction \big\{ f = (f_1, f_2) \in \operatorname{dom} T_{\max}^\Omega : f_2 \in H_0^1(\Omega;\mathbb{C}^2) \big\}.$$

This operator has the explicit representation

$$\mathcal{A}_m^\Omega = \begin{pmatrix} mc^2 I_2 & \widetilde{A} \\ \widetilde{A}^* & -mc^2 I_2 \end{pmatrix}, \tag{5.27}$$

where $\widetilde{A}$ is

$$\widetilde{A} f = -i\sigma \cdot \nabla f, \quad \operatorname{dom} \widetilde{A} = H_0^1(\Omega;\mathbb{C}^2),$$

and $\sigma = (\sigma_1, \sigma_2, \sigma_3)$ is the family of $\mathbb{C}^{2\times 2}$-valued Pauli matrices from (3.2). We claim that $\mathcal{A}_m^\Omega$ is self-adjoint. For that purpose it suffices to consider $m = 0$, as $mc^2\beta$ is a bounded self-adjoint perturbation.

Indeed $\mathcal{A}_0^\Omega$ is symmetric, as we have for $f = (f_1, f_2) \in \operatorname{dom} \mathcal{A}_0^\Omega$

$$(\mathcal{A}_0^\Omega f, f)_\Omega = (\widetilde{A} f_2, f_1)_\Omega + (\widetilde{A}^* f_1, f_2)_\Omega = 2\operatorname{Re}(\widetilde{A} f_2, f_1)_\Omega \in \mathbb{R}.$$

Next, it holds for $f = (f_1, f_2) \in \operatorname{dom} (\mathcal{A}_0^\Omega)^*$ and $g = (g_1, g_2) \in \operatorname{dom} \mathcal{A}_0^\Omega$

$$\big((\mathcal{A}_0^\Omega)^* f, g\big)_\Omega = \big(f, \mathcal{A}_0^\Omega g\big)_\Omega = (f_1, \widetilde{A} g_2)_\Omega + (f_2, \widetilde{A}^* g_1)_\Omega. \tag{5.28}$$

Choosing $g_1 = 0$ we get from (5.28)

$$\big(\big((\mathcal{A}_0^\Omega)^* f\big)_2, g_2\big)_\Omega = (f_1, \widetilde{A} g_2)_\Omega$$

and hence $f_1 \in \operatorname{dom} \widetilde{A}^*$ and $\widetilde{A}^* f_1 = \big((\mathcal{A}_0^\Omega)^* f\big)_2$. Similarly, choosing $g_2 = 0$ we obtain from (5.28) that $f_2 \in \operatorname{dom} \widetilde{A}$ and $\widetilde{A} f_2 = \big((\mathcal{A}_0^\Omega)^* f\big)_1$. Therefore, we conclude $f \in \operatorname{dom} \mathcal{A}_0^\Omega$ and $(\mathcal{A}_0^\Omega)^* f = \mathcal{A}_0^\Omega f$, that means $\mathcal{A}_0^\Omega$ is self-adjoint.

Step 2: We show that $A_1^\Omega \subset \mathcal{A}_m^\Omega$. Since A_1^Ω is essentially self-adjoint by Theorem 5.4.3 this yields then $\mathcal{A}_m^\Omega = \overline{A_1^\Omega}$. We prove that $f \in \operatorname{dom} T^\Omega$ fulfills

$$f \in \operatorname{dom} A_1^\Omega \quad \text{if and only if} \quad (\beta - I_4) f|_{\partial\Omega} = 0. \tag{5.29}$$

This yields then the claim of this step. To see (5.29) recall that the boundary condition of A_1^Ω reads

$$0 = \Gamma_1^\Omega f - \Gamma_0^\Omega f = P_+(\beta - I_4)f|_{\partial\Omega}. \tag{5.30}$$

Because of (1.2) it holds $P_+\beta = \beta P_-$ and hence, using $\beta^2 = I_4$ we see that (5.30) is equivalent to

$$0 = \beta P_-(\beta - I_4)f|_{\partial\Omega}. \tag{5.31}$$

Since β is invertible, we deduce (5.29) from (5.30) and (5.31).

Step 3: Eventually we show that mc^2 is an eigenvalue of $\mathcal{A}_m^\Omega$ of infinite multiplicity. Note that $\widetilde{A}$ is the upper right corner of the minimal operator $T_{\min}^\Omega$ from (3.11) and similarly $\widetilde{A}^*$ is the upper right corner of the maximal operator $T_{\max}^\Omega$. Hence $\widetilde{A}$ is a symmetric operator with infinite deficiency indices. Moreover $\ker\widetilde{A} = \{0\}$, as $T_{\min}^\Omega$ is simple by Lemma 3.1.2. Therefore $\dim\ker\widetilde{A}^* = \infty$.

Finally, picking any $f_1 \in \ker\widetilde{A}^*$ we deduce from (5.27) that $f := (f_1, 0)$ is an eigenfunction of $\mathcal{A}_m^\Omega$ and eigenvalue mc^2. This yields the claimed result of this theorem. □

5.4.1 Dirac operators on domains with variable critical boundary values

Finally, we would like to state several remarks on the operator A_τ^Ω, if $\tau : \partial\Omega \to \mathbb{R}$ is a Lipschitz continuous function in the critical case, that means if there are some $x \in \partial\Omega$ such that $\tau(x)^2 = 1$. We have seen already in Proposition 5.4.1 that A_τ^Ω is symmetric, but not self-adjoint. If τ fulfills some suitable assumptions, then one can still show similarly as in Section 5.4 that A_τ^Ω is essentially self-adjoint, compute the self-adjoint realization and provide some spectral properties of this operator as in Theorem 5.4.3.

The crucial result in Section 5.4 is Proposition 5.4.2 – all following main results are based on this. The critical point here is to prove that $\Theta_\tau^{0,\Omega} \subset \overline{\Theta_\tau^{1,\Omega}}$, the other steps in the proof can be done similarly as for constant τ. With some suitable assumptions on τ one can modify the verification of $\Theta_\tau^{0,\Omega} \subset \overline{\Theta_\tau^{1,\Omega}}$ for more general τ. This consideration is based on the fact that any $\varphi \in \operatorname{dom}\Theta_\tau^{0,\Omega}$ fulfills

$$(\tau^2 - 1)\varphi \in \mathcal{G}_\Omega^{1/2}. \tag{5.32}$$

Hence, if we assume that τ is such that for all $\varphi \in \mathcal{G}_\Omega^{-1/2}$ which satisfy (5.32) there is a sequence $\varphi_n \in \mathcal{G}^{1/2}$ with

$$\varphi_n \to \varphi \text{ in } \mathcal{G}_\Omega^{-1/2} \quad \text{and} \quad (\tau^2 - 1)\varphi_n \to (\tau^2 - 1)\varphi \text{ in } \mathcal{G}_\Omega^{1/2}, \tag{5.33}$$

as $n \to \infty$, then one could also verify $\Theta_\tau^{0,\Omega} \subset \overline{\Theta_\tau^{1,\Omega}}$ similarly as in the proof of Proposition 5.4.2 with just little modifications. One only must be careful that a non-constant τ

does not commute with $\mathcal{C}_\mu^{-1/2}$ and hence with $\widetilde{M}^\Omega(\mu)$. But due to Proposition 3.2.3 the commutator of $\mathcal{C}_\mu^{-1/2}$ with any Lipschitz continuous function is a bounded operator from $H^{-1/2}(\partial\Omega;\mathbb{C}^4)$ to $H^{1/2}(\partial\Omega;\mathbb{C}^4)$, which allows to prove the desired claim.

Having the analogue of Proposition 5.4.2 one can then proceed as for constant interaction strengths: in the same way as in Theorem 5.4.3 it follows that A_τ^Ω is essentially self-adjoint and that the self-adjoint closure is given by

$$\overline{A_\tau^\Omega} f := (-ic\alpha\cdot\nabla + mc^2\beta)f,$$
$$\operatorname{dom}\overline{A_\tau^\Omega} := \{f \in \operatorname{dom} T_{\max}^\Omega : \tau\widetilde{\Gamma}_0^\Omega f = \widetilde{\Gamma}_1^\Omega f\}.$$

Moreover, if for all $\varphi \in \mathcal{G}_\Omega^{-1/2}$ satisfying (5.32) it holds (5.33), then the spectral properties of $\overline{A_\tau^\Omega}$ can be deduced in a similar way as in Theorem 5.4.3 and we get that:

(i) For $\lambda \in \mathbb{C}\setminus\mathbb{R}$ it holds

$$(\overline{A_\tau^\Omega} - \lambda)^{-1} = (T_{\mathrm{MIT}}^\Omega - \lambda)^{-1} + \widetilde{\gamma}^\Omega(\lambda)\big(\tau - \widetilde{M}^\Omega(\lambda)\big)^{-1}\gamma^\Omega(\overline{\lambda})^*.$$

(ii) If Ω is unbounded, then $(-\infty,-mc^2]\cup[mc^2,\infty) \subset \sigma_{\mathrm{ess}}(A_\tau^\Omega)$ and $\lambda \in (-mc^2,mc^2)\cap\sigma_{\mathrm{p}}(\overline{A_\tau^\Omega})$ if and only if $0 \in \sigma_{\mathrm{p}}(\tau - \widetilde{M}^\Omega(\lambda))$.

(iii) If Ω is bounded, then λ is an eigenvalue of $\overline{A_\tau^\Omega}$ if and only if there exists a $\varphi \in \mathcal{G}_\Omega$ such that

$$\lim_{\varepsilon\searrow 0} i\varepsilon\big[\iota_+^\Omega(\widetilde{M}^\Omega(\lambda+i\varepsilon) - \tau)(\iota_-^\Omega)^{-1}\big]^{-1}\varphi \neq 0.$$

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