A CLASS OF SINGULAR PERTURBATIONS OF THE DIRAC OPERATOR: BOUNDARY TRIPLETS AND WEYL FUNCTIONS

JUSSI BEHRNDT, MARKUS HOLZMANN, CHRISTIAN STELZER, AND GEORG STENZEL

Dedicated to our friend and colleague Seppo Hassi on the occasion of his 60th birthday!

Abstract. In this note we provide boundary triplets and Weyl functions for singular perturbations of Dirac operators, and apply them to investigate Dirac operators with Lorentz scalar δ-shell interactions supported on points in $\mathbb{R}$, curves in $\mathbb{R}^2$, and surfaces in $\mathbb{R}^3$. In the one-dimensional situation such a singular interaction is a rank two perturbation of the free Dirac operator and can easily be treated with an ordinary boundary triplet. In the multidimensional situation δ-shell interactions lead to infinite dimensional perturbations and here it is more natural to apply generalized and quasi boundary triplets when proving self-adjointness and spectral properties of the perturbed Dirac operator. Some of the abstract techniques in this note are closely related and inspired by the notion of boundary relations introduced by Seppo Hassi and his coauthors in [23].

1. Introduction

Singular perturbations of self-adjoint operators play an important role in the description of idealized quantum systems, where a localized short-range potential is often replaced by a more singular model potential. More precisely, assume that A_0 is a self-adjoint differential operator in an L^2-Hilbert space which is viewed as the Hamiltonian of an unperturbed quantum system and suppose that V is some potential such that the formal sum $A_V = A_0 + V$ describes the quantum system under investigation. Standard operator theory techniques ensure that for potentials V belonging to certain function spaces the perturbed operator A_V is again self-adjoint; we refer the reader to the monographs of Reed and Simon [48, 49, 50, 51] or Kato [40]. However, a detailed spectral analysis of A_V is typically very difficult, and for this reason the potential V is often replaced by an idealized perturbation term of δ-type, which is then regarded as an approximation of the real model [5, 31]. On the one hand this procedure may simplify the spectral analysis considerably [1, 16, 19, 39], but on the other hand it may lead to new technical difficulties in the mathematically rigorous definition of the Hamiltonian itself.

In the case that A_0 is the Laplacian in an L^2-space and the δ-potential is supported on hypersurfaces in $\mathbb{R}^d$ (e.g., curves in $\mathbb{R}^2$, or surfaces in $\mathbb{R}^3$) the standard quadratic form approach is useful. In this situation, roughly speaking, the perturbed operator $A_\tau = A_0 + \tau\delta_\Sigma$ is viewed as the self-adjoint operator corresponding to the form

$$\mathfrak{a}[f,g] = (\nabla f, \nabla g)_{L^2} + \int_\Sigma \tau\, f|_\Sigma\, \overline{g|_\Sigma}\, dx, \tag{1.1}$$

where $(\nabla f, \nabla g)_{L^2}$ is the quadratic form defined on the Sobolev space H^1 associated with the Laplacian, and the singular perturbation is encoded in the additive form perturbation with Σ denoting the support of the δ-distribution, τ is some real (position dependent) coefficient, and $f|_\Sigma$ and $g|_\Sigma$ denote the traces of the Sobolev space functions f, g defined in an appropriate way. Of course one has to impose certain assumptions on the support Σ of the δ-potential and the coefficient τ to ensure that $\mathfrak{a}$ in (1.1) is a densely defined closed semibounded form (which then gives rise to a self-adjoint operator A_τ); we refer to [19, 31, 32, 37, 52] for a detailed treatment and further references. A different approach to the operator A_τ is via extension theory techniques in general, and boundary triplet methods in particular (see the recent monograph [9] and [21, 22, 23, 24, 25, 26, 27] by Seppo Hassi and his coauthors for an extensive treatment of boundary triplets and further developments). For the case of point interactions it is well known what type of transmission or jump conditions the functions in the domain of A_τ satisfy; cf. [1] for a comprehensive treatment of point interactions. In the case that the δ-distribution is supported on a hypersurface we refer to [16], where quasi boundary triplets were used for the first time to define A_τ as a self-adjoint restriction of a Laplacian that is decoupled along the support Σ. As in the case of point interactions also in the multidimensional setting one ends up with transmission and jump conditions for the functions in the domain of A_τ along the support Σ of the δ-distribution, see also [8, 17, 42]. In conclusion, for the case that A_0 is the Laplacian (or some more general semibounded Schrödinger operator) nowadays one may efficiently apply form techniques or boundary triplet methods to define and study the perturbed operator A_τ – depending on the particular problem under consideration one method may prove more useful than the other.

Now assume that the unperturbed operator A_0 is the Dirac operator instead of the Laplacian or the Schrödinger operator. While the Dirac operator describes a similar physical system as the Laplace operator including relativistic effects (see Section 3 for more details), the mathematical situation is entirely different: The free Dirac operator A_0 is not semibounded from below and hence standard quadratic form methods are not applicable. Therefore, it is most natural to try to apply boundary triplet techniques, since these methods do not require any type of semiboundedness of the operators under consideration. In fact, Dirac operators with singular interactions supported on points and spheres were already treated with direct methods in [1, 30, 35], but for more general supports of the singular potential only recently a series of papers was published [2, 3, 4], which in turn led to our publications [6, 10, 12, 13] employing the quasi boundary triplet technique. We also emphasize the recent papers [7, 11, 38, 43, 45, 46] where closely related techniques were used to study Dirac operators with δ-shell interactions.

The main objective of this small note is to provide boundary triplets for Dirac operators with Lorentz scalar interactions supported on a point in the one-dimensional case, and supported on curves and surfaces in the two- and three-dimensional situation. This operator is formally given by

$$A_\tau = A_0 + \tau \alpha_0 \delta_\Sigma,$$

where α_0 is a Dirac matrix defined in Section 3, and $\tau \alpha_0 \delta_\Sigma$ describes the Lorentz scalar δ-shell interaction supported on Σ. The one-dimensional setting with a single point interaction is particularly easy to treat and we discuss in Section 4 a possible choice of an ordinary boundary triplet, which was also used in [46]. We compute the corresponding γ-field and Weyl function, and give an expression for the resolvent of the singularly perturbed one-dimensional Dirac operator. In the multidimensional setting one observes typical analytic difficulties with trace maps and integration by parts formulas on maximal operator domains (similar as for the Laplacian or more general elliptic operators; cf. [14, 15]). It is convenient to extend the notion of ordinary boundary triplets in such a way that these analytic difficulties can be circumvented. As in the case of symmetric second order elliptic operators the concepts of quasi boundary triplets and generalized boundary triplets are useful and fit in this setting very well. In the present manuscript we allow some flexibility in the domain of the boundary maps and obtain a family of quasi boundary triplets that reduce to a generalized boundary triplet in the limit case, where the parameter describing regularity of the operator domain is minimal; cf. Theorem 5.3. As in the one-dimensional situation we provide the corresponding γ-fields and Weyl functions, we discuss the self-adjointness of the operator A_τ and list some of its spectral properties. An interesting issue in the multidimensional setting is the regularity of the support Σ of the Lorentz scalar δ-perturbation: From C^2-curves and hypersurfaces treated earlier in [2, 3, 6, 7, 10, 45] and piecewise C^2-curves studied in [47] we make a substantial step towards more rough supports, and discuss in Theorem 5.4 the case that Σ is the boundary of a bounded Lipschitz domain.

2. Ordinary, generalized, and quasi boundary triplets

In this section we briefly recall basic definitions of ordinary and generalized boundary triplets, quasi boundary triplets, and some related techniques in extension and spectral theory of symmetric and self-adjoint operators in Hilbert spaces. The concepts will be presented such that they can be applied directly to Dirac operators with singular interactions in the next sections. We refer the reader to [9, 14, 15, 20, 28, 29, 36] for more details on boundary triplet techniques.

Throughout this section $\mathcal{H}$ denotes a complex Hilbert space with inner product $(\cdot,\cdot)_\mathcal{H}$ and S is a densely defined closed symmetric operator with adjoint S^*.

Definition 2.1. Let T be a linear operator in $\mathcal{H}$ such that $\overline{T} = S^*$. A triplet $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ consisting of a Hilbert space $\mathcal{G}$ and linear mappings $\Gamma_0, \Gamma_1 : \operatorname{dom} T \to \mathcal{G}$ is called a *quasi boundary triplet* for S^* if the following holds:

(i) For all $f, g \in \operatorname{dom} T$ the abstract Green's identity
$$(Tf, g)_\mathcal{H} - (f, Tg)_\mathcal{H} = (\Gamma_1 f, \Gamma_0 g)_\mathcal{G} - (\Gamma_0 f, \Gamma_1 g)_\mathcal{G}$$
is true.

(ii) The range of $\Gamma = (\Gamma_0, \Gamma_1)^\top$ is dense in $\mathcal{G} \times \mathcal{G}$.

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

If (i) and (iii) hold, and the mapping $\Gamma_0 : \operatorname{dom} T \to \mathcal{G}$ is surjective, then $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ is called *generalized boundary triplet*; if (i) and (iii) hold, and the mapping $\Gamma = (\Gamma_0, \Gamma_1)^\top : \operatorname{dom} T \to \mathcal{G} \times \mathcal{G}$ is surjective, then $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ is called *ordinary boundary triplet.*

We remark that the above (non-standard) definition of generalized and ordinary boundary triplets is equivalent to the usual one given in, e.g., [9, 20, 28, 29, 36], see [14, Corollary 3.2 and Corollary 3.7]. In particular, if $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ is an ordinary boundary triplet, then $T = S^*$. Note that a quasi boundary triplet, generalized boundary triplet, or ordinary boundary triplet for S^* exists if and only if the defect numbers $\dim \ker (S^* \pm i)$ coincide, i.e. if and only if S admits self-adjoint extensions in $\mathcal{H}$. Moreover, the operator T in Definition 2.1 is in general not unique.

Next, we recall the definition of the γ-field and the Weyl function associated with the quasi boundary triplet $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$. These mappings will allow us to describe spectral properties of self-adjoint extensions of S. Let $A_0 = T \upharpoonright \ker \Gamma_0$. Then the direct sum decomposition

$$\operatorname{dom} T = \operatorname{dom} A_0 \dot{+} \ker (T - \lambda) = \ker \Gamma_0 \dot{+} \ker (T - \lambda), \qquad \lambda \in \rho(A_0), \tag{2.1}$$

holds. The definition of the γ-field and Weyl function for quasi boundary triplets is in accordance with the one for ordinary and generalized boundary triplets in [28, 29].

Definition 2.2. Assume that T is a linear operator in $\mathcal{H}$ satisfying $\overline{T} = S^*$ and let $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ be a quasi boundary triplet for S^*. Then the corresponding γ-field γ and Weyl function M are defined by

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

and

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

respectively.

From (2.1) we get that the γ-field is well defined and that $\operatorname{ran} \gamma(\lambda) = \ker (T - \lambda)$ holds for all $\lambda \in \rho(A_0)$. Moreover, $\operatorname{dom} \gamma(\lambda) = \operatorname{ran} \Gamma_0$ is dense in $\mathcal{G}$ by Definition 2.1. With the help of the abstract Green's identity in Definition 2.1 (i) one verifies that

$$\gamma(\lambda)^* = \Gamma_1 (A_0 - \overline{\lambda})^{-1}, \qquad \lambda \in \rho(A_0); \tag{2.2}$$

this is a bounded and everywhere defined operator from $\mathcal{H}$ to $\mathcal{G}$. Therefore, $\gamma(\lambda)$ is a (in general not everywhere defined) bounded operator; cf. [14, Proposition 2.6] or [15, Proposition 6.13]. If $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ is a generalized or ordinary boundary triplet, then $\gamma(\lambda)$ is automatically bounded and everywhere defined.

Next, we state some useful properties of the Weyl function M corresponding to the quasi boundary triplet $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$; see, e.g, [14, Proposition 2.6] for proofs of these statements. For any $\lambda \in \rho(A_0)$ the operator $M(\lambda)$ is densely defined in $\mathcal{G}$ with $\operatorname{dom} M(\lambda) = \operatorname{ran} \Gamma_0$ and $\operatorname{ran} M(\lambda) \subset \operatorname{ran} \Gamma_1$. Next, for all $\lambda, \mu \in \rho(A_0)$ and $\varphi \in \operatorname{ran} \Gamma_0$ one has

$$M(\lambda)\varphi - M(\mu)^*\varphi = (\lambda - \overline{\mu})\gamma(\mu)^*\gamma(\lambda)\varphi. \tag{2.3}$$

Therefore, we see that $M(\lambda) \subset M(\overline{\lambda})^*$ for any $\lambda \in \rho(A_0)$ and hence $M(\lambda)$ is a closable, but in general unbounded linear operator in $\mathcal{G}$. If $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ is a generalized or ordinary boundary triplet, then $M(\lambda)$ is bounded and everywhere defined.

In the main part of the paper we are going to use ordinary boundary triplets, generalized boundary triplets, quasi boundary triplets, and their Weyl functions to define and study self-adjoint extensions of the underlying symmetry S. Let again T be a linear operator in $\mathcal{H}$ such that $\overline{T} = S^*$, let $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ be a quasi boundary triplet for S^*, and let ϑ be a linear operator in $\mathcal{G}$. Then we define the extension A_ϑ of S by

$$A_\vartheta = T \upharpoonright \ker (\Gamma_1 - \vartheta \Gamma_0), \tag{2.4}$$

i.e. $f \in \operatorname{dom} T$ belongs to $\operatorname{dom} A_\vartheta$ if and only if f satisfies $\Gamma_1 f = \vartheta \Gamma_0 f$. If ϑ is a symmetric operator in $\mathcal{G}$, then Green's identity implies

$$(A_\vartheta f, g)_\mathcal{H} - (f, A_\vartheta g)_\mathcal{H} = (\vartheta \Gamma_0 f, \Gamma_0 g)_\mathcal{G} - (\Gamma_0 f, \vartheta \Gamma_0 g)_\mathcal{G} = 0 \tag{2.5}$$

for all $f, g \in \operatorname{dom} A_\vartheta$ and hence the extension A_ϑ is symmetric in $\mathcal{H}$.

Of course, one is mostly interested in the self-adjointness of A_ϑ. If $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ is an ordinary boundary triplet, then the situation is simple: Here one has a one-to-one correspondence between self-adjoint realizations A_ϑ as in (2.4) and self-adjoint operators and relations ϑ in $\mathcal{G}$. In particular, if ϑ is a self-adjoint operator in $\mathcal{G}$, then A_ϑ is self-adjoint in $\mathcal{H}$, see, e.g. [9, Theorem 2.1.3] for more details.

If $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ is a generalized or a quasi boundary triplet, then the self-adjointness of ϑ does, in general, not imply the self-adjointness of A_ϑ, or vice versa. However, the following theorem, where we also state an abstract version of the Birman-Schwinger principle and a Krein type resolvent formula for canonical extensions A_ϑ, will allow us to give conditions for the self-adjointness of A_ϑ; for the proof we refer to [14, Theorem 2.8] or [15, Theorem 6.16].

Theorem 2.3. *Let T be a linear operator in $\mathcal{H}$ satisfying $\overline{T} = S^*$, let $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ be a quasi boundary triplet for S^* with $A_0 = T \upharpoonright \ker \Gamma_0$, and denote the associated γ-field and Weyl function by γ and M, respectively. Let A_ϑ be the extension of S associated with an operator ϑ in $\mathcal{G}$ as in* (2.4)*. Then the following holds for all $\lambda \in \rho(A_0)$:*

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

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

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

(iii) *If* $\lambda \notin \sigma_\mathrm{p}(A_\vartheta)$*, then*

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

holds for all $g \in \operatorname{ran}(A_\vartheta - \lambda)$*.*

Assertion (ii) of the previous theorem shows how the self-adjointness of an extension A_ϑ can be proven, if $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ is a generalized or a quasi boundary triplet. If ϑ is symmetric in $\mathcal{G}$, then A_ϑ is symmetric in $\mathcal{H}$ by (2.5), and hence A_ϑ is self-adjoint if, in addition, $\operatorname{ran}(A_\vartheta \mp i) = \mathcal{H}$. According to Theorem 2.3 (ii) the latter is the case, if $\operatorname{ran} \gamma(\mp i)^* \subset \operatorname{ran}(\vartheta - M(\pm i))$.

3. Some facts about Dirac operators

In this section, a brief introduction to Dirac operators will be presented. These operators correspond to the right-hand side of the Dirac equation. The free Dirac equation was derived by P. Dirac when linearising the relativistic energy-momentum relationship of the energy E and the momentum $p = (p_1, \dots, p_d)$ given by

$$E^2 = \sum_{j=1}^d p_j^2 + m^2.$$

Here and in the subsequent sections, d is the space dimension and $m > 0$ is the mass of the particle. Furthermore, the speed of light c and Planck's constant $\hbar$ are set to one for simplicity. This can always be realised by a suitable choice of units. The usual linearisation approach, as it is carried out for instance in [53], corresponds to

$$\left(E - \sum_{j=1}^{d} \alpha_j p_j - m\alpha_0\right)\left(E + \sum_{j=1}^{d} \alpha_j p_j + m\alpha_0\right) = 0 \tag{3.1}$$

with matrices $\alpha_j \in \mathbb{C}^{N\times N}$, where $N = 2^{[(d+1)/2]}$ and $[\cdot]$ is the Gauss bracket. For the cases relevant to us we have $N = 2$ for $d \in \{1,2\}$ and $N = 4$ for $d = 3$. A comparison with the energy-momentum relationship above shows that the matrices α_j must be chosen such that they satisfy the anti-commutation relations

$$\alpha_k\alpha_j + \alpha_j\alpha_k = 2\delta_{kj} I_N \quad \text{for all} \quad k, j \in \{0, 1, \dots, d\}, \tag{3.2}$$

where I_n denotes the $n \times n$-identity matrix. For $d \in \{1,2\}$ the matrices α_j can be chosen as the Pauli spin matrices

$$\alpha_1 = \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \alpha_2 = \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \text{and } \alpha_0 = \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

and for $d = 3$ as the so-called Dirac matrices

$$\alpha_j = \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix} \quad \text{and} \quad \alpha_0 = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}.$$

If one now applies the usual substitution rules $i\frac{\partial}{\partial t}$ and $-i\frac{\partial}{\partial x_j}$ for E and p_j in one of the factors in (3.1), one obtains the free Dirac equation

$$i\frac{\partial}{\partial t}\Psi = \left(-i\sum_{j=1}^{d} \alpha_j \frac{\partial}{\partial x_j} + m\alpha_0\right)\Psi,$$

which describes a particle with spin 1/2, such as an electron, that moves in $\mathbb{R}^d$. Here and in the following we use for $x = (x_1, \dots, x_d) \in \mathbb{R}^d$ the notation

$$\alpha \cdot x := \sum_{j=1}^{d} \alpha_j x_j \quad \text{and} \quad \alpha \cdot \nabla := \sum_{j=1}^{d} \alpha_j \frac{\partial}{\partial x_j}.$$

As in the case of the Schrödinger equation, one now defines the free Dirac operator as the right-hand side of the free Dirac equation by

$$A_0 f = (-i\alpha \cdot \nabla + m\alpha_0) f, \qquad \operatorname{dom} A_0 = H^1(\mathbb{R}^d; \mathbb{C}^N). \tag{3.3}$$

With the help of the Fourier transform it is not difficult to verify that A_0 is self-adjoint in $L^2(\mathbb{R}^d; \mathbb{C}^N)$ with purely essential spectrum

$$\sigma(A_0) = (-\infty, -m] \cup [m, \infty); \tag{3.4}$$

cf. [53] or [54]. From a physical point of view there are possible energy states of the system that are negative and these energies are not bounded from below. This led to the discovery of anti-particles, as, e.g., in the case of the electron, the positron.

To derive an explicit representation of the resolvent $(A_0 - \lambda)^{-1}$ for $\lambda \in \rho(A_0)$, one uses that (3.2) implies the relation

$$(A_0 - \lambda)(A_0 + \lambda) = \left(-\Delta + m^2 - \lambda^2\right) I_N,$$

where $-\Delta$ is the free Laplace operator defined on $\operatorname{dom}(-\Delta) = H^2(\mathbb{R}^d)$. This implies

$$(A_0 - \lambda)^{-1} = \big(-i\alpha \cdot \nabla + m\alpha_0 + \lambda I_N\big)(-\Delta + m^2 - \lambda^2)^{-1} I_N. \tag{3.5}$$

Using the well-known form of the resolvent of $-\Delta$, one finds that $(A_0-\lambda)^{-1}$ is an integral operator in $L^2(\mathbb{R}^d;\mathbb{C}^N)$. In order to describe the integral kernel $G_{\lambda,d}(x-y)$, we write K_j for the modified Bessel functions of the second kind and

$$k(\lambda)=\sqrt{\lambda^2-m^2} \quad \text{and } \zeta=\frac{\lambda+m}{k(\lambda)}=\frac{\lambda+m}{\sqrt{\lambda^2-m^2}}; \tag{3.6}$$

here $\sqrt{z}$ is chosen for $z\in\mathbb{C}\setminus[0,\infty)$ such that $\operatorname{Im}\sqrt{z}>0$. For $d\in\{1,2,3\}$ the integral kernel $G_{\lambda,d}$ is explicitly given by

$$\begin{aligned} G_{\lambda,1}(x)&=\frac{i}{2}e^{ik(\lambda)|x|}\begin{pmatrix}\zeta & \operatorname{sgn}(x)\\ \operatorname{sgn}(x) & \zeta^{-1}\end{pmatrix},\\ G_{\lambda,2}(x)&=\frac{k(\lambda)}{2\pi}K_1\big(-ik(\lambda)|x|\big)\frac{\sigma\cdot x}{|x|}+\frac{1}{2\pi}K_0\big(-ik(\lambda)|x|\big)\big(\lambda I_2+m\sigma_3\big),\\ G_{\lambda,3}(x)&=\left(\lambda I_4+m\alpha_0+(1-ik(\lambda)|x|)\frac{i(\alpha\cdot x)}{|x|^2}\right)\frac{1}{4\pi|x|}e^{ik(\lambda)|x|}; \end{aligned} \tag{3.7}$$

cf. [1, 13, 53, 54].

Next, external potential fields are to be considered in which the particle moves. Since we are studying relativistic effects, these potentials must be invariant under Lorentz transformations. For a given scalar potential Φ_s the quantity $V=\Phi_s\alpha_0$ is Lorentz invariant as shown in [53]. This motivates the following formal ansatz for the Dirac operator of a relativistic quantum particle with spin 1/2 moving in an external field consisting of a scalar potential Φ_s:

$$A=A_0+\Phi_s\alpha_0.$$

Of particular interest are strongly localized fields which only have an effect in a small neighbourhood of a set $\Sigma\subset\mathbb{R}^d$ with measure 0. An example for a field of this kind is the quark confinement inside a nucleon in form of the MIT bag model. To describe these strongly localized fields it is often a useful simplification to replace them by δ-potentials which are supported on Σ. In the following we consider a Lorentz scalar potential which is strongly localized in a neighbourhood of the hypersurface $\Sigma\subset\mathbb{R}^d$ and approximate it by a δ-potential supported on Σ. Applying the formal ansatz above for the Dirac operator yields the formal expression

$$A_\tau=A_0+\tau\alpha_0\delta_\Sigma \tag{3.8}$$

with interaction strength $\tau\in\mathbb{R}$. In the following sections, this operator will be defined in a mathematically rigorous way and its properties will be studied. Recall from (3.4) that the free Dirac operator A_0 is not bounded from below and hence the usual form approach to construct self-adjoint realizations with singular perturbations is not applicable.

4. One-dimensional Dirac operators with Lorentz scalar δ-point interactions

In this section, one-dimensional Dirac operators with Lorentz scalar δ-interactions supported on $\Sigma=\{0\}$ will be investigated. The following results are well known, see for instance [46], but are presented here for the sake of completeness. In particular, the methods used and the results obtained in the discussion will serve as a motivation for the analysis of two- and three-dimensional Dirac operators in the following section.

As already mentioned in the previous section, it is well known that the free Dirac operator

$$A_0 f = -i\sigma_1 \frac{\mathrm{d}}{\mathrm{d}x} f + m\sigma_3 f, \qquad \operatorname{dom} A_0 = H^1\left(\mathbb{R};\mathbb{C}^2\right),$$

is self-adjoint in the Hilbert space $L^2(\mathbb{R},\mathbb{C}^2)$. In accordance with (3.8), Lorentz scalar δ-interactions shall now be considered, which are represented by the formal expression

$$A_\tau = A_0 + \tau\sigma_3\delta_\Sigma. \tag{4.1}$$

Here $\tau \in \mathbb{R}$ corresponds to the constant interaction strength. Following the usual construction of self-adjoint realizations of the expression above as in [1], one first defines the symmetric operator

$$\begin{aligned} Sf &:= \left(-i\sigma_1 \frac{\mathrm{d}}{\mathrm{d}x} f_+ + m\sigma_3 f_+\right) \oplus \left(-i\sigma_1 \frac{\mathrm{d}}{\mathrm{d}x} f_- + m\sigma_3 f_-\right), \\ \operatorname{dom} S &:= H_0^1\left((0,\infty);\mathbb{C}^2\right) \oplus H_0^1((-\infty,0);\mathbb{C}^2). \end{aligned}$$

Here the orthogonal decomposition $L^2(\mathbb{R};\mathbb{C}^2) = L^2((0,\infty);\mathbb{C}^2) \oplus L^2((-\infty,0);\mathbb{C}^2)$, as well as the notation $f = f_+ \oplus f_-$ for a function $f \in L^2(\mathbb{R};\mathbb{C}^2)$ is used. It can be shown that the adjoint operator S^* acts in the same way as S, but has the larger domain $\operatorname{dom} S^* = H^1((0,\infty);\mathbb{C}^2) \oplus H^1((-\infty,0);\mathbb{C}^2)$. In the next step, self-adjoint extensions of S are defined by restricting S^* to a suitable domain of definition. This domain is characterised by imposing certain coupling conditions on $\Sigma = \{0\}$, which are found by a formal integration of the expression (4.1). In the present case the coupling conditions have the form

$$\begin{aligned} i\left(f_2(0+) - f_2(0-)\right) &= \frac{\tau}{2}\left(f_1(0+) + f_1(0-)\right), \\ i\left(f_1(0+) - f_1(0-)\right) &= -\frac{\tau}{2}\left(f_2(0+) + f_2(0-)\right). \end{aligned} \tag{4.2}$$

Next, we define the two linear mappings $\Gamma_0, \Gamma_1 : \operatorname{dom} S^* \to \mathbb{C}^2$ by the assignments

$$\Gamma_0 f = -i\begin{pmatrix} f_2(0+) - f_2(0-) \\ f_1(0+) - f_1(0-)\end{pmatrix} \quad \text{and} \quad \Gamma_1 f = \frac{1}{2}\begin{pmatrix} f_1(0+) + f_1(0-) \\ f_2(0+) + f_2(0-)\end{pmatrix}. \tag{4.3}$$

Using these boundary maps one obtains the equivalent representation

$$\Gamma_0 f + \tau\sigma_3\Gamma_1 f = 0, \qquad f \in \operatorname{dom} S^*,$$

of the above coupling conditions.

Proposition 4.1. *The triplet $\{\mathbb{C}^2, \Gamma_0, \Gamma_1\}$ is an ordinary boundary triplet for S^*.*

Proof. Integration by parts and a straightforward computation shows that the abstract Green's identity in Definition 2.1 is valid. If one defines the function

$$f(x) = \frac{i}{2}\begin{pmatrix} c_2 \\ c_1 \end{pmatrix} \operatorname{sgn}(x) e^{-|x|} + \begin{pmatrix} c_3 \\ c_4 \end{pmatrix} e^{-|x|}, \quad x \in \mathbb{R},$$

for a given vector $(c_1, c_2, c_3, c_4) \in \mathbb{C}^4$, then $f \in \operatorname{dom} S^*$ and the surjectivity of the mapping $(\Gamma_0, \Gamma_1)^\top : \operatorname{dom} S^* \to \mathbb{C}^4$ follows. This shows (ii) in Definition 2.1. Finally, to show that Definition 2.1 (iii) holds, notice that the restriction $A_0 = S^* \upharpoonright \ker \Gamma_0$ corresponds to the free Dirac operator. □

Using the ordinary boundary triplet from Proposition 4.1, one can now define the operator

$$A_\tau = S^* \upharpoonright \ker(\Gamma_0 + \tau\sigma_3\Gamma_1),$$

which is interpreted as the realisation of the formal expression (4.1) on the basis of the coupling conditions (4.2). Due to $\tau \in \mathbb{R}$ it follows immediately that A_τ is a self-adjoint operator in $L^2(\mathbb{R};\mathbb{C}^2)$; see the discussion before Theorem 2.3. Note that in this case ϑ^{-1} corresponds to $-\tau\sigma_3$, which is self-adjoint.

Next, we derive an explicit resolvent representation of A_τ and characterise its spectrum. For this purpose, the first step is to determine the γ-field and the Weyl function of the ordinary boundary triplet from Proposition 4.1. To simplify the presentation, we first define the two functions

$$f_1(x) = \frac{i}{2}\begin{pmatrix} \zeta \\ \operatorname{sgn}(x) \end{pmatrix} e^{ik(\lambda)|x|} \quad \text{and } f_2(x) = \frac{i}{2}\begin{pmatrix} \operatorname{sgn}(x) \\ \zeta^{-1} \end{pmatrix} e^{ik(\lambda)|x|}$$

with $k(\lambda)$ and ζ defined as in (3.6). Note that these functions form a basis of $\ker(S^* - \lambda)$ for all $\lambda \in \rho(A_0)$ and are mapped to the basis vectors $(1,0)$ and $(0,1)$ of $\mathbb{C}^2$ by Γ_0. A simple computation now shows that the γ-field is given by

$$\left[\gamma(\lambda)\begin{pmatrix} \xi_1 \\ \xi_2 \end{pmatrix}\right](x) = \xi_1 f_1(x) + \xi_2 f_2(x) = \frac{i}{2} e^{ik(\lambda)|x|}\begin{pmatrix} \zeta & \operatorname{sgn}(x) \\ \operatorname{sgn}(x) & \zeta^{-1} \end{pmatrix}\begin{pmatrix} \xi_1 \\ \xi_2 \end{pmatrix}$$

for $(\xi_1, \xi_2) \in \mathbb{C}^2$ and $x \in \mathbb{R}$, while the Weyl function corresponds to the matrix

$$M(\lambda) = \frac{i}{2}\begin{pmatrix} \zeta & 0 \\ 0 & \zeta^{-1} \end{pmatrix}.$$

Note that the x-dependent part in the representation of the γ-field corresponds to the Green's function of the free Dirac operator. This will remain valid also in the multidimensional considerations in the next sections. Using the above representations of the γ-field and the Weyl function the next result follows from Theorem 2.3.

Proposition 4.2. *For all $\lambda \in \rho(A_\tau) \cap \rho(A_0)$ and $f \in L^2(\mathbb{R};\mathbb{C}^2)$ the resolvent formula*

$$\begin{aligned}(A_\tau - \lambda)^{-1} f(x) &= (A_0 - \lambda)^{-1} f(x) \\ &+ \frac{\tau}{2\,(2 + i\tau\zeta)}\left(\begin{pmatrix} \zeta \\ -\operatorname{sgn}(\cdot) \end{pmatrix} e^{ik(\lambda)|\cdot|}, \overline{f}\right)_{L^2(\mathbb{R};\mathbb{C}^2)} \begin{pmatrix} \zeta \\ \operatorname{sgn}(x) \end{pmatrix} e^{ik(\lambda)|x|} \\ &- \frac{\tau\zeta}{2\,(2\zeta - i\tau)}\left(\begin{pmatrix} -\operatorname{sgn}(\cdot) \\ \zeta^{-1} \end{pmatrix} e^{ik(\lambda)|\cdot|}, \overline{f}\right)_{L^2(\mathbb{R};\mathbb{C}^2)} \begin{pmatrix} \operatorname{sgn}(x) \\ \zeta^{-1} \end{pmatrix} e^{ik(\lambda)|x|}\end{aligned}$$

is valid for all $x \in \mathbb{R}$. Furthermore, the spectrum of A_τ is given by

$$\sigma_{\mathrm{ess}}(A_\tau) = (-\infty, -m] \cup [m, \infty)$$

$$\sigma_{\mathrm{disc}}(A_\tau) = \begin{cases} \emptyset & , \text{ if } \tau \geq 0 \\ \left\{\pm m\frac{4-\tau^2}{4+\tau^2}\right\} & , \text{ if } \tau < 0. \end{cases}$$

Proof. From Theorem 2.3 (iii) the representation

$$(A_\tau - \lambda)^{-1} f = (A_0 - \lambda)^{-1} f - \gamma(\lambda)\tau\sigma_3(I + \tau M(\lambda)\sigma_3)^{-1}\gamma(\overline{\lambda})^* f$$

follows for all $\lambda \in \rho(A_\tau) \cap \rho(A_0)$. After a simple calculation using the above expressions for the γ-field and the Weyl function one obtains the claimed resolvent representation for all $f \in L^2(\mathbb{R};\mathbb{C}^2)$. The statement about the essential spectrum follows from the fact that both A_τ and A_0 are self-adjoint extensions of the operator S, which has the finite defect indices $(2,2)$. It remains to show the claim about the discrete spectrum. Notice first that $\sigma_{\mathrm{disc}}(A_\tau) \subseteq (-m,m) \subseteq \rho(A_0)$. Thus, it follows from Theorem 2.3 (i) that $\lambda \in \sigma_{\mathrm{disc}}(A_\tau)$ if and only if $0 \in \sigma(I + \tau M(\lambda)\sigma_3)$. The eigenvalues of this matrix can be determined quite elementarily and one obtains the defining equations

$$2 + i\tau\zeta = 0 \quad \text{or} \quad 2\zeta - i\tau = 0.$$

Due to the choice of the complex square root in the definitions of ζ and $k(\lambda)$ it follows in the case that the first equation is valid that an eigenvalue exists if and only if $\tau < 0$. This eigenvalue is then given by $\lambda_1 = m(4-\tau^2)/(4+\tau^2)$. If the second equation holds, then a similar reasoning yields the eigenvalue $\lambda_2 = -\lambda_1$. $\square$

5. Boundary triplets for two- and three-dimensional Dirac operators with singular interactions

In this section we use similar boundary mappings as in Section 4 to construct boundary triplets for Dirac operators with δ-shell interactions in $\mathbb{R}^2$ and $\mathbb{R}^3$. However, by translating the boundary mappings in (4.3) directly to the higher dimensional setting one obtains a generalized or quasi boundary triplet instead of an ordinary boundary triplet. Before we can introduce the boundary triplets, some preliminaries related to function spaces and trace theorems are needed. For smooth surfaces similar boundary triplets and Sobolev spaces were used in [6, 7, 10, 38] and [13, 18, 45], respectively; it is one of the main goals in this note to extend these constructions to closed Lipschitz smooth hypersurfaces. As an application we prove that Dirac operators with Lorentz scalar δ-shell interactions supported on general compact Lipschitz hypersurfaces are self-adjoint.

5.1. **Sobolev spaces for Dirac operators and related trace theorems.** As in Section 3 the space dimension is denoted by $d \in \{2,3\}$ and $N := 2^{[(d+1)/2]}$, where $[\cdot]$ is the Gauss bracket. Consequently, we have $N = 2$ for $d = 2$ and $N = 4$ for $d = 3$. Let $\alpha_0, \dots, \alpha_d$ be the $d+1$ anti-commuting $\mathbb{C}^{N\times N}$-valued Dirac matrices defined in Section 3.

Throughout this subsection let $\Omega \subset \mathbb{R}^d$ be a bounded or unbounded Lipschitz domain with compact boundary and denote by ν the unit normal vector field at $\partial\Omega$. For $s \in [0,1]$ we define the space

$$H^s_\alpha(\Omega;\mathbb{C}^N) := \big\{ f \in H^s(\Omega;\mathbb{C}^N) : (\alpha\cdot\nabla) f \in L^2(\Omega;\mathbb{C}^N) \big\},$$

where the derivatives are understood in the distributional sense and $H^s(\Omega;\mathbb{C}^N)$ is the standard L^2-based Sobolev space of order s of $\mathbb{C}^N$-valued functions, and endow it with the norm

$$\|f\|^2_{H^s_\alpha(\Omega;\mathbb{C}^N)} := \|f\|^2_{H^s(\Omega;\mathbb{C}^N)} + \|(\alpha\cdot\nabla) f\|^2_{L^2(\Omega;\mathbb{C}^N)}.$$

One can show with standard techniques that $H^s_\alpha(\Omega;\mathbb{C}^N)$ is a Hilbert space and that $C_0^\infty(\overline{\Omega};\mathbb{C}^N)$ is dense in $H^s_\alpha(\Omega;\mathbb{C}^N)$; cf. [18, Lemma 2.1], [10, Lemma 3.2], or [45, Proposition 2.12] for similar arguments. Moreover, with the help of the Fourier transform it is not difficult to see that $H^s_\alpha(\mathbb{R}^d;\mathbb{C}^N) = H^1(\mathbb{R}^d;\mathbb{C}^N)$ for any $s \in [0,1]$. In the following lemma we state a trace theorem for $H^s_\alpha(\Omega;\mathbb{C}^N)$ for $s \geq \frac{1}{2}$.

Lemma 5.1. *For $s \in [\frac{1}{2}, 1]$ the map $C_0^\infty(\overline{\Omega}; \mathbb{C}^N) \ni f \mapsto f|_{\partial\Omega}$ extends to a unique continuous operator $\gamma_D : H_\alpha^s(\Omega; \mathbb{C}^N) \to H^{s-1/2}(\partial\Omega; \mathbb{C}^N)$.*

Proof. For $s \in (\frac{1}{2}, 1]$ the claim follows from the classical trace theorem [44, Theorem 3.38], as $H_\alpha^s(\Omega; \mathbb{C}^N)$ is continuously embedded in $H^s(\Omega; \mathbb{C}^N)$. For $s = \frac{1}{2}$ we consider for $s_1, s_2 \in \mathbb{R}$ the Hilbert space

$$H_\Delta^{s_1,s_2}(\Omega; \mathbb{C}^N) := \big\{ f \in H^{s_1}(\Omega; \mathbb{C}^N) : -\Delta f \in H^{s_2}(\Omega; \mathbb{C}^N) \big\} \tag{5.1}$$

endowed with the norm

$$\|f\|^2_{H_\Delta^{s_1,s_2}(\Omega;\mathbb{C}^N)} := \|f\|^2_{H^{s_1}(\Omega;\mathbb{C}^N)} + \|\Delta f\|^2_{H^{s_2}(\Omega;\mathbb{C}^N)}.$$

It follows from [34, Lemma 3.1] that there exists a continuous trace map from $H_\Delta^{1/2,-1}(\Omega)$ to $L^2(\partial\Omega)$. Since (3.2) implies $(\alpha \cdot \nabla)^2 = -\Delta$ in the distributional sense, $H_\alpha^{1/2}(\Omega; \mathbb{C}^N)$ is continuously embedded in $H_\Delta^{1/2,-1}(\Omega; \mathbb{C}^N)$. This yields the claim also for $s = \frac{1}{2}$. □

Using Lemma 5.1 and the fact that $C_0^\infty(\overline{\Omega}; \mathbb{C}^N)$ is dense in $H_\alpha^s(\Omega; \mathbb{C}^N)$ one can show for all $f, g \in H_\alpha^s(\Omega; \mathbb{C}^N)$, $s \in [\frac{1}{2}, 1]$, the following integration by parts formula:

$$\int_\Omega i(\alpha \cdot \nabla) f \cdot \overline{g} dx = \int_{\partial\Omega} i(\alpha \cdot \nu) f \cdot \overline{g} d\sigma + \int_\Omega f \cdot \overline{i(\alpha \cdot \nabla) g} dx. \tag{5.2}$$

In the construction of boundary triplets for Dirac operators with singular interactions some families of integral operators related to the fundamental solution $G_{\lambda,d}$ given in (3.7) are required. Let $\Sigma \subset \mathbb{R}^d$ be a closed bounded Lipschitz hypersurface and let Ω_+ be the bounded Lipschitz domain with $\partial\Omega_+ = \Sigma$, let ν be the unit normal vector field at Σ pointing outwards of Ω_+, and let $\Omega_- := \mathbb{R}^d \setminus \overline{\Omega_+}$. We introduce for $\lambda \notin (-\infty, -m] \cup [m, \infty)$ the potential operator $\Phi_\lambda : L^2(\Sigma; \mathbb{C}^N) \to L^2(\mathbb{R}^d; \mathbb{C}^N)$ by

$$\Phi_\lambda \varphi(x) := \int_\Sigma G_{\lambda,d}(x - y) \varphi(y) \mathrm{d}\sigma(y), \quad \varphi \in L^2(\Sigma; \mathbb{C}^N),\ x \in \mathbb{R}^d \setminus \Sigma, \tag{5.3}$$

and the strongly singular boundary integral operator $\mathcal{C}_\lambda : L^2(\Sigma; \mathbb{C}^N) \to L^2(\Sigma; \mathbb{C}^N)$ acting as

$$\mathcal{C}_\lambda \varphi(x) := \lim_{\varepsilon \searrow 0} \int_{\Sigma \setminus B(x,\varepsilon)} G_{\lambda,d}(x - y) \varphi(y) \mathrm{d}\sigma(y), \quad \varphi \in L^2(\Sigma; \mathbb{C}^N),\ x \in \Sigma, \tag{5.4}$$

where $B(x, \varepsilon)$ is the ball of radius ε centered at x. Both operators Φ_λ and $\mathcal{C}_\lambda$ are well defined and bounded, see [2, Lemma 3.3] and the references there. Moreover, for $\lambda \in (-m, m)$ the operator $\mathcal{C}_\lambda$ is self-adjoint in $L^2(\Sigma; \mathbb{C}^N)$. In the next lemma we improve the mapping properties for Φ_λ.

Lemma 5.2. *For any $\lambda \in \rho(A_0)$ the operator Φ_λ gives rise to a bounded map*

$$\Phi_\lambda : L^2(\Sigma; \mathbb{C}^N) \to H_\alpha^{1/2}(\mathbb{R}^d \setminus \Sigma; \mathbb{C}^N).$$

Proof. Let $\mathrm{SL}(\mu) = (-\Delta - \mu)^{-1} \gamma_D'$ be the single layer potential for $-\Delta - \mu$, where γ_D' is the dual of the Dirichlet trace operator. Using that (3.2) implies $(\alpha \cdot \nabla)^2 = \Delta$ in the distributional sense one gets

$$\Phi_\lambda = \big(- i\alpha \cdot \nabla + m\alpha_0 + \lambda I_N \big) \mathrm{SL}(\lambda^2 - m^2) I_N,$$

see also (3.5). Since $\mathrm{SL}(\lambda^2 - m^2) : L^2(\Sigma) \to H^{3/2,0}_\Delta(\mathbb{R}^d \setminus \Sigma)$ is bounded, where $H^{3/2,0}_\Delta(\mathbb{R}^d \setminus \Sigma)$ is defined by (5.1) (this follows, e.g., from [33, Equation (2.127)]), the claimed result follows. □

Finally, we note that for $\varphi \in L^2(\Sigma; \mathbb{C}^N)$ the trace of $\Phi_\lambda \varphi$, which is well defined by Lemmas 5.1 and 5.2, is given by

$$\gamma_D^\pm \Phi_\lambda \varphi = \mp \frac{i}{2}(\alpha \cdot \nu)\varphi + \mathcal{C}_\lambda \varphi, \tag{5.5}$$

where $\gamma_D^\pm$ denotes the trace operator for $\Omega_\pm$; this can be shown in the same way as in [2, Lemma 3.3] or [13, Proposition 3.4].

5.2. **Quasi boundary triplets and generalized boundary triplets for Dirac operators with singular interactions.** In this subsection we follow ideas from Section 4 and introduce a family of quasi boundary triplets for Dirac operators; similar constructions can also be found in [6, 10]. Let $\Omega_+ \subset \mathbb{R}^d$ be a bounded Lipschitz domain, set $\Omega_- := \mathbb{R}^d \setminus \overline{\Omega_+}$ and $\Sigma := \partial\Omega_+ = \partial\Omega_-$. We denote by ν the unit normal vector field at Σ that is pointing outwards of Ω_+. In the following we will often denote the restriction of a function f defined on $\mathbb{R}^d$ onto $\Omega_\pm$ by $f_\pm$.

We introduce for $s \in [0,1]$ the operators $T^{(s)}$ in $L^2(\mathbb{R}^d; \mathbb{C}^N)$ by

$$\begin{aligned} T^{(s)} f &:= (-i(\alpha \cdot \nabla) + m\alpha_0) f_+ \oplus (-i(\alpha \cdot \nabla) + m\alpha_0) f_-, \\ \operatorname{dom} T^{(s)} &:= H^s_\alpha(\Omega_+; \mathbb{C}^N) \oplus H^s_\alpha(\Omega_-; \mathbb{C}^N), \end{aligned}$$

and $S := T^{(s)} \upharpoonright H^1_0(\mathbb{R}^d \setminus \Sigma; \mathbb{C}^N)$, which is given more explicitly by

$$Sf = (-i(\alpha \cdot \nabla) + m\alpha_0) f, \qquad \operatorname{dom} S = H^1_0(\mathbb{R}^d \setminus \Sigma; \mathbb{C}^N).$$

The operator S is densely defined, closed, and symmetric. Using standard arguments and distributional derivatives one verifies that

$$S^* = T^{(0)} \qquad \text{and} \qquad (T^{(0)})^* = S.$$

Next, we introduce for $s \in [\frac{1}{2}, 1]$ the mappings $\Gamma_0^{(s)}, \Gamma_1^{(s)} : \operatorname{dom} T^{(s)} \to L^2(\Sigma; \mathbb{C}^N)$ by

$$\Gamma_0^{(s)} f := i(\alpha \cdot \nu)(f_+|_\Sigma - f_-|_\Sigma) \quad \text{and} \quad \Gamma_1^{(s)} f := \frac{1}{2}(f_+|_\Sigma + f_-|_\Sigma), \tag{5.6}$$

and note that $\Gamma_0^{(s)}$ and $\Gamma_1^{(s)}$ are well defined due to Lemma 5.1. In order to characterize the range of $\Gamma_0^{(s)}$, we introduce the space

$$H^s_\alpha(\Sigma; \mathbb{C}^N) := \big\{ \varphi \in L^2(\Sigma; \mathbb{C}^N) : (\alpha \cdot \nu)\varphi \in H^s(\Sigma; \mathbb{C}^N) \big\},$$

where $H^s(\Sigma; \mathbb{C}^N)$ denotes the standard Sobolev space on Σ of $\mathbb{C}^N$-valued functions. If Σ is $C^{1,s+\varepsilon}$-smooth for some $\varepsilon > 0$, then $H^s_\alpha(\Sigma; \mathbb{C}^N) = H^s(\Sigma; \mathbb{C}^N)$, cf. [12, Lemma A.2]. In the following theorem we show that the mappings $\Gamma_0^{(s)}$ and $\Gamma_1^{(s)}$ in (5.6) give rise to a quasi boundary triplet for S^* and we compute the associated γ-field and Weyl function. Recall that A_0 is the free Dirac operator defined in (3.3) and that Φ_λ and $\mathcal{C}_\lambda$ are the mappings introduced in (5.3) and (5.4), respectively.

Theorem 5.3. *Let $s \in [\frac{1}{2}, 1]$. Then the following holds:*

(i) *The triplet* $\{L^2(\Sigma;\mathbb{C}^N),\Gamma_0^{(s)},\Gamma_1^{(s)}\}$ *is a quasi boundary triplet for* $S^*=\overline{T^{(s)}}$ *with* $T^{(s)}\upharpoonright\ker\Gamma_0^{(s)}=A_0$*, and one has*

$$\operatorname{ran}\Gamma_0^{(s)}=H_\alpha^{s-1/2}(\Sigma;\mathbb{C}^N). \tag{5.7}$$

In particular, $\{L^2(\Sigma;\mathbb{C}^N),\Gamma_0^{(1/2)},\Gamma_1^{(1/2)}\}$ *is a generalized boundary triplet.*

(ii) *For* $\lambda\in\rho(A_0)=\mathbb{C}\setminus((-\infty,-m]\cup[m,\infty))$ *the values* $\gamma^{(s)}(\lambda)$ *of the* γ*-field are given by*

$$\gamma^{(s)}(\lambda)=\Phi_\lambda\upharpoonright H_\alpha^{s-1/2}(\Sigma;\mathbb{C}^N).$$

Each $\gamma^{(s)}(\lambda)$ *is a densely defined bounded operator from the Hilbert space* $L^2(\Sigma;\mathbb{C}^N)$ *to* $L^2(\mathbb{R}^d;\mathbb{C}^N)$ *and an everywhere defined bounded operator from* $H_\alpha^{s-1/2}(\Sigma;\mathbb{C}^N)$ *to* $H_\alpha^s(\mathbb{R}^d\setminus\Sigma;\mathbb{C}^N)$*. Moreover,*

$$\gamma^{(s)}(\lambda)^*:L^2(\mathbb{R}^d;\mathbb{C}^N)\to L^2(\Sigma;\mathbb{C}^N)$$

is compact.

(iii) *For* $\lambda\in\rho(A_0)=\mathbb{C}\setminus((-\infty,-m]\cup[m,\infty))$ *the values* $M^{(s)}(\lambda)$ *of the Weyl function are given by*

$$M^{(s)}(\lambda)=\mathcal{C}_\lambda\upharpoonright H_\alpha^{s-1/2}(\Sigma;\mathbb{C}^N).$$

Each $M^{(s)}(\lambda)$ *is a densely defined bounded operator in* $L^2(\Sigma;\mathbb{C}^N)$ *and a bounded everywhere defined operator from* $H_\alpha^{s-1/2}(\Sigma;\mathbb{C}^N)$ *to* $H^{s-1/2}(\Sigma;\mathbb{C}^N)$*.*

Proof. Let $s\in[\frac12,1]$ be fixed. First, we show that $\{L^2(\Sigma;\mathbb{C}^N),\Gamma_0^{(s)},\Gamma_1^{(s)}\}$ is a quasi boundary triplet. For this we note that $\overline{T^{(s)}}=T^{(0)}=S^*$, as $C_0^\infty(\overline{\Omega_\pm};\mathbb{C}^N)$ is dense in $H_\alpha^0(\Omega_\pm;\mathbb{C}^N)$ and the norm in $H_\alpha^s(\mathbb{R}^3\setminus\Sigma;\mathbb{C}^N)$ and the graph norm induced by $T^{(0)}$ are equivalent. Next, we verify that Green's identity in Definition 2.1 (i) is fulfilled. For this let $f=f_+\oplus f_-$, $g=g_+\oplus g_-\in\operatorname{dom}T^{(s)}=H_\alpha^s(\Omega_+;\mathbb{C}^N)\oplus H_\alpha^s(\Omega_-;\mathbb{C}^N)$. Then integration by parts (5.2) applied in $\Omega_\pm$ yields

$$\begin{aligned}\big((-i(\alpha\cdot\nabla)+m\alpha_0)f_\pm,g_\pm\big)_{L^2(\Omega_\pm;\mathbb{C}^N)}-\big(f_\pm,(-i(\alpha\cdot\nabla)+m\alpha_0)g_\pm\big)_{L^2(\Omega_\pm;\mathbb{C}^N)}\\ =\pm\big(-i(\alpha\cdot\nu)f_\pm|_\Sigma,g_\pm|_\Sigma\big)_{L^2\Sigma;\mathbb{C}^N)},\end{aligned}$$

where it is used that $-\nu$ is the normal vector field pointing outwards of Ω_-. By adding these two formulas for Ω_+ and Ω_- one arrives at Green's identity.

Next, we show that $T^{(s)}\upharpoonright\ker\Gamma_0^{(s)}=A_0$. As the free Dirac operator A_0 is self-adjoint, this shows that $T^{(s)}\upharpoonright\ker\Gamma_0^{(s)}$ is self-adjoint. The inclusion $A_0\subset T^{(s)}\upharpoonright\ker\Gamma_0^{(s)}$ is clear. To verify the converse inclusion, let $f\in\ker\Gamma_0^{(s)}$. Then Green's identity yields for any $\varphi\in C_0^\infty(\mathbb{R}^d;\mathbb{C}^N)$

$$\big(f,-i(\alpha\cdot\nabla)\varphi\big)_{L^2(\mathbb{R}^3;\mathbb{C}^N)}=\big((T^{(s)}-m\alpha_0)f,\varphi\big)_{L^2(\mathbb{R}^3;\mathbb{C}^N)}. \tag{5.8}$$

Hence, $(\alpha\cdot\nabla)f\in L^2(\mathbb{R}^d;\mathbb{C}^N)$, which shows $f\in H_\alpha^s(\mathbb{R}^d;\mathbb{C}^N)=H^1(\mathbb{R}^d;\mathbb{C}^N)=\operatorname{dom}A_0$. Therefore, we conclude that $T^{(s)}\upharpoonright\ker\Gamma_0^{(s)}=A_0$ holds.

It remains to prove that $\operatorname{ran}(\Gamma_0^{(s)},\Gamma_1^{(s)})$ is dense in $L^2(\Sigma;\mathbb{C}^N)\times L^2(\Sigma;\mathbb{C}^N)$. For this, we prove

$$\operatorname{ran}(\Gamma_0^{(s)}\upharpoonright\ker\Gamma_1^{(s)})=H_\alpha^{1/2}(\Sigma;\mathbb{C}^N) \tag{5.9}$$

and

$$\operatorname{ran}(\Gamma_1^{(s)}\upharpoonright\ker\Gamma_0^{(s)})=H^{1/2}(\Sigma;\mathbb{C}^N). \tag{5.10}$$

To see the inclusion "$\subset$" in (5.9) we note that any function $f \in \ker \Gamma_1^{(s)}$ satisfies $f_+|_\Sigma = -f_-|_\Sigma$. One can show as in (5.8) that $f_+ \oplus (-f_-) \in H^s_\alpha(\mathbb{R}^d;\mathbb{C}^N) = H^1(\mathbb{R}^d;\mathbb{C}^N)$ and thus, $f \in H^1(\Omega_+;\mathbb{C}^N) \oplus H^1(\Omega_-;\mathbb{C}^N)$. Therefore, the definition of $\Gamma_0^{(s)}$ yields the claimed inclusion. For the converse inclusion let $\varphi \in H^{1/2}_\alpha(\Sigma;\mathbb{C}^N)$. Choose $f_\pm \in H^1(\Omega_\pm;\mathbb{C}^N)$ such that $f_\pm|_\Sigma = \mp\frac{i}{2}(\alpha\cdot\nu)\varphi$. Then $f \in \ker \Gamma_1^{(s)}$ and $\Gamma_0^{(s)} f = \varphi$. Since this can be done for all $\varphi \in H^{1/2}_\alpha(\Sigma;\mathbb{C}^N)$, we have shown (5.9).

To verify (5.10) note that the inclusion "$\subset$" follows from $\ker \Gamma_0^{(s)} = H^1(\mathbb{R}^d;\mathbb{C}^N)$ and the definition of $\Gamma_1^{(s)}$. For the converse inclusion let $\varphi \in H^{1/2}(\Sigma;\mathbb{C}^N)$. Choose $f \in H^1(\mathbb{R}^d;\mathbb{C}^N)$ such that $f|_\Sigma = \varphi$. Then $f \in \ker \Gamma_0^{(s)}$ and $\Gamma_1^{(s)} f = \varphi$. Since this can be done for all $\varphi \in H^{1/2}(\Sigma;\mathbb{C}^N)$, we have verified (5.10). Hence, we have shown that $\{L^2(\Sigma;\mathbb{C}^N), \Gamma_0^{(s)}, \Gamma_1^{(s)}\}$ is indeed a quasi boundary triplet for all $s \in [\frac{1}{2}, 1]$. Thus, besides formula (5.7) assertion (i) is shown. Equation (5.7) will be proved together with items (ii) and (iii).

Next, we show that $\gamma^{(s)}(\lambda)^*$ is compact for all s. Formula (2.2) implies that $\gamma^{(s)}(\lambda)^* = \Gamma_1^{(s)}(A_0 - \overline{\lambda})^{-1}$. Since $(A_0 - \overline{\lambda})^{-1} : L^2(\mathbb{R}^d;\mathbb{C}^N) \to H^1(\mathbb{R}^d;\mathbb{C}^N)$ is bounded, we see that $\gamma^{(s)}(\lambda)^*$ is actually independent of s and furthermore, that $\gamma^{(s)}(\lambda)^* : L^2(\mathbb{R}^d;\mathbb{C}^N) \to H^{1/2}(\Sigma;\mathbb{C}^N)$ is also bounded. Since $H^{1/2}(\Sigma;\mathbb{C}^N)$ is compactly embedded in $L^2(\Sigma;\mathbb{C}^N)$, the claimed compactness of $\gamma^{(s)}(\lambda)^*$ follows.

In the next step, we show items (ii) and (iii) and (5.7) for $s = \frac{1}{2}$. Consider for $\varphi \in L^2(\Sigma;\mathbb{C}^N)$ the function $f_\lambda := \Phi_\lambda \varphi$. Then $f_\lambda \in H^{1/2}_\alpha(\mathbb{R}^d \setminus \Sigma;\mathbb{C}^N) = \operatorname{dom} T^{(1/2)}$ by Lemma 5.2 and by (5.5) we get $\Gamma_0^{(1/2)} f_\lambda = \varphi$. Therefore, $\operatorname{ran} \Gamma_0^{(1/2)} = L^2(\Sigma;\mathbb{C}^N)$, which is (5.7) for $s = \frac{1}{2}$. Moreover, as $G_{\lambda,d}$ in (3.7) is a fundamental solution for the Dirac equation the definition of Φ_λ shows that

$$\big(T^{(1/2)} - \lambda\big) f_\lambda = 0 \quad \text{in } \mathbb{R}^d \setminus \Sigma.$$

Hence, $\gamma^{(1/2)}(\lambda) = \Phi_\lambda$. Eventually, using the definition of $\Gamma_1^{(1/2)}$ and (5.5) we conclude $M^{(1/2)}(\lambda) = \mathcal{C}_\lambda$ and thus, $M^{(1/2)}(\lambda)$ is bounded in $L^2(\Sigma;\mathbb{C}^N)$. This shows all claims for $s = \frac{1}{2}$.

Next, we prove (ii) and (iii) for $s = 1$. First $\operatorname{dom} T^{(1)} = H^1(\mathbb{R}^d \setminus \Sigma;\mathbb{C}^N)$, the definition of $\Gamma_0^{(1)}$, and (5.9) imply $\operatorname{ran} \Gamma_0^{(1)} = H^{1/2}_\alpha(\Sigma;\mathbb{C}^N)$. As $\{L^2(\Sigma;\mathbb{C}^N), \Gamma_0^{(1)}, \Gamma_1^{(1)}\}$ is a restriction of the triplet for $s = \frac{1}{2}$ we deduce from the already shown results that

$$\gamma^{(1)}(\lambda) = \gamma^{(1/2)}(\lambda) \restriction \operatorname{ran} \Gamma_0^{(1)} = \Phi_\lambda \restriction H^{1/2}_\alpha(\Sigma;\mathbb{C}^N)$$

and

$$M^{(1)}(\lambda) = M^{(1/2)}(\lambda) \restriction \operatorname{ran} \Gamma_0^{(1)} = \mathcal{C}_\lambda \restriction H^{1/2}_\alpha(\Sigma;\mathbb{C}^N).$$

Using the closed graph theorem and the fact that $H^{1/2}_\alpha(\Sigma;\mathbb{C}^N)$ and $H^1(\mathbb{R}^d \setminus \Sigma;\mathbb{C}^N)$ are boundedly embedded in $L^2(\Sigma;\mathbb{C}^N)$ and $L^2(\mathbb{R}^d;\mathbb{C}^N)$, respectively, one gets that

$$\gamma^{(1)}(\lambda) : \operatorname{ran} \Gamma_0^{(1)} = H^{1/2}_\alpha(\Sigma;\mathbb{C}^N) \to \operatorname{dom} T^{(1)} = H^1(\mathbb{R}^d \setminus \Sigma;\mathbb{C}^N)$$

is bounded as well. The mapping properties of the trace map yield that also

$$M^{(1)}(\lambda) : \operatorname{ran} \Gamma_0^{(1)} = H^{1/2}_\alpha(\Sigma;\mathbb{C}^N) \to \operatorname{ran} \Gamma_1^{(1)} = H^{1/2}(\Sigma;\mathbb{C}^N)$$

is bounded. Hence, all claimed statements for $s = 1$ are shown.

In order to obtain the claimed results for $s \in (\frac{1}{2}, 1)$, we note first that an interpolation argument shows that $\Phi_\lambda : H^{s-1/2}(\Sigma;\mathbb{C}^N) \to H^s_\alpha(\mathbb{R}^d \setminus \Sigma;\mathbb{C}^N) = \operatorname{dom} T^{(s)}$ is bounded. Together with (5.5) this shows that $\operatorname{ran}\Gamma_0^{(s)} = H_\alpha^{s-1/2}(\Sigma;\mathbb{C}^N)$, i.e. (5.7) for $s \in (\frac{1}{2}, 1)$. Hence, we have $\gamma^{(s)}(\lambda) = \Phi_\lambda \upharpoonright H_\alpha^{s-1/2}(\Sigma;\mathbb{C}^N)$ and the trace theorem shows that $M^{(s)}(\lambda) = \Gamma_1^{(s)}\gamma^{(s)}(\lambda) : H_\alpha^{s-1/2}(\Sigma;\mathbb{C}^N) \to H^{s-1/2}(\Sigma;\mathbb{C}^N)$ is bounded. Thus, all claims are proved. □

In the next theorem we study the self-adjointness of a Dirac operator A_τ with a Lorentz scalar δ-shell interaction of strength $\tau \in \mathbb{R} \setminus \{0\}$, which is formally given by $-i(\alpha \cdot \nabla) + m\alpha_0 + \tau\alpha_0\delta_\Sigma$. In a similar way as in (4.2) we define A_τ by

$$A_\tau := T^{(1/2)} \upharpoonright \ker \big(\Gamma_0^{(1/2)} + \tau\alpha_0\Gamma_1^{(1/2)}\big).$$

The operator A_τ is given more explicitly by

$$\begin{aligned} A_\tau f &= (-i(\alpha\cdot\nabla) + m\alpha_0)f_+ \oplus (-i(\alpha\cdot\nabla) + m\alpha_0)f_-, \\ \operatorname{dom} A_\tau &= \left\{ f \in H_\alpha^{1/2}(\mathbb{R}^d\setminus\Sigma;\mathbb{C}^N) : i(\alpha\cdot\nu)(f_+|_\Sigma - f_-|_\Sigma) + \frac{\tau}{2}\alpha_0(f_+|_\Sigma + f_-|_\Sigma) \right\}, \end{aligned}$$

and it was investigated under various assumptions in [7, 13, 38, 47]. In the following theorem we show, for the first time, the self-adjointness of A_τ, when the interaction support $\Sigma \subset \mathbb{R}^d$ is an arbitrary closed bounded Lipschitz smooth hypersurface.

Theorem 5.4. *For any $\tau \in \mathbb{R}\setminus\{0\}$ the operator A_τ is self-adjoint in $L^2(\mathbb{R}^d;\mathbb{C}^N)$ and the following holds:*

(i) *For $\lambda \in \rho(A_\tau)$ the resolvent of A_τ is given by*

$$(A_\tau - \lambda)^{-1} = (A_0 - \lambda)^{-1} - \Phi_\lambda \left(\frac{1}{\tau}\alpha_0 + \mathcal{C}_\lambda\right)^{-1} \Phi_{\bar\lambda}^*.$$

(ii) $\sigma_{\mathrm{ess}}(A_\tau) = \sigma_{\mathrm{ess}}(A_0) = (-\infty, -m] \cup [m, \infty)$.

(iii) *$\sigma_{\mathrm{disc}}(A_\tau)$ is finite and $\lambda \in \sigma_{\mathrm{disc}}(A_\tau)$ if and only if $0 \in \sigma_{\mathrm{p}}(\frac{1}{\tau}\alpha_0 + \mathcal{C}_\lambda)$.*

Remark 5.5. By Theorem 5.4 the operator A_τ is self-adjoint defined on a subset of $H_\alpha^{1/2}(\mathbb{R}^d\setminus\Sigma;\mathbb{C}^N)$. If Σ is a smooth hypersurface, then it is known that A_τ is self-adjoint and $\operatorname{dom} A_\tau \subset H^1(\mathbb{R}^d\setminus\Sigma;\mathbb{C}^N)$, see [13, 38]. However, for more general Lipschitz smooth hypersurfaces this smoothness in the operator domain can not be expected, as it is shown explicitly in [41, Remark 1.9] in the two-dimensional setting for polygonal domains.

Proof of Theorem 5.4. In order to show the self-adjointness of A_τ, it suffices, according to Theorem 2.3 and the following discussion, to verify

$$\begin{aligned} \operatorname{ran}\big(\Gamma_1^{(1/2)}(A_0 \pm i)^{-1}\big) = H^{1/2}(\Sigma;\mathbb{C}^N) &\subset \operatorname{ran}\left(\frac{1}{\tau}\alpha_0 + M_{\pm i}^{(1/2)}\right) \\ &= \operatorname{ran}\left(\frac{1}{\tau}\alpha_0 + \mathcal{C}_{\pm i}\right). \end{aligned} \tag{5.11}$$

In order to see this, we prove that $\frac{1}{\tau}\alpha_0 + \mathcal{C}_{\pm i}$ is bijective in $L^2(\Sigma;\mathbb{C}^N)$. First, we note that $\frac{1}{\tau}\alpha_0 + \mathcal{C}_{\pm i}$ is injective, as otherwise the symmetric operator A_τ would have the non-real eigenvalue $\pm i$ by Theorem 2.3. Next, by (2.3) we have that

$$\mathcal{C}_{\pm i} = M^{(1/2)}(\pm i) = M^{(1/2)}(0) \pm i\gamma^{(1/2)}(0)^*\gamma^{(1/2)}(\pm i) = \mathcal{C}_0 + \mathcal{K}_{\pm i}$$

and note that $\mathcal{K}_{\pm i} = \pm i\gamma^{(1/2)}(0)^*\gamma^{(1/2)}(\pm i)$ is compact in $L^2(\Sigma;\mathbb{C}^N)$ due to Theorem 5.3 (ii). Next, we compute

$$\left(\frac{1}{\tau}\alpha_0 + \mathcal{C}_{\pm i}\right)^2 = \frac{1}{\tau^2}I_N + \mathcal{C}_0^2 + \frac{1}{\tau}\big(\alpha_0\mathcal{C}_{\pm i} + \mathcal{C}_{\pm i}\alpha_0\big) + \mathcal{K}_{\pm i}^2 + \mathcal{C}_0\mathcal{K}_{\pm i} + \mathcal{K}_{\pm i}\mathcal{C}_0.$$

Since $\mathcal{C}_0$ is self-adjoint, the operator $\frac{1}{\tau^2} I_N + \mathcal{C}_0^2$ is a strictly positive self-adjoint operator and hence it is a Fredholm operator with index zero. Next, due to the anti-commutation relation (3.2) it is not difficult to see that

$$\frac{1}{\tau}\big(\alpha_0 \mathcal{C}_{\pm i} + \mathcal{C}_{\pm i}\alpha_0\big) = \frac{1}{\tau}(2m \pm 2i\alpha_0)\mathcal{S}(-m^2-1),$$

where $\mathcal{S}(\nu)$ is the single layer boundary integral operator for $-\Delta - \nu$. According to [39, Lemma 3.4] the latter operator is compact. Since also $\mathcal{K}_{\pm i}$ is compact, we conclude that $\big(\frac{1}{\tau}\alpha_0 + \mathcal{C}_{\pm i}\big)^2$ must be a Fredholm operator with index zero. Since $\frac{1}{\tau}\alpha_0 + \mathcal{C}_{\pm i}$ is injective, we conclude that $\big(\frac{1}{\tau}\alpha_0 + \mathcal{C}_{\pm i}\big)^2$ is also injective and hence, as it has Fredholm index zero, it must be surjective. Therefore $\frac{1}{\tau}\alpha_0 + \mathcal{C}_{\pm i}$ is also bijective. This shows that (5.11) holds and thus, A_τ is self-adjoint.

Next, by Theorem 2.3 the claimed resolvent formula in (i) holds for $\lambda = \pm i$. The map $\frac{1}{\tau}\alpha_0 + \mathcal{C}_{\pm i}$ is bijective and hence boundedly invertible. This, the mapping properties of $\Phi_{\pm i}$ and $\Phi^*_{\mp i}$ from Theorem 5.3, and Krein's resolvent formula imply assertion (ii). The resolvent formula in item (i) for $\lambda \in \rho(A_\tau)$ is now a direct consequence of Theorem 2.3. The fact that $\sigma_{\mathrm{disc}}(A_\tau)$ is finite can be shown in the same way as in [13, Proposition 3.8], while the Birman Schwinger principle in (iii) follows again directly from Theorem 2.3 and the representation of $M^{(1/2)}(\lambda)$ from Theorem 5.3. □

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Institut für Angewandte Mathematik, Technische Universität Graz, Steyrergasse 30, 8010 Graz, Austria

Email address: behrndt@tugraz.at, holzmann@math.tugraz.at, christian.stelzer09@gmail.at, gstenzel@math.tugraz.at