ON DIRAC OPERATORS WITH ELECTROSTATIC δ-SHELL INTERACTIONS OF CRITICAL STRENGTH

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ABSTRACT. In this paper we prove that the Dirac operator A_η with an electrostatic δ-shell interaction of critical strength $\eta = \pm 2$ supported on a C^2-smooth compact surface Σ is self-adjoint in $L^2(\mathbb{R}^3; \mathbb{C}^4)$, we describe the domain explicitly in terms of traces and jump conditions in $H^{-1/2}(\Sigma; \mathbb{C}^4)$, and we investigate the spectral properties of A_η. While the non-critical interaction strengths $\eta \neq \pm 2$ have received a lot of attention in the recent past, the critical case $\eta = \pm 2$ remained open. Our approach is based on abstract techniques in extension theory of symmetric operators, in particular, boundary triples and their Weyl functions.

1. INTRODUCTION

Dirac operators with electrostatic δ-shell interactions attracted a lot of attention in the recent past, see [3, 4, 5, 7, 30, 31, 33] or the related papers [2, 12, 13]. From the physical point of view they are the relativistic counterpart of Schrödinger operators with δ-potentials, which are used as idealized models for Schrödinger operators with strongly localized regular potentials, cf. [1, 6, 22, 29] and the references therein. On the other hand Dirac operators with electrostatic δ-shell interactions are also interesting from the mathematical point of view, since it can be expected that their spectral properties depend on the geometry of the interaction support and/or the interaction strength; such effects are studied in the monograph [24] and, e.g., in [14, 21, 22, 23, 25] for Schrödinger operators with δ-potentials.

The mathematical study of Dirac operators with singular interactions supported on a set of measure zero started in the 1980s. In the one-dimensional case several results as, e.g., a description of the spectrum, an explicit resolvent formula, the approximation by Dirac operators with squeezed potentials and their convergence in the nonrelativistic limit were deduced in [1, 17, 27, 34, 35]. Making use of these results and a decomposition into spherical harmonics J. Dittrich, P. Exner, and P. Šeba studied the Dirac operator in $\mathbb{R}^3$ with a singular perturbation supported on a sphere in [20]. The investigation of the Dirac operator in $\mathbb{R}^3$ with singular perturbations supported on more general surfaces was initiated only recently in the pioneering paper [3] by N. Arrizabalaga, A. Mas, and L. Vega, where a new approach to extension theory of symmetric operators was employed; this research was continued in [4, 5, 30, 31]. A different approach using the abstract theory of quasi boundary triples and their Weyl functions from [9, 10] was proposed by P. Exner, V. Lotoreichik, and the authors of the present paper in [7].

In what follows we fix some notations and describe several already obtained results to set up the problem treated in this paper. Let us choose units such that the Planck constant $\hbar$ and the speed of light are both equal to one. The free Dirac operator A_0 in $L^2(\mathbb{R}^3; \mathbb{C}^4)$ is given by

$$A_0 f := -i \sum_{j=1}^{3} \alpha_j \partial_j f + m\beta f, \qquad \operatorname{dom} A_0 = H^1(\mathbb{R}^3; \mathbb{C}^4),$$

where the Dirac matrices $\alpha_1, \alpha_2, \alpha_3$ and β are defined by (1.2) below. The operator A_0 describes the motion of a free spin-$\frac{1}{2}$ particle with mass $m > 0$ in $\mathbb{R}^3$ taking relativistic effects into account. Furthermore, let Σ be the boundary of a bounded C^2-smooth domain $\Omega_+ \subset \mathbb{R}^3$ and let $\Omega_- := \mathbb{R}^3 \setminus \overline{\Omega_+}$. The Dirac operator with an electrostatic δ-shell interaction of strength $\eta \in \mathbb{R}$ supported on Σ is formally given by

$$A_\eta = A_0 + \eta I_4 \delta_\Sigma;$$

here I_4 stands for the identity matrix in $\mathbb{C}^{4 \times 4}$. In a mathematically rigorous form $A_\eta, \eta \neq \pm 2$, is defined in [3, 7] as a particular self-adjoint extension of the symmetric operator

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

Observe that S is the restriction of the free Dirac operator to functions that vanish on Σ. Roughly speaking, a function $f \in \operatorname{dom} S^*$ belongs to $\operatorname{dom} A_\eta$ if the traces of $f_\pm := f \restriction \Omega_\pm$ satisfy the jump condition

$$(1.1) \qquad \frac{\eta}{2}\big(f_+|_\Sigma + f_-|_\Sigma\big) = -i\alpha \cdot \nu\big(f_+|_\Sigma - f_-|_\Sigma\big),$$

where ν is the outer unit normal vector field of Ω_+; cf. Definition 5.1 for more details. Concerning the basic spectral properties of A_η in the non-critical case $\eta \neq \pm 2$ the following theorem is known from [3, 7] and Proposition 5.2.

Theorem 1.1. *For $\eta \in \mathbb{R} \setminus \{\pm 2\}$ the operator A_η is self-adjoint in $L^2(\mathbb{R}^3; \mathbb{C}^4)$ and the following properties hold:*

(i) $\operatorname{dom} A_\eta \subset H^1(\mathbb{R}^3 \setminus \Sigma; \mathbb{C}^4)$;

(ii) *the essential spectrum of A_η is given by*

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

(iii) *the discrete spectrum of A_η in the gap $(-m, m)$ is finite.*

For an interaction strength $\eta \in \mathbb{R} \setminus \{\pm 2\}$ also various other results for the operator A_η are known, as, e.g., an abstract version of the Birman-Schwinger principle [4, 7], an isoperimetric inequality [5], the existence and completeness of the wave operators for the pair $\{A_\eta, A_0\}$, the convergence in the nonrelativistic limit [7], and the approximation by Dirac operators with squeezed potentials including Klein's paradox [31].

We emphasize that in all papers [3, 4, 5, 7, 30, 31] the critical interaction strengths $\eta = \pm 2$ were excluded. This situation is more difficult to handle with extension theoretic techniques and remained open so far. It is the goal of this paper to fill this gap. Our main result can be summarized as follows; cf. Theorem 5.5, Theorem 5.7, and Theorem 5.9 for more details.

Theorem 1.2. *The Dirac operator with an electrostatic δ-shell interaction of critical strength $\eta = \pm 2$ is self-adjoint in $L^2(\mathbb{R}^3; \mathbb{C}^4)$, its domain is not contained in $H^1(\mathbb{R}^3 \setminus \Sigma; \mathbb{C}^4)$, the set $(-\infty, -m] \cup [m, \infty)$ belongs to the essential spectrum and essential spectrum may also appear in $(-m, m)$.*

In fact, it will turn out in Theorem 5.5 that the operator $A_{\pm 2}$ is essentially self-adjoint in $L^2(\mathbb{R}^3; \mathbb{C}^4)$ and hence, its closure is self-adjoint. Here $A_{\pm 2}$ is defined with the help of a suitable quasi boundary triple in a similar way as in [7] on functions satisfying the jump condition (1.1) in $H^{1/2}(\Sigma; \mathbb{C}^4)$. Our techniques, based on special transformations of quasi boundary triples to ordinary boundary triples and vice versa in the spirit of [11], allow us to give an explicit description of the domain of the self-adjoint operator $\overline{A_{\pm 2}}$. More precisely, we show that $f \in \operatorname{dom} S^*$ belongs to the domain of the self-adjoint Dirac operator $\overline{A_{\pm 2}}$ with critical interaction strength if and only if the traces of f satisfy the jump condition in (1.1) in $H^{-1/2}(\Sigma; \mathbb{C}^4)$ and that $\operatorname{dom} \overline{A_{\pm 2}}$ is not contained in $H^1(\mathbb{R}^3 \setminus \Sigma; \mathbb{C}^4)$. Thus the functions in $\operatorname{dom} \overline{A_{\pm 2}}$ are less regular than those in $\operatorname{dom} A_\eta$, $\eta \in \mathbb{R} \setminus \{\pm 2\}$, which indicates one of the key difficulties in the treatment of the critical interaction strengths ± 2. We would like to point out that a result of the same type as Theorem 5.5 was obtained recently in [33] by T. Ourmières-Bonafos and L. Vega. In the present paper we also investigate the spectral properties of the self-adjoint operators $\overline{A_{\pm 2}}$. As one may expect the set $(-\infty, -m] \cup [m, \infty)$ belongs to the essential spectrum – the proof of this fact is based on the usage of suitable singular sequences – but it is less intuitive that also in the interval $(-m, m)$ essential spectrum may appear. For the case that the interaction support Σ contains a flat part we prove in Theorem 5.9 that the point 0 belongs to $\sigma_{\mathrm{ess}}(\overline{A_{\pm 2}})$ and at the same time it turns out that in this situation the functions in $\operatorname{dom} \overline{A_{\pm 2}}$ do not possess any Sobolev regularity of positive order. We remark that a similar effect occurs in the study of indefinite Laplacians; cf. [8, 16].

The paper is organized as follows: In Section 2 we provide some statements from the theory of quasi and ordinary boundary triples that are needed to prove our main results. Section 3 contains then some preliminary considerations on the free Dirac operator in $\mathbb{R}^3$ and a maximal Dirac operator in $\mathbb{R}^3 \setminus \Sigma$, while in Section 4 boundary triples suitable for Dirac operators with singular interactions are studied. Section 5 contains our main results: Theorem 5.5, Theorem 5.7, and Theorem 5.9.

Notations. The positive constant m stands for the mass of the particle. The identity matrix in $\mathbb{C}^{n \times n}$ is denoted by I_n. Furthermore, $\alpha_1, \alpha_2, \alpha_3$ and β are the Dirac matrices

$$(1.2) \qquad \alpha_j := \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix} \quad \text{and} \quad \beta := \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix},$$

where σ_j are the Pauli spin matrices

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

The Dirac matrices satisfy the anti-commutation relations

$$(1.3) \qquad \alpha_j \alpha_k + \alpha_k \alpha_j = 2\delta_{jk} \quad \text{and} \quad \alpha_j \beta + \beta \alpha_j = 0, \quad j, k \in \{1, 2, 3\}.$$

For vectors $x = (x_1, x_2, x_3)^\top$ we employ the notation $\alpha \cdot x := \sum_{j=1}^{3} \alpha_j x_j$.

The open ball of radius R centered at x is denoted by $B(x, R)$. Moreover, $\Omega_+ \subset \mathbb{R}^3$ is a C^2-smooth bounded domain and we set $\Omega_- := \mathbb{R}^3 \setminus \overline{\Omega_+}$ and $\Sigma := \partial \Omega_+$. For an open set $\Omega \subset \mathbb{R}^3$ we write $C_c^\infty(\Omega; \mathbb{C}^4)$ for the space of all infinitely many times differentiable vector valued functions with four components and compact support, and $C^\infty(\overline{\Omega}; \mathbb{C}^4) := \{f \restriction \Omega : f \in C_c^\infty(\mathbb{R}^3; \mathbb{C}^4)\}$. In a similar way, if Ω is an open subset of $\mathbb{R}^3$ or if $\Omega = \Sigma$, then $L^2(\Omega; \mathbb{C}^4)$ denotes the space of vector valued functions, where each of the four components is square integrable, and we write $(\cdot, \cdot)_\Omega$ for the corresponding inner product. If $\Omega = \Sigma$, then these L^2-spaces are equipped with the Hausdorff measure σ, otherwise with the standard Lebesgue measure. Eventually, we use the symbol $H^s(\Omega; \mathbb{C}^4)$ for Sobolev spaces of order $s \geq 0$ and $H_0^1(\Omega; \mathbb{C}^4)$ for the closure of $C_c^\infty(\Omega; \mathbb{C}^4)$ with respect to the H^1-norm. For more details on Sobolev and other function spaces, see, e.g., [32].

The Laplace-Beltrami operator on Σ acting on $\mathbb{C}^4$-vector valued functions will be denoted by $-\Delta_\Sigma$. The operator $(I_4 - \Delta_\Sigma)^s : H^{2s}(\Sigma; \mathbb{C}^4) \to L^2(\Sigma; \mathbb{C}^4)$ is bijective and continuous for any $s \in [-1, 1]$. Finally, we are going to use the following expression for the duality product for the pair $H^{1/2}(\Sigma; \mathbb{C}^4)$ and its dual space $H^{-1/2}(\Sigma; \mathbb{C}^4)$:

$$(\varphi, \psi)_{1/2 \times -1/2} := \left((I_4 - \Delta_\Sigma)^{1/4} \varphi, (I_4 - \Delta_\Sigma)^{-1/4} \psi\right)_\Sigma$$

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

2. Quasi and ordinary boundary triples

In this section we give a short introduction to ordinary boundary triples, quasi boundary triples, and some related techniques in extension and spectral theory of symmetric and self-adjoint operators in Hilbert spaces. We formulate the results in a way such that they can be applied directly in the main part of the paper in the analysis of Dirac operators with singular interactions. In order to get a detailed overview of the concept of ordinary and quasi boundary triples and applications to partial differential operators we refer the reader to [9, 10, 15, 18, 19, 28].

Throughout this section $\mathcal{H}$ is always a complex Hilbert space with inner product $(\cdot, \cdot)_\mathcal{H}$ and S denotes a densely defined, closed and symmetric operator with adjoint S^*. We start with the definition of quasi and ordinary boundary triples.

Definition 2.1. *Assume that T is a linear operator in $\mathcal{H}$ such that $\overline{T} = S^*$. A triple $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ 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 triple *for S^* if the following conditions hold:*

   (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 satisfied.
   (ii) *$\Gamma = (\Gamma_0, \Gamma_1)^\top : \operatorname{dom} T \to \mathcal{G} \times \mathcal{G}$ has dense range.*
   (iii) *$A_0 := T \restriction \ker \Gamma_0$ is a self-adjoint operator in $\mathcal{H}$.*

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 triple.

We point out that the above (non-standard) definition of ordinary boundary triples is equivalent to the usual one in, e.g., [15, 18, 28], see [9, Corollary 3.2]. In particular, if $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ is an ordinary boundary triple, then T coincides with S^*. Note that a quasi boundary triple or ordinary boundary triple 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 $\mathcal{H}$, and that the operator T in Definition 2.1 is in general not unique.

Let $T \subset \overline{T} = S^*$ and let $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ be a quasi boundary triple for S^*. Then

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

and the mapping $\Gamma = (\Gamma_0, \Gamma_1)^\top : \operatorname{dom} T \to \mathcal{G} \times \mathcal{G}$ is closable; cf. [9]. Next, we are going to introduce the γ-field and the Weyl function associated to the quasi boundary triple $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$; as we will see one can describe spectral properties of self-adjoint extensions of S with the help of these operators. In the following let $A_0 = T \upharpoonright \ker \Gamma_0$. Then the direct sum decomposition

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

holds. The definition of the γ-field and Weyl function for quasi boundary triples is in accordance with the one for ordinary boundary triples in [18].

Definition 2.2. *Let* T *be a linear operator in* $\mathcal{H}$ *such that* $\overline{T} = S^*$ *and let* $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ *be a quasi boundary triple 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.

Because of (2.1) the γ-field is well-defined and one has $\operatorname{ran} \gamma(\lambda) = \ker(T - \lambda)$ for any $\lambda \in \rho(A_0)$. Note that $\operatorname{dom} \gamma(\lambda) = \operatorname{ran} \Gamma_0$ is dense in $\mathcal{G}$ by Definition 2.1. Making use of the abstract Green's formula (Definition 2.1 (i)) one can show that

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

this is a bounded and everywhere defined operator from $\mathcal{H}$ to $\mathcal{G}$. Thus $\gamma(\lambda)$ is a (in general not everywhere defined) bounded operator; cf. [9, Proposition 2.6] or [10, Proposition 6.13]. In the special case that $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ is an ordinary boundary triple $\gamma(\lambda)$ is automatically bounded and everywhere defined. Next, one has for all $\lambda, \mu \in \rho(A_0)$ and all $\varphi \in \operatorname{ran} \Gamma_0$

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

see [9, Proposition 2.6]. In particular, the mapping $\lambda \mapsto \gamma(\lambda)\varphi$ is holomorphic on $\rho(A_0)$ for any fixed $\varphi \in \operatorname{ran} \Gamma_0$.

Next, we state some useful properties of the Weyl function M corresponding to the quasi boundary triple $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$; the proofs of these statements can be found in [9, Proposition 2.6]. The definition of M implies that

$$M(\lambda)\Gamma_0 f_\lambda = \Gamma_1 f_\lambda, \qquad f_\lambda \in \ker(T - \lambda), \ \lambda \in \rho(A_0).$$

In particular, for any $\lambda \in \rho(A_0)$ the linear operator $M(\lambda)$ is densely defined in $\mathcal{G}$ with dom $M(\lambda) = \operatorname{ran} \Gamma_0$ and $\operatorname{ran} M(\lambda) \subset \operatorname{ran} \Gamma_1$. For $\lambda, \mu \in \rho(A_0)$ and $\varphi \in \operatorname{ran} \Gamma_0$ one has

$$M(\lambda)\varphi - M(\mu)^*\varphi = (\lambda - \overline{\mu})\gamma(\mu)^*\gamma(\lambda)\varphi. \tag{2.4}$$

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 $\mathcal{G}$. In the special case that $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ is an ordinary boundary triple $M(\lambda)$ is bounded and everywhere defined. Equation (2.4) also yields that for any $\varphi \in \operatorname{ran} \Gamma_0$ the $\mathcal{G}$-valued function $\lambda \mapsto M(\lambda)\varphi$ is analytic on $\rho(A_0)$.

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

$$A_\vartheta = T \upharpoonright \ker(\Gamma_1 - \vartheta\Gamma_0), \tag{2.5}$$

i.e. $f \in \operatorname{dom} T$ belongs to dom A_ϑ 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

$$(A_\vartheta f, g)_{\mathcal{H}} - (f, A_\vartheta g)_{\mathcal{H}} = (\vartheta\Gamma_0 f, \Gamma_0 g)_{\mathcal{G}} - (\Gamma_0 f, \vartheta\Gamma_0 g)_{\mathcal{G}} = 0 \tag{2.6}$$

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

In the following theorem we state an abstract version of the Birman-Schwinger principle and a Krein type resolvent formula for canonical extensions A_ϑ; for the proof of this result, see [9, Theorem 2.8] or [10, Theorem 6.16].

Theorem 2.3. *Let T be a linear operator in $\mathcal{H}$ such that $\overline{T} = S^*$, let $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ be a quasi boundary triple for S^* with $A_0 = T \upharpoonright \ker \Gamma_0$, and denote the corresponding γ-field and Weyl function by γ and M, respectively. Let A_ϑ be the canonical extension of S associated to an operator ϑ in $\mathcal{G}$ as in (2.5). Then the following assertions hold 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, it holds that*

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

(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*

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

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. Namely, if ϑ is symmetric in $\mathcal{G}$ then A_ϑ is symmetric in $\mathcal{H}$ by (2.6), 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 equivalent to $\operatorname{ran} \gamma(\mp i)^* \subset \operatorname{ran}(\vartheta - M(\pm i))$.

In the special case that $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ is an ordinary boundary triple the situation is simpler as the next well-known proposition states. We note that the converse in Proposition 2.4 holds if ϑ in (2.5) is allowed to be a linear relation (multivalued operator).

Proposition 2.4. *Let S be a densely defined closed symmetric operator in $\mathcal{H}$ and assume that $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ is an ordinary boundary triple for S^*. Let ϑ be an operator in $\mathcal{G}$ and let A_ϑ be defined by (2.5). If ϑ is (essentially) self-adjoint in $\mathcal{G}$ then A_ϑ is (essentially) self-adjoint in $\mathcal{H}$.*

In what follows we describe a particular transformation procedure of quasi boundary triples to ordinary boundary triples from [11] which will be useful later in this paper. 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^*. Define the spaces

$$(2.7) \qquad \mathscr{G}_0 := \operatorname{ran}(\Gamma_0 \upharpoonright \ker \Gamma_1) \quad \text{and} \quad \mathscr{G}_1 := \operatorname{ran}(\Gamma_1 \upharpoonright \ker \Gamma_0).$$

We will often assume that $\mathscr{G}_1$ is dense in $\mathcal{G}$. In this case, we denote by $\mathscr{G}_1'$ the dual space of $\mathscr{G}_1$ with respect to any norm $\|\cdot\|_{\mathscr{G}_1}$ such that $(\mathscr{G}_1, \|\cdot\|_{\mathscr{G}_1})$ is a reflexive Banach space continuously embedded into $\mathcal{G}$; such a norm exists, see [11, Proposition 2.9], and all norms with this property are equivalent, cf. [11, Proposition 2.10]. Analogous statements hold if $\mathscr{G}_0$ is dense in $\mathcal{G}$ and $T \upharpoonright \ker \Gamma_1$ is self-adjoint, and hence we can employ a similar notation in this case as well.

First, it turns out that the boundary mapping Γ_0 or Γ_1 can be extended to $\operatorname{dom} S^*$, if the set $\mathscr{G}_1$ or $\mathscr{G}_0$, respectively, is dense in $\mathcal{G}$; cf. [11, Proposition 2.10 and Corollary 2.11]. In the following we write $\|\cdot\|_{S^*}$ for the graph norm induced by S^*.

Proposition 2.5. *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^*, and let $\mathscr{G}_0, \mathscr{G}_1$ be as in (2.7). Then the following assertions are true:*

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

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

(ii) *If $\mathscr{G}_0$ is dense in $\mathcal{G}$ and $A_\infty := T \upharpoonright \ker \Gamma_1$ is self-adjoint then Γ_1 admits a unique, surjective and continuous extension*

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

Under the assumptions of the previous proposition also the γ-field and the Weyl function associated to the quasi boundary triple $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ can be extended; cf. [11, Definition 2.14] and the corresponding discussion.

Proposition 2.6. *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^*, and let $A_0 = T \upharpoonright \ker \Gamma_0$. Denote the corresponding γ-field and Weyl function by γ and M, respectively. Assume that $\mathscr{G}_0$ and $\mathscr{G}_1$ defined by (2.7) are dense in $\mathcal{G}$ and that $A_\infty := T \upharpoonright \ker \Gamma_1$ is self-adjoint. Then the following assertions hold for all $\lambda \in \rho(A_0)$:*

(i) *The values of the γ-field admit continuous extensions*

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

(ii) *The values of the Weyl function $M(\lambda)$ admit continuous extensions*

$$\widetilde{M}(\lambda) = \widetilde{\Gamma}_1 \widetilde{\gamma}(\lambda) : \mathscr{G}_1' \to \mathscr{G}_0'.$$

Making use of the extended boundary mapping $\widetilde{\Gamma}_0$ one can transform the originally given quasi boundary triple $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ to an ordinary boundary triple, see [11,

Theorem 2.12]. In order to introduce this ordinary boundary triple fix some iso-morphisms $\iota_+ : \mathscr{G}_1 \to \mathcal{G}$ and $\iota_- : \mathscr{G}_1' \to \mathcal{G}$ which satisfy

$$(\iota_- x', \iota_+ x)_{\mathcal{G}} = (x', x)_{\mathscr{G}_1' \times \mathscr{G}_1}$$

for all $x \in \mathscr{G}_1$ and $x' \in \mathscr{G}_1'$, where $(\cdot, \cdot)_{\mathscr{G}_1' \times \mathscr{G}_1}$ denotes the duality product of the pair $\mathscr{G}_1'$ and $\mathscr{G}_1$.

Theorem 2.7. *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^* with $A_0 = T \upharpoonright \ker \Gamma_0$. Assume that $\mathscr{G}_1$ defined by* (2.7) *is dense in $\mathcal{G}$ and that there exists $\mu \in \rho(A_0) \cap \mathbb{R}$. Define the mappings $\Upsilon_0, \Upsilon_1 : \operatorname{dom} S^* \to \mathcal{G}$ by*

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

where $\widetilde{\Gamma}_0$ is the extension of the boundary mapping Γ_0 from Proposition 2.5 *(i). Then $\{\mathcal{G}, \Upsilon_0, \Upsilon_1\}$ is an ordinary boundary triple for S^* such that the self-adjoint operators $T \upharpoonright \ker \Gamma_0$ and $S^* \upharpoonright \ker \Upsilon_0$ coincide.*

We remark that the γ-field β and the Weyl function $\mathcal{M}$ associated to the boundary triple $\{\mathcal{G}, \Upsilon_0, \Upsilon_1\}$ are given by

$$(2.8) \qquad \beta(\lambda) = \widetilde{\gamma}(\lambda) \iota_-^{-1} \quad \text{and} \quad \mathcal{M}(\lambda) = \iota_+ \big(\widetilde{M}(\lambda) - \widetilde{M}(\mu)\big) \iota_-^{-1}$$

for $\lambda \in \rho(A_0)$ and $\mu \in \mathbb{R} \cap \rho(A_0)$ chosen as in Theorem 2.7; cf. [11, eq. (2.17)].

Finally, let ϑ be a linear operator in $\mathcal{G}$ and let A_ϑ be the canonical extension of S defined via (2.5) and the quasi boundary triple $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$. Consider the linear operator

$$(2.9) \qquad \begin{aligned} &\Theta(\vartheta) = \iota_+ \big(\vartheta - M(\mu)\big) \iota_-^{-1}, \\ &\operatorname{dom} \Theta(\vartheta) = \big\{ \varphi \in \mathcal{G} : \iota_-^{-1} \varphi \in \operatorname{dom}(\vartheta - M(\mu)) \text{ and } (\vartheta - M(\mu)) \iota_-^{-1} \varphi \in \mathscr{G}_1 \big\}, \end{aligned}$$

in $\mathcal{G}$. If $\{\mathcal{G}, \Upsilon_0, \Upsilon_1\}$ is the ordinary boundary triple in Theorem 2.7 then one verifies

$$\ker(\Gamma_1 - \vartheta \Gamma_0) = \ker\big(\Upsilon_1 - \Theta(\vartheta)\Upsilon_0\big);$$

cf. [11, Corollary 3.5]. Together with Proposition 2.4 the next corollary follows immediately; again a converse statement is true if ϑ and $\Theta(\vartheta)$ are allowed to be linear relations.

Corollary 2.8. *Let ϑ, $\Theta(\vartheta)$ and A_ϑ be as above and assume that the assumptions in Theorem* 2.7 *are satisfied. If $\Theta(\vartheta)$ is (essentially) self-adjoint in $\mathcal{G}$ then the operator A_ϑ is (essentially) self-adjoint in $\mathcal{H}$.*

In this context we also note that for some self-adjoint operator Θ acting in $\mathcal{G}$ and its corresponding extension $A_\Theta = S^* \upharpoonright \ker(\Upsilon_1 - \Theta \Upsilon_0)$ one has

$$(2.10) \qquad \lambda \in \sigma(A_\Theta) \cap \rho(A_0) \quad \text{if and only if} \quad 0 \in \sigma(\Theta - \mathcal{M}(\lambda)),$$

$$(2.11) \qquad \lambda \in \sigma_{\mathrm{p}}(A_\Theta) \cap \rho(A_0) \quad \text{if and only if} \quad 0 \in \sigma_{\mathrm{p}}(\Theta - \mathcal{M}(\lambda)),$$

and

$$(2.12) \qquad \lambda \in \sigma_{\mathrm{disc}}(A_\Theta) \cap \rho(A_0) \quad \text{if and only if} \quad 0 \in \sigma_{\mathrm{disc}}(\Theta - \mathcal{M}(\lambda));$$

cf. [18, 19] and [15, Theorem 1.29 and Theorem 3.3]. Moreover, for $\lambda \in \rho(A_0) \cap \rho(A_\Theta)$ we have

$$(2.13) \qquad (A_\Theta - \lambda)^{-1} = (A_0 - \lambda)^{-1} + \beta(\lambda)\big(\Theta - \mathcal{M}(\lambda)\big)^{-1} \beta(\bar{\lambda})^*;$$

see [18, 19] and [11, Section 3] for more details.

3. The free and the maximal Dirac operator

In this section we first recall the definition and some standard properties of the free Dirac operator, which will be of importance in our further considerations. Then we introduce and discuss the maximal Dirac operator in $\mathbb{R}^3 \setminus \Sigma$, where Σ is the boundary of a bounded C^2-domain.

Let us choose units such that the speed of light and the Planck constant $\hbar$ are both equal to one. Then, the free Dirac operator is given by

$$(3.1) \quad A_0 f := -i \sum_{j=1}^{3} \alpha_j \partial_j f + m\beta f = -i\alpha \cdot \nabla f + m\beta f, \quad \text{dom} A_0 = H^1(\mathbb{R}^3; \mathbb{C}^4),$$

where the Dirac matrices $\alpha_1, \alpha_2, \alpha_3$ and β are defined by (1.2) and we require $m > 0$. If $-\Delta$ denotes the self-adjoint Laplace operator in $L^2(\mathbb{R}^3; \mathbb{C})$ defined on $H^2(\mathbb{R}^3; \mathbb{C})$ then

$$(3.2) \quad A_0^2 = (-\Delta + m^2)I_4, \quad \text{dom} A_0^2 = H^2(\mathbb{R}^3; \mathbb{C}^4);$$

cf. [37, Korollar 20.2] for $m = 1$. In the above formula the symbol $(-\Delta + m^2)I_4$ is understood as a 4×4 diagonal block operator, where each diagonal entry acts as $-\Delta + m^2$. Next, it is well-known that A_0 is self-adjoint in $L^2(\mathbb{R}^3; \mathbb{C}^4)$ and that the spectrum of A_0 is

$$(3.3) \quad \sigma(A_0) = (-\infty, -m] \cup [m, \infty),$$

see [36] or [37, Chapter 20]. Furthermore, for $\lambda \notin \sigma(A_0)$ the resolvent of A_0 is given by

$$(3.4) \quad (A_0 - \lambda)^{-1} f(x) = \int_{\mathbb{R}^3} G_\lambda(x - y) f(y) \mathrm{d}y, \quad x \in \mathbb{R}^3, \ f \in L^2(\mathbb{R}^3; \mathbb{C}^4),$$

where the integral kernel G_λ is a $\mathbb{C}^{4 \times 4}$-valued function of the form

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

cf. [36, Section 1.E] or [4, Lemma 2.1]. In the above formula the square root is defined such that $\operatorname{Im} \sqrt{\lambda^2 - m^2} > 0$ for $\lambda \notin \sigma(A_0)$.

Let Σ be the boundary of the bounded C^2-domain Ω_+ and let $\Omega_- := \mathbb{R}^3 \setminus \overline{\Omega_+}$. We will make use of the decomposition $L^2(\mathbb{R}^3; \mathbb{C}^4) = L^2(\Omega_+; \mathbb{C}^4) \oplus L^2(\Omega_-; \mathbb{C}^4)$ and split functions $f \in L^2(\mathbb{R}^3; \mathbb{C}^4)$ in the form $f = f_+ \oplus f_-$, where $f_\pm := f \upharpoonright \Omega_\pm \in L^2(\Omega_\pm; \mathbb{C}^4)$. Furthermore, we define the subspaces $\mathcal{D}_\pm$ of $L^2(\Omega_\pm; \mathbb{C}^4)$ by

$$\mathcal{D}_\pm := \left\{ f_\pm \in L^2(\Omega_\pm; \mathbb{C}^4) : (-i\alpha \cdot \nabla + m\beta) f_\pm \in L^2(\Omega_\pm; \mathbb{C}^4) \right\},$$

where all derivatives are understood in the distributional sense, and we endow $\mathcal{D}_\pm$ with the natural norms

$$(3.6) \quad \|f_\pm\|_{\mathcal{D}_\pm}^2 := \|f_\pm\|_{\Omega_\pm}^2 + \left\| (-i\alpha \cdot \nabla + m\beta) f_\pm \right\|_{\Omega_\pm}^2, \quad f_\pm \in \mathcal{D}_\pm.$$

Now, we define the maximal Dirac operator $T_{\max}$ in $L^2(\mathbb{R}^3; \mathbb{C}^4)$ by

$$(3.7) \quad \begin{aligned} T_{\max} f &:= (-i\alpha \cdot \nabla + m\beta) f_+ \oplus (-i\alpha \cdot \nabla + m\beta) f_-, \\ \text{dom} T_{\max} &:= \mathcal{D}_+ \oplus \mathcal{D}_-. \end{aligned}$$

The operator $T_{\max}$ turns out to be the adjoint of the symmetric restriction of A_0 on functions vanishing on Σ.

Proposition 3.1. *Define the linear operator S by*

$$(3.8) \qquad\qquad S := A_0 \restriction H_0^1(\mathbb{R}^3 \setminus \Sigma; \mathbb{C}^4)$$

and let $T_{\max}$ be as above. Then S is a densely defined, closed, symmetric operator such that $S^* = T_{\max}$ holds.

Proof. Since $C_c^\infty(\mathbb{R}^3 \setminus \Sigma; \mathbb{C}^4) \subset \operatorname{dom} S$ and $S \subset A_0$ it is clear that S is densely defined and symmetric. Moreover S is closed since $H_0^1(\mathbb{R}^3 \setminus \Sigma; \mathbb{C}^4)$ is a closed subspace of $H^1(\mathbb{R}^3; \mathbb{C}^4)$ and the graph norm of A_0 is equivalent to the $H^1(\mathbb{R}^3; \mathbb{C}^4)$-norm, see, e.g., [37, Satz 20.1].

Next we show $S^* \subset T_{\max}$. For that, let $f \in \operatorname{dom} S^*$ and $g_+ \in C_c^\infty(\Omega_+; \mathbb{C}^4)$. Then $g := g_+ \oplus 0 \in \operatorname{dom} S$ and

$$\big((S^*f)_+, g_+\big)_{\Omega_+} = (S^*f, g)_{\mathbb{R}^3} = (f, Sg)_{\mathbb{R}^3} = \big(f_+, (-i\alpha \cdot \nabla + m\beta)g_+\big)_{\Omega_+}.$$

Since this holds for any $g_+ \in C_c^\infty(\Omega_+; \mathbb{C}^4)$, the distribution $(-i\alpha \cdot \nabla + m\beta)f_+$ exists in $L^2(\Omega_+; \mathbb{C}^4)$ and is equal to $(S^*f)_+$. Similarly, one verifies $(-i\alpha \cdot \nabla + m\beta)f_- = (S^*f)_-$ in the distributional sense. This yields $f \in \mathcal{D}_+ \oplus \mathcal{D}_- = \operatorname{dom} T_{\max}$ and $T_{\max}f = S^*f$.

It remains to prove that $T_{\max} \subset S^*$. Let $f \in \operatorname{dom} T_{\max}$ and $g \in C_c^\infty(\mathbb{R}^3 \setminus \Sigma; \mathbb{C}^4)$. Then we have

$$\begin{aligned}
\big(f_+, (Sg)_+\big)_{\Omega_+} &= \big(f_+, (-i\alpha \cdot \nabla + m\beta)g_+\big)_{\Omega_+} \\
&= \big((-i\alpha \cdot \nabla + m\beta)f_+, g_+\big)_{\Omega_+} = \big((T_{\max}f)_+, g_+\big)_{\Omega_+}
\end{aligned}$$

and similarly $(f_-, (Sg)_-)_{\Omega_-} = \big((T_{\max}f)_-, g_-\big)_{\Omega_-}$. Summing up these two equations yields

$$(f, Sg)_{\mathbb{R}^3} = (T_{\max}f, g)_{\mathbb{R}^3}.$$

A density argument shows that this remains valid for any $g \in H_0^1(\mathbb{R}^3 \setminus \Sigma; \mathbb{C}^4) = \operatorname{dom} S$ and hence $f \in \operatorname{dom} S^*$ and $S^*f = T_{\max}f$. This completes the proof of this proposition. $\qquad\square$

The next lemma implies that smooth functions are dense in $\operatorname{dom} T_{\max}$ equipped with the graph norm. The proof follows the strategy in [12, Lemma 2.1]; a similar result can also be found in [33, Proposition 2.12].

Lemma 3.2. *The space $C^\infty(\overline{\Omega_\pm}; \mathbb{C}^4)$ is dense in $\mathcal{D}_\pm$ with respect to the norm $\|\cdot\|_{\mathcal{D}_\pm}$ in (3.6).*

Proof. We show this statement for $\mathcal{D}_-$, the assertion for $\mathcal{D}_+$ follows in almost the same way. Assume that $f \in \mathcal{D}_-$ satisfies

$$(3.9) \qquad \big(f, g\big)_{\Omega_-} + \big((-i\alpha \cdot \nabla + m\beta)f, (-i\alpha \cdot \nabla + m\beta)g\big)_{\Omega_-} = 0$$

for all $g \in C^\infty(\overline{\Omega_-}; \mathbb{C}^4)$. Since this is true, in particular, for any $g \in C_c^\infty(\Omega_-; \mathbb{C}^4)$, it follows that the distribution $(-i\alpha \cdot \nabla + m\beta)^2 f$ exists in $L^2(\Omega_-; \mathbb{C}^4)$ and coincides with $-f$.

Next, we claim that

$$(3.10) \qquad\qquad (-i\alpha \cdot \nabla + m\beta)f \in H_0^1(\Omega_-; \mathbb{C}^4).$$

To see this, let A_0 be the free Dirac operator in (3.1), let $h \in C_c^\infty(\mathbb{R}^3; \mathbb{C}^4)$ and choose a smooth cutoff function $\chi : \mathbb{R}^3 \to [0, 1]$ satisfying $\chi \equiv 1$ in $B(0, 1)$ and $\chi \equiv 0$ in $\mathbb{R}^3 \setminus B(0, 2)$. Set $\chi_l := \chi(\cdot/l)$, $l \in \mathbb{N}$. Then $(\chi_l A_0^{-1} h) \upharpoonright \Omega_- \in C^\infty(\overline{\Omega_-}; \mathbb{C}^4)$ converges to $(A_0^{-1} h)_-$ in $H^1(\Omega_-; \mathbb{C}^4)$ as $l \to \infty$. Making use of (3.9), we conclude that

$$
\begin{aligned}
\left(A_0^{-1}(0 \oplus -f), h\right)_{\mathbb{R}^3} &= -\left(f, (A_0^{-1}h)_-\right)_{\Omega_-} = -\lim_{l \to \infty} \left(f, (\chi_l A_0^{-1}h)_-\right)_{\Omega_-} \\
&= \lim_{l \to \infty} \left((-i\alpha \cdot \nabla + m\beta)f, (-i\alpha \cdot \nabla + m\beta)(\chi_l A_0^{-1}h)_-\right)_{\Omega_-} \\
&= \left((-i\alpha \cdot \nabla + m\beta)f, (-i\alpha \cdot \nabla + m\beta)(A_0^{-1}h)_-\right)_{\Omega_-} \\
&= \left(0 \oplus (-i\alpha \cdot \nabla + m\beta)f, h\right)_{\mathbb{R}^3}.
\end{aligned}
$$

Since this is true for any $h \in C_c^\infty(\mathbb{R}^3; \mathbb{C}^4)$ it follows that

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

Moreover, the trace of $0 \oplus (-i\alpha \cdot \nabla + m\beta)f$ at Σ is equal to zero. This yields (3.10).

From (3.10) it is clear that there exists a sequence $(h_n) \subset C_c^\infty(\Omega_-; \mathbb{C}^4)$ such that $h_n \to (-i\alpha \cdot \nabla + m\beta)f$ in $H^1(\Omega_-; \mathbb{C}^4)$. Integration by parts yields finally that

$$
\begin{aligned}
0 &\le \left((-i\alpha \cdot \nabla + m\beta)f, (-i\alpha \cdot \nabla + m\beta)f\right)_{\Omega_-} = \lim_{n \to \infty} \left(h_n, (-i\alpha \cdot \nabla + m\beta)f\right)_{\Omega_-} \\
&= \lim_{n \to \infty} \left((-i\alpha \cdot \nabla + m\beta)h_n, f\right)_{\Omega_-} = \left((-i\alpha \cdot \nabla + m\beta)^2 f, f\right)_{\Omega_-} \\
&= \left(-f, f\right)_{\Omega_-} \le 0.
\end{aligned}
$$

Thus, $f = 0$ and hence $C^\infty(\overline{\Omega_-}; \mathbb{C}^4)$ is dense in $\mathcal{D}_-$. $\qquad \square$

4. Boundary triples for Dirac operators with δ-shell interactions

In this section we first provide a quasi boundary triple which is convenient to study Dirac operators with singular interactions supported on Σ. In a slightly different way this quasi boundary triple was already introduced in [7]. Although only C^∞-smooth surfaces Σ were considered in [7] the relevant results below remain valid for C^2-surfaces. The main purpose is then to extend and transform this quasi boundary triple to an ordinary boundary triple as explained in Section 2; cf. [11].

First, we define the operator $T := T_{\max} \upharpoonright H^1(\mathbb{R}^3 \setminus \Sigma; \mathbb{C}^4)$, that is,

(4.1)
$$
\begin{aligned}
Tf &:= (-i\alpha \cdot \nabla + m\beta)f_+ \oplus (-i\alpha \cdot \nabla + m\beta)f_-, \\
\operatorname{dom} T &:= H^1(\mathbb{R}^3 \setminus \Sigma; \mathbb{C}^4) = H^1(\Omega_+; \mathbb{C}^4) \oplus H^1(\Omega_-; \mathbb{C}^4),
\end{aligned}
$$

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

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

Since Σ is C^2-smooth, it follows that the normal vector field ν is differentiable and hence, $\Gamma_0 f, \Gamma_1 f \in H^{1/2}(\Sigma; \mathbb{C}^4)$ for $f \in \operatorname{dom} T$ by the trace theorem.

It can be deduced from [7] that $\{L^2(\Sigma; \mathbb{C}^4), \Gamma_0, \Gamma_1\}$ is a quasi boundary triple for $\overline{T}$ (see [7, Remark 3.3]). For the convenience of the reader we give a direct and simple proof here.

Theorem 4.1. *Let S be given by* (3.8) *and let the mappings T, Γ_0 and Γ_1 be as in* (4.1) *and* (4.2)*, respectively. Then $\{L^2(\Sigma; \mathbb{C}^4), \Gamma_0, \Gamma_1\}$ is a quasi boundary triple for $T_{\max} = S^* = \overline{T}$ with*

$$(4.3) \qquad \operatorname{ran}(\Gamma_0, \Gamma_1)^\top = H^{1/2}(\Sigma; \mathbb{C}^4) \times H^{1/2}(\Sigma; \mathbb{C}^4),$$

and $T \restriction \ker \Gamma_0$ is the free Dirac operator A_0 in (3.1)*.*

Proof. Observe first that $\overline{T} = T_{\max}$ since $C^\infty(\overline{\Omega_+}; \mathbb{C}^4) \oplus C^\infty(\overline{\Omega_+}; \mathbb{C}^4)$ is dense in $\operatorname{dom} T_{\max}$ with respect to the graph norm by Lemma 3.2. Hence also the space $H^1(\Omega_+; \mathbb{C}^4) \oplus H^1(\Omega_+; \mathbb{C}^4)$ is dense in $\operatorname{dom} T_{\max}$ with respect to the graph norm and thus $\overline{T} = T_{\max}$. Moreover, S is closed and $S^* = T_{\max}$ by Proposition 3.1.

Next it will be shown that Green's identity holds. For this let $f = f_+ \oplus f_-$, $g = g_+ \oplus g_- \in \operatorname{dom} T = H^1(\Omega_+; \mathbb{C}^4) \oplus H^1(\Omega_-; \mathbb{C}^4)$. Using $(-i\alpha_j)^* = i\alpha_j$, $j \in \{1, 2, 3\}$, we get by integration by parts

$$\big((-i\alpha \cdot \nabla + m\beta)f_\pm, g_\pm\big)_{\Omega_\pm} - \big(f_\pm, (-i\alpha \cdot \nabla + m\beta)g_\pm\big)_{\Omega_\pm} = \pm\big(-i\alpha \cdot \nu f_\pm|_\Sigma, g_\pm|_\Sigma\big)_\Sigma;$$

note that the normal vector field ν always points inside Ω_-, hence there is a different sign on the right hand side. By adding these two formulae for Ω_+ and Ω_-, we obtain

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

i.e. Green's identity in Definition 2.1 (i) is valid.

To prove the range property (4.3) consider $\varphi, \psi \in H^{1/2}(\Sigma; \mathbb{C}^4)$. By the trace theorem and $(\alpha \cdot \nu)^2 = I_4$ there exists $g_+ \in H^1(\Omega_+; \mathbb{C}^4)$ and $h \in H^1(\mathbb{R}^3; \mathbb{C}^4)$ such that

$$i\alpha \cdot \nu g_+|_\Sigma = \varphi \quad \text{and} \quad h|_\Sigma = \psi - \frac{1}{2}g_+|_\Sigma.$$

Then $f := (g_+ \oplus 0) + h$ belongs to $\operatorname{dom} T = H^1(\mathbb{R}^3 \setminus \Sigma; \mathbb{C}^4)$ and satisfies

$$\Gamma_0 f = i\alpha \cdot \nu g_+|_\Sigma + i\alpha \cdot \nu(h_+|_\Sigma - h_-|_\Sigma) = \varphi \quad \text{and} \quad \Gamma_1 f = \frac{1}{2}g_+|_\Sigma + h|_\Sigma = \psi.$$

This implies (4.3) and hence item (ii) in Definition 2.1. Finally, since $\ker \Gamma_0 = H^1(\mathbb{R}^3; \mathbb{C}^4)$ the restriction $T \restriction \ker \Gamma_0$ coincides with the free Dirac operator A_0 which is self-adjoint. Therefore, $\{L^2(\Sigma; \mathbb{C}^4), \Gamma_0, \Gamma_1\}$ is a quasi boundary triple for S^*. $\qquad\square$

Next we provide the γ-field and Weyl function associated to the quasi boundary triple in Theorem 4.1.

Proposition 4.2. *Let $\{L^2(\Sigma; \mathbb{C}^4), \Gamma_0, \Gamma_1\}$ be the quasi boundary triple in Theorem 4.1, let $\lambda \in \rho(A_0) = \mathbb{C} \setminus ((-\infty, -m] \cup [m, \infty))$ and let G_λ be the integral kernel of the resolvent of the free Dirac operator in* (3.5)*. Then the following statements hold.*

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

$$\gamma(\lambda)\varphi(x) = \int_\Sigma G_\lambda(x - y)\varphi(y)\mathrm{d}\sigma(y), \quad x \in \mathbb{R}^3, \ \varphi \in H^{1/2}(\Sigma; \mathbb{C}^4).$$

Each $\gamma(\lambda)$ is a densely defined and bounded operator from $L^2(\Sigma; \mathbb{C}^4)$ to $L^2(\mathbb{R}^3; \mathbb{C}^4)$ and an everywhere defined bounded operator from $H^{1/2}(\Sigma; \mathbb{C}^4)$

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

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

(ii) *The values* $M(\lambda) : L^2(\Sigma; \mathbb{C}^4) \to L^2(\Sigma; \mathbb{C}^4)$ *of the Weyl function are defined on* $H^{1/2}(\Sigma; \mathbb{C}^4)$ *and given by*

$$M(\lambda)\varphi(x) := \lim_{\varepsilon \searrow 0} \int_{|x-y|>\varepsilon} G_\lambda(x-y)\varphi(y)\mathrm{d}\sigma(y), \quad x \in \Sigma, \ \varphi \in H^{1/2}(\Sigma; \mathbb{C}^4).$$

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

Proof. Since the triple $\{L^2(\Sigma; \mathbb{C}^4), \Gamma_0, \Gamma_1\}$ in Theorem 4.1 is a restriction of the quasi boundary triple considered in [7], the γ-field, the Weyl function and the adjoint γ-field are restrictions of the corresponding operators there; their explicit computation can be found in [7, Proposition 3.4]. By definition and from [7, Proposition 3.4] it is also clear that $\gamma(\lambda)$ and $M(\lambda)$ are defined on $\operatorname{ran}\Gamma_0 = H^{1/2}(\Sigma; \mathbb{C}^4)$ and are bounded operators in the respective L^2-spaces. Moreover, by Definition 2.2 we have $\operatorname{ran}\gamma(\lambda) = \ker(T-\lambda) \subset H^1(\mathbb{R}^3\setminus\Sigma; \mathbb{C}^4)$ and $\operatorname{ran}M(\lambda) \subset \operatorname{ran}\Gamma_1 \subset H^{1/2}(\Sigma; \mathbb{C}^4)$.

To see that $\gamma(\lambda) : H^{1/2}(\Sigma; \mathbb{C}^4) \to H^1(\mathbb{R}^3 \setminus \Sigma; \mathbb{C}^4)$ is bounded it suffices to show that $\gamma(\lambda)$ is closed. Assume that $(\varphi_n) \subset H^{1/2}(\Sigma; \mathbb{C}^4)$ is a sequence such that

$$\varphi_n \to \varphi \quad \text{in } H^{1/2}(\Sigma; \mathbb{C}^4) \quad \text{and} \quad \gamma(\lambda)\varphi_n \to f \quad \text{in } H^1(\mathbb{R}^3 \setminus \Sigma; \mathbb{C}^4).$$

Clearly, $\varphi \in H^{1/2}(\Sigma; \mathbb{C}^4) = \operatorname{dom}\gamma(\lambda)$ and $\varphi_n \to \varphi$ in $L^2(\Sigma; \mathbb{C}^4)$. Since $\gamma(\lambda)$ is bounded in the respective L^2-spaces, we have $\gamma(\lambda)\varphi_n \to \gamma(\lambda)\varphi$ in $L^2(\mathbb{R}^3; \mathbb{C}^4)$. This implies $\gamma(\lambda)\varphi = f$ and therefore $\gamma(\lambda) : H^{1/2}(\Sigma; \mathbb{C}^4) \to H^1(\mathbb{R}^3\setminus\Sigma; \mathbb{C}^4)$ is closed and everywhere defined, and hence bounded.

Finally, since $\gamma(\lambda) : H^{1/2}(\Sigma; \mathbb{C}^4) \to H^1(\mathbb{R}^3 \setminus \Sigma; \mathbb{C}^4)$ is bounded, the continuity of the operator $M(\lambda) = \Gamma_1\gamma(\lambda)$ in $H^{1/2}(\Sigma; \mathbb{C}^4)$ follows from the continuity of the trace map. $\qquad\square$

Recall that $M(\lambda)$ is injective for any $\lambda \in \mathbb{C} \setminus \big((-\infty, -m] \cup [m, \infty)\big)$ and that its inverse is given by

$$(4.4) \qquad\qquad\qquad M(\lambda)^{-1} = -4\alpha \cdot \nu M(\lambda)\alpha \cdot \nu.$$

In particular, $M(\lambda)$ is bijective in $H^{1/2}(\Sigma; \mathbb{C}^4)$. For $\lambda \in (-m, m)$ equation (4.4) follows from the known identity $-4(M(\lambda)\alpha \cdot \nu)^2 = I_4$, which is stated, e.g., in [4, Lemma 2.2 (ii)] (note that $M(\lambda) = C_\sigma^\lambda$ in the notation of [4, Lemma 2.2]). For $\lambda \in \mathbb{C} \setminus \mathbb{R}$ the above formula (4.4) follows then by an analytic continuation argument.

Next we extend and transform the quasi boundary triple from Theorem 4.1 to an ordinary boundary triple for S^* using Proposition 2.5 and Theorem 2.7. Recall from (2.7) that $\mathscr{G}_0$ and $\mathscr{G}_1$ are defined by

$$(4.5) \qquad \mathscr{G}_0 := \operatorname{ran}(\Gamma_0 \upharpoonright \ker\Gamma_1) \quad \text{and} \quad \mathscr{G}_1 := \operatorname{ran}(\Gamma_1 \upharpoonright \ker\Gamma_0).$$

Lemma 4.3. *Let* $\{L^2(\Sigma; \mathbb{C}^4), \Gamma_0, \Gamma_1\}$ *be the quasi boundary triple in Theorem 4.1. Then the operator* $A_\infty := T \upharpoonright \ker\Gamma_1$ *is self-adjoint, the spaces* $\mathscr{G}_0$ *and* $\mathscr{G}_1$ *in (4.5) are*

$$(4.6) \qquad\qquad\qquad \mathscr{G}_0 = \mathscr{G}_1 = H^{1/2}(\Sigma; \mathbb{C}^4),$$

and Γ_0 *and* Γ_1 *have surjective extensions*

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

which are continuous with respect to the graph norm of $T_{\max}$.

Proof. First, it will be shown that A_∞ is self-adjoint. Because of Green's formula (Definition 2.1 (i)) we see immediately that A_∞ is symmetric. To prove that A_∞ is self-adjoint it suffices to check $\operatorname{ran} A_\infty = L^2(\mathbb{R}^3; \mathbb{C}^4)$, which by Theorem 2.3 (ii) is the case if and only if $\operatorname{ran} \gamma(0)^* \subset \operatorname{ran} M(0)$. The latter inclusion holds since $\operatorname{ran} \gamma(0)^* = \operatorname{ran} \Gamma_1 A_0^{-1} = H^{1/2}(\Sigma; \mathbb{C}^4)$ by (2.2) and (4.4) yields that $M(0)$ is bijective in $H^{1/2}(\Sigma; \mathbb{C}^4)$. Therefore A_∞ is self-adjoint.

In order to show (4.6) let $\varphi \in H^{1/2}(\Sigma; \mathbb{C}^4)$ and choose functions $f_\pm \in H^1(\Omega_\pm; \mathbb{C}^4)$ with $f_\pm|_\Sigma = \mp \frac{1}{2} i\alpha \cdot \nu\varphi$. Then $f = f_+ \oplus f_- \in \ker \Gamma_1$ and $\Gamma_0 f = \varphi$, and hence $\mathscr{G}_0 = H^{1/2}(\Sigma; \mathbb{C}^4)$. To show the claim on $\mathscr{G}_1$ consider $\varphi \in H^{1/2}(\Sigma; \mathbb{C}^4)$ and choose $f \in H^1(\mathbb{R}^3; \mathbb{C}^4)$ with $f|_\Sigma = \varphi$. Then $f \in \ker \Gamma_0$ and $\Gamma_1 f = f|_\Sigma = \varphi$. Hence (4.6) is shown.

The last assertion on the surjective extensions of Γ_0 and Γ_1 is now an immediate consequence of Proposition 2.5. $\qquad\square$

Next we discuss the extensions of the γ-field and the Weyl function of the quasi boundary triple $\{L^2(\Sigma; \mathbb{C}^4), \Gamma_0, \Gamma_1\}$.

Proposition 4.4. *Let* $\{L^2(\Sigma; \mathbb{C}^4), \Gamma_0, \Gamma_1\}$ *be the quasi boundary triple from Theorem 4.1 with corresponding γ-field γ and Weyl function M. Then the following assertions hold for all $\lambda \in \rho(A_0)$:*

(i) *The values of the γ-field admit continuous extensions*

$$\widetilde{\gamma}(\lambda) = \left(\widetilde{\Gamma}_0 \upharpoonright \ker(T_{\max} - \lambda)\right)^{-1} : H^{-1/2}(\Sigma; \mathbb{C}^4) \to L^2(\mathbb{R}^3; \mathbb{C}^4).$$

(ii) *The values of the Weyl function admit continuous extensions*

$$\widetilde{M}(\lambda) = \widetilde{\Gamma}_1 \left(\widetilde{\Gamma}_0 \upharpoonright \ker(T_{\max} - \lambda)\right)^{-1} : H^{-1/2}(\Sigma; \mathbb{C}^4) \to H^{-1/2}(\Sigma; \mathbb{C}^4).$$

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

(4.7) $$\left(\varphi, \widetilde{M}(\lambda)\psi\right)_{1/2 \times -1/2} = \left(M(\overline{\lambda})\varphi, \psi\right)_{1/2 \times -1/2}.$$

(iii) *The operators*

$$\widetilde{M}(\lambda)^2 - \frac{1}{4} I_4 : H^{-1/2}(\Sigma; \mathbb{C}^4) \to H^{1/2}(\Sigma; \mathbb{C}^4)$$

are well-defined and bounded. In particular, $M(\lambda)^2 - \frac{1}{4} I_4$ is compact in $H^{1/2}(\Sigma; \mathbb{C}^4)$.

Proof. Proposition 2.6 implies the existence and continuity of $\widetilde{\gamma}(\lambda)$ and $\widetilde{M}(\lambda)$ in (i) and (ii). In order to show (4.7) let $\varphi, \psi \in H^{1/2}(\Sigma; \mathbb{C}^4)$. Making use of (2.4) we find

$$\begin{aligned}
\left(\varphi, \widetilde{M}(\lambda)\psi\right)_{1/2 \times -1/2} &= \left((I_4 - \Delta_\Sigma)^{1/4}\varphi, (I_4 - \Delta_\Sigma)^{-1/4}\widetilde{M}(\lambda)\psi\right)_\Sigma \\
&= \left(\varphi, M(\lambda)\psi\right)_\Sigma = \left(M(\overline{\lambda})\varphi, \psi\right)_\Sigma \\
&= \left((I_4 - \Delta_\Sigma)^{1/4} M(\overline{\lambda})\varphi, (I_4 - \Delta_\Sigma)^{-1/4}\psi\right)_\Sigma \\
&= \left(M(\overline{\lambda})\varphi, \psi\right)_{1/2 \times -1/2}.
\end{aligned}$$

A density argument yields (4.7).

To prove item (iii) we first consider the case $\lambda = 0$. Note that equation (4.4) and $(\alpha \cdot \nu)^2 = I_4$ imply

$$(4.8) \qquad M(0)^2 - \frac{1}{4} I_4 = M(0)\alpha \cdot \nu \big(\alpha \cdot \nu M(0) + M(0)\alpha \cdot \nu \big).$$

According to [33, Proposition 2.8] the operator

$$(4.9) \qquad \mathcal{A} := \alpha \cdot \nu M(0) + M(0)\alpha \cdot \nu : H^{1/2}(\Sigma; \mathbb{C}^4) \to H^{1/2}(\Sigma; \mathbb{C}^4)$$

admits a bounded extension $\widetilde{\mathcal{A}} : H^{-1/2}(\Sigma; \mathbb{C}^4) \to H^{1/2}(\Sigma; \mathbb{C}^4)$. This and (4.8) show assertion (iii) for $\lambda = 0$.

Let now $\lambda \in \rho(A_0)$ be arbitrary. The identity (2.4) yields for $\varphi \in H^{1/2}(\Sigma; \mathbb{C}^4)$

(4.10)
$$\left(M(\lambda)^2 - \frac{1}{4} \right) \varphi = \big(M(0) + \lambda \gamma(0)^* \gamma(\lambda) \big)^2 \varphi - \frac{1}{4}\varphi$$

$$= \left(M(0)^2 - \frac{1}{4} \right) \varphi + \lambda M(0)\gamma(0)^* \gamma(\lambda)\varphi + \lambda \gamma(0)^* \gamma(\lambda) M(0)\varphi$$

$$+ \big(\lambda \gamma(0)^* \gamma(\lambda) \big)^2 \varphi.$$

From (2.2) we get

$$\operatorname{ran} \gamma(0)^* = \operatorname{ran} \big(\Gamma_1 A_0^{-1} \big) = H^{1/2}(\Sigma; \mathbb{C}^4).$$

Hence, the closed graph theorem implies that $\gamma(0)^* : L^2(\mathbb{R}^3; \mathbb{C}^4) \to H^{1/2}(\Sigma; \mathbb{C}^4)$ is continuous. Using item (i) of this proposition we see that $\gamma(0)^* \gamma(\lambda)$ admits the continuous extension

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

Moreover, since $M(0)$ has the continuous extension $\widetilde{M}(0)$ in $H^{-1/2}(\Sigma; \mathbb{C}^4)$ and $M(0)^2 - \frac{1}{4} I_4$ has a continuous extension from $H^{-1/2}(\Sigma; \mathbb{C}^4)$ to $H^{1/2}(\Sigma; \mathbb{C}^4)$ by the previous considerations, equation (4.10) yields finally the statement of assertion (iii) for all $\lambda \in \rho(A_0)$.

Finally, since Σ is compact, the embedding $\iota : H^{1/2}(\Sigma; \mathbb{C}^4) \to H^{-1/2}(\Sigma; \mathbb{C}^4)$ is compact. Therefore, the mapping

$$M(\lambda)^2 - \frac{1}{4} = \left(\widetilde{M}(\lambda)^2 - \frac{1}{4} \right) \iota$$

is compact in $H^{1/2}(\Sigma; \mathbb{C}^4)$. $\qquad\qquad\square$

Eventually, we provide a transformation of the quasi boundary triple from Theorem 4.1 to an ordinary boundary triple. This is an immediate consequence of Theorem 2.7 for the special choice $\iota_\pm = (I_4 - \Delta_\Sigma)^{\pm 1/4}$ and $\mu = 0 \in \rho(A_0)$, but for the convenience of the reader we provide also a short direct proof. In order to define the transformed boundary mappings recall that the direct sum decomposition

$$(4.11) \qquad\qquad \operatorname{dom} T_{\max} = \operatorname{dom} A_0 \dot{+} \ker T_{\max}$$

holds, as $0 \in \rho(A_0)$.

Theorem 4.5. *Let S be the symmetric operator in* (3.8) *with adjoint $S^* = T_{\max}$ in* (3.7). *Moreover, let $\{L^2(\Sigma; \mathbb{C}^4), \Gamma_0, \Gamma_1\}$ be the quasi boundary triple from Theorem 4.1, let $\widetilde{\Gamma}_0$ be the extension of Γ_0 from Lemma 4.3, and define the mappings $\Upsilon_0, \Upsilon_1 : \operatorname{dom} T_{\max} \to L^2(\mathbb{R}^3; \mathbb{C}^4)$ by*

$$\Upsilon_0 f := (I_4 - \Delta_\Sigma)^{-1/4} \widetilde{\Gamma}_0 f \quad and \quad \Upsilon_1 f := (I_4 - \Delta_\Sigma)^{1/4} \Gamma_1 f_0,$$

where $f = f_0 + f_1 \in \operatorname{dom} A_0 \dotplus \ker T_{\max} = \operatorname{dom} T_{\max}$. Then $\{L^2(\Sigma; \mathbb{C}^4), \Upsilon_0, \Upsilon_1\}$ is an ordinary boundary triple for $S^* = T_{\max}$ with $S^* \upharpoonright \ker \Upsilon_0 = T \upharpoonright \ker \Gamma_0 = A_0$.

Proof. First we verify that Green's identity is true. Assume that $f, g \in \operatorname{dom} T \subset \operatorname{dom} T_{\max}$ and decompose these functions with respect to (4.11) as $f = f_0 + f_1$ and $g = g_0 + g_1$ with $f_0, g_0 \in \operatorname{dom} A_0$ and $f_1, g_1 \in \ker T$. Using the self-adjointness of the free Dirac operator A_0 and $T f_1 = T g_1 = 0$ we deduce then

$$(Tf, g)_{\mathbb{R}^3} - (f, Tg)_{\mathbb{R}^3} = (A_0 f_0, g_0)_{\mathbb{R}^3} + (T f_0, g_1)_{\mathbb{R}^3} - (f_0, A_0 g_0)_{\mathbb{R}^3} - (f_1, T g_0)_{\mathbb{R}^3}$$
$$= (T f_0, g_1)_{\mathbb{R}^3} - (f_0, T g_1)_{\mathbb{R}^3} + (T f_1, g_0)_{\mathbb{R}^3} - (f_1, T g_0)_{\mathbb{R}^3}.$$

Employing now Theorem 4.1 and $\Gamma_0 f_0 = \Gamma_0 g_0 = 0$, as $f_0, g_0 \in \operatorname{dom} A_0 = \ker \Gamma_0$, we get

$$(Tf, g)_{\mathbb{R}^3} - (f, Tg)_{\mathbb{R}^3}$$
$$= (\Gamma_1 f_0, \Gamma_0 g_1)_\Sigma - (\Gamma_0 f_0, \Gamma_1 g_1)_\Sigma + (\Gamma_1 f_1, \Gamma_0 g_0)_\Sigma - (\Gamma_0 f_1, \Gamma_1 g_0)_\Sigma$$
$$= (\Gamma_1 f_0, \Gamma_0 g)_\Sigma - (\Gamma_0 f, \Gamma_1 g_0)_\Sigma.$$

The self-adjointness of $(I_4 - \Delta_\Sigma)^{\pm 1/4}$ implies eventually

$$(Tf, g)_{\mathbb{R}^3} - (f, Tg)_{\mathbb{R}^3} = \left((I_4 - \Delta_\Sigma)^{1/4} \Gamma_1 f_0, (I_4 - \Delta_\Sigma)^{-1/4} \Gamma_0 g\right)_\Sigma$$
$$- \left((I_4 - \Delta_\Sigma)^{-1/4} \Gamma_0 f, (I_4 - \Delta_\Sigma)^{1/4} \Gamma_1 g_0\right)_\Sigma$$
$$= (\Upsilon_1 f, \Upsilon_0 g)_\Sigma - (\Upsilon_0 f, \Upsilon_1 g)_\Sigma.$$

Since $C^\infty(\overline{\Omega_+}; \mathbb{C}^4) \oplus C^\infty(\overline{\Omega_+}; \mathbb{C}^4) \subset \operatorname{dom} T$ is dense in $\operatorname{dom} T_{\max}$ by Lemma 3.2 and $\widetilde{\Gamma}_0, \Gamma_1$ are continuous with respect to the graph norm by Lemma 4.3 we conclude that Green's identity holds for all $f, g \in \operatorname{dom} T_{\max}$.

To see that (Υ_0, Υ_1) is surjective let $\varphi, \psi \in L^2(\Sigma; \mathbb{C}^4)$ arbitrary, but fixed. Since $\operatorname{ran} \widetilde{\Gamma}_0 = H^{-1/2}(\Sigma; \mathbb{C}^4)$ by Lemma 4.3 there exists $g \in \operatorname{dom} \widetilde{\Gamma}_0 = \operatorname{dom} T_{\max}$ such that

$$\Upsilon_0 g = (I_4 - \Delta_\Sigma)^{-1/4} \widetilde{\Gamma}_0 g = \varphi.$$

Next, choose some $h \in \operatorname{dom} A_0$ which satisfies

$$\Upsilon_1 h = (I_4 - \Delta_\Sigma)^{1/4} \Gamma_1 h = \psi - \Upsilon_1 g.$$

Since $h \in \operatorname{dom} A_0 = \ker \Gamma_0$ we have, in particular, $\Upsilon_0 h = 0$. Thus, the function $f := g + h \in \operatorname{dom} T_{\max}$ fulfills $\Upsilon_0 f = \varphi$ and $\Upsilon_1 f = \psi$, which shows that (Υ_0, Υ_1) is surjective.

It remains to show that $T_{\max} \upharpoonright \ker \Upsilon_0$ is self-adjoint. With the help of Green's identity, which is already proved, it is easy to see that $T_{\max} \upharpoonright \ker \Upsilon_0$ is symmetric. Moreover, the self-adjoint free Dirac operator is contained in $T_{\max} \upharpoonright \ker \Upsilon_0$. Thus, these operators must coincide. Therefore, the triple $\{L^2(\Sigma; \mathbb{C}^4), \Upsilon_0, \Upsilon_1\}$ fulfills all conditions to be an ordinary boundary triple for $S^* = T_{\max}$ in the sense of Definition 2.1 and the proof of this theorem is finished. $\square$

5. DIRAC OPERATORS WITH ELECTROSTATIC δ-SHELL INTERACTIONS

In this section we define and investigate Dirac operators A_η with δ-shell interactions supported on the closed and bounded C^2-surface $\Sigma \subset \mathbb{R}^3$ with interaction strength $\eta \in \mathbb{R}$. In particular, we treat the case of the critical interaction strength $\eta = \pm 2$, for which self-adjointness and other spectral properties of $A_{\pm 2}$ were not obtained so far. The strategy is as follows: Using the quasi boundary triple from Theorem 4.1 and the transformed ordinary boundary triple from Theorem 4.5 with the corresponding transformed parameter $\Theta_1(\pm 2)$, cf. (2.9), we identify the closure of $A_{\pm 2}$ with the closure of $\Theta_1(\pm 2)$, which turns out to be self-adjoint in $L^2(\Sigma; \mathbb{C}^4)$. Making use of the corresponding Weyl functions and by constructing suitable singular sequences we prove some spectral results for $\overline{A_{\pm 2}}$ in Theorem 5.7.

We start with the definition of Dirac operators with an electrostatic δ-shell interaction of constant strength.

Definition 5.1. *Let $\{L^2(\Sigma; \mathbb{C}^4), \Gamma_0, \Gamma_1\}$ be the quasi boundary triple from Theorem 4.1 for $S^* = T_{\max} = \overline{T}$ with T in (4.1) and let $\eta \in \mathbb{R}$. Then the Dirac operator A_η with an electrostatic δ-shell interaction of strength η is defined by*

$$(5.1) \qquad A_\eta := T \restriction \ker(\Gamma_0 + \eta \Gamma_1),$$

that is,

$$A_\eta f = (-i\alpha \cdot \nabla + m\beta)f_+ \oplus (-i\alpha \cdot \nabla + m\beta)f_-,$$

$$\operatorname{dom} A_\eta = \left\{ f = f_+ \oplus f_- \in \operatorname{dom} T : \tfrac{\eta}{2}(f_+|_\Sigma + f_-|_\Sigma) = -i\alpha \cdot \nu(f_+|_\Sigma - f_-|_\Sigma) \right\}.$$

It follows immediately from (5.1) and Green's identity that A_η is symmetric for any $\eta \in \mathbb{R}$. In the following proposition we prove that A_η is self-adjoint for $\eta \neq \pm 2$; similar results have been obtained in [3, 7], but the approach used here also yields an additional regularity result for the functions in $\operatorname{dom} A_\eta$.

Proposition 5.2. *Let $\eta \in \mathbb{R} \setminus \{\pm 2\}$ and let A_η be defined as in Definition 5.1. Then A_η is self-adjoint and $\operatorname{dom} A_\eta \subset H^1(\mathbb{R}^3 \setminus \Sigma; \mathbb{C}^4)$.*

Proof. Let $\eta \in \mathbb{R} \setminus \{\pm 2\}$ be fixed and assume $\eta \neq 0$ (note that A_0 is the self-adjoint free Dirac operator). In order to show that the symmetric operator A_η is self-adjoint we verify $\operatorname{ran}(A_\eta - \lambda) = L^2(\mathbb{R}^3; \mathbb{C}^4)$ for all $\lambda \in \mathbb{C} \setminus \mathbb{R}$. For $\lambda \in \mathbb{C} \setminus \mathbb{R}$ we have $\lambda \notin \sigma_p(A_\eta)$ since A_η is symmetric. Hence, by Theorem 2.3 (ii) the operator $A_\eta - \lambda$ is surjective if $\operatorname{ran} \gamma(\overline{\lambda})^* \subset \operatorname{ran}\left(-\tfrac{1}{\eta} I_4 - M(\lambda)\right)$. Observe first that

$$\operatorname{ran} \gamma(\overline{\lambda})^* = \operatorname{ran}\left(\Gamma_1 (A_0 - \lambda)^{-1}\right) = H^{1/2}(\Sigma; \mathbb{C}^4)$$

by (2.2). To show that $H^{1/2}(\Sigma; \mathbb{C}^4) \subset \operatorname{ran}\left(-\tfrac{1}{\eta} I_4 - M(\lambda)\right)$ we note that

$$(5.2) \qquad \left(-\frac{1}{\eta} I_4 - M(\lambda)\right)\left(-\frac{1}{\eta} I_4 + M(\lambda)\right) = \left(\frac{1}{\eta^2} - \frac{1}{4}\right) I_4 + K(\lambda)$$

with $K(\lambda) := \tfrac{1}{4} I_4 - M(\lambda)^2$. By Proposition 4.4 (iii) the operator $K(\lambda)$ is compact in $H^{1/2}(\Sigma; \mathbb{C}^4)$. Moreover (5.2) is an injective operator as otherwise one of the symmetric operators $A_{\pm \eta}$ would have the non-real eigenvalue λ; cf. Theorem 2.3 (i). Thus, Fredholm's alternative and (5.2) yield

$$H^{1/2}(\Sigma; \mathbb{C}^4) = \operatorname{ran}\left(\left(\frac{1}{\eta^2} - \frac{1}{4}\right) I_4 + K(\lambda)\right) \subset \operatorname{ran}\left(-\frac{1}{\eta} I_4 - M(\lambda)\right).$$

From this and the above considerations it follows that A_η is self-adjoint for $\eta \in \mathbb{R} \setminus \{\pm 2\}$. The inclusion dom $A_\eta \subset H^1(\mathbb{R}^3 \setminus \Sigma; \mathbb{C}^4)$ is clear from (5.1). $\qquad \square$

Now we turn our attention to the critical case $\eta = \pm 2$ in Definition 5.1.

Proposition 5.3. *The operators*

$$(5.3) \qquad A_{\pm 2} = T \upharpoonright \ker(\Gamma_0 \pm 2\Gamma_1) = T \upharpoonright \ker\left(\Gamma_1 \pm \tfrac{1}{2}\Gamma_0\right)$$

are symmetric in $L^2(\mathbb{R}^3; \mathbb{C}^4)$ but not self-adjoint.

Proof. First, it follows from Green's identity (Definition 2.1 (i)) that $A_{\pm 2}$ are both symmetric. Now assume that A_2 is self-adjoint; the same argument applies to A_{-2}. Then $\operatorname{ran}(A_2 - \lambda) = L^2(\mathbb{R}^3; \mathbb{C}^4)$ for any $\lambda \in \mathbb{C} \setminus \mathbb{R}$ and hence Theorem 2.3 (ii) yields

$$(5.4) \qquad \operatorname{ran}\gamma(\overline{\lambda})^* = H^{1/2}(\Sigma; \mathbb{C}^4) \subset \operatorname{ran}\left(-\frac{1}{2}I_4 - M(\lambda)\right).$$

Since $\lambda \notin \sigma_{\mathrm{p}}(A_2)$ it follows that $-\frac{1}{2}I_4 - M(\lambda)$ is bijective in $H^{1/2}(\Sigma; \mathbb{C}^4)$.

We claim that (5.4) also implies $\operatorname{ran}\left(\frac{1}{2}I_4 - M(\lambda)\right) = H^{1/2}(\Sigma; \mathbb{C}^4)$. In fact, for $\varphi \in H^{1/2}(\Sigma; \mathbb{C}^4)$ we have $-2M(\lambda)\,\alpha \cdot \nu\,\varphi \in H^{1/2}(\Sigma; \mathbb{C}^4)$ since Σ is C^2-smooth and $M(\lambda)$ maps $H^{1/2}(\Sigma; \mathbb{C}^4)$ into $H^{1/2}(\Sigma; \mathbb{C}^4)$; cf. Proposition 4.2 (ii). By (5.4) there exists $\psi \in H^{1/2}(\Sigma; \mathbb{C}^4)$ such that

$$-2M(\lambda)\,\alpha \cdot \nu\,\varphi = \left(-\frac{1}{2} - M(\lambda)\right)\psi.$$

Applying on both sides $M(\lambda)\alpha \cdot \nu$ and using $(\alpha \cdot \nu)^2 = I_4$ and $(M(\lambda)\alpha \cdot \nu)^2 = -\frac{1}{4}I_4$ (see (4.4)) we find

$$\frac{1}{2}\varphi = -2(M(\lambda)\alpha \cdot \nu)^2\varphi = \left(-\frac{1}{2}M(\lambda)\alpha \cdot \nu - M(\lambda)\alpha \cdot \nu M(\lambda)(\alpha \cdot \nu)^2\right)\psi,$$

which is equivalent to $\varphi = \left(\frac{1}{2} - M(\lambda)\right)\alpha \cdot \nu\,\psi$, i.e. $\varphi \in \operatorname{ran}\left(\frac{1}{2}I_4 - M(\lambda)\right)$. We have shown $\operatorname{ran}\left(\frac{1}{2}I_4 - M(\lambda)\right) = H^{1/2}(\Sigma, \mathbb{C}^4)$, and as $\lambda \notin \sigma_{\mathrm{p}}(A_{-2})$ it follows that $\frac{1}{2}I_4 - M(\lambda)$ is bijective in $H^{1/2}(\Sigma; \mathbb{C}^4)$.

Since $-\frac{1}{2}I_4 - M(\lambda)$ and $\frac{1}{2}I_4 - M(\lambda)$ are both bijective on $H^{1/2}(\Sigma; \mathbb{C}^4)$ also $M(\lambda)^2 - \frac{1}{4}I_4$ is bijective on $H^{1/2}(\Sigma; \mathbb{C}^4)$. On the other hand, $M(\lambda)^2 - \frac{1}{4}I_4$ is compact in $H^{1/2}(\Sigma; \mathbb{C}^4)$ by Proposition 4.4 (iii). Hence, this operator can not be surjective; a contradiction. Therefore A_2 is not self-adjoint in $L^2(\mathbb{R}^3; \mathbb{C}^4)$. $\qquad \square$

In the following we complement Proposition 5.3, show that $A_{\pm 2}$ in (5.3) is essentially self-adjoint and determine the closure $\overline{A_{\pm 2}}$. For this we shall also consider the ordinary boundary triple $\{L^2(\Sigma; \mathbb{C}^4), \Upsilon_0, \Upsilon_1\}$ in Theorem 4.5 with γ-field

$$(5.5) \qquad \beta(\lambda) = \widetilde{\gamma}(\lambda)(I_4 - \Delta_\Sigma)^{1/4}, \qquad \lambda \in \rho(A_0),$$

and Weyl function

$$(5.6) \qquad \mathcal{M}(\lambda) = (I_4 - \Delta_\Sigma)^{1/4}\big(\widetilde{M}(\lambda) - \widetilde{M}(0)\big)(I_4 - \Delta_\Sigma)^{1/4}, \qquad \lambda \in \rho(A_0).$$

The corresponding parameter (here $\vartheta = \mp\frac{1}{2}$ by (5.3)) in Corollary 2.8 is then given by

$$\Theta_1(\pm 2) := -(I_4 - \Delta_\Sigma)^{1/4}\left(\pm\frac{1}{2} + M(0)\right)(I_4 - \Delta_\Sigma)^{1/4},$$

$$\operatorname{dom}\Theta_1(\pm 2) := H^1(\Sigma; \mathbb{C}^4),$$

that is,

$$(5.7) \qquad\qquad A_{\pm 2} = T_{\max} \upharpoonright \ker\left(\Upsilon_1 - \Theta_1(\pm 2)\Upsilon_0\right).$$

Clearly, $\Theta_1(\pm 2)$ is symmetric in $L^2(\Sigma; \mathbb{C}^4)$. Our next goal is to prove that $\Theta_1(\pm 2)$ is essentially self-adjoint and that $\overline{\Theta_1(\pm 2)}$ coincides with the maximal operator

$$(5.8)$$

$$\Theta_{\max}(\pm 2)\varphi := -(I_4 - \Delta_\Sigma)^{1/4}\left(\pm\frac{1}{2} + \widetilde{M}(0)\right)(I_4 - \Delta_\Sigma)^{1/4}\varphi,$$

$$\operatorname{dom}\Theta_{\max}(\pm 2) := \left\{\varphi \in L^2(\Sigma; \mathbb{C}^4) : \left(\pm\frac{1}{2} + \widetilde{M}(0)\right)(I_4 - \Delta_\Sigma)^{1/4}\varphi \in H^{1/2}(\Sigma; \mathbb{C}^4)\right\}.$$

Lemma 5.4. *The operator $\Theta_1(\pm 2)$ is essentially self-adjoint in $L^2(\Sigma; \mathbb{C}^4)$ and $\overline{\Theta_1(\pm 2)} = \Theta_{\max}(\pm 2)$. In particular, $\Theta_{\max}(\pm 2)$ is self-adjoint.*

Proof. We prove the statement for $\eta = 2$, the case $\eta = -2$ is analogous. For the convenience of the reader we divide the proof in three steps.

Step 1. We check first that $\Theta_{\max}(2)$ is closed. For this let $(\varphi_n) \subset \operatorname{dom}\Theta_{\max}(2)$ such that $\varphi_n \to \varphi \in L^2(\Sigma; \mathbb{C}^4)$ and $\Theta_{\max}(2)\varphi_n \to \psi \in L^2(\Sigma; \mathbb{C}^4)$ as $n \to \infty$. Since $(I_4 - \Delta_\Sigma)^{-1/4} : L^2(\Sigma; \mathbb{C}^4) \to H^{1/2}(\Sigma; \mathbb{C}^4)$ is an isomorphism we find

$$(5.9) \qquad -\left(\frac{1}{2} + \widetilde{M}(0)\right)(I_4 - \Delta_\Sigma)^{1/4}\varphi_n \to (I_4 - \Delta_\Sigma)^{-1/4}\psi, \quad n \to \infty,$$

with respect to the $H^{1/2}$-norm, and hence also with respect to the $H^{-1/2}$-norm. On the other hand, since $(I_4 - \Delta_\Sigma)^{1/4} : L^2(\Sigma; \mathbb{C}^4) \to H^{-1/2}(\Sigma; \mathbb{C}^4)$ and $\widetilde{M}(0)$ is continuous in $H^{-1/2}(\Sigma; \mathbb{C}^4)$ by Proposition 4.4 (ii) we obtain

$$-\left(\frac{1}{2} + \widetilde{M}(0)\right)(I_4 - \Delta_\Sigma)^{1/4}\varphi_n \to -\left(\frac{1}{2} + \widetilde{M}(0)\right)(I_4 - \Delta_\Sigma)^{1/4}\varphi, \quad n \to \infty,$$

with respect to the $H^{-1/2}$-norm. Combining this with (5.9) the last observation leads to

$$-\left(\frac{1}{2} + \widetilde{M}(0)\right)(I_4 - \Delta_\Sigma)^{1/4}\varphi = (I_4 - \Delta_\Sigma)^{-1/4}\psi \in H^{1/2}(\Sigma; \mathbb{C}^4).$$

Therefore, $\varphi \in \operatorname{dom}\Theta_{\max}(2)$ and $\Theta_{\max}(2)\varphi = \psi$. Thus, $\Theta_{\max}(2)$ is closed.

Step 2. Let us now show the inclusion

$$(5.10) \qquad\qquad \Theta_{\max}(2) \subset \overline{\Theta_1(2)};$$

together with $\Theta_1(2) \subset \Theta_{\max}(2)$ and $\Theta_{\max}(2)$ closed from *Step 1* this yields

$$(5.11) \qquad\qquad \Theta_{\max}(2) = \overline{\Theta_1(2)}.$$

To prove (5.10) let $\varphi \in \operatorname{dom}\Theta_{\max}(2)$ and choose a sequence $(\psi_n) \subset H^1(\Sigma; \mathbb{C}^4)$ such that $\psi_n \to \varphi$ in $L^2(\Sigma; \mathbb{C}^4)$ as $n \to \infty$. We define

$$\varphi_n := \varphi + (I_4 - \Delta_\Sigma)^{-1/4} \left(\widetilde{M}(0) - \frac{1}{2} \right) (I_4 - \Delta_\Sigma)^{1/4}(\varphi - \psi_n).$$

It follows from

$$\varphi_n = (I_4 - \Delta_\Sigma)^{-1/4} \left(\frac{1}{2} + \widetilde{M}(0) \right) (I_4 - \Delta_\Sigma)^{1/4}\varphi$$

$$+ (I_4 - \Delta_\Sigma)^{-1/4} \left(\frac{1}{2} - M(0) \right) (I_4 - \Delta_\Sigma)^{1/4}\psi_n,$$

$\left(\frac{1}{2} + \widetilde{M}(0) \right)(I_4 - \Delta_\Sigma)^{1/4}\varphi \in H^{1/2}(\Sigma; \mathbb{C}^4)$ for $\varphi \in \operatorname{dom}\Theta_{\max}(2)$, Proposition 4.2 and the mapping properties of $(I_4 - \Delta_\Sigma)^{-1/4}$ that $\varphi_n \in H^1(\Sigma; \mathbb{C}^4) = \operatorname{dom}\Theta_1(2)$. Moreover, since $\widetilde{M}(0)$ is continuous in $H^{-1/2}(\Sigma; \mathbb{C}^4)$ we obtain

$$\varphi_n - \varphi = (I_4 - \Delta_\Sigma)^{-1/4} \left(\widetilde{M}(0) - \frac{1}{2} \right) (I_4 - \Delta_\Sigma)^{1/4}(\varphi - \psi_n) \to 0, \quad n \to \infty,$$

in $L^2(\Sigma; \mathbb{C}^4)$. Finally, since $\widetilde{M}(0)^2 - \frac{1}{4}I_4 : H^{-1/2}(\Sigma; \mathbb{C}^4) \to H^{1/2}(\Sigma; \mathbb{C}^4)$ is continuous by Proposition 4.4 (iii) we have

$$\Theta_{\max}(2)(\varphi-\varphi_n) = (I_4-\Delta_\Sigma)^{1/4} \left(\widetilde{M}(0)^2 - \frac{1}{4} \right) (I_4-\Delta_\Sigma)^{1/4}(\varphi-\psi_n) \to 0, \quad n \to \infty,$$

in $L^2(\Sigma; \mathbb{C}^4)$. In particular, as $\Theta_1(2) \subset \Theta_{\max}(2)$ we have $\Theta_1(2)\varphi_n \to \Theta_{\max}(2)\varphi$ as $n \to \infty$, and hence $\varphi \in \operatorname{dom}\overline{\Theta_1(2)}$ and $\overline{\Theta_1(2)}\varphi = \Theta_{\max}(2)\varphi$, i.e. (5.10) holds.

Step 3. Since $\Theta_1(2)$ is symmetric it follows from (5.11) that $\overline{\Theta_1(2)} = \Theta_{\max}(2)$ is a symmetric operator. It is also clear from (5.11) that $\Theta_1(2)^* = \Theta_{\max}(2)^*$. In order to conclude that $\Theta_{\max}(2)$ is self-adjoint it suffices to show the inclusion

$$(5.12) \qquad\qquad\qquad \Theta_1(2)^* \subset \Theta_{\max}(2).$$

For this let $\psi \in \operatorname{dom}\Theta_1(2)^*$ and $\varphi \in H^1(\Sigma; \mathbb{C}^4) = \operatorname{dom}\Theta_1(2)$. Making use of (4.7) we compute

$$\left(\Theta_1(2)^*\psi, \varphi \right)_\Sigma = \left(\psi, \Theta_1(2)\varphi \right)_\Sigma$$

$$= \left(\psi, -(I_4 - \Delta_\Sigma)^{1/4} \left(\tfrac{1}{2} + M(0) \right) (I_4 - \Delta_\Sigma)^{1/4}\varphi \right)_\Sigma$$

$$= \left((I_4 - \Delta_\Sigma)^{1/4}\psi, - \left(\tfrac{1}{2} + M(0) \right) (I_4 - \Delta_\Sigma)^{1/4}\varphi \right)_{-1/2 \times 1/2}$$

$$= \left(- \left(\tfrac{1}{2} + \widetilde{M}(0) \right) (I_4 - \Delta_\Sigma)^{1/4}\psi, (I_4 - \Delta_\Sigma)^{1/4}\varphi \right)_{-1/2 \times 1/2}$$

$$= \left(- (I_4 - \Delta_\Sigma)^{-1/4} \left(\tfrac{1}{2} + \widetilde{M}(0) \right) (I_4 - \Delta_\Sigma)^{1/4}\psi, (I_4 - \Delta_\Sigma)^{1/2}\varphi \right)_\Sigma.$$

Since this is true for any $\varphi \in H^1(\Sigma; \mathbb{C}^4) = \operatorname{dom}(I_4 - \Delta_\Sigma)^{1/2}$ we conclude

$$-(I_4 - \Delta_\Sigma)^{-1/4} \left(\tfrac{1}{2} + \widetilde{M}(0) \right) (I_4 - \Delta_\Sigma)^{1/4}\psi \in \operatorname{dom}\left((I_4 - \Delta_\Sigma)^{1/2} \right)^* = H^1(\Sigma; \mathbb{C}^4)$$

and using the self-adjointness of $(I_4 - \Delta_\Sigma)^{1/2}$ we find

$$-(I_4 - \Delta_\Sigma)^{1/2} \left((I_4 - \Delta_\Sigma)^{-1/4} \left(\tfrac{1}{2} + \widetilde{M}(0) \right) (I_4 - \Delta_\Sigma)^{1/4}\psi \right) = \Theta_1(2)^*\psi.$$

This implies $\psi \in \operatorname{dom}\Theta_{\max}(2)$ and $\Theta_1(2)^*\psi = \Theta_{\max}(2)\psi$, and hence (5.12) holds. $\qquad\square$

In the following theorem we conclude that the symmetric operator $A_{\pm 2}$ is essentially self-adjoint and provide the domain of its closure, which is the proper self-adjoint realization of the Dirac operator with an electrostatic δ-shell interaction of strength ± 2. For that recall the definitions of the maximal Dirac operator $T_{\max}$ from (3.7), the extended boundary mappings $\widetilde{\Gamma}_0, \widetilde{\Gamma}_1$ in Lemma 4.3, and of the ordinary boundary triple $\{L^2(\Sigma; \mathbb{C}^4), \Upsilon_0, \Upsilon_1\}$ in Theorem 4.5.

Theorem 5.5. *The operator $A_{\pm 2}$ in (5.1) is essentially self-adjoint in $L^2(\mathbb{R}^3; \mathbb{C}^4)$ and the self-adjoint closure is given by*

$$(5.13) \qquad \overline{A_{\pm 2}} = T_{\max} \restriction \ker\left(\Upsilon_1 - \Theta_{\max}(\pm 2)\Upsilon_0\right) = T_{\max} \restriction \ker\left(\widetilde{\Gamma}_0 \pm 2\widetilde{\Gamma}_1\right).$$

Furthermore, $A_{\pm 2} \subsetneq \overline{A_{\pm 2}}$ and $\operatorname{dom} \overline{A_{\pm 2}} \not\subset H^1(\mathbb{R}^3 \setminus \Sigma; \mathbb{C}^4)$.

Proof. It follows from Lemma 5.4 and (5.7) that $A_{\pm 2}$ is essentially self-adjoint; cf. Corollary 2.8. Furthermore, since $\{L^2(\Sigma; \mathbb{C}^4), \Upsilon_0, \Upsilon_1\}$ is an ordinary boundary triple the closure $\overline{A_{\pm 2}}$ corresponds to the closure of the parameter $\Theta_1(\pm 2)$, that is,

$$\overline{A_{\pm 2}} = T_{\max} \restriction \ker\left(\Upsilon_1 - \Theta_{\max}(\pm 2)\Upsilon_0\right),$$

and $\overline{A_{\pm 2}}$ is self-adjoint in $L^2(\mathbb{R}^3; \mathbb{C}^4)$; cf. Lemma 5.4 and Corollary 2.8. The second equality in (5.13) can be checked directly and also follows from [11, Corollary 3.8]. The last assertions are consequences of Proposition 5.3. $\qquad\square$

Remark 5.6. The boundary condition $\pm 2\widetilde{\Gamma}_1 f = -\widetilde{\Gamma}_0 f$ for $f \in \operatorname{dom} T_{\max}$ in Theorem 5.5 is understood in $H^{-1/2}(\Sigma; \mathbb{C}^4)$ and with traces interpreted in $H^{-1/2}(\Sigma; \mathbb{C}^4)$ (cf. [33, Proposition 2.1]) it has the more explicit form

$$\pm(f_+|_\Sigma + f_-|_\Sigma) = -i\alpha \cdot \nu(f_+|_\Sigma - f_-|_\Sigma), \qquad f \in \operatorname{dom} T_{\max},$$

which is in accordance with Definition 5.1.

In the next theorem we discuss some spectral properties of the self-adjoint operator $\overline{A_{\pm 2}}$; the results complement those for A_η, $\eta \neq \pm 2$, from Theorem 1.1. We point out that, in contrast to the non-critical case $\eta \neq \pm 2$, in the critical case $\eta = \pm 2$ the interval $(-m, m)$ may contain essential spectrum, see also Theorem 5.9 below.

Theorem 5.7. *The following assertions hold for the self-adjoint operators $\overline{A_{\pm 2}}$:*

  (i) $(-\infty, -m] \cup [m, \infty) \subset \sigma_{\mathrm{ess}}(\overline{A_{\pm 2}})$;
 (ii) $\lambda \in (-m, m) \cap \sigma_{\mathrm{p}}(\overline{A_{\pm 2}})$ *if and only if* $0 \in \sigma_{\mathrm{p}}\left(1 \pm 2\widetilde{M}(\lambda)\right)$;
(iii) $\sigma_{\mathrm{disc}}(\overline{A_2}) = \sigma_{\mathrm{disc}}(\overline{A_{-2}})$ *and* $\sigma_{\mathrm{ess}}(\overline{A_2}) = \sigma_{\mathrm{ess}}(\overline{A_{-2}})$;
 (iv) *For $\lambda \in \rho(\overline{A_{\pm 2}})$ it holds that*

$$(\overline{A_{\pm 2}} - \lambda)^{-1} = (A_0 - \lambda)^{-1} \mp \widetilde{\gamma}(\lambda)\left(1 \pm 2\widetilde{M}(\lambda)\right)^{-1} 2\gamma(\bar{\lambda})^*.$$

Proof. (i) We verify the inclusion $(-\infty, -m] \cup [m, \infty) \subset \sigma_{\mathrm{ess}}(\overline{A_2})$; the inclusion for the strength -2 can be verified in the same way. For $\lambda \in (-\infty, -m] \cup [m, \infty)$ fixed we construct a singular sequence as follows. First of all, since Σ is compact we can choose $R > 0$ such that $\Sigma \subset B(0, R)$. Next, let $\chi \in C_c^\infty(\mathbb{R})$ be a cutoff function satisfying $\chi(r) = 1$ for $|r| < \frac{1}{2}$ and $\chi(r) = 0$ for $|r| > 1$ and set $x_n := (R + n^2)e_1$, where $e_1 = (1, 0, 0)^\top$. We define

$$(5.14) \quad \psi_n^\lambda(x) := \frac{1}{n^{3/2}}\chi\left(\frac{1}{n}|x - x_n|\right)e^{i\sqrt{\lambda^2 - m^2}x \cdot e_1}\left(\sqrt{\lambda^2 - m^2}\alpha_1 + m\beta + \lambda\right)\zeta,$$

where $\zeta \in \mathbb{C}^4$ is chosen such that $\left(\sqrt{\lambda^2 - m^2}\alpha_1 + m\beta + \lambda\right)\zeta \neq 0$. By construction we have $\operatorname{supp}\psi_n^\lambda \cap \Sigma = \emptyset$ and thus $\psi_n^\lambda \in \operatorname{dom} S \subset \operatorname{dom} \overline{A_2}$; cf. (3.8). Moreover, it holds

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

and since the supports of the ψ_n^λ are pairwise disjoint, the sequence (ψ_n^λ) converges weakly to zero. A straightforward computation shows

$$(\overline{A_2} - \lambda)\psi_n^\lambda(x) = (S - \lambda)\psi_n^\lambda(x)$$
$$= -\frac{i}{n^{5/2}}e^{i\sqrt{\lambda^2 - m^2}x \cdot e_1}\chi'\left(\frac{1}{n}|x - x_n|\right)\alpha \cdot \frac{x - x_n}{|x - x_n|}\left(\sqrt{\lambda^2 - m^2}\alpha_1 + m\beta + \lambda\right)\zeta$$
$$+ \frac{1}{n^{3/2}}\chi\left(\frac{1}{n}|x - x_n|\right)e^{i\sqrt{\lambda^2 - m^2}x \cdot e_1}$$
$$\cdot \left(\sqrt{\lambda^2 - m^2}\alpha_1 + m\beta - \lambda\right)\left(\sqrt{\lambda^2 - m^2}\alpha_1 + m\beta + \lambda\right)\zeta.$$

Note that $\left(\sqrt{\lambda^2 - m^2}\alpha_1 + m\beta - \lambda\right)\left(\sqrt{\lambda^2 - m^2}\alpha_1 + m\beta + \lambda\right) = 0$ by (1.3). Hence, we have

$$\|(\overline{A_2} - \lambda)\psi_n^\lambda\| \leq \frac{C}{n}\left(\int_{B(0,1)} |\chi'(|y|)|^2 \mathrm{d}y\right)^{1/2}$$

and therefore, $(\overline{A_2} - \lambda)\psi_n^\lambda \to 0$. Thus (ψ_n^λ) is a singular sequence for $\overline{A_2}$ and λ and hence $\lambda \in \sigma_{\mathrm{ess}}(\overline{A_2})$.

Assertions (ii) and (iv) follow from (2.11), (2.13), and the special form of the γ-field, Weyl function and $\Theta_{\max}(2)$ in (5.5), (5.6), and (5.8); cf. also [11, Corollary 3.14].

It remains to prove item (iii). Since $(-\infty, -m] \cup [m, \infty) \subset \sigma_{\mathrm{ess}}(\overline{A_{\pm 2}})$ by (i), it suffices to consider the case $\lambda \in (-m, m)$. Assume that $\lambda \in \sigma_{\mathrm{disc}}(\overline{A_2})$. Note first that the Birman Schwinger principle (2.12) implies

$$(5.15) \qquad\qquad 0 \in \sigma_{\mathrm{disc}}(\Theta_{\max}(2) - \mathcal{M}(\lambda)).$$

A simple calculation using (4.4) shows

$$-2M(\lambda)\alpha \cdot \nu\left(\frac{1}{2}I_4 + M(\lambda)\right) = -\left(-\frac{1}{2}I_4 + M(\lambda)\right)\alpha \cdot \nu,$$

where the operators $M(\lambda)$ and $\alpha \cdot \nu$ are both bijective in $H^{1/2}(\Sigma; \mathbb{C}^4)$. Hence we have

$$(5.16) \qquad -\left(\frac{1}{2}I_4 + \widetilde{M}(\lambda)\right)\left(2M(\lambda)\alpha \cdot \nu\right)' = -(\alpha \cdot \nu)'\left(-\frac{1}{2}I_4 + \widetilde{M}(\lambda)\right)$$

with bijective operators $(2M(\lambda)\alpha \cdot \nu)'$ and $(\alpha \cdot \nu)'$ in $H^{-1/2}(\Sigma; \mathbb{C}^4)$. From (5.16) we conclude

$$(5.17) \qquad \dim\ker(\Theta_{\max}(-2) - \mathcal{M}(\lambda)) = \dim\ker(\Theta_{\max}(2) - \mathcal{M}(\lambda))$$

and since $\operatorname{ran}(\Theta_{\max}(2) - \mathcal{M}(\lambda))$ is closed it follows from (5.16) that $\operatorname{ran}(\Theta_{\max}(-2) - \mathcal{M}(\lambda))$ is closed; thus we have

$$(5.18) \qquad\qquad 0 \in \sigma_{\mathrm{disc}}(\Theta_{\max}(-2) - \mathcal{M}(\lambda))$$

and hence $\lambda \in \sigma_{\text{disc}}(\overline{A_{-2}})$. In the same way one can show that $\lambda \in \sigma_{\text{disc}}(\overline{A_{-2}})$ implies $\lambda \in \sigma_{\text{disc}}(\overline{A_2})$.

Finally, we prove $\rho(\overline{A_2}) \cap (-m, m) = \rho(\overline{A_{-2}}) \cap (-m, m)$. By exclusion and the previous considerations this implies then $\sigma_{\text{ess}}(\overline{A_2}) = \sigma_{\text{ess}}(\overline{A_{-2}})$. Again, we only verify that $\rho(\overline{A_2}) \cap (-m, m) \subset \rho(\overline{A_{-2}}) \cap (-m, m)$, the other inclusion follows by symmetry.

Let $\lambda \in \rho(\overline{A_2}) \cap (-m, m)$. Then, by (2.10) we have that $0 \in \rho(\Theta_{\max}(2) - \mathcal{M}(\lambda))$. This implies that $\frac{1}{2} + \widetilde{M}(\lambda)$ is injective and that $H^{1/2}(\Sigma; \mathbb{C}^4) \subset \text{ran}\left(\frac{1}{2} + \widetilde{M}(\lambda)\right)$. Using equation (5.16) we deduce that $-\frac{1}{2} + \widetilde{M}(\lambda)$ is injective and that $H^{1/2}(\Sigma; \mathbb{C}^4) \subset \text{ran}\left(-\frac{1}{2} + \widetilde{M}(\lambda)\right)$, i.e. $0 \in \rho(\Theta_{\max}(-2) - \mathcal{M}(\lambda))$. Using again (2.10) we find $\lambda \in \rho(\overline{A_{-2}})$. $\square$

Remark 5.8. The functions ψ_n^λ in (5.14) are constructed as a solution of the equation $(-i\alpha \cdot \nu + m\beta)f = 0$ times a cutoff function such that $\text{supp}\,\psi_n^\lambda \cap \Sigma = \emptyset$. Because of the last property ψ_n^λ is contained in the domain of the symmetric operator S in (3.8), and hence (ψ_n^λ) is a singular sequence for any self-adjoint extension of S at λ. This implies that the set $(-\infty, -m] \cup [m, \infty)$ is contained in the essential spectrum of any self-adjoint extension of S; cf. [7, Theorem 4.4 (i)].

Note that Theorem 5.7 does not state that the spectrum of $\overline{A_{\pm 2}}$ in $(-m, m)$ is purely discrete; in fact essential spectrum may appear in the gap as well. In the special case when the interaction support contains a flat part it turns out in the next theorem that $0 \in \sigma_{\text{ess}}(\overline{A_{\pm 2}})$. Moreover, the functions in dom $\overline{A_{\pm 2}}$ do not possess any Sobolev regularity (of positive order); cf. Theorem 5.5.

Theorem 5.9. *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. Then the following assertions hold for the self-adjoint operators* $\overline{A_{\pm 2}}$:

(i) $0 \in \sigma_{\text{ess}}(\overline{A_{\pm 2}})$;
(ii) dom $\overline{A_{\pm 2}} \not\subset H^s(\mathbb{R}^3 \setminus \Sigma; \mathbb{C}^4)$ *for all $s > 0$.*

Proof. (i) The proof of this item is shown in an indirect way and is split into four steps. Again we restrict ourselves to the case $\eta = 2$. Let us assume that

$$0 \in \rho(\overline{A_2}) \cup \sigma_{\text{disc}}(\overline{A_2}) \tag{5.19}$$

and consider the operator $\Xi : L^2(\Sigma; \mathbb{C}^4) \to L^2(\Sigma; \mathbb{C}^4)$ defined by

$$\Xi\varphi := (I_4 - \Delta_\Sigma)^{1/4}\left(\widetilde{M}(0)^2 - \frac{1}{4}\right)(I_4 - \Delta_\Sigma)^{1/4}\varphi, \quad \varphi \in L^2(\Sigma; \mathbb{C}^4). \tag{5.20}$$

Step 1. Observe first that the operator Ξ is bounded and self-adjoint in $L^2(\Sigma; \mathbb{C}^4)$. In fact, $\widetilde{M}(0)^2 - \frac{1}{4}I_4 : H^{-1/2}(\Sigma; \mathbb{C}^4) \to H^{1/2}(\Sigma; \mathbb{C}^4)$ is bounded by Proposition 4.4 (iii) and hence Ξ is well defined and bounded in $L^2(\Sigma; \mathbb{C}^4)$. Moreover, since $M(0)$ is symmetric by (2.4) we have

$$\left(\Xi\varphi, \varphi\right) = \left(\left(M(0)^2 - \frac{1}{4}\right)(I_4 - \Delta_\Sigma)^{1/4}\varphi, (I_4 - \Delta_\Sigma)^{1/4}\varphi\right) \in \mathbb{R}$$

for $\varphi \in H^1(\Sigma; \mathbb{C}^4)$. By a density argument this extends to all $\varphi \in L^2(\Sigma; \mathbb{C}^4)$, so that Ξ is self-adjoint in $L^2(\Sigma; \mathbb{C}^4)$.

Step 2. We claim that the direct sum decomposition

$$(5.21) \qquad \ker \Xi = \ker \Theta_{\max}(2) \dotplus \ker \Theta_{\max}(-2)$$

holds. In particular, together with (5.17) for $\lambda = 0$, $\mathcal{M}(0) = 0$ and assumption (5.19) this implies that $\dim \ker \Xi < \infty$. Note first that the sum in (5.21) is direct since $\ker(\frac{1}{2} + \widetilde{M}(0)) \cap \ker(\frac{1}{2} - \widetilde{M}(0)) = \{0\}$. Next, the inclusion

$$(5.22) \qquad \ker \Theta_{\max}(2) \dotplus \ker \Theta_{\max}(-2) \subset \ker \Xi$$

follows easily from

$$
\begin{aligned}
(5.23) \qquad \Xi &= (I_4 - \Delta_\Sigma)^{1/4} \left(\frac{1}{2} + \widetilde{M}(0) \right) \left(-\frac{1}{2} + \widetilde{M}(0) \right) (I_4 - \Delta_\Sigma)^{1/4} \\
&= (I_4 - \Delta_\Sigma)^{1/4} \left(-\frac{1}{2} + \widetilde{M}(0) \right) \left(\frac{1}{2} + \widetilde{M}(0) \right) (I_4 - \Delta_\Sigma)^{1/4}.
\end{aligned}
$$

Furthermore, (5.23) also yields

$$\left(\widetilde{M}(0) - \frac{1}{2} \right) (I_4 - \Delta_\Sigma)^{1/4} \big(\ker \Xi \ominus \ker \Theta_{\max}(-2) \big) \subset \ker \left(\frac{1}{2} + \widetilde{M}(0) \right),$$

where $\ker \Xi \ominus \ker \Theta_{\max}(-2)$ denotes the orthogonal complement of $\ker \Theta_{\max}(-2)$ in the closed subspace $\ker \Xi$ of $L^2(\Sigma; \mathbb{C}^4)$. Since the operator

$$(\widetilde{M}(0) - \frac{1}{2})(I_4 - \Delta_\Sigma)^{1/4} \restriction \big(\ker \Xi \ominus \ker \Theta_{\max}(-2) \big)$$

is injective and $(I_4 - \Delta_\Sigma)^{1/4}$ is an isomorphism we find

$$
\begin{aligned}
\dim \ker \Xi &\leq \dim \ker \left(\frac{1}{2} + \widetilde{M}(0) \right) + \dim \ker \left(\frac{1}{2} - \widetilde{M}(0) \right) \\
&= \dim \ker \Theta_{\max}(2) + \dim \ker \Theta_{\max}(-2),
\end{aligned}
$$

which together with (5.22) implies (5.21).

Step 3. Now we consider the restriction of the self-adjoint operator Ξ onto the invariant subspace $\mathscr{H} := (\ker \Xi)^\perp$. From the above considerations it is clear that $\Xi \restriction_{\mathscr{H}}$ is a bounded, self-adjoint and injective operator in $\mathscr{H}$. We claim that the operator $(\Xi \restriction_{\mathscr{H}})^{-1}$ is bounded and everywhere defined in $\mathscr{H}$.

In the following let $P_\pm$ be the orthogonal projectors onto $\ker \Theta_{\max}(\pm 2)$ and observe that the self-adjoint operators

$$\Theta_{\max}(\pm 2) \restriction_{(1 - P_\pm) L^2(\Sigma; \mathbb{C}^4)}$$

are boundedly invertible in $(1 - P_\pm) L^2(\Sigma; \mathbb{C}^4)$; this follows from (5.19), Theorem 5.7 (iii) and (2.12). We shall denote these restrictions by $\Theta_{\max}^\pm(\pm 2)$. Let $\varphi \in \operatorname{ran} \Xi \subset \mathscr{H}$ and choose $\psi \in \mathscr{H}$ such that $\varphi = \Xi \psi$. It is easy to see that

$$\psi_\pm := -(I_4 - \Delta_\Sigma)^{-1/4} \left(\mp \frac{1}{2} + \widetilde{M}(0) \right) (I_4 - \Delta_\Sigma)^{1/4} \psi \in \operatorname{dom} \Theta_{\max}(\pm 2)$$

satisfy $\varphi = \Xi \psi = \Theta_{\max}(\pm 2) \psi_\pm$. Then we have $\psi_\pm = \Theta_{\max}^\pm(\pm 2)^{-1} \varphi + P_\pm \psi_\pm$ and hence

$$(5.24) \quad (\Xi \restriction_{\mathscr{H}})^{-1} \varphi = \psi = \psi_+ - \psi_- = \Theta_{\max}^+(2)^{-1} \varphi - \Theta_{\max}^-(-2)^{-1} \varphi + P_+ \psi_+ - P_- \psi_-.$$

Since $P_-\psi_- - P_+\psi_+ \in \ker \Xi = \mathscr{H}^\perp$ by (5.21) we find

$$\|(\Xi\restriction_{\mathscr{H}})^{-1}\varphi\|^2 \leq \|(\Xi\restriction_{\mathscr{H}})^{-1}\varphi\|^2 + \|P_-\psi_- - P_+\psi_+\|^2$$
$$= \left\|(\Xi\restriction_{\mathscr{H}})^{-1}\varphi + (P_-\psi_- - P_+\psi_+)\right\|^2$$
$$= \left\|\Theta_{\max}^+(2)^{-1}\varphi - \Theta_{\max}^-(-2)^{-1}\varphi\right\|^2$$

and as $\Theta_{\max}^\pm(\pm 2)^{-1}$ are bounded it follows that $(\Xi\restriction_{\mathscr{H}})^{-1}$ is bounded in $\mathscr{H}$. As $(\Xi\restriction_{\mathscr{H}})^{-1}$ is self-adjoint in $\mathscr{H}$ it is clear that it is defined on $\mathscr{H}$.

Step 4. Now we show that the assumption on $\Sigma_0 \subset \Sigma$ implies that there are infinitely many linearly independent functions which do not belong to the range of the operator Ξ in (5.20). This is a contradiction to the fact that $\dim \ker \Xi$ is finite and that $\Xi\restriction_{\mathscr{H}}$ is boundedly invertible with an inverse defined on all of $\mathscr{H}$; thus (5.19) can not be true.

As in the proof of Proposition 4.4 (iii) consider

$$\mathcal{A} = M(0)\alpha\cdot\nu + \alpha\cdot\nu M(0)$$

in $H^{1/2}(\Sigma;\mathbb{C}^4)$ and recall that this operator admits a bounded extension $\widetilde{\mathcal{A}} : H^{-1/2}(\Sigma;\mathbb{C}^4) \to H^{1/2}(\Sigma;\mathbb{C}^4)$; cf. [33, Proposition 2.8] or (4.9) and the discussion afterwards. Since $M(0)^2 - \frac{1}{4}I_4 = M(0)\alpha\cdot\nu\mathcal{A}$ (see the proof of Proposition 4.4 (iii)) a density argument leads to

$$\widetilde{M}(0)^2 - \frac{1}{4}I_4 = M(0)\alpha\cdot\nu\widetilde{\mathcal{A}}.$$

Since $M(0)$ and $\alpha\cdot\nu$ are bijective in $H^{1/2}(\Sigma;\mathbb{C}^4)$ and $(I_4-\Delta_\Sigma)^{1/4}$ is an isomorphism, we see by comparing with (5.20) that infinitely many linearly independent functions do not belong to $\operatorname{ran}\Xi$ if and only if infinitely many linearly independent functions do not belong to $\operatorname{ran}\widetilde{\mathcal{A}}$. This statement will be shown now.

Making use of (1.3) we see that $\mathcal{A}$ is an integral operator of the form

$$(5.25) \qquad \mathcal{A}\varphi(x) = \int_\Sigma K(x,z)\varphi(z)\mathrm{d}\sigma(z)$$

with integral kernel

$$K(x,z) = G_0(x-z)\alpha\cdot(\nu(z)-\nu(x)) + \frac{ie^{-m|x-z|}}{2\pi|x-z|^3}(1+m|x-z|)\nu(x)\cdot(x-z),$$

where G_0 is the Green's function for the resolvent of A_0 given by (3.5). Note that $|K(x,z)| \leq C|x-z|^{-1}$ and hence the integral operator in (5.25) is not singular (see also [3, equation (22) and Lemma 3.5] and [26, Proposition 3.11]). Let $\Sigma_1 \subset \Sigma$ such that $\overline{\Sigma_1} \subset \Sigma_0$. Note that $K(x,z) = 0$, if $x,z \in \Sigma_0$. Let $U_1 \subset \mathbb{R}^2$ and $\phi : U_1 \to \mathbb{R}^3$ be a linear affine function which parametrizes Σ_1, i.e. $\operatorname{ran}\phi = \Sigma_1$, and let $\varphi \in H^{1/2}(\Sigma;\mathbb{C}^4)$ be fixed. Since ν is constant on Σ_0 and $\overline{\Sigma_1} \subset \Sigma_0$, we see that the mapping $U_1 \ni u \mapsto K(\phi(u),z)$ is C^∞-smooth for any $z \in \Sigma$ and the mapping $\Sigma \ni z \mapsto K(\phi(u),z)$ 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

$$\partial_{u_j}(\mathcal{A}\varphi)(\phi(u)) = \int_\Sigma \partial_{u_j}K(\phi(u),z)\varphi(z)\mathrm{d}\sigma(z), \qquad j \in \{1,2\}.$$

Let us denote the elements of the 4×4-matrix $K(x,z)$ by $K_{lm}(x,z)$ and the elements of $\varphi(x) \in \mathbb{C}^4$ by $\varphi_m(x)$, $l,m \in \{1,2,3,4\}$. Then the last observation implies, in

particular, that

$$\|\partial_{u_j}\mathcal{A}\varphi\|^2_{L^2(\Sigma_1;\mathbb{C}^4)} = C_1 \int_{U_1} \left|\partial_{u_j}\mathcal{A}\varphi(\phi(u))\right|^2 \mathrm{d}u$$

$$= C_1 \int_{U_1} \left|\int_\Sigma \partial_{u_j} K(\phi(u),z)\varphi(z)\mathrm{d}\sigma(z)\right|^2 \mathrm{d}u$$

$$= C_1 \int_{U_1} \sum_{m,l=1}^{4} \left|\left(\partial_{u_j} K_{lm}(\phi(u),\cdot),\varphi_m\right)_{1/2\times-1/2}\right|^2 \mathrm{d}u$$

$$\leq C_1 \int_{U_1} \|\partial_{u_j} K(\phi(u),\cdot)\|^2_{H^{1/2}(\Sigma;\mathbb{C}^4)}\|\varphi\|_{H^{-1/2}(\Sigma;\mathbb{C}^4)}\mathrm{d}u$$

$$= C_2 \|\varphi\|_{H^{-1/2}(\Sigma;\mathbb{C}^4)}.$$

By continuity we obtain from this observation that $\widetilde{\mathcal{A}}\varphi|_{\Sigma_1} \in H^1(\Sigma_1;\mathbb{C}^4)$ for any $\varphi \in H^{-1/2}(\Sigma;\mathbb{C}^4)$. Thus, any $\psi \in H^{1/2}(\Sigma;\mathbb{C}^4)$ with $\psi|_{\Sigma_1} \notin H^1(\Sigma_1;\mathbb{C}^4)$ is not contained in ran $\mathcal{A}$. Hence, there are infinitely many linearly independent functions in $H^{1/2}(\Sigma;\mathbb{C}^4)$ that are not contained in ran $\widetilde{\mathcal{A}}$. The proof of item (i) is complete.

(ii) We show that $\mathrm{dom}\,\overline{A_2} \subset H^s(\mathbb{R}^3 \setminus \Sigma;\mathbb{C}^4)$ for some $s > 0$ implies that the resolvent difference $(\overline{A_2} - \lambda)^{-1} - (A_0 - \lambda)^{-1}$ is compact for $\lambda \in \mathbb{C} \setminus \mathbb{R}$. Since $\sigma_{\mathrm{ess}}(A_0) = (-\infty,-m] \cup [m,\infty) \neq \sigma_{\mathrm{ess}}(\overline{A_2})$ this is a contradiction.

For $s \in [0,1]$ consider the Hilbert spaces

$$\mathcal{H}^s := H^s(\mathbb{R}^3 \setminus \Sigma;\mathbb{C}^4) \cap \mathrm{dom}\,T_{\max}$$

equipped with the norms

$$\|f\|^2_{\mathcal{H}^s} := \|f\|^2_{H^s(\mathbb{R}^3\setminus\Sigma;\mathbb{C}^4)} + \|T_{\max}f\|^2_{L^2(\mathbb{R}^3;\mathbb{C}^4)}, \qquad f \in \mathcal{H}^s.$$

Then, the trace mappings $\Gamma_j^1 := \Gamma_j : H^1(\mathbb{R}^3 \setminus \Sigma;\mathbb{C}^4) = \mathcal{H}^1 \to H^{1/2}(\Sigma;\mathbb{C}^4)$ and $\Gamma_j^0 := \widetilde{\Gamma}_j : \mathrm{dom}\,T_{\max} = \mathcal{H}^0 \to H^{-1/2}(\Sigma;\mathbb{C}^4)$ are continuous for $j \in \{0,1\}$. By interpolation we get that also

$$\Gamma_j^s := \widetilde{\Gamma}_j \upharpoonright \mathcal{H}^s : \mathcal{H}^s \to H^{s-1/2}(\Sigma;\mathbb{C}^4)$$

is continuous for any $s \in [0,1]$.

Let us assume now that $\mathrm{dom}\,\overline{A_2} = \ker\left(\Upsilon_1 - \Theta_{\max}(2)\Upsilon_0\right) \subset \mathcal{H}^s$ for some $s > 0$. Then we have $\mathrm{dom}\,\Theta_{\max}(2) \subset H^s(\Sigma;\mathbb{C}^4)$ as $\Upsilon_0 = (I_4 - \Delta_\Sigma)^{-1/4}\widetilde{\Gamma}_0$. Let β and $\mathcal{M}$ be the γ-field and Weyl function corresponding to $\{L^2(\Sigma;\mathbb{C}^4),\Upsilon_0,\Upsilon_1\}$; cf. (5.5) and (5.6). For $\lambda \in \mathbb{C} \setminus \mathbb{R}$ we have

$$\mathrm{ran}\left(\Theta_{\max}(2) - \mathcal{M}(\lambda)\right)^{-1} = \mathrm{dom}\left(\Theta_{\max}(2) - \mathcal{M}(\lambda)\right) \subset H^s(\Sigma;\mathbb{C}^4)$$

and $\left(\Theta_{\max}(2) - \mathcal{M}(\lambda)\right)^{-1}$ is continuous in $L^2(\Sigma;\mathbb{C}^4)$. It follows that the operator

$$\left(\Theta_{\max}(2) - \mathcal{M}(\lambda)\right)^{-1} : L^2(\Sigma;\mathbb{C}^4) \to H^s(\Sigma;\mathbb{C}^4)$$

is closed and hence continuous. As the embedding $\iota_s : H^s(\Sigma;\mathbb{C}^4) \to L^2(\Sigma;\mathbb{C}^4)$ is compact we conclude that $(\Theta_{\max}(2)-\mathcal{M}(\lambda))^{-1}$ is a compact operator in $L^2(\Sigma;\mathbb{C}^4)$. Eventually (2.13) yields that

$$(\overline{A_2} - \lambda)^{-1} - (A_0 - \lambda)^{-1} = \beta(\lambda)\left(\Theta_{\max}(2) - \mathcal{M}(\lambda)\right)^{-1}\beta(\overline{\lambda})^*, \quad \lambda \in \mathbb{C} \setminus \mathbb{R},$$

is a compact operator in $L^2(\mathbb{R}^3;\mathbb{C}^4)$. This completes the proof. $\qquad\square$

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