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Spectral analysis of Dirac operators on bounded domains

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Title: Spectral analysis of Dirac operators on bounded domains

Abstract This thesis is devoted to the spectral study of two types of perturbation of the Dirac operator, which are singular from the point of view of scaling.

In the first part of this thesis, we consider the coupling of the Dirac operator with a combination of delta-shell interactions of electrostatic, Lorentz scalar, and magnetic type supported either on regular compact surfaces or locally deformed hyperplanes. We develop an approach based on regularization techniques that will allow us to describe the self-adjoint realization of the perturbed Dirac operator for any combination of the coupling constants. We then investigate the qualitative spectral properties of the various models using a Birman-Schwinger principle and a Krein-type formula relating the resolvent of the perturbed operator to that of the free Dirac operator, and we pay special attention to the case of critical combinations of coupling constants and those that give rise to the phenomenon of confinement.

In the second part, we study the coupling of the Dirac operator with non-critical combinations of delta interactions supported on non-regular compact surfaces. We first generalize the results obtained in the context of regular surfaces to the case of surfaces locally coincident with the graph of a Lipschitz function whose gradient is bounded and has vanishing mean oscillations. For this we use some techniques from harmonic analysis, potential theory and Fredholm's theory. Moreover, in the case of Hölder surfaces, we show how the smoothness of the surface supporting the delta interactions affects the Sobolev regularity of the domain of the operator under consideration. In a second step, we investigate delta-interactions supported on surfaces satisfying certain weak topological conditions. We first study the Dirac operator coupled with the electrostatic and Lorentz scalar delta-shell interactions supported on uniformly rectifiable surfaces. Under certain conditions on the coupling constants, we prove the self-adjointness fo the perturbed operator and we establish several spectral properties in the Lipschitz case. In particular, we determine the essential spectrum of the perturbed operator and we show that at most a finite number of eigenvalues can appear in the gap. Moreover, we fit these results to other delta-shell interactions and derive several models of Dirac operators that give rise to the confinement phenomenon.

In the third part of this thesis, we are concerned the study of the pseudodifferential properties of Poincaré-Steklov (PS) operators associated with the Dirac operator with the MIT bag boundary condition. First, we show that the PS operators fit well into the framework of classical pseudodifferential operators. Then, we study the PS operators from the point of view of semiclassical pseudodifferential operators, where the semiclassical parameter is given by the inverse of the mass. In particular, using some regularity properties of the MIT bag operator, we show that the PS operators are zero-order semiclassical pseudodifferential operators, and we determine their semiclassical principal symbols. In a second step, we study the Dirac operator coupled with a potential depending on an additional mass and supported outside a regular domain. When the additional mass is large enough, using the symbolic calculus and the properties of the PS operators, we establish a Krein-type formula relating the resolvent of the perturbed operator to that of the MIT bag operator. With its help, we show that the perturbed operator converges in the norm resolvent sense towards the MIT bag operator and give a sharp estimate of the convergence rate.

Keywords: Spectral analysis, Dirac operators, self-adjoint extensions, shell interactions, quantum confinement, Poincaré-Steklov operators, the MIT bag model, h-Pseudodifferential operators, large coupling limits.

Titre: Analyse spectrale d'opérateurs de Dirac sur des domaines bornés

Résumé Cette thèse est consacrée à l'étude spectrale de deux types de perturbations de l'opérateur libre de Dirac en dimension 3, qui sont singulières d'un point de vue de changement d'échelle.

Dans la première partie, nous nous intéressons au couplage de l'opérateur de Dirac avec une combinaison de delta interactions du type électrostatique, scalaire de Lorentz et magnétique, qui sont supportés soit sur des surfaces régulières et compactes ou sur des perturbations locales et régulières de l'hyperplan. Nous développons une approche basée sur des techniques de régularisations qui nous permettra de décrire pour toute combinaison des constantes d'interactions la réalisation auto-adjoint de l'opérateur considéré. Ensuite, nous étudions les propriétés spectrales qualitatives des différents modèles à l'aide d'un principe de Birman-Schwinger et une formule de Krein qui relie la résolvante de l'opérateur perturbé avec celle de l'opérateur libre de Dirac, et nous portons une attention particulière au cas des combinaisons critiques de constantes de couplage et à celles qui donnent lieu au phénomène de confinement.

Dans la deuxième partie, nous étudions le couplage de l'opérateur de Dirac avec une combinaison de delta interactions non critiques supportées sur des surfaces compactes non régulières. Dans un premier temps, nous généralisons les résultats obtenus dans le cadre des surfaces régulières au cas des surfaces qui coïncident localement avec le graphe d'une fonction dont le gradient est borné et a des oscillations moyennes nulles. Pour cela, nous utilisons des techniques d'analyse harmonique et la théorie du potentiel. De plus, nous mettons en lumière l'influence de la régularité de la surface supportant les delta interactions sur la régularité Sobolev du domaine de l'opérateur sous considération dans le cas des surfaces Hölderienne. Dans un second temps, nous considérons le cas de delta interactions supportées sur des surfaces satisfaisant certaines conditions topologiques faibles. Nous étudions d'abord l'opérateur de Dirac couplé avec les delta interactions électrostatique et scalaire de Lorentz supportées sur des surfaces uniformément rectifiables. Sous certains conditions sur les constantes de couplages, nous prouvons que l'opérateur perturbé est auto-adjoint et nous établissons plusieurs propriétés spectrales dans le cas Lipschitzienne. En particulier, on détermine le spectre essentiel de l'opérateur perturbé et on démontre qu'au plus un nombre fini de valeurs propres peut apparaître. Puis, nous adaptons ces résultats à d'autres interactions et nous dérivons plusieurs model d'opérateur de Dirac qui donnent lieu au phénomène de confinement.

Dans la troisième partie de cette thèse, nous nous intéressons à l'étude des propriétés pseudodifférentiel d'opérateurs de Poincaré-Steklov (PS) associés à l'opérateur de Dirac avec la condition au bord dite MIT bag. Dans un premier temps, nous montrons que ces derniers s'inscrivent bien dans le cadre des opérateurs pseudodifférentiel classiques. Ensuite, nous étudions les opérateurs PS d'un point de vue d'opérateurs pseudodifférentiel semiclassique, où le paramètre semi-classique est donné par l'inverse de la masse. En particulier, à l'aide de certaines propriétés de régularités de l'opérateur MIT bag, nous montrons que les opérateurs PS sont des pseudo semi-classique d'ordre zéro et nous déterminons également leurs symboles principaux semi-classique. Dans un second temps, nous étudions le couplage de l'opérateur de Dirac avec un potentiel supporté à l'extérieur d'un domaine régulier et qui dépend d'une masse supplémentaire. Quand cette dernière est suffisamment grande, en utilisant le calcul symbolique et les propriétés des opérateurs PS, nous établissons une formule de Krein reliant la résolvante de l'opérateur perturbé avec celle de l'opérateur MIT bag. De plus, nous montrons que l'opérateur perturbé converge au sens de la norme de la résolvante vers l'opérateur MIT bag et nous donnons une estimation précise du taux de convergence.

Mots-clés: Analyse spectrale, opérateurs de Dirac, extensions auto-adjointes, δ-interactions, opérateurs de Poincaré-Steklov, le model MIT bag, opérateurs h-Pseudodifferentiel, couplage

fort.

Título: Análisis espectral de operadores de Dirac en dominios acotados

Resumen Esta tesis está dedicada al estudio espectral de dos tipos de perturbaciones del operador libre de Dirac en dimensión 3, que son singulares desde el punto de vista de la escala.

En la primera parte, nos interesa el acoplamiento del operador de Dirac con una combinación de interacciones delta del tipo electrostático, escalar de Lorentz y magnético, que se apoyan bien en superficies regulares y compactas o en perturbaciones locales y regulares del hiperplano. Desarrollamos una aproximación basada en técnicas de regularización que nos permitirá describir para cualquier combinación de constantes de interacción la realización autoadjunta del operador considerado. A continuación, estudiamos las propiedades espectrales cualitativas de los diferentes modelos con la ayuda de un principio de Birmann-Schwinger y una fórmula de Krein que relaciona el resolvente del operador perturbado con el del operador libre de Dirac, y prestamos especial atención al caso de las combinaciones críticas de constantes de acoplamiento y a las que dan lugar al fenómeno de confinamiento.

En la segunda parte, estudiamos el acoplamiento del operador de Dirac con una combinación de interacciones no críticas delta soportadas en superficies compactas no regulares. En primer lugar, generalizamos los resultados obtenidos en el marco de las superficies regulares al caso de las superficies que coinciden localmente con la gráfica de una función cuyo gradiente está acotado y tiene oscilaciones medias nulas. Para ello, utilizamos técnicas de análisis armónico y la teoría del potencial. Además, destacamos la influencia de la regularidad de la superficie que soporta las interacciones delta en la regularidad de Sobolev del dominio del operador considerado en el caso de las superficies hölderianas. En un segundo paso, consideramos el caso de las interacciones delta soportadas en superficies que satisfacen ciertas condiciones topológicas débiles. En primer lugar, estudiamos el operador de Dirac acoplado con las interacciones electrostáticas delta y escalares de Lorentz soportadas en superficies uniformemente rectificables. Bajo ciertas condiciones sobre las constantes de acoplamiento, demostramos que el operador perturbado es autoadjunto y establecemos varias propiedades espectrales en el caso Lipschitziano. En particular, determinamos el espectro esencial del operador perturbado y mostramos que a lo sumo puede aparecer un número finito de valores propios. A continuación, adaptamos estos resultados a otras interacciones y derivamos varios modelos de operadores de Dirac que dan lugar al fenómeno de confinamiento.

En la tercera parte de esta tesis, estudiamos las propiedades pseudodiferenciales de los operadores de Poincaré-Steklov (PS) asociados al operador de Dirac con la condición de bolsa MIT. En primer lugar, mostramos que estos operadores encajan bien en el marco de los operadores pseudodiferenciales clásicos. A continuación, estudiamos los operadores PS desde el punto de vista de los operadores pseudodiferenciales semiclásicos, donde el parámetro semiclásico viene dado por la inversa de la masa. En particular, utilizando algunas propiedades de regularidad del MIT operador , mostramos que los operadores PS son pseudo-semiclásicos de orden cero y también determinamos sus símbolos principales semiclásicos. En un segundo paso, estudiamos el acoplamiento del operador de Dirac con un potencial soportado fuera de un dominio regular y que depende de una masa adicional. Cuando este último es lo suficientemente grande, utilizando el cálculo simbólico y las propiedades de los operadores PS, establecemos una fórmula de Krein que relaciona el resolvente del operador perturbado con el del MIT operador . Además, mostramos que el operador perturbado converge en el sentido de la norma del resolvente al del MIT operador y damos una estimación precisa de la tasa de convergencia.

Palabras clave: Análisis espectral, operadores de Dirac, extensiones autoadjuntas, δ-interacciones, operadores de Poincar'e-Steklov, el modelo del MIT bag, acoplamiento fuerte, operadores h-Pseudodiferenciales.

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Contents

Introduction

This introduction presents the context of δ-interactions for Dirac operators and Dirac operators on domains treated in this thesis. We first review the existing literature on the subject, then we briefly present our contributions.

The intertwining of mathematics with physics has led to their evolution over the centuries, and has resulted in a vast development of mathematics as well as many fields in physics. The development of the theory of (special and general) relativity and the theory of quantum mechanics made the beginning of the 20th century a turning point in the history of physics. Indeed, on the one hand, the relativistic Pythagorean energy relation $E = \sqrt{c^2p^2 + m^2c^4}$ (here E, p, $m > 0$ and c denote the energy, the momentum, the mass and the speed of light, respectively) of the special theory of relativity coherently describes the physical phenomena involving speeds close to that of light. On the other hand, with its fundamental Schrödinger equation, the theory of quantum mechanics describes the structure and the evolution in time and space of physical phenomena at the scale of the atom and below. Very quickly, physicists noticed that Schrödinger's equation does not respect covariance, a principle arising from special relativity, which leads them to the following question: *can we unify quantum mechanics and special relativity in order to describe the evolution of particles moving at great speeds (i.e., close to that of light)?*. Relativistic quantum mechanics thus began with the arrival of the Klein-Gordon equation. Indeed, starting from the classical relativistic energy-momentum relation $E^2 = c^2p^2 + m^2c^4$, and using the operators associated with the energy and the momentum, i.e.,

$$E \longrightarrow i\hbar\partial_t, \quad p \longrightarrow -i\hbar\nabla,$$

where $\hbar$ is the Planck's constant and ∇ is the gradient in $\mathbb{R}^3$, we end up with the Klein-Gordon equation

$$i\hbar\partial_t^2\psi(t,x) = (-c^2\hbar^2\Delta + m^2c^4)\psi(t,x), \quad t \in \mathbb{R},\ x \in \mathbb{R}^3,$$

where, ψ denotes the wave function and Δ is the Laplace operator. However, the Klein-Gordon equation is not consistent with a quantum mechanical interpretation since it has a second time derivative and does not have an L^2-conservation law. Indeed, to formulate an equation consistent with a quantum mechanical interpretation, one needs an equation that conserve the L^2-norm of the solution and such that the wave function at time $t = 0$ determines the wave function at all times. Paul Dirac then looked for a way to modify the Klein-Gordon equation to obtain an equation containing a first order derivative in time, like the Schrödinger equation, while respecting the covariance from the point of view of special relativity. The first step in his approach consists in setting a linear Hamiltonian in the time derivatives. It is normal to believe that the dependence of the Hamiltonian on the spatial derivatives will also be linear. With these considerations, we get the following equation

$$i\hbar\partial_t\psi(t,x) = -ic\hbar(\alpha_1\partial_{x_1} + \alpha_2\partial_{x_2} + \alpha_3\partial_{x_3})\psi(t,x) + \beta mc^2\psi(t,x), \quad t \in \mathbb{R},\ x \in \mathbb{R}^3,$$

where $\alpha = (\alpha_1, \alpha_2, \alpha_3)$ and β have to be determined from the energy-momentum relation. We then see that it is impossible for the coefficients α_j and β to be scalars, but it is possible if α_j and β are 4×4 matrices satisfying $\alpha_j^2 = \beta^2 = I_4$ and the anticommutation relationship

$$\alpha_j \alpha_k = -\alpha_k \alpha_j \text{ for } j \neq k, \quad \text{and} \quad \alpha_j \beta = -\beta \alpha_j.$$

Using the Pauli matrices $\sigma = (\sigma_1, \sigma_2, \sigma_3)$ defined by

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{0.0.1}$$

Dirac introduced the standard representation

$$\alpha_k = \begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{pmatrix} \text{ for } k = 1, 2, 3, \quad \beta = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}, \tag{0.0.2}$$

which satisfies the above relations. Thus, he introduced the equation which bears his name "*the Dirac equation*":

$$i\partial_t \varphi(t, x) = H\varphi(t, x), \quad \varphi(\cdot, x) : \mathbb{R}^3 \to \mathbb{C}^4,$$

which describes the motion of a free massive particle of spin-1/2 in $\mathbb{R}^3$ (typically relativistic electron or positron). Since then the Dirac equation has played an important role in several areas of physics and mathematics and has plenty of applications in quantum mechanics.

It is well-know that the study of spectral properties of an operators gives fundamental informations from point of view of quantum mechanics, since when the particle is subjected to the action of an external potential V, the linear Dirac equation $(H+V)\varphi = \lambda\varphi$ appears when looking for bound states of the particle; cf. [103] for example. The dynamical properties of the considered quantum system can be derived from the understanding of the spectral features of the resulting Hamiltonian.

In contrast to the Schrödinger operator, in which the free operator $-\Delta$ is nonnegative, the free Dirac operator H is unbounded both above and below, and its spectrum is $\mathrm{Sp}(H) = (-\infty, -m] \cup [m, \infty)$. Hence, one cannot define the Friedrich's extension for symmetric perturbations of H since they are not bounded below, and this creates challenges in the analysis of perturbations for the Dirac operator.

The aim of this doctoral thesis is to investigate the spectral properties of some particular perturbation of the Dirac operator $H = -i\alpha \cdot \nabla + m\beta$ (where from now on, we use the units $c = \hbar = 1$), which are singular from the point of view of scaling, and Dirac operators on domains of $\mathbb{R}^3$ with special boundary conditions.

In the first part of this thesis, we study several Dirac operators with δ-interactions supported on the boundaries of domains. Formally, for Ω an open set of $\mathbb{R}^3$, these operators act on $L^2(\mathbb{R}^3)^4$ and are defined by the following common (differential) expression

$$H_{a,\tau} := H + V_{a,\tau} = H + A_{a,\tau}\delta_{\partial\Omega}, \tag{0.0.3}$$

where $A_{a,\tau}$ is a bounded invertible, self-adjoint operator in $L^2(\partial\Omega)^4$, which depends on parameters $(a, \tau) \in \mathbb{R} \times \mathbb{R}^n$, $n \geqslant 1$, and the δ-potential is the Dirac distribution supported on $\partial\Omega$.

In the second part, we focus on the study of the spectral asymptotic of the coupling of the Dirac operator with a large mass potential supported on the exterior of a domain $\Omega \subset \mathbb{R}^3$, and we study its connection with the Dirac operator on Ω with the MIT bag boundary condition. There, the operator we are interested on acts on $L^2(\mathbb{R}^3)^4$, and is defined by the formal expression:

$$H_M := H + M\beta 1_{\mathbb{R}^3\setminus\overline{\Omega}}. \tag{0.0.4}$$

Shell interactions for Dirac operators. The study of Dirac operators coupled with interactions supported on sets of zero Lebesgue measure has a long story. As far as we know, in three dimension, [48] is first paper providing a rigorous mathematical analysis of relativistic shell interactions of the form (0.0.3), where J. Dittrich, P. Exner and P. Šeba studied in the case of the sphere (i.e., $\partial\Omega = \mathbb{S}^2_r$) the Dirac operator with electrostatic and Lorentz scalar δ-sphere interactions, defined by the expression:

$$H_{\epsilon,\mu} := H + (\epsilon I_4 + \mu\beta)\delta_{\partial\Omega}, \quad (\epsilon,\mu) \in \mathbb{R}^2.$$

Here, ϵI_4 is the electrostatic potential and $\mu\beta$ is the Lorentz scalar potential. In [48], the operators $H_{\epsilon,\mu}$ was defined as follows

$$H_{\epsilon,\mu}\phi = H\phi \quad \text{for } \phi \in C_0^\infty(\mathbb{R}^3 \setminus \mathbb{S}^2_r, \mathbb{C}^2) =: C_0^\infty(\mathbb{R}^3 \setminus \mathbb{S}^2_r)^4.$$

After reducing the problem to the one-dimensional case by using the spherical symmetry and the decomposition into spherical harmonics, the authors proved the essential self-adjointness of $H_{\epsilon,\mu}$ and constructed its self-adjoint extension for any $\epsilon, \mu \in \mathbb{R}$ such that $\epsilon^2 - \mu^2 \neq 4$. Moreover, they pointed out that under the assumption $\epsilon^2 - \mu^2 = -4$, the spherical shell (i.e., the boundary of Ω) becomes impenetrable barrier between the two regions Ω and $\mathbb{R}^3 \setminus \overline{\Omega}$. Physically, this means that at the time $t = 0$, if the particle in consideration (an electron for example) is in the region Ω (respectively in $\mathbb{R}^3 \setminus \overline{\Omega}$), then during the evolution in time, it cannot cross the surface $\partial\Omega$ to join the region $\mathbb{R}^3 \setminus \overline{\Omega}$ (respectively Ω) for all $t > 0$. Mathematically, this means that the Dirac operator in consideration decouples into a direct sum of two Dirac operators acting respectively on Ω and $\mathbb{R}^3 \setminus \overline{\Omega}$, with appropriate boundary conditions. In particular, when $\epsilon = 0$ and $\mu = 2$, this phenomenon has been known to physicists since the 1970's (cf.[44] and [70] for example); and its mathematical model described by the so-called Dirac operator with the MIT boundary conditions (see below for its rigorous definition). Shortly afterwards and independently, in his paper [49], F. Dominguez-Adame also considered the operator $H_{\epsilon,\mu}$ in the spherical case with a special attention to the study of bound and scattering states. A decade later, J. Shabani and A. Vyabandi [98] took over the spectral analysis of the Dirac operator $H_{\epsilon,\mu}$. In particular, they proved a resolvent formula for $H_{\epsilon,\mu}$ and studied the scattering theory of this model. Moreover, they investigated the non-relativistic limit, proving that the non-relativistic limit of $H_{\epsilon,0}$ and $H_{0,\mu}$ (i.e., when $\mu = 0$ and $\epsilon = 0$, respectively) yield the Schrödinger operator with δ-interactions.

Since the arguments used in the papers cited above are specific to δ-sphere interactions, it is not possible to extend them to more general domains. Because of that (but not only), the study of relativistic δ-interactions supported on general surfaces has known a long period of silence (24 years !), unlike its non-relativistic counterpart (i.e., Schrödinger operators with δ-shell interactions) where the approach involving a quadratic form is available to tackle such a problem. Indeed, to the best of our knowledge, since the publication of [48, 49], and apart from J. Shabani and A. Vyabandi paper [98], and the paper [5] where N. Arrizabalaga studied the self-adjointness of the Dirac operator with purely electrostatic δ-sphere interactions (i.e., $H_{\epsilon,0}$) via Hardy-Dirac inequalities, no progress has been made in the study of the spectral properties of Dirac operators with δ-interactions supported on general surfaces. This obstacle was finally broken by the arrival of the paper [10], where N. Arrizabalaga, A. Mas and L.

Vega developed a new strategy based on Fredholm theory and integral operators to prove the self-adjointness and to study the spectral properties of the Dirac operator coupled with a singular measure valued potential with respect to the Lebesgue measure. Indeed, instead of using Von Neuman's classical approach, in [10] the authors argued as follows. For Σ a closed surface in $\mathbb{R}^3$ (satisfying some assumption, e.g., Σ preserves Markov's inequality, Σ is locally the graph of a Lipschitz function from $\mathbb{R}^2$ to $\mathbb{R}^3$), σ is 2-dimensional Hausdorff measure restricted to Σ, and for V a generic $L^2(\Sigma,\sigma)^4$-valued potential, they considered the operator $T = H + V$ and looked for a domain $\mathscr{D} \subset L^2(\mathbb{R}^3)^4$ such that $(T, \mathscr{D})$ is self-adjoint. By assumption, for any $\varphi \in \mathscr{D}$, one has

$$V\varphi = -g \text{ for some } g \in L^2(\Sigma,\sigma)^4 \quad \text{and} \quad T\varphi = G \in L^2(\mathbb{R}^3)^4, \tag{0.0.5}$$

in the sense of distributions. From this, one see that $H\varphi = G + g\sigma$ must be satisfied in the sense of distributions, and thus φ must be expressed by taking the convolution of $G + g\sigma$ with the fondamental solution of H. This means that $\mathscr{D}$ is a subdomain of

$$X = \{\phi * (G + g) : G \in L^2(\mathbb{R}^3)^4 \text{ and } g \in L^2(\Sigma,\sigma)^4\},$$

where ϕ is given by

$$\phi(x) = \frac{e^{-m|x|}}{4\pi|x|}\left(m\beta + (1 + m|x|)i\alpha \cdot \frac{x}{|x|^2}\right), \quad \text{for all } x \in \mathbb{R}^3 \setminus \{0\}. \tag{0.0.6}$$

Since the mapping $L^2(\mathbb{R}^3)^4 \ni G \longmapsto \phi * G$ defines the resolvent of H, and H defined in the first order Sobolev space $H^1(\mathbb{R}^3)^4$ is a self-adjoint operator, we see that

$$X = \{u + \phi * g : u \in H^1(\mathbb{R}^3)^4 \text{ and } g \in L^2(\Sigma,\sigma)^4\}, \tag{0.0.7}$$

and under the above assumption on Σ, the trace of u, $u_{|\Sigma}$, belongs to $L^2(\Sigma,\sigma)^4$, and it was shown in [10] that the mapping defined for $g \in L^2(\Sigma)^4$ by $\Phi[g] = \phi * g$, is indeed bounded from $L^2(\Sigma)^4$ to $L^2(\mathbb{R}^3)^4$. In order to ensure the self-adjointness of T, one needs to imposing some linear relations between $u_{|\Sigma}$ and g. One of these possibilities which was obtained in [10] reads as follows

Theorem 0.0.1. *[10, Theorem 2.1.] Given an operator $\Lambda : L^2(\Sigma,\sigma)^4 \longrightarrow L^2(\Sigma,\sigma)^4$ bounded, self-adjoint and with closed range. Define the domain*

$$\mathrm{dom}(T) = \left\{u + \phi * g : u \in H^1(\mathbb{R}^3)^4, g \in L^2(\Sigma)^4, u_{|\Sigma} = -\Lambda[g]\right\} \subset L^2(\mathbb{R}^3)^4.$$

If $V(u + \phi * g) = -g\sigma$ for $(u + \phi * g) \in \mathrm{dom}(T)$, then $T = H + V\sigma$ defined on $\mathrm{dom}(T)$ is essentially self-adjoint. Moreover, if Λ is Fredholm, then $(T, \mathrm{dom}(T))$ is self-adjoint.

The above theorem means in particular that, given V such that $V(u + \phi * g) = -g\sigma$, if we can find a suitable Fredholm and self-adjoint operator $\Lambda : L^2(\Sigma,\sigma)^4 \longrightarrow L^2(\Sigma,\sigma)^4$ such that $u_{|\Sigma} = -\Lambda[g]$, then $(T, \mathrm{dom}(T))$ is self-adjoint.

It is worth mentioning that, since the fundamental solution ϕ behaves like $|x|^{-2}$ when $|x|$ goes to 0, the mapping Φ has a jump at Σ. Indeed, it was shown in [10] that for Ω a smooth bounded domain with

$$\Omega_+ := \Omega \quad \Omega_- = \mathbb{R}^3 \setminus \overline{\Omega_+} \quad \text{and} \quad \Sigma := \partial\Omega,$$

and assuming that the δ-interactions are supported on Σ, then the nontangential limit $\Phi|^{\mathrm{nt}}_{\Omega_\pm}$ exists and is bounded in $L^2(\Sigma)^4$ and satisfies the following *Plemelj-Sokhotski* jump formula

$$\Phi|^{\mathrm{nt}}_{\Omega_\pm} = \mp\frac{i}{2}(\alpha \cdot N) + \mathscr{C}_\Sigma, \quad ((\alpha \cdot N)\mathscr{C}_\Sigma)^2 = -\frac{1}{4}I_4, \tag{0.0.8}$$

where N is the unit normal vector field at Σ which points outwards of Ω, and $\mathscr{C}_\Sigma$ is the Cauchy operator associated with H, defined for $g \in L^2(\Sigma)^4$ as the principal value $\mathscr{C}_\Sigma[g] = \mathrm{pv}(\phi * g)$. With the above properties in hand, for $\varphi = u + \Phi[g] \in X$, the authors defined the expression $\varphi\delta_\Sigma)$ as the distribution

$$\varphi\delta_\Sigma = \frac{1}{2}(\varphi|^{\mathrm{nt}}_{\Omega_+} + \varphi|^{\mathrm{nt}}_{\Omega_-}) = u_{|\Sigma} + \mathscr{C}_\Sigma[g].$$

Then, as an application of Theorem 0.0.1, the authors dealt in [10, 11] with the Dirac operator $H_{\epsilon,\mu}$ when the δ-interactions are supported on the boundary of a bounded C^2-smooth domain, and they proved that $H_{\epsilon,\mu}$ is self-adjoint when $\epsilon^2 - \mu^2 \neq 4$. Moreover, they have showed that the confinement stills occur when $\epsilon^2 - \mu^2 = -4$, generalizing the result of [48] for sufficiently regular surfaces. The same authors continued the spectral study of $H_{\epsilon,\mu}$, proving several symmetry relations on the point spectrum (where the algebraic identity (0.0.8) for the Cauchy-type operators play an important role), and showing an adapted Birman-Schwinger principle which gives a criterion for the existence of point spectrum in the gap $(-m, m)$. Moreover, in the case of the sphere, a deeper study of the point spectrum of $H_{\epsilon,\mu}$ had been carried out by the same authors in [11]. The study was then continued in [12] where an isoperimetric-type inequality for the admissible range of ϵ's for which $H_{\epsilon,0}$ (i.e., in the purely electrostatic case) generates pure point spectrum in $(-m, m)$ was obtained.

Since then, the mathematical study of Dirac operators gained a lot of attention and different approaches based on self-adjoint extensions of symmetric operators have been adapted and developed. Namely, the abstract theory of quasi boundary triples and their Weyl functions proposed by J. Behrndt, P. Exner, M. Holzmann and V. Lotoreichik in [16], where they studied the Dirac operators with electrostatic δ-shell interactions. The theory of quasi boundary triples is a systematic approach that gives suitable framework to describe self-adjoint extensions of a symmetric operator, study its self-adjointness and spectral properties. Using this approach, the authors of [16] were able to recover the result of [10] concerning the spectral properties of the operator $H_{\epsilon,0}$, proving the self-adjointness for all $\epsilon \neq \pm 2$. Moreover, they noticed that functions in $\mathrm{dom}(H_{\epsilon,0})$ have the H^1-Sobolev regularity, and they obtained a Krein-type resolvent formula, allowing them to study the scattering theory and asymptotic properties of the model.

We mention that the case $\epsilon = \pm 2$ (known as the critical interaction strengths) has been only considered in [10] when the δ-interactions are supported in an hyperplan (i.e., $\Sigma = \mathbb{R}^2 \times \{0\}$ for example), and it turned out that $H_{\pm 2,0}$ is essentially self-adjoint and the domain of $\overline{H_{\pm 2,0}}$ is completely different from the case $\epsilon \neq \pm 2$, moreover, the authors showed that 0 is an eigenvalue of $\overline{H_{\pm 2,0}}$ with infinite multiplicity. This gap has been covered for general bounded C^2-smooth domains by T. Ourmières-Bonafos and L. Vega in [90] and by J. Behrndt and M. Holzmann in [19] with different approaches. Indeed, in this particular case, it turns out that the restriction of $H_{\pm 2,0}$ on $H^1(\mathbb{R}^3 \setminus \Sigma)^4$ is essentially self-adjoint, and functions in the domain of the closure do not have the H^1-Sobolev regularity, and therefore, less regular comparing to the non critical case. Moreover, in [19] it is shown that if $\Sigma = \partial\Omega_+$ contains a flat part, then the point 0 belongs to the essential spectrum of $\overline{H_{\pm 2,0}}$, generalizing in this sense the result obtained in [10] in the case of hyperplans. A similar phenomenon appears when studying the operator $H_{\epsilon,\mu}$. In fact, in this case, the critical combinations of coupling constants are $\epsilon^2 - \mu^2 = 4$. The self-adjointness in this critical case was proved for the two dimensional analogue of $H_{\epsilon,\mu}$ in [22], where J. Behrndt, M. Holzmann, T. Ourmières-Bonafos and K. Pankrashkin considered δ-interactions supported on a smooth closed curve. Furthermore, by making use of complex analysis and periodic pseudodifferential operators techniques, they showed that

$$\mathrm{Sp_{ess}}(\overline{H_{\epsilon,\mu}}) = \big(-\infty, -m\big] \cup \left\{-\frac{m\mu}{\epsilon}\right\} \cup \big[m, +\infty\big). \tag{0.0.9}$$

Since 2014 (date of publication [10]), the literature around Dirac operators with δ-interactions supported on smooth compact surfaces has been enriched with the contribution of several authors, and several progresses have been made on this subject. The coupling $H + (\epsilon I_4 + \eta(\alpha \cdot N))\delta_\Sigma$ in the non critical case (i.e., $\epsilon^2 - \eta^2 \neq 4$) had been explored in [78], where the author used an appropriate change of gauge (given by a discontinuous gauge function across Σ) to prove that the latter operator is unitarily equivalent to the coupling $(H + \epsilon' I_4 \delta_\Sigma)$ for some $\epsilon' \neq \pm 2$; moreover, he also performed a spectral study of coupling $H + \lambda(\alpha \cdot N)\delta_\Sigma$ when λ is a C^1-smooth function along the boundary Σ. In [66] the eigenvalue asymptotics of Dirac operators with Lorentz scalar δ-interactions (when $\mu \neq \pm 2$) as the mass becomes large have been investigated, showing that the behaviour of the individual eigenvalues and their total number are governed by an effective Schrödinger operator on the boundary with an external Yang-Mills potential and a curvature-induced potential. In [20] a limiting absorption principle for the Dirac operator $H_{\epsilon,\mu}$ is obtained, and the completeness for the scattering couple $(H_{\epsilon,\mu}, H)$ $(\epsilon^2 - \mu^2 \neq 4)$ and a representation formula for the corresponding scattering matrix is shown. We also mention the survey [91] where the state of the art on the subject and the results obtained before 2020 are gathered and discussed.

We emphasize that the intentions related to the intensive study of relativistic δ-interactions are due not only to the mathematical challenges just mentioned above, but also for their applications in various areas of physics. On one hand, similarly to its non-relativistic counterpart, from the mathematical physics point of view, δ-shell potential are often used as idealized models for strongly localized electric or magnetic potentials. This fact has been proved mathematically in [79, 80], where A. Mas and F. Pizzichillo used the approach of [10, 11] and proved that $H_{\epsilon,0}$ and $H_{0,\mu}$ can be approximated in the strong resolvent sense by Dirac operators coupled with squeezed electrostatic and scalar potentials, respectively. However, the recovered coupling constant in the limit does depend nonlinearly on the potential, a phenomenon that was observed in [97], where P. Šeba studied the one dimensional version of this problem. We also mention that the exact solvability of relativistic quantum Hamiltonians describing such models has been (see, e.g., [48, 98, 49]) and still remains an interesting and open theoretical question for general surfaces. On the other hand, it is known that strong scalar coupling confine relativistic particles at high energies inside a bag (i.e., a bounded region of $\mathbb{R}^3$), and they are described by Dirac operators acting on domains; cf. [39, 44, 70]. In particular, when $\mu = 2$ the Dirac operator $H_{0,\mu}$ gives rise to the MIT bag operator mentioned above, and describes the confinement of quarks in 3D (dimension three). More recently, 2-dimensional massless Dirac operators on domains with boundary conditions have been used to describe the evolution of quasi-particles in *Dirac materials*, cf. [39]. All these physical motivations made the mathematical study of Dirac operators with δ-shell interactions a very important subject. Moreover, as already mentioned above, for some particular values of the parameters the phenomenon of confinement arises. Thereby, the Dirac operator under consideration decouples into the orthogonal sum of two Dirac operators acting respectively on $L^2(\Omega_+)^4$ and $L^2(\Omega_-)^4$, with appropriate boundary conditions, and this crucially gives the link between Dirac operators with boundary conditions and the Dirac operators with δ-interactions.

In the following two parts of this introduction, we will describe our main results from Chapters 2 and 3 on the study of Dirac operators with δ-shell interactions, which correspond to the results obtained in [29] and [30], respectively.

The case of smooth non-compact interaction supports (Chapter 2). For me, as a first step to get into this business, I considered in [29] δ-interactions supported on C^2-smooth (non) compact surfaces and I have taken up the strategy of [10] with the initial motivation of, on the one hand, closing the gap concerning self-adjointness in the critical case and, on the other hand, understanding the role played by the operator Λ (from Theorem 0.0.1) in both the critical and non-critical cases. My second motivation was to tackle the problem of characterizing the essential spectrum of the Dirac operator $H_{\epsilon,\mu}$ in the critical case in the three-dimensional case. Indeed, as I mentioned above the techniques used in [22] to prove (0.0.9) are specific to the bidimensional case and are no longer available in the three dimensional case. So I asked my self the following question:

(Q1) Given a smooth domain $\Omega \subset \mathbb{R}^3$ (bounded or not), and assuming that $\overline{H_{\epsilon,\mu}}$ is self-adjoint when $\epsilon^2 - \mu^2 = 4$, does (0.0.9) holds true?

Notice that when ϵ and μ run through the whole branch of the hyperbola $\epsilon^2 - \mu^2 = 4$ the point $-m\mu/\epsilon$ can take any value in the gap $(-m, m)$.

Let us now present the context we consider in Chapter 2 and summarize the main results obtained there. We assume that the open set Ω satisfies one of the following hypotheses:

(1) Ω is a C^2-bounded domain.

(2) $\Omega := \Omega_\nu := \{(x,t) \in \mathbb{R}^2 \times \mathbb{R} : t > \nu\phi(x)\}$, where $\nu \in \mathbb{R}$ and $\phi : \mathbb{R}^2 \to \mathbb{R}$ is a C^2-smooth, compactly supported function.

We mention that the consideration of the assumption (2) was inspired by [51], where in the same setting the Schrödinger operator with δ-shell interactions was considered.
As before, we use the notations

$$\Omega_+ := \Omega \quad \Omega_- = \mathbb{R}^3 \setminus \overline{\Omega_+} \quad \text{and} \quad \Sigma := \partial\Omega,$$

and we let N donotes the unit normal vector field at Σ which points outwards of Ω_+, and δ_Σ denotes the Dirac distribution supported on Σ.

We investigate in Chapter 2 the self-adjointness character and the spectral properties of the free Dirac operator H (in $\mathbb{R}^3$) coupled with combinations of the following singular potentials:

$$V_\epsilon = \epsilon I_4 \delta_\Sigma, \quad V_\mu = \mu\beta\delta_\Sigma, \quad V_\eta = \eta(\alpha \cdot N)\delta_\Sigma, \quad \epsilon, \mu, \eta \in \mathbb{R},$$
$$V_\zeta = \zeta\gamma_5\delta_\Sigma := -i\zeta\alpha_1\alpha_2\alpha_3\delta_\Sigma, \quad V_\upsilon = i\upsilon\beta\,(\alpha \cdot N)\,\delta_\Sigma, \quad \zeta, \upsilon \in \mathbb{R}.$$

To be precise, our main objective in Chapter 2 is to study the spectral properties and the phenomenon of the confinement of the following couplings:

$$\begin{aligned} H_\kappa &:= H + (\epsilon I_4 + \mu\beta + \eta(\alpha \cdot N))\delta_{\partial\Omega}, \quad \kappa := (\epsilon, \mu, \eta) \in \mathbb{R}^3, \\ H_{\zeta,\upsilon} &:= H + (-i\zeta\alpha_1\alpha_2\alpha_3 + i\upsilon\beta\,(\alpha \cdot N))\,\delta_{\partial\Omega}, \quad (\zeta, \upsilon) \in \mathbb{R}^2. \end{aligned} \tag{0.0.10}$$

We recall that the coupling constants ϵ, μ, η and υ represent the constants strength of the electrostatic, Lorentz scalar, magnetic and anomalous magnetic potentials, respectively. We will see later that the singular interaction given by the coupling constant ζ can be considered as an interactions of electrostatic type.

Now, we define on $L^2(\Sigma)^4$ the bounded linear operators

$$\begin{aligned}\Lambda_{\kappa,\pm} &= \frac{1}{\epsilon^2-\mu^2-\eta^2}(\epsilon I_4 \mp (\mu\beta+\eta(\alpha\cdot N))) \pm \mathscr{C}_\Sigma,\\ \Lambda_{(\zeta,\upsilon),\pm} &= \frac{1}{\zeta^2+\upsilon^2}(\zeta\gamma_5 + i\upsilon\beta(\alpha\cdot N)) \pm \mathscr{C}_\Sigma,\end{aligned} \tag{0.0.11}$$

for all $(\epsilon,\mu,\eta)\in\mathbb{R}^3$ such that $\epsilon^2-\mu^2-\eta^2\neq 0$, and for all $(\zeta,\upsilon)\in\mathbb{R}^2\setminus\{(0,0)\}$, respectively. Then, following the strategy of [10], we define the Dirac operators $H_\bullet$, $\bullet=\kappa$ or (ζ,υ), on the domain

$$\operatorname{dom}(H_\bullet) = \left\{u+\Phi[g] : u\in H^1(\mathbb{R}^3)^4, g\in L^2(\Sigma)^4, u_{|\Sigma} = -\Lambda_{\bullet,+}[g]\right\},$$

where for $g\in L^2(\Sigma)^4$, $\Phi[g]=(\phi * g)$ with ϕ as in (0.0.6).

In a first step of Chapter 2, we study the self-adjointness character of H_κ when Ω_+ satisfies the assumption (1) or (2). We begin by proving that H_κ is self-adjoint when $\epsilon^2-\mu^2-\eta^2\neq 4$ (i.e., in the non-critical case), and we show that $\operatorname{dom}(H_\kappa)\subset H^1(\mathbb{R}^3\setminus\partial\Omega)^4$, which means that functions in $\operatorname{dom}(H_\kappa)$ have a Sobolev regularity. When $\epsilon^2-\mu^2-\eta^2=4$, which is actually the critical case, we show that H_κ defined on $\operatorname{dom}(H_\kappa)$ is essentially self-adjoint (i.e., $\overline{H_\kappa}$ is self-adjoint). More precisely, in Section 2.2 we prove that

Theorem 0.0.2. *The following statements hold true:*

(i) If $\epsilon^2-\mu^2-\eta^2\neq 4$, then H_κ is self-adjoint and we have

$$\operatorname{dom}(H_\kappa) = \left\{u+\Phi[g] : u\in H^1(\mathbb{R}^3)^4, g\in H^{1/2}(\Sigma)^4, u_{|\Sigma} = -\Lambda_{\kappa,+}[g]\right\}.$$

(ii) If $\epsilon^2-\mu^2-\eta^2 = 4$, then H_κ is essentially self-adjoint and we have

$$\operatorname{dom}(\overline{H_\kappa}) = \left\{u+\Phi[g] : u\in H^1(\mathbb{R}^3)^4, g\in H^{-1/2}(\Sigma)^4, u_{|\Sigma} = -\tilde{\Lambda}_{\kappa,+}[g]\right\}.$$

where $\tilde{\Lambda}_{\kappa,\pm}$ is the continuous extension of $\Lambda_{\kappa,\pm}$ defined from $H^{-1/2}(\Sigma)^4$ into itself.

To prove this result we develop in Section 2.2 a strategy close to the one of [90], it is based essentially on the fact that the anticommutators of the Cauchy operator $\mathscr{C}_\Sigma$ with β or with $(\alpha\cdot N)$ have a regularizing effect. Indeed, as we will see in Section 2.2, the operator $\Lambda_{\kappa,\mp}\Lambda_{\kappa,\pm}$ involves the above anticommutators and it turns out that in the non-critical case, the regularization effect of these anticommutator pushes $\Lambda_{\kappa,+}$ to regularize the functions in $\operatorname{dom}(H_\kappa^*)$ to have the H^1-Sobolev regularity. In the critical case, the regularization property of the anticommutators play a crucial role in proof of the inclusion $\operatorname{dom}(H_\kappa^*)\subset\operatorname{dom}(\overline{H_\kappa})$, but in contrast to non-critical case, it doesn't push $\Lambda_{\kappa,+}$ to regularizes functions in $\operatorname{dom}(H_\kappa^*)$.

As a second step, we turn in Section 2.3 to the spectral study of H_κ, and we pay a special attention to the case where Ω_+ satisfies the second assumption, and we show several spectral properties of H_κ. Namely, using Fourier analysis, compactness and suitable localization arguments, we compute precisely the essential spectrum of H_κ in the non-critical case, cf. Theorem 2.3.3 (for the sake of readability, we don't want to write it here). More precisely, under certain conditions on the sign of the parameters ϵ,μ,η and $\epsilon^2-\mu^2-\eta^2\neq 4$, it turns out in Theorem 2.3.3 that the continuous spectrum emerge in the gap $(-m,m)$ (e.g., $\mathrm{Sp}_{\mathrm{ess}}(H_\kappa)=\mathbb{R}$, when $\mu=-2$ and $\epsilon=\eta=0$), in contrast to the case when Ω_+ satisfies the first assumption where we prove in Theorem 2.3.2 that $\mathrm{Sp}_{\mathrm{ess}}(H_\kappa)=(-\infty,-m]\cup[m,+\infty)$ and that $\mathrm{Sp}_{\mathrm{disc}}(H_\kappa)\cap(-m,m)$ is finite.

In the critical case, we give a complete characterization of the essential spectrum of $\overline{H_\kappa}$ when Ω_+ satisfies the second assumption. More precisely, we prove that

Theorem 0.0.3. *Let $\kappa = (\epsilon, \mu, \eta) \in \mathbb{R}^3$ be such that $\epsilon^2 - \mu^2 - \eta^2 = 4$, and assume that Ω_+ satisfies the second assumption, then it holds that*

$$\mathrm{Sp}_{\mathrm{ess}}(\overline{H_\kappa}) = (-\infty, -m] \cup \left\{-\frac{m\mu}{\epsilon}\right\} \cup [m, +\infty),$$

and the equality $\mathrm{Sp}(\overline{H_\kappa}) = \mathrm{Sp}_{\mathrm{ess}}(\overline{H_\kappa})$ holds true for $\Sigma = \mathbb{R}^2 \times \{0\}$

This theorem answers positively to the question (Q1) and generalizes the result of [22] to this kind of surfaces. We remark that even after adding the perturbation by the potential V_η, the point which appears in the gap remains the same (see the discussion after Theorem 2.3.4 for more details).

The proofs of the above results are based on a Krein-type resolvent formula and an adapted Birman-Schwinger principle that we prove in Proposition 2.3.1 and Theorem 2.3.1, combined with sophisticated compactness and localization arguments of some nonlocal operators on the boundary when Ω_+ satisfies the second assumption.

The last part of Chapter 2 is devoted to the spectral study of the Dirac operator $H_{\zeta,\upsilon}$. There, we adapte the strategy developed in Section 2.2 for the operator H_κ, and we show in Theorems 2.4.1 and 2.4.2 that $H_{\zeta,\upsilon}$ is self-adjoint for all possible combinations of interaction strengths, and we prove in the critical case (i.e., $\zeta^2 + \upsilon^2 = 4$) that $\mathrm{dom}(\overline{H_{\zeta,\upsilon}}) \not\subset H^s(\mathbb{R}^3 \setminus \Sigma)^4$ for any $s > 0$.

The spectral properties of $H_{\zeta,\upsilon}$ obviously depend on the interaction strengths and are significantly different whether Ω_+ satisfies the assumption (1) or (2). Thereby, we choose to discuss the most important ones here.

Theorem 0.0.4. *If $\zeta^2 + \upsilon^2 = 4$, then $\overline{H_{\zeta,\upsilon}}$ induce confinement, and the following hold:*

(i) If $\zeta = 0$, then $\mathrm{Sp}_{\mathrm{ess}}(\overline{H_{\zeta,\upsilon}}) = (-\infty, -m] \cup [m, +\infty)$. Moreover, $-m$ and m are eigenvalues of $\overline{H_{0,\upsilon}}$ with infinite multiplicities.

(ii) If $\zeta = 0$, Ω_+ satisfies the assumption (1), and $\{\lambda_j\}_{j\in\mathbb{N}^*}$ is the sequence of eigenvalues of the Dirichlet Laplacian $(-\Delta)$ in Ω_+, counted with their multiplicities. Then, for all $j \in \mathbb{N}^*$, $\lambda_j^{\pm}(m) = \pm\sqrt{m^2 + \lambda_j}$ is an embedded eigenvalue of $\overline{H_{\zeta,\upsilon}}$ with finite multiplicity.

(iii) If $\upsilon = 0$ and Ω_+ satisfies the assumption (2), then $\mathrm{Sp}_{\mathrm{ess}}(\overline{H_{\zeta,\upsilon}}) = (-\infty, -m] \cup \{0\} \cup [m, +\infty)$.

Theorem 0.0.4 reveals an interesting phenomenon concerning the confinement in contrast to what we have seen before, and actually this is one of the main motivations for considering the coupling $H_{\zeta,\upsilon}$. Indeed, the operator $H_{\zeta,\upsilon}$ induces in the critical case the confinement with a loss of regularity in the operator domain, and such effects have not been known before. Moreover, in one hand $H_{\pm\zeta,0}$ coincides with the Dirac operator coupled with the electrostatic δ-interactions of strengths $\mp\zeta$. On the other hand, the inner part of $\overline{H_{0,\pm\upsilon}}$ acting on Ω_+ coincides with the so-called Dirac operator with *zig-zag* boundary condition, one of the quantum dot boundary conditions describing the graphene. We note that the presence of embedded eigenvalues expressed in terms of the Dirichlet eigenvalues is due the boundary condition. The proof of assertions (i) and (ii) in Theorem 0.0.4 is based on some symmetry relations of the spectrum and quadratic forms techniques.

Finally, we mention that the two-dimensional analogue of the anomalous magnetic potential was introduced and studied at the same time in [41], and similar results have been obtained.

The case of rough interaction supports (Chapter 3). A very important issue that arises when we study δ-shell interactions of the form (0.0.3) is the regularity of the surface $\partial\Omega$. As far as we know, apart from the paper [10], all the works dealing with the study of three-dimensional Dirac operators with δ-shell interactions have been carried out for C^2-smooth domains. Nevertheless, thanks to the properties of Φ and $\{\alpha \cdot N, \mathscr{C}_{\partial\Omega}\}$, these results can be generalized (in the non-critical case) without difficulty to $C^{1,\omega}$-smooth domains for $\omega \in (1/2, 1)$ as we will see below.

In 2D, the self-adjointness of the coupling $H + V_\mu$ (in the massless case) was proved in [92], when $|\mu| < 2$, and $\partial\Omega$ is a closed curve with finitely many corners and piecewise smooth. We also mention the works [42, 76], where the self-adjointness of the Dirac operator with infinite mass boundary conditions on sectors and wedges have been studied. It is worth mentioning that the techniques used in the papers previously cited depend significantly on the canonical identification $\mathbb{R}^2 \simeq \mathbb{C}$, and the nature of the problem. Consequently, if Ω is a general Lipschitz domain, then the strategies of [42, 76, 92] cannot be used to prove the self-adjointness of Dirac operator coupled with the usual δ-interactions, especially in 3D and this problem remains open.

As already mentioned, far less attention has been paid to the spectral study of Dirac operators with δ-interactions supported on rough surfaces (and Dirac operators acting in rough domains with boundary conditions), yet this context is the most relevant from the point of view of physics (especially when the domain involves corners), for two principal reasons. Firstly, although in the study of quarks physicists often use simplified geometries in their experiments (such as spherical bags for optimization reasons), quarks appear to be confined in nature independently of the geometry of the bag. The 2D situation is more illustrative and the most famous example is the *graphene*. In fact, the graphene consists of a layer of carbon atoms arranged in a honeycomb lattice, and recently experiments have shown that Dirac materials share this structure (see e.g. [105]), which justify the consideration of corner domains. The second reason which justify the consideration of much more rough domains is due to the deformation of Dirac materials. A concrete example that illustrates this is the deformation of monolayer graphene, we refer to [77] where it was shown that a very rough geometry appears under chemical vapor deposition (see panels (a) and (b) in Figure 1. of [77]).

Recall the Dirac operator $H_{a,\tau} = H + A_{a,\tau}\delta_{\partial\Omega}$ defined in (0.0.3). In view of the discussion above, one can ask naturally the following questions:

(Q1) Until what extent the results on self-adjointness of $H_{a,\tau}$ (at least when $A_{a,\tau}$ is one of the usual δ-interactions) also hold for non smooth domains (Lipschitz for example)?

(Q2) If $H_{a,\tau}$ is self-adjoint, can we characterize its (essential/discrete) spectrum?

(Q3) In the non-critical case, is it possible to characterize the dependence of the Sobolev regularity of the domain of $H_{a,\tau}$ through the regularity of Ω?

Clearly, the above questions are interconnected and depend on the regularity of Ω and on the operator $A_{a,\tau}$.

The main goal of Chapter 3 is to generalize the result of Chapter 2 and to study questions (Q1),(Q2) and (Q3) under the weakest geometric assumptions on Ω (i.e., possibly for non-Lipschitz domains). Also, being motivated by the confinement phenomenon, the second goal of Chapter 3 is to derive some important models of Dirac operators that generate this phenomenon. However, in the study of the spectral properties we are not going to do a whole catalog, but we will take as a reference the operator H_κ defined previously in (0.0.10), whose spectral properties have been discussed above for a critical and non-critical parameter when Ω is a C^2-smooth domain. Once we understand how to answer the questions (Q1),(Q2) and (Q3) for the operator H_κ, we will look at

$$\begin{aligned} H_{\tilde{\mu}} &= H + V_{\tilde{v}} = H + i\tilde{\mu}\gamma_5\beta\delta_\Sigma, \quad \tilde{\mu} \in \mathbb{R}, \\ H_{\tilde{v}} &= H + V_{\tilde{v}} = H + i\tilde{v}\gamma_5\beta(\alpha\cdot N)\delta_\Sigma, \quad \tilde{v} \in \mathbb{R}, \end{aligned} \tag{0.0.12}$$

and also to the families of Dirac operators given by:

$$\begin{aligned} (-m, m) \ni a &\longmapsto H_{a,\lambda} = H + \lambda C_\Sigma^a \delta_\Sigma, \quad \lambda \in \mathbb{R}\setminus\{0\}, \\ (-m, m) \ni a &\longmapsto H_{a,\lambda'} = H + \lambda'(\alpha\cdot N) C_\Sigma^a (\alpha\cdot N)\delta_\Sigma, \quad \lambda' \in \mathbb{R}\setminus\{0\}, \end{aligned} \tag{0.0.13}$$

where $\mathscr{C}_\Sigma^a$ is the Cauchy operator associated with $(H-a)$. We will see that $H_{\tilde{\mu}}$, $H_{\tilde{v}}$, $H_{a,\lambda}$ and $H_{a,\lambda'}$ induce confinement, with some new boundaries conditions.

Let us now describe the main results of Chapter 3 and explain the strategy used there. First of all, we shall always distinguish between the critical and non-critical parameters. In the critical case, the self-adjointness of $H_{a,\tau}$ requires in general the C^2-smoothness, we are therefore particularly interested in what happens in the non critical case for non-smooth domains. Nevertheless, we provide in Theorem 3.1.2 a systematic approach that generalize the strategy developed in Section 2.2 in order to prove the self-adjointness of $H_{a,\tau}$ in the critical case. Moreover, in order to take into account the confinement phenomenon in the later situation, we give in Propositions 3.1.3 and 3.1.4 a sufficient condition on the operator $A_{a,\tau}$ so that $H_{a,\tau}$ generates confinement in the critical and non-critical case, respectively.

In order to tackle the questions (Q1),(Q2) and (Q3) under the weakest geometric assumptions on Ω, we will follow the strategy of [10]. Before going into more details, let us first explain why we have chosen to use the strategy developed in [10]. Indeed, there are several reasons prompt us to choose to work with the strategy of [10], we cite here:

- For functions in $H^1(\mathbb{R}^3)$, one can give meaning to the trace on $\partial\Omega$ for a very large class of surfaces (Ahlfors-David regular surfaces). If Ω is a non Lipschitz domain, then this becomes a real obstacle if we work with transmission conditions, see the discussion in the beginning of Subsection 3.1.3.

- For non-critical combinations of coupling constants, the main result of [10] (i.e., Theorem 0.0.1) gives us a powerful tool to prove the self-adjointness of $H_{a,\tau}$ (recall that it suffices to show that $\Lambda_{\tau,+}$ is Fredholm to prove the self-adjointness of $H_{a,\tau}$), in addition, we can easily extend it to more rough surfaces (see Theorem 3.1.1 for its generalization).

- In order to study the Sobolev regularity of $\mathrm{dom}(H_{a,\tau})$, it is sufficient to study the regularity properties of the mapping Φ and the Sobolev regularity of the singular part of $\varphi \in \mathrm{dom}(H_{a,\tau})$ (i.e., the function g with $\varphi = u + \Phi[g]$).

Since our strategy is based on the same set of techniques and in order to simplify our exposition, we are going to summarize our main results concerning the Dirac operator H_κ. As before, with $\Lambda_{\kappa,+}$ as in (0.0.11), we define the operator H_κ on the domain

$$\mathrm{dom}(H_\kappa) = \left\{u + \Phi[g] : u \in H^1(\mathbb{R}^3)^4, g \in L^2(\partial\Omega)^4, u_{|\partial\Omega} = -\Lambda_{\kappa,+}[g]\right\},$$

In Section 3.2, our main purpose is to identify some situations where $\Lambda_{\kappa,+}$ gives rise to a Fredholm operator. As we will see throughout Chapters 2 and 3, the anticommutators $\{\alpha\cdot N, \mathscr{C}_{\partial\Omega}\}$ play a central role in our study. Indeed, as already mentioned, the operator $\Lambda_{\kappa,\pm}\Lambda_{\kappa,\mp}$ involves the anticommutators $\{\alpha\cdot N, \mathscr{C}_{\partial\Omega}\}$, and we will see that the compactness on $L^2(\partial\Omega)^4$ of $\{\alpha\cdot N, \mathscr{C}_{\partial\Omega}\}$ implies that $\Lambda_{\kappa,+}$ is a Fredholm operator. It is worth pointing out that for bounded C^1-smooth domains, the compactness of $\{\alpha\cdot N, \mathscr{C}_{\partial\Omega}\}$ have been established in [10, Lemma 3.5 and Remark 3.6], so one may ask whether this property is still true for less regular domains. Actually, this question was formulated in the survey [91] as follows:

(Q4) Given a bounded Lipschitz domain Ω, what is the necessary regularity on $\partial\Omega$ so that the anticommutator $\{\alpha\cdot N, \mathscr{C}_{\partial\Omega}\}$ gives rise to a compact operator on $L^2(\partial\Omega)^4$?

In this direction, we investigate the regularity and the geometric properties of the domain Ω which ensures this compactness property. Looking closely at the anticommutator $\{\alpha\cdot N, \mathscr{C}_{\partial\Omega}\}$, we observe that it involves a matrix version of the principal value of the harmonic double-layer K, its adjoint K^* and the commutators $[N_k, R_j]$, where R_j are the Riesz transforms (see (3.2.4) for the precise definitions). Hence the situation is more clear. In fact, from the harmonic analysis and geometric measure theory point of view, it is shown that the boundedness of Riesz transforms characterizes the uniform rectifiability of $\partial\Omega$; cf. [88], for example. In addition, functional analytic properties of the Riesz transforms (such as the identity $\sum_{j=1}^3 R_j^2 = -I$) and the analogue version of the strongly singular part of $(\alpha\cdot N)C_{\partial\Omega}$ in the Clifford algebra $\mathcal{C}l_3$, i.e., the Cauchy-Clifford operator (especially its self-adjointness and compactness character) are strongly related to the regularity and geometric properties of the domain Ω. For more details we refer to [61] and [63].

Using the materials provided in [63], it turns out in Theorem 3.2.2 that the answer to the question (Q4) is:

Theorem 0.0.5. *Let Ω be a bounded Lipschitz domain, and let $z\in\rho(H)$. Then, $\{\alpha\cdot N, \mathscr{C}^z_{\partial\Omega}\}$ is compact in $L^2(\Sigma)^4$ if and only if $N\in \mathrm{VMO}(\partial\Omega, \mathrm{dS})^3$. Here $\mathrm{VMO}(\partial\Omega, \mathrm{dS})^3$ is space of functions with vanishing mean oscillation on $\partial\Omega$.*

Once we have established that, we use a characterization of Fredholm operators to prove that $\Lambda_{\kappa,+}$ is Fredholm, and we show in Subsection 3.2.1 the following result:

Theorem 0.0.6. *Assume that Ω is a bounded Lipschitz domain with $N\in \mathrm{VMO}(\partial\Omega, \mathrm{dS})^3$, and let $\kappa=(\epsilon,\mu,\eta)\in\mathbb{R}^3$ be such that $\epsilon^2-\mu^2-\eta^2\neq 0,4$. Then, H_κ defined on $\mathrm{dom}(H_\kappa)$ is self-adjoint, and we have*

(i) $\mathrm{Sp}_{\mathrm{ess}}(H_\kappa) = (-\infty,-m]\cup[m,\infty)$.

(ii) $\mathrm{Sp}_{\mathrm{disc}}(H_\kappa)\cap(-m,m)$ *is finite.*

In addition to this result, we prove several qualitative spectral properties as in the C^2-smooth case. The proof of the assertions (i) and (ii) in Theorem 0.0.6 are based on a Krein-type resolvent formula (that we prove in Proposition 3.1.1, which is valid in the Lipschitz case), the fact that $\mathrm{dom}(H_\kappa)\subset H^{1/2}(\mathbb{R}^3\setminus\partial\Omega)^4$ and quadratic forms techniques.

At this stage, it is clear that if we restrict ourselves to the Lipschitz setting, then beyond the class of Lipschitz domains with VMO normals (which contains C^1-smooth domains), the compactness arguments mentioned previously are no longer valid. So, in order to go further in our study and to be able to consider situations that are close to the physical reality, we change the strategy and we turn to the invertibility arguments which are rather valid for a large class of domains. Indeed, we investigate the case of bounded uniformly rectifiable domains (aka UR domains). Uniform rectifiability is a natural quantitative analogue of rectifiability, which is intimately connected with the boundedness properties of singular integral operators. As already mentioned, the L^2-boundedness of Riesz transforms characterizes the uniform rectifiability of $\partial\Omega$, and more precisely, uniformly rectifiable surfaces is the most general setting on which all Calderón-Zygmund operators with odd and smooth kernels are bounded in $L^2(\partial\Omega)$.

In Subsection 3.2.3, we study the spectral properties of H_κ in the setting of bounded uniformly rectifiable domains, and we focus on the case $\kappa = (\epsilon, \mu, 0)$, i.e., the Dirac operator with electrostatic and Lorentz scalar δ-interactions $H_{\epsilon,\mu}$. There, as a first step, we prove the following:

Theorem 0.0.7. *Assume that Ω is a bounded uniformly rectifiable domain and let $\epsilon, \mu \in \mathbb{R}$ be such that $0 < |\epsilon^2 - \mu^2| < 1/\|\mathscr{C}_{\partial\Omega}\|^2_{L^2(\partial\Omega)^4 \to L^2(\partial\Omega)^4}$, then $H_{\epsilon,\mu}$ is self-adjoint. In particular, if Ω is Lipschitz and there is $z_0 \in \mathbb{C} \setminus \mathbb{R}$ such that $|\epsilon^2 - \mu^2| < 1/\|\mathscr{C}^{z_0}_{\partial\Omega}\|^2_{L^2(\partial\Omega)^4 \to L^2(\partial\Omega)^4}$, then it holds that*

$$\mathrm{Sp}_{\mathrm{ess}}(H_{\epsilon,\mu}) = (-\infty, -m] \cup [m, +\infty).$$

Although the quantitative assumption on the parameters assumed in Theorem 0.0.7 gives us a sufficient condition to guarantee the self-adjointness of $H_{\epsilon,\mu}$, but unfortunately it is very restricted and it does not allow to make a more advanced spectral study. To get around this problem, we impose a better quantitative assumption than the previous one involving the strongly singular par of the Cauchy operator. Indeed, let W be the Cauchy operator associated with the massless Dirac operator $-i(\sigma\cdot\nabla)$, defined for $h \in L^2(\partial\Omega)^2$ as the principal value $W[g] = \mathrm{pv}(\tilde{\phi} * g)$, where for $x \in \mathbb{R}^3 \setminus \{0\}$, $\tilde{\phi}(x) = -i(\sigma \cdot x)/|x|^3$ is the fundamental solution of $-i(\sigma \cdot \nabla)$. Then, the main result of Subsection 3.2.3 reads as follows:

Theorem 0.0.8. *Let Ω be a uniformly rectifiable domain. Assume that ϵ and μ satisfy one of the following assumptions:*

$$\text{(a) } 16\|W\|^2_{L^2(\Sigma)^2 \to L^2(\Sigma)^2} < \epsilon^2 - \mu^2, \qquad \text{(b) } \epsilon^2 - \mu^2 < 1/\|W\|^2_{L^2(\Sigma)^2 \to L^2(\Sigma)^2}.$$

Then $H_{\epsilon,\mu}$ is self-adjoint. In particular, $H_{\epsilon,\mu}$ generates confinement when $\epsilon^2 - \mu^2 = -4$. Moreover, if Ω is Lipschitz, then

(i) $\mathrm{Sp}_{\mathrm{ess}}(H_{\epsilon,\mu}) = (-\infty, -m] \cup [m, \infty)$.

(ii) $\mathrm{Sp}_{\mathrm{disc}}(H_{\epsilon,\mu}) \cap (-m, m)$ *is finite.*

(iii) $C_0 := \sup_{a \in [-m,m]} \|\mathscr{C}^a_\Sigma\| < \infty$. *Moreover,* $\mathrm{Sp}_{\mathrm{disc}}(H_{\epsilon,\mu}) \cap (-m, m) = \emptyset$ *either if* $|\epsilon - \mu| < 1/C_0$ *and* $|\epsilon + \mu| < 1/C_0$, *or if* $|\epsilon - \mu| > 4C_0$ *and* $|\epsilon + \mu| > 4C_0$.

(iv) If $\epsilon = 0$ *and* $\mu > 0$, *then* $\mathrm{Sp}_{\mathrm{disc}}(H_{\epsilon,\mu}) \cap (-m, m) = \emptyset$.

This result clearly generalizes the known results on the spectral properties of the Dirac operator $H_{\epsilon,\mu}$. Moreover, it shows that the phenomenon is still occur under the condition $\epsilon^2 - \mu^2 = -4$ even in this very general framework.

Having established the above results and in order to give an answer to question (Q3), we consider the class of Hölder's domains $C^{1,\omega}$, with $\omega \in (0, 1)$. In Subsection 3.2.2 we show the following result.

Theorem 0.0.9. *Let $\kappa = (\epsilon, \mu, \eta) \in \mathbb{R}^3$ be such that $\epsilon^2 - \mu^2 - \eta^2 \neq 0, 4$. Then we have:*

(i) If Ω is $C^{1,\omega}$-smooth and $\omega \leqslant 1/2$, then for all $s < \omega$, we have

$$\mathrm{dom}(H_\kappa) \subset \Big\{ u + \Phi[g] : u \in H^1(\mathbb{R}^3)^4, g \in H^s(\partial\Omega)^4, u_{|\partial\Omega} = -\Lambda_{\kappa,+}[g] \Big\} \subset H^{1/2+s}(\mathbb{R}^3 \setminus \partial\Omega)^4.$$

(ii) If Ω is $C^{1,\omega}$-smooth and $\omega > 1/2$, then

$$\mathrm{dom}(H_\kappa) = \Big\{u + \Phi[g] : u \in H^1(\mathbb{R}^3)^4, g \in H^{1/2}(\partial\Omega)^4, u_{|\partial\Omega} = -\Lambda_{\kappa,+}[g]\Big\} \subset H^1(\mathbb{R}^3 \setminus \partial\Omega)^4.$$

From this result, we clearly see how the Sobolev regularity of $\mathrm{dom}(H_\kappa)$ depends on the smoothness of Ω. The proof of Theorem 0.0.9 is based on the regularization property of the anticommutator $\{\alpha \cdot N, \mathscr{C}_{\partial\Omega}\}$ (see Lemma 3.2.3) and the mapping Φ as well as the regularization effect of the operators $\Lambda_{\kappa,+}$.

Finally, the above compactness and invertibility arguments are then applied to the spectral study of the Dirac operators given by (0.0.12) and (0.0.13), and the their spectral study is performed in Subsection 3.2.4 and Section 3.3, respectively.

We end this part of the introduction by noting that we recently learned (more precisely, when the paper [40] appeared on arXiv) that the Dirac operator with Lorentz scalar δ-interactions supported on compact Lipschitz surfaces was being considered in the paper [24], and that similar results have been obtained there.

In the following, we address the second topic of this thesis, which we discuss in Chapter 4.

Poincaré-Steklov operators and large mass Dirac operators (Chapter 4). The study of boundary integral operators has been the motivation behind the development of several tools and branches in mathematics, e.g., Fredholm theory, Singular integral and Pseudodifferential operators. Moreover, it turned out that functional analytic and spectral properties of some of these operators are strongly related to the regularity and geometric properties of surfaces. Two typical examples are the Neumann-Poincaré (NP) operator (also known as the harmonic double layer) and the Dirichlet-to-Neumann (DtN) operator. Indeed, in the classical setting of a bounded domain $\Omega \subset \mathbb{R}^d$ with smooth boundary (C^1-smooth for example), it is well-known that the NP operator is compact operator in $L^2(\partial\Omega)$ ($1 < p < \infty$), cf. [52]. Generally, this compactness property fails when Ω is less regular, however, as we have seen before, it has been shown that the compactness criterion in $L^2(\partial\Omega)$ of the NP operator (and the commutators of the Riesz transforms with the outward normal) characterizes the class of regular Semmes-Kening-Toro domains, see [63] for details. We also mention that, from the viewpoint of the spectral theory, it was shown that the asymptotic behaviour of the eigenvalues of the NP operator involve some topological properties of surface $\partial\Omega$ (in the case of smooth domains), such as the Willmore energy and the Euler characteristic, see, e.g., **??**. In the same vein, the eigenvalue problem for the DtN operator, called the Steklov problem, occurs in many applications which makes the subject especially appealing. We mention that several geometric properties of the DtN eigenvalue (such as isoperimetric inequalities, spectral asymptotics and geometric invariants) are closely related to the theory of minimal surfaces [54], as well as the problem of determining a complete Riemannian manifold with boundary from the Cauchy data of harmonic functions, see [75] (see also the survey [57] for further details).

The main goal of Chapter 4 is to introduce a Poincaré-Steklov map for the Dirac operator (i.e., an analogue of the Dirichlet-to-Neumann map for the Laplace operator) and to study its (semiclassical) pseudodifferential properties. Our main motivation for considering this operator arises from the fact that it is naturally related to the Dirac operator with the MIT bag boundary condition, $H_{\mathrm{MIT}}(m)$, which will be rigorously defined below, and in particular, from the key role it plays in the study of the large mass problem that we are going to formulate in question (Q5) below.

Let $\Omega \subset \mathbb{R}^3$ be a domain with a compact smooth boundary $\partial\Omega$, set $\Omega_i = \Omega$ and $\Omega_e = \mathbb{R}^3 \backslash \overline{\Omega}$, let n be the outward unit normal to Ω, and define the projections $P_\pm := (I_4 \mp i\beta(\alpha\cdot n))/2$ along the boundary $\partial\Omega$. Similarly to the Dirichlet and Neumann traces Γ_D and Γ_N, we introduce the following trace mappings

$$\Gamma_\pm = P_\pm \Gamma_D : H^1(\Omega)^4 \longrightarrow P_\pm H^{1/2}(\partial\Omega)^4. \tag{0.0.14}$$

We investigate in Chapter 4 the specific case of the Poincaré-Steklov (PS for short) operator, $\mathscr{A}_m$, defined by

$$\mathscr{A}_m : P_- H^{1/2}(\partial\Omega)^4 \longrightarrow P_+ H^{1/2}(\partial\Omega)^4, \quad g \longmapsto \mathscr{A}_m(g) = \Gamma_+ U_z(g), \tag{0.0.15}$$

where for $z \in \rho(H_{\mathrm{MIT}}(m))$, $U_z(g) \in H^1(\Omega)^4$ is the unique solution of the following elliptic boundary problem:

$$\begin{cases} (H - z)U_z(g) = 0, & \text{in } \Omega, \\ \Gamma_- U_z(g) = g, & \text{on } \partial\Omega. \end{cases} \tag{0.0.16}$$

Let us now briefly describe our main results concerning the properties of the operators $\mathscr{A}_m$. The pseudodifferential character of $\mathscr{A}_m$ is the central element of discussion in Sections 4.3 and 4.4. To begin with, we show in Section 4.3 that $\mathscr{A}_m$ fits into the framework of pseudodifferential operators and we focus in particular on the case where the mass m is fixed. Working on local coordinates and denoting by $\nabla_{\partial\Omega}$ and $\Delta_{\partial\Omega}$ the surface gradient and the Laplace-Beltrami operator on $\partial\Omega$, respectively, we prove in Sections 4.3 the following result:

Theorem 0.0.10. *For any fixed $m > 0$ and $z \in \rho(D_m)$, the Poincaré-Steklov operator $\mathscr{A}_m$ is a classical homogeneous pseudodifferential operators of order 0, and it holds that*

$$\mathscr{A}_m = S \cdot \left(\frac{\nabla_{\partial\Omega} \wedge n}{\sqrt{-\Delta_{\partial\Omega}}} \right) P_- \mod OpS^{-1}(\partial\Omega),$$

where $S = i(\alpha \wedge \alpha)/2$ denotes the spin angular momentum.

From this result, one may ask if there is a link between $\mathscr{A}_m$ and the Cauchy operator associated with $(H - z)$ (which we denote here by $\mathscr{C}_{z,m}$). In fact, the familiar reader with the Cauchy operator $\mathscr{C}_{z,m}$ may recognize that the Riesz operator on $\partial\Omega$ coincides with $\nabla_{\partial\Omega}(-\Delta_{\partial\Omega})^{-1/2}$, and comes essentially from the singular part of the Cauchy operator $\mathscr{C}_{z,m}$ (i.e., the operator W from Theorem 0.0.8). Indeed, as we will see in Section 4.3, for $z \in \rho(D_m)$ we have an explicit solution of the system (0.0.16), and in this case, the PS operator takes the layer potential form:

$$\mathscr{A}_m = -P_+ \beta \left(\beta/2 + \mathscr{C}_{z,m} \right)^{-1} P_-, \tag{0.0.17}$$

So the starting point of the proof of Theorem 0.0.10 is to analyze the pseudodifferential properties of the Cauchy operator. In this sense, we show that $2\mathscr{C}_{z,m}$ is equal, modulo $OpS^{-1}(\partial\Omega)$, to $\alpha \cdot (\nabla_{\partial\Omega}(-\Delta_{\partial\Omega})^{-1/2})$. Then, the explicit layer potential description of $\mathscr{A}_m$ and the symbol calculus allow us to prove the pseudodifferential character of $\mathscr{A}_m$ and to trap its principal symbol.

While the above strategy allows us to capture the pseudodifferential character of $\mathscr{A}_m$, unfortunately, it does not allow us to trace the dependence on the parameter m, and it imposes also a restriction on z (i.e., $z \in \rho(D_m)$), whereas $\mathscr{A}_m$ is well defined for any $z \in \rho(H_{\mathrm{MIT}}(m))$. In Section 4.4, we address the m-dependence of the pseudodifferential properties of $\mathscr{A}_m$ for any $z \in \rho(H_{\mathrm{MIT}}(m))$. Since in our application we mainly deal with large masses m, we treat this problem from the semiclassical point of view by using $h = 1/m \in (0, 1]$ as a semiclassical parameter, and we show the following result:

Theorem 0.0.11. *Let $h \in (0,1]$ and let $\mathscr{A}^h := \mathscr{A}_m$. Then, for $h_0 > 0$ sufficiently small and for any $h < h_0$, $\mathscr{A}^h$ is a h-pseudodifferential operator of order 0, and it holds that*

$$\mathscr{A}^h = S \cdot \left(\frac{h\nabla_{\partial\Omega} \wedge n}{\sqrt{-h^2\Delta_{\partial\Omega} + I} + I} \right) P_- \quad \mathrm{mod}\ h\,Op^h\mathcal{S}^{-1}(\partial\Omega).$$

The main idea to prove Theorem 0.0.11 is to use the system (0.0.16) instead of the explicit formula (0.0.17), and it is based on the following two steps. The first step is to construct a local approximate solution for (the pushforward of) the system (0.0.16) of the form

$$U^h(\tilde{x}, x_3) = \int_{\mathbb{R}^2} A^h(\tilde{x}, \xi, x_3) e^{iy\cdot\xi} \tilde{g}(\xi) \mathrm{d}\xi, \quad (\tilde{x}, x_3) \in \mathbb{R}^2 \times [0, \infty),$$

where A^h belongs to a specific (tangential) symbol class and admits an asymptotic expansion of the form

$$A^h(\tilde{x}, \xi, x_3) \sim \sum_{j \geq 0} h^j A_j(\tilde{x}, \xi, x_3),$$

so that, for each $x_3 > 0$, $U^h(\cdot, x_3)$ is a h-pseudodifferential operator of order 0. The second step is to show that when applying the trace mapping Γ_+ to the pull-back of $U^h(\cdot, 0)$, it coincides locally with $\mathscr{A}^h$ modulo a regularizing and negligible operator. It is at this precise point that the properties of the MIT bag operator become crucial, in particular, the regularization property of its resolvent (see Theorem 0.0.12 below) that allows us to achieve this second step, as it will be seen in Section 4.4.

We recall that the Dirac operator with the MIT bag boundary condition on Ω_i, or simply the MIT bag operator, is the operator $(H_{\mathrm{MIT}}(m), \mathrm{dom}(H_{\mathrm{MIT}}(m)))$ defined by

$$H_{\mathrm{MIT}}(m)\psi = H\psi, \quad \text{for all } \psi \in \mathrm{dom}(H_{\mathrm{MIT}}(m)) := \left\{ \psi \in H^1(\Omega_i)^4 : P_- t_{\partial\Omega}\psi = 0 \text{ on } \partial\Omega \right\}. \tag{0.0.18}$$

This operator corresponds to the inner part of the Dirac operator $H_{\epsilon,\mu}$ acting on Ω in the confining case $\mu = 2$ and $\epsilon = 0$. We mention that direct proofs of the self-adjointness of $H_{\mathrm{MIT}}(m)$ have been established in [7, 8, 90, 94], we refer also to [21] where special boundary conditions similar to the ones in the MIT bag model were investigated. In the same vein, the bidimensional analogue of $H_{\mathrm{MIT}}(m)$ (in the massless case, i.e., $m = 0$), known as the Dirac operator with the infinite mass boundary condition, was treated in [26, 27].

In Section 4.2, we briefly discuss the basic spectral properties of $H_{\mathrm{MIT}}(m)$ when Ω_i is a domain with compact Lipschitz boundary (see Theorem 4.2.1) and we establish some regularity results concerning the regularization property of the resolvent and the Sobolev regularity of the eigenfunctions of $H_{\mathrm{MIT}}(m)$. In particular, we prove the following result:

Theorem 0.0.12. *Let $k \geqslant 1$ be an integer and assume that Ω_i is C^{2+k}-smooth. Given $0 \neq \phi \in \mathrm{dom}(H_{MIT})$. If ϕ satisfies $(H - z)\phi = f$ in Ω_i, with $f \in H^k(\Omega_i)^4$ and $z \in \rho(H_{MIT}(m))$, then $\phi \in H^{1+k}(\Omega)^4$.*

Let M be a nonnegative real, and consider in $\mathbb{R}^3$ the Dirac operator $H_M = H + M\beta 1_{\Omega_e}$, where 1_{Ω_e} is the characteristic function of Ω_e. By Kato-Rellich theorem and Weyl's theorem, we easily see that H_M defined on $\mathrm{dom}(H_M) := H^1(\mathbb{R}^3)^4$ is self-adjoint, and that

$$\mathrm{Sp}_{\mathrm{ess}}(H_M) = (-\infty, -(m + M)] \cup [m + M, +\infty),$$
$$\mathrm{Sp}(H_M) \cap (-(m + M), m + M) \text{ is purely discrete.}$$

Recently it turned out that there is a close relation between the MIT bag operator and the Dirac operator H_M. In [6, 87] it was shown that, in the limite $M \to \infty$, any eigenvalue of $H_{\rm MIT}(m)$ is a limit of eigenvalues of H_M, similar result in higher dimension have been obtained [87] (see also [98] for the two-dimensional setting). Moreover, for $m = 0$, it is shown in [14] that the bidimensional analogue of H_M convergences to the bidimensional analogue of $H_{\rm MIT}(0)$ (i.e., $m = 0$) in the norm resolvent sense with a convergence rate of $\mathcal{O}(M^{-1/2})$. We point out that these results fits with similar well-known results for the stationary Schrödinger operator, for more details we refer to [34] and the references therein.

After reviewing briefly the connection between the Dirac operators H_M and $H_{\rm MIT}(m)$, namely the fact that (at least on a purely formal level) $H_M = H_{\rm MIT}(m)$ when $M = \infty$, it seems reasonable to ask the following questions about the intermediate values of M:

(Q6) Let $M_0 > 0$ be large enough, fix $M \geqslant M_0$ and $z \in \rho(H_{\rm MIT}(m)) \cap \rho(H_M)$. Given $f \in L^2(\mathbb{R}^3)^4$ and $U \in H^1(\mathbb{R}^3)^4$, what is the boundary value problem on Ω_i whose solutions closely approximate those of $(H + M\beta 1_{\Omega_e} - z)U = f$?

Notice that the answer to this question becomes trivial if one establishes an explicit formula for the resolvent of the operator H_M. In fact, having in mind the connection between H_M and $H_{\rm MIT}(m)$, in [31] V. Bruneau, M. Zreik and myself addressed the following problem: *for M sufficiently large, is it possible to relate the resolvents of H_M and $H_{MIT}(m)$ via a Krein-type resolvent formula?* When trying to solve this question, it turned out that it was necessary to invert in $H^{1/2}(\partial\Omega)^4$ operators of the form $(I_4 + K_M)$, where K_M is uniformly bounded in $\mathscr{L}(H^{1/2}(\partial\Omega)^4)$ with respect to M, and involves the Poincaré-Steklov operators. We mention that the standard arguments do not allow us to ensure the invertibility of (I_4+K_M), which led us to consider the h-pseudodifferential properties of the PS operators (with $h = 1/M$ being the semiclassical parameter) in order to overcome this obstacle. In the end of the day, we establish in Theorem 4.5.1 a Krein-type resolvent formula for H_M in terms of the resolvent of $H_{\rm MIT}(m)$ and prove a Birman-Schwinger principle relating the eigenvalues of H_M in the gap $(-(m+M), m+M)$ with a spectral property of certain bounded operators in $H^{1/2}(\partial\Omega)^4$, see Theorem 4.5.1 for the precise statement. With the help of these tools, we show in Corollary 4.5.1 that there is a $1/M$-pseudodifferential operators of order 0, $\Xi^-_M(z)$, such that for U as in question (Q5), $U_{|\Omega_i}$ satisfies the following elliptic problem

$$\begin{cases} (H - z)U_{|\Omega_i} = f & \text{in } \Omega_i, \\ \quad \Gamma_- U_{|\Omega_i} = \Xi^-_M(z)\Gamma_+(H_{\rm MIT}(m) - z)^{-1}(f_{|\Omega_i}) & \text{on } \partial\Omega, \\ \quad \Gamma_+ U_{|\Omega_i} = \Gamma_+(H_{\rm MIT}(m) - z)^{-1}(f_{|\Omega_i}) + \mathscr{A}_m \Gamma_- U & \text{on } \partial\Omega. \end{cases}$$

Moreover, using the Krein-type resolvent formula from Theorem 4.5.1, the boundedness properties of PS operators between Sobolev spaces and the regularity estimates of some layer potential carried out in Proposition 4.5.1, we establish in Section 4.5 an asymptotic expansion in $\mathscr{L}(L^2(\mathbb{R}^3)^4)$ for the resolvent of H_M in terms of the resolvent of $H_{\rm MIT}(m)$, and we give a sharp estimate for the convergence rate, which reads as follows:

Theorem 0.0.13. *Let r_{Ω_i} be the restriction operator on Ω_i, and let e_{Ω_i} be the extension operator by 0 on Ω_e. Then, the resolvent H_M admits an asymptotic expansion in $\mathscr{L}(L^2(\mathbb{R}^3)^4)$ of the form:*

$$(H_M - z)^{-1} = e_{\Omega_i}(H_{MIT}(m) - z)^{-1} r_{\Omega_i} + \frac{1}{M} K_M(z) + \frac{1}{M} L_M(z) \tag{0.0.19}$$

where $K_M(z)$ and $L_M(z)$ are bounded from $L^2(\mathbb{R}^3)^4$ into itself uniformly with respect to M, and we have

$$r_{\Omega_i} K_M(z) e_{\Omega_i} = 0 = r_{\Omega_e} K_M(z) e_{\Omega_e}.$$

In particular, it holds that

$$\left\|(H_M - z)^{-1} - e_{\Omega_i}(H_{MIT}(m) - z)^{-1} r_{\Omega_i}\right\|_{\mathcal{B}(L^2(\mathbb{R}^3)^4)} = \mathcal{O}\left(\frac{1}{M}\right).$$

Introduction (french)

L'équation de Dirac

$$i\partial_t \varphi(t,x) = H\varphi(t,x), \quad \varphi(\cdot,x) : \mathbb{R}^3 \to \mathbb{C}^4,$$

où $H = -i\alpha\cdot\nabla + m\beta$ est l'opérateur libre de Dirac dans $\mathbb{R}^3$, est utilisé en mécanique quantique relativiste pour décrire la dynamique de particules élémentaires de spins demi-entiers.

Ces dernières années, l'étude mathématique des perturbations singulières de l'opérateur de Dirac a connu un rebond considérable et a attiré beaucoup d'attention. D'une part, cet intérêt vient du fait que certains de ces opérateurs de Dirac ont été récemment associés à l'évolution des quasi-particules dans les nouveaux matériaux dites de Dirac tel que le graphène. D'autre part, cela est dû aux défis mathématiques que représente l'étude des opérateurs de Dirac, que se soit d'un point d'EDP ou d'analyse.

Dans cette thèse, nous nous intéressons à l'étude spectrale de deux types de perturbation de l'opérateur libre de Dirac en dimension 3, qui sont singulières du point de vue de changement d'échelle, ainsi qu'à l'étude des opérateurs de Dirac agissant sur des domaines avec des conditions aux bords issues du phénomène de confinement. Plus précisément, nous considérons dans la première partie de cette thèse des opérateurs de Dirac formellement définis par l'expression différentielle

$$H_\tau := H + V_\tau = H + A_\tau \delta_\Sigma,$$

où Σ est une surface (compacte ou non-compacte) de l'espace euclidienne $\mathbb{R}^3$ qui le divise en deux ouverts $\Omega_\pm$, A_τ est un opérateur borné, inversible et auto-adjoint dans $L^2(\Sigma)^4$ et qui dépend d'un paramètre $\tau \in \mathbb{R}^n$ avec $n \geqslant 1$. Ici δ est la distribution de Dirac supporté sur Σ. Ce type de perturbation est souvent appelée opérateurs de Dirac avec δ-interactions.

Afin de simplifier l'illustration de nos résultat concernant l'étude spectrale de l'opérateur H_τ, nous nous restreignons dans la suite au cas où H_τ est donné par le couplage de l'opérateur de Dirac avec une combinaison de delta interactions électrostatique et scalaire de Lorentz, qui est définit par

$$H_{\epsilon,\mu} := H + (\epsilon I_4 + \mu\beta)\delta_\Sigma, \quad (\epsilon,\mu) \in \mathbb{R}^2.$$

Ici ϵ et μ désignes respectivement les amplitudes des potentiels électrostatique et scalaire de Lorentz.

La littérature concernant l'étude spectrale de l'opérateur de Dirac $H_{\epsilon,\mu}$ est très riche. En particulier, plusieurs progrès ont été réalisés dans le cas où Σ est une surface compacte de régularité C^2, on cite par exemple [48, 10, 11, 16, 17] où l'auto-adjonction a été prouvé et différents aspects de l'opérateur ont été analysés quand les paramètres ϵ et μ satisfont la condition $\epsilon^2 - \mu^2 \neq 4$. Il s'avère que le cas $\epsilon^2 - \mu^2 = 4$ (que nous appelons cas critique) est plus délicat à analyser et les propriétés de l'opérateur $H_{\epsilon,\mu}$ sont totalement différentes en comparaison avec le cas non-critique $\epsilon^2 - \mu^2 \neq 4$. En effet, contrairement au cas non-critique, la restriction de l'opérateur $H_{\epsilon,\mu}$ sur l'espace de Sobolev $H^1(\mathbb{R}\setminus\Sigma)^4$ n'est pas auto-adjointe mais plutôt essentiellement auto-adjointe, voir [90, 19, 22]. De plus, il a été remarqué dans [10] et [19] que si Σ est un hyperplan ou une surface compacte de régularité C^2 et qui contient une partie plate alors le point 0 appartient au spectre essentiel de $\overline{H_{\epsilon,0}}$ (c'est-à-dire quand $\mu=0$). Dans [22] à l'aide des techniques d'analyse complexe et d'opérateurs pseudodifférentiels périodiques ont été utilisés pour donner une caractérisation complète du spectre essentiel de $\overline{H_{\epsilon,\mu}}$ dans le cas 2-dimensionnel quand Σ une courbe C^∞-compacte, et il s'est avéré que

$$\mathrm{Sp}_{\mathrm{ess}}(\overline{H_{\epsilon,\mu}})=(-\infty,-m]\cup\left\{-\frac{m\mu}{\epsilon}\right\}\cup[m,+\infty).$$

Cependant, la caractérisation complète du spectre essentiel de $\overline{H_{\epsilon,\mu}}$ dans le cas de la dimension trois reste encore une question ouverte et a été l'une des motivations du chapitre 2.

Toute au long de cette thèse, nous suivons la terminologie développée dans [10] pour définir rigoureusement l'opérateur $H_{\epsilon,\mu}$. Ainsi, nous définissons $H_{\epsilon,\mu}$ sur le domaine

$$\mathrm{dom}(H_{\epsilon,\mu})=\left\{u+\Phi[g]: u\in H^1(\mathbb{R}^3)^4, g\in L^2(\Sigma)^4, u_{|\Sigma}=-\Lambda_+[g]\right\},$$

où il agit au sens des distributions de la manière suivante :

$$H_{\epsilon,\mu}(u+\Phi[g])=Hu,\quad \forall u+\Phi[g]\in\mathrm{dom}(H_{\epsilon,\mu}).$$

Ici Φ est une solution fondamental de l'opérateur libre de Dirac, et $\Lambda_\pm$ un opérateur borné de $L^2(\Sigma)^4$ dans lui même et qui est défini par la formule

$$\Lambda^a_\pm=\frac{1}{\epsilon^2-\mu^2}(\epsilon I_4\mp(\mu\beta))\pm\mathscr{C}^a_\Sigma,\quad \epsilon^2\neq\mu^2,$$

où $a\in(-m,m)$ et $\mathscr{C}^a_\Sigma$ est l'opérateur de Cauchy associé à l'opérateur de Dirac $(H-a)$.

L'objectif du chapitre 2 est d'étudier les propriétés spectrales de l'opérateur de Dirac $H_{\epsilon,\mu}$ quand la surface Σ satisfait l'une des hypothèses suivantes :

(1) Σ est le bord d'un ouvert borné de classe C^2.

(2) $\Sigma:=\Sigma_\nu:=\{(x,t)\in\mathbb{R}^2\times\mathbb{R}: t>\nu\phi(x)\}$, où $\nu\in\mathbb{R}$ et $\phi:\mathbb{R}^2\to\mathbb{R}$ est une fonction à support compact et de régularité C^2.

Nos contributions principales portent essentiellement sur l'étude du cas des surfaces qui satisfont l'hypothèse (2). Néanmoins, nous développerons une approche uniforme basée sur des techniques de régularisations qui nous permettra de décrire pour toute combinaison des constantes d'interactions la réalisation auto-adjoint de l'opérateur de Dirac $H_{\epsilon,\mu}$ quand Σ satisfait l'hypothèse (1) ou (2). Plus précisément, la stratégie que nous développerons repose essentiellement sur le fait que les anti-commutateurs $\{\beta,\mathscr{C}_\Sigma\}$ et $\{(\alpha\cdot N),\mathscr{C}_\Sigma\}$ (où N est le vecteur normal sur Σ) ont un effet régularisant. Comme on le verra au long de cette thèse, les opérateurs $\Lambda^0_\mp\Lambda^0_\pm$ font intervenir ces anti-commutateurs ce qui fait que l'opérateur Λ^0_+ force les fonctions dans $\mathrm{dom}(H^*_{\epsilon,\mu})$ pour avoir la régularité H^1-Sobolev, et ainsi nous permettra de montrer que $H_{\epsilon,\mu}$ est auto-adjoint dans le cas non-critique. Dans le cas critique, la propriété de régularisation des anti-commutateurs joue un rôle crucial dans la preuve de l'inclusion $\mathrm{dom}(H^*_{\epsilon,\mu})\subset\mathrm{dom}(\overline{H_{\epsilon,\mu}})$, mais contrairement au cas non critique, cette propriété ne permet pas à l'opérateur Λ^0_+ de régulariser les fonctions dans $\mathrm{dom}(H^*_{\epsilon,\mu})$, et induit ainsi une perte de régularité de Sobolev des fonctions dans $\mathrm{dom}(\overline{H_{\epsilon,\mu}})$. Plus précisément nous montrons que

Theorem 0.0.14. *Soit $H_{\epsilon,\mu}$ comme ci-dessus, alors les assertions suivantes sont vraies :*

(i) Si $\epsilon^2 - \mu^2 \neq 4$, alors $H_{\epsilon,\mu}$ est auto-adjoint et on a

$$\mathrm{dom}(H_{\epsilon,\mu}) = \Big\{ u + \Phi[g] : u \in H^1(\mathbb{R}^3)^4, g \in H^{1/2}(\Sigma)^4, u_{|\Sigma} = -\Lambda_+^0[g] \Big\}.$$

(ii) Si $\epsilon^2 - \mu^2 = 4$, alors $H_{\epsilon,\mu}$ est essentiellement auto-adjoint et on a

$$\mathrm{dom}(\overline{H_{\epsilon,\mu}}) = \Big\{ u + \Phi[g] : u \in H^1(\mathbb{R}^3)^4, g \in H^{-1/2}(\Sigma)^4, u_{|\Sigma} = -\tilde{\Lambda}_+^0[g] \Big\}.$$

où $\tilde{\Lambda}_\pm^0$ est l'extension continues de $\Lambda_\pm^0$ définie de $H^{-1/2}(\Sigma)^4$ dans $H^{-1/2}(\Sigma)^4$.

Nous complémentons notre étude en mettant en évidence dans section 2.2.2 la relation entre l'auto-adjonction de $H_{\epsilon,\mu}$ et l'opérateur Λ_+^0, qui est l'idée principale derrière le concept des quasi boundary triples utilisé dans [16, 19, 17, 22].

Ensuite, nous étudions les propriétés spectrales qualitatives de l'opérateur $H_{\epsilon,\mu}$. En particulier, nous effectuerons une étude détaillée du spectre de $H_{\epsilon,\mu}$ quand Σ satisfait l'hypothèse (2) dans le cas critique ou non-critique. Dans un premier temps, nous montrons un principe de Birman-Schwinger adapté à notre contexte qui relie le spectre de l'opérateur de Dirac $\overline{H_{\epsilon,\mu}}$ dans la gap $(-m, m)$ avec les propriétés spectrales des opérateurs Λ_+^a. Ce principe nous permettra de déduire en particulier l'existence des valeurs propres pour l'opérateur $\overline{H_{\epsilon,\mu}}$ dans la gap $(-m, m)$. Nous montrons aussi une formule de Krein reliant la résolvante de l'opérateur $\overline{H_{\epsilon,\mu}}$ avec celle de l'opérateur libre de Dirac, voir Proposition 2.3.1 et Théorème 2.3.1 pour plus de détails. Avec ces deux outils en main, et à l'aide des arguments de compacité et de localisation de certains opérateurs non locaux que nous développons dans les lemmes 2.3.2 et 2.3.3 , nous donnons dans les théorèmes 2.3.3 et 2.3.4 une caractérisation complète du spectre essentiel de $\overline{H_{\epsilon,\mu}}$ pour toute combinaison des constantes d'interactions lorsque Σ satisfait la seconde hypothèse. En particulier, nous remarquons que dans le cas non-critique, et contrairement au cas des surfaces compactes, le spectre essentiel émerge dans la gap $(-m, m)$, voir le théorème 2.3.3. Dans le cas critique, nous montrons que le spectre essentiel $\overline{H_{\epsilon,\mu}}$ est donné par

$$\mathrm{Sp}_{\mathrm{ess}}(\overline{H_{\epsilon,\mu}}) = \big(-\infty, -m\big] \cup \Big\{-\frac{m\mu}{\epsilon}\Big\} \cup \big[m, +\infty\big),$$

ce qui rejoint le résultat obtenu dans [22].

La difficulté la plus importante qui se pose lorsque nous étudions le couplage de l'opérateur de Dirac avec des δ-interactions est la régularité de la surface Σ qui supporte ces dernières. Comme on le notera dans le chapitre 2, la régularité C^2 de la surface Σ s'avère essentiel pour montrer l'auto-adjonction de l'opérateur $H_{\epsilon,\mu}$. Ainsi, l'objectif principal du chapitre 3 est de généraliser les résultats obtenus dans le chapitre 2 au cas des surfaces compactes non régulières pour des combinaisons de constantes d'interactions non-critiques, c'est-à-dire $\epsilon^2 - \mu^2 \neq 4$. Pour cela, nous utilisons des techniques d'analyse harmonique et la théorie du potentiel. Dans un premier temps, nous généralisons les résultats obtenus dans le cadre des surfaces régulières au cadre des surfaces qui coïncident localement avec le graphe d'une fonction Lipschitzienne dont les oscillations sont nulles en moyenne, c'est-à-dire $N \in L^\infty(\Sigma) \cap VMO(\Sigma)$. Dans ce cas, nos principaux résultats peuvent être grossièrement résumés comme suit :

- L'opérateur $H_{\epsilon,\mu}$ est auto-adjoint et $\mathrm{dom}(H_{\epsilon,\mu}) \subset H^{1/2}(\mathbb{R}^3 \setminus \Sigma)^4$.
- $\mathrm{Sp}_{\mathrm{ess}}(H_{\epsilon,\mu}) = (-\infty, -m] \cup [m, \infty)$.

- $\mathrm{Sp}_{\mathrm{disc}}(H_{\epsilon,\mu}) \cap (-m,m)$ is finite.

De plus, nous mettons en lumière l'influence de la régularité de la surface supportant les delta interactions sur la régularité Sobolev du domaine de l'opérateur sous considération dans le cas des surfaces Hölderienne. En effet, dans la section 3.2.2, après avoir étudié les propriétés de régularisations de l'anti-commutateur $\{\alpha \cdot N, \mathscr{C}_\Sigma\}$ (voir le lemme 3.2.3) et l'opérateur Φ ainsi que l'effet de régularisation de l'opérateur Λ_+, nous montrons que

- Si Σ est de classe $C^{1,\omega}$ avec $\omega \leqslant 1/2$, alors pour tout $s < \omega$ on a

$$\mathrm{dom}(H_{\epsilon,\mu}) \subset \Big\{u + \Phi[g] : u \in H^1(\mathbb{R}^3)^4, g \in H^s(\Sigma)^4, u_{|\Sigma} = -\Lambda_+[g]\Big\} \subset H^{1/2+s}(\mathbb{R}^3 \setminus \Sigma)^4.$$

- Si Σ est de classe $C^{1,\omega}$ avec $\omega > 1/2$, alors

$$\mathrm{dom}(H_{\epsilon,\mu}) = \Big\{u + \Phi[g] : u \in H^1(\mathbb{R}^3)^4, g \in H^{1/2}(\Sigma)^4, u_{|\Sigma} = -\Lambda_+[g]\Big\} \subset H^1(\mathbb{R}^3 \setminus \Sigma)^4.$$

Ce résultat montre clairement comment la régularité de la surface Σ affecte la régularité Sobolev de $\mathrm{dom}(H_{\epsilon,\mu})$.

Dans un second temps, nous considérons le cas de delta interactions supportées sur des surfaces satisfaisant certaines conditions topologiques faibles. Plus précisément, nous étudions dans la section 3.2.3 les propriétés spectrales de l'opérateur de Dirac $H_{\epsilon,\mu}$ dans le cadre de surfaces uniformément rectifiables. Sous certains conditions sur les constantes de couplages, nous montrons que l'opérateur $H_{\epsilon,\mu}$ est auto-adjoint et nous établissons plusieurs propriétés spectrales qualitatives dans le cas lipschitzienne. Plus précisément, on supposons que ϵ et μ satisfont l'une des hypothèses suivantes :

$$\text{(a) } 16\|W\|^2_{L^2(\Sigma)^2 \to L^2(\Sigma)^2} < \epsilon^2 - \mu^2, \quad \text{(b) } \epsilon^2 - \mu^2 < 1/\|W\|^2_{L^2(\Sigma)^2 \to L^2(\Sigma)^2},$$

où W est la partie singulière de l'opérateur de Cauchy $\mathscr{C}_\Sigma$, nous montrons que $H_{\epsilon,\mu}$ est auto-adjoint. Si on suppose de plus que Σ est lipschitzienne, nous montrons alors que les assertions suivantes sont vraies :

- $\mathrm{Sp}_{\mathrm{ess}}(H_{\epsilon,\mu}) = (-\infty, -m] \cup [m, \infty)$.
- $\mathrm{Sp}_{\mathrm{disc}}(H_{\epsilon,\mu}) \cap (-m,m)$ is finite.
- $C_0 := \sup_{a \in [-m,m]} \|\mathscr{C}^a_\Sigma\| < \infty$. De plus, $\mathrm{Sp}_{\mathrm{disc}}(H_{\epsilon,\mu}) \cap (-m,m) = \emptyset$ soit si $|\epsilon - \mu| < 1/C_0$ et $|\epsilon + \mu| < 1/C_0$, ou bien si $|\epsilon - \mu| > 4C_0$ et $|\epsilon + \mu| > 4C_0$.
- Si $\epsilon = 0$ et $\mu > 0$, alors $H_{\epsilon,\mu}$ n'a pas de spectre discret dans la gap $(-m,m)$.

Nous mentionnons que le chapitre 3 ne porte pas seulement sur l'étude de l'opérateur de Dirac $H_{\epsilon,\mu}$, mais plutôt plusieurs couplages de l'opérateur de Dirac avec des combinaisons de potentiels singuliers de types électrostatique et magnétiques ainsi que le couplage de l'opérateur de Dirac avec des potentiels singuliers qui font intervenir l'opérateur de Cauchy $\mathscr{C}^a_\Sigma$ pour $a \in (-m,m)$. De plus, nous dérivons plusieurs model d'opérateur de Dirac qui donnent lieu au phénomène de confinement.

Dans le chapitre 4 qui est la deuxième partie de cette thèse, nous nous intéressons à l'étude des propriétés pseudodifférentiel de l'analogue de l'opérateur de Dirichlet-Neumann pour l'opérateur de Dirac. Nous étudions en particulier les opérateurs de Poincaré-Steklov (PS) associés à l'opérateur de Dirac avec la condition au bord dite MIT bag défini par

$$H_{\mathrm{MIT}}(m)\psi = H\psi, \quad \text{pour tout} \psi \in \mathrm{dom}(H_{\mathrm{MIT}}(m)) := \Big\{\psi \in H^1(\Omega)^4 : P_- t_\Sigma \psi = 0 \text{ sur } \Sigma\Big\}. \tag{0.0.20}$$

Ici Ω est un ouvert borné de $\mathbb{R}^3$ dont la frontière Σ est régulière, et $P_\pm := (I_4 \mp i\beta(\alpha\cdot n))/2$ sont des projections toutes au long de la frontière Σ. Nous mentionnons que l'opérateur $H_{\mathrm{MIT}}(m)$ est auto-adjoint avec un spectre discret, et correspond à la partie intérieure de l'opérateur de Dirac $H_{\epsilon,\mu}$ agissant sur Ω dans le cas du confinement avec paramètres $\mu = 2$ et $\epsilon = 0$ (voir aussi [7, 8, 90, 94] pour une preuve directe de l'auto-adjonction de $H_{\mathrm{MIT}}(m)$).

Plus concrètement, nous considérons l'opérateur Poincaré-Steklov $\mathscr{A}_m$ défini par

$$\mathscr{A}_m : P_- H^{1/2}(\Sigma)^4 \longrightarrow P_+ H^{1/2}(\Sigma)^4, \quad g \longmapsto \mathscr{A}_m(g) = P_+ t_\Sigma U_z(g), \tag{0.0.21}$$

où pour $z \in \rho(H_{\mathrm{MIT}}(m))$, $U_z(g) \in H^1(\Omega)^4$ est l'unique solution du problème elliptic suivant :

$$\begin{cases} (H - z)U_z(g) = 0, & \text{dans } \Omega, \\ P_- t_\Sigma U_z(g) = g, & \text{sur } \Sigma. \end{cases}$$

Dans un premier temps, nous montrons que pour tout $z \in \rho(H)$ et tout $m > 0$ fixes, l'opérateur Poincaré-Steklov $\mathscr{A}_m$ s'inscrivit bien dans le cadre des opérateurs pseudodifférentiel classiques, et que

$$\mathscr{A}_m = S \cdot \left(\frac{\nabla_\Sigma \wedge n}{\sqrt{-\Delta_\Sigma}}\right) P_- \quad \mathrm{mod}\ Op\mathcal{S}^{-1}(\Sigma),$$

où $S = i(\alpha \wedge \alpha)/2$ désigne le moment angulaire de spin. La preuve de ce résultat repose essentiellement sur le calcul symbolique et le fait que pour $z \in \rho(H)$, nous obtenons facilement une formule explicite de l'opérateur $\mathscr{A}_m$ faisant intervenir l'opérateur de Cauchy $\mathscr{C}_\Sigma^z$, voir théorème 4.3.1.

Dans un second temps, nous considérons le cas de grandes masses $m > 0$, et nous nous intéressons à l'étude des propriétés des opérateurs Poincaré-Steklov d'un point de vue d'opérateurs pseudodifférentiel semiclassique avec $1/m$ comme paramètre semiclassique. Nous mentionnons que l'étude semiclassique des opérateurs PS est motivé par la question suivante:

- Soit $M_0 > 0$ suffisamment grand, et fixons $M \geqslant M_0$ et $z \in \rho(H_{\mathrm{MIT}}(m)) \cap \rho(H)$. Étant donné $f \in L^2(\mathbb{R}^3)^4$ et $U \in H^1(\mathbb{R}^3)^4$, quel est le problème aux limites sur Ω dont les solutions se rapprochent étroitement de celles de $(H + M\beta 1_{\mathbb{R}^3\setminus\overline{\Omega}} - z)U = f$?

Cette question nous amène à l'étude spectrale de l'opérateur de Dirac $H_M = H + M\beta 1_{\mathbb{R}^3\setminus\overline{\Omega}}$, où $1_{\mathbb{R}^3\setminus\overline{\Omega}}$ est la fonction caractéristique de $\mathbb{R}^3 \setminus \overline{\Omega}$. En effet, la question ci-dessus qui peut être vue comme un problème d'EDP, se ramène simplement à un problème spectral pour l'opérateur H_M, à savoir obtenir une formule explicite de sa résolvante, et plus précisément une formule de type Krein reliant la résolvante de H_M avec la résolvante d'un opérateur de référence. Puisque il a été prouvé dans [14] que l'opérateur H_M converge au sens de la norme de la résolavante vers l'opérateur $H_{\mathrm{MIT}}(m)$ quand $M \to \infty$, cela fait du ce dernier le candidat idéal pour être l'opérateur de référence. Ainsi, pour d'obtenir cette formule de résolvante, il s'avère que la considération des opérateurs Poincaré-Steklov d'un point de vue d'opérateurs pseudodifférentiel semiclassique est essentiel. Dans cette direction, nous montrons dans le théorème 4.4.1 que pour tout $z \in \rho(H_{\mathrm{MIT}}(m))$ et $m > 0$ suffisamment grand, $\mathscr{A}_m$ est un opérateur $1/m$-pseudodifférentiel d'ordre 0, et on a :

$$\mathscr{A}_m = S \cdot \left(\frac{\nabla_\Sigma \wedge n}{\sqrt{-\Delta_\Sigma + m^2} + m}\right) P_- \quad \mathrm{mod}\ \frac{1}{m} Op^{1/m}\mathcal{S}^{-1}(\Sigma).$$

Pour prouver ce résultat, nous utilisons les propriétés spectrales de l'opérateur de Dirac $H_{\mathrm{MIT}}(m)$ que nous montrons dans la section 4.2, et qui jouent un rôle crucial pour prouver le résultat ci-dessus, notamment les propriétés de régularisation de la résolvante de $H_{\mathrm{MIT}}(m)$, voir le théorème 4.2.2.

En utilisant les propriétés pseudodifférentiel semiclassique des opérateurs de Poincaré-Steklov, on arrive finalement à relie les résolvantes des opérateurs de Dirac H_M et $H_{\mathrm{MIT}}(m)$, voir le théorème 4.5.1 pour la formule explicite. Ainsi, nous obtenons la réponse à la question que nous avons posé ci-dessus. En effet, comme corollaire de la formule de résolvante nous dans le corollaire 4.5.1 qu'il existe un opérateur $1/M$-pseudodifferential d'ordre 0, $\Xi_M^-(z)$, tel que la restriction de U, noté par $U_{|\Omega}$, satisfait le problème elliptique suivant :

$$\begin{cases} (H-z)U_{|\Omega_i} = f & \text{dans } \Omega, \\ \quad P_- t_\Sigma U_{|\Omega} = \Xi_M^-(z) P_+ t_\Sigma (H_{\mathrm{MIT}}(m) - z)^{-1}(f_{|\Omega}) & \text{sur } \Sigma, \\ \quad P_+ t_\Sigma U_{|\Omega} = P_+ t_\Sigma (H_{\mathrm{MIT}}(m) - z)^{-1}(f_{|\Omega}) + \mathscr{A}_m P_- t_\Sigma U & \text{sur } \Sigma, \end{cases}$$

De plus, nous montrons que l'opérateur perturbé converge au sens de la norme de la résolvante vers l'opérateur MIT bag et nous donnons une estimation précise du taux de convergence, voir la proposition 4.5.1.

Introducción (spanish)

La ecuación de Dirac

$$i\partial_t \varphi(t,x) = H\varphi(t,x), \quad \varphi(\cdot,x) : \mathbb{R}^3 \to \mathbb{C}^4,$$

donde $H = -i\alpha\cdot\nabla + m\beta$ es el operador libre de Dirac en $\mathbb{R}^3$, se utiliza en la mecánica cuántica relativista para describir la dinámica de las partículas elementales de espines semienteros.

En esta tesis estamos interesados en el estudio espectral de dos tipos de perturbaciones del operador libre de Dirac en dimensión 3, que son singulares desde el punto de vista del cambio de escala, así como en el estudio de los operadores de Dirac que actúan sobre dominios con condiciones de borde derivadas del fenómeno de confinamiento. Más concretamente, consideramos en la primera parte de esta tesis los operadores de Dirac definidos formalmente por la expresión diferencial

$$H_\tau := H + V_\tau = H + A_\tau \delta_\Sigma,$$

donde Σ es una superficie (compacta o no compacta) del espacio euclidiano $\mathbb{R}^3$ que lo divide en dos espacios abiertos $\Omega_\pm$, A_τ es un operador acotado, invertible y autoadjunto en $L^2(\Sigma)^4$ y que depende de un parámetro $\tau \in \mathbb{R}^n$ con $n \geqslant 1$. Aquí δ es la distribución de Dirac soportada en Σ. Este tipo de perturbación se suele denominar operadores de Dirac con δ-interacciones.

Para simplificar la ilustración de nuestros resultados relativos al estudio espectral del operador H_τ, nos limitamos en lo que sigue al caso en que H_τ está dado por el acoplamiento del operador de Dirac con una combinación de interacciones delta electrostáticas y escalares de Lorentz, que se define por

$$H_{\epsilon,\mu} := H + (\epsilon I_4 + \mu\beta)\delta_\Sigma, \quad (\epsilon,\mu) \in \mathbb{R}^2.$$

Aquí ϵ y μ denotan las magnitudes de los potenciales electrostáticos y escalares de Lorentz respectivamente.

La literatura relativa al estudio espectral del operador de Dirac $H_{\epsilon,\mu}$ es muy rica. En particular, se han hecho varios avances en el caso en que Σ es una superficie compacta de regularidad C^2, se cita por ejemplo [48, 10, 11, 16, 17] donde se ha demostrado la autoadjunto y se han analizado diferentes aspectos del operador cuando los parámetros ϵ y μ satisfacen la condición $\epsilon^2 - \mu^2 \neq 4$. Resulta que el caso $\epsilon^2 - \mu^2 = 4$ (que llamamos el caso crítico) es más delicado de analizar y las propiedades del operador $H_{ep,\mu}$ son totalmente diferentes en comparación con el caso no crítico $\epsilon^2 - \mu^2 \neq 4$. En efecto, a diferencia del caso no crítico, la restricción del operador $H_{\epsilon,\mu}$ sobre el espacio de Sobolev $H^1(\mathbb{R}^3 \setminus \Sigma)^4$ no es autoadjunto sino esencialmente autoadjunto, véase [90, 19, 22]. Además, se observó en [10] y [19] que si Σ es un hiperplano o superficie compacta de regularidad C^2 y que contiene una parte plana entonces el punto 0 pertenece al espectro esencial de $\overline{H_{\epsilon,0}}$ (es decir, cuando $\mu = 0$). En [22] se utilizaron técnicas de análisis complejo y operadores pseudodiferenciales periódicos para dar una caracterización completa del espectro esencial de $\overline{H_{ep,\mu}}$ en el caso de 2-dimensiones cuando Σ una curva C^∞-compacta, y resultó que

$$\mathrm{Sp}_{\mathrm{ess}}(\overline{H_{\epsilon,\mu}}) = (-\infty, -m] \cup \left\{-\frac{m\mu}{\epsilon}\right\} \cup [m, +\infty).$$

Sin embargo, la caracterización completa del espectro esencial de $\overline{H_{ep,\mu}}$ en el caso de la dimensión tres sigue siendo una cuestión abierta y fue una de las motivaciones del capítulo 2.

A lo largo de esta tesis, seguimos la terminología desarrollada en [10] para definir rigurosamente el operador $H_{\epsilon,\mu}$. Por lo tanto, definimos $H_{\epsilon,\mu}$ en el dominio

$$\mathrm{dom}(H_{\epsilon,\mu}) = \left\{u + \Phi[g] : u \in H^1(\mathbb{R}^3)^4, g \in L^2(\Sigma)^4, u_{|\Sigma} = -\Lambda_+[g]\right\},$$

El objetivo del capítulo 2 es estudiar las propiedades espectrales del operador de Dirac $H_{\epsilon,\mu}$ cuando la superficie Σ satisface una de las siguientes hipótesis:

(1) Σ es el borde de un abierto acotado de clase C^2.

(2) $\Sigma := \Sigma_\nu := \{(x,t) \in \mathbb{R}^2 \times \mathbb{R} : t > \nu\phi(x)\}$, onde $\nu \in \mathbb{R}$ y $\phi : \mathbb{R}^2 \to \mathbb{R}$ es una función con soporte compacto y regularidad C^2. .

Nuestras principales aportaciones se refieren al estudio del caso de las superficies que satisfacen la hipótesis (2). No obstante, desarrollaremos una aproximación uniforme basada en técnicas de regularización que nos permitirá describir para cualquier combinación de constantes de interacción la realización autoadjunta del operador de Dirac $H_{\epsilon,\mu}$ cuando Σ satisface la hipótesis (1) o (2). Más concretamente, la estrategia que desarrollaremos se basa esencialmente en el hecho de que los anticomutadores $\{\beta, \mathscr{C}_S\}$ y $\{(\alpha \cdot N), \mathscr{C}_S\}$ (donde N es el vector normal en Σ) tienen un efecto regularizador. Como veremos a lo largo de esta tesis, los operadores $\Lambda^0_\mp\Lambda^0_\pm$ implican estos anticomutadores lo que hace que el operador Λ^0_+ fuerce funciones en $\mathrm{dom}(H^*_{\epsilon,\mu})$ para tener H^1-regularidad de Sobolev, y así nos permitirá demostrar que $H_{\epsilon,\mu}$ es autoadjunto en el caso no crítico. En el caso crítico, la propiedad de regularización anticomutador juega un papel crucial en la prueba de inclusión $\mathrm{dom}(H^*_{\epsilon,\mu}) \subset \mathrm{dom}(\overline{H_{\epsilon,\mu}})$, pero a diferencia del caso no crítico, esta propiedad no permite que el operador Λ^0_+ regularice las funciones en $\mathrm{dom}(H^*_{\epsilon,\mu})$, y por tanto induce una pérdida de regularidad de Sobolev de las funciones en $\mathrm{dom}(\overline{H_{\epsilon,\mu}})$. Más concretamente, demostramos que

Theorem 0.0.15. *Sea $H_{\epsilon,\mu}$ como arriba, entonces las siguientes afirmaciones son verdaderas:*

(i) Si $\epsilon^2 - \mu^2 \neq 4$, entonces $H_{\epsilon,\mu}$ es autoadjunto y tenemos

$$\mathrm{dom}(H_{\epsilon,\mu}) = \left\{u + \Phi[g] : u \in H^1(\mathbb{R}^3)^4, g \in H^{1/2}(\Sigma)^4, u_{|\Sigma} = -\Lambda^0_+[g]\right\}.$$

(ii) Si $\epsilon^2 - \mu^2 = 4$, entonces $H_{\epsilon,\mu}$ es esencialmente autoadjunto y tenemos

$$\mathrm{dom}(\overline{H_{\epsilon,\mu}}) = \left\{u + \Phi[g] : u \in H^1(\mathbb{R}^3)^4, g \in H^{-1/2}(\Sigma)^4, u_{|\Sigma} = -\tilde{\Lambda}^0_+[g]\right\}.$$

donde $\tilde{\Lambda}^0_\pm$ es la extensión continua de $\Lambda^0_\pm$ definida desde $H^{-1/2}(\Sigma)^4$ en $H^{-1/2}(\Sigma)^4$.

Completamos nuestro estudio destacando en la sección 2.2.2 la relación entre la autoadjunción de $H_{\epsilon,\mu}$ y el operador Λ^0_+, que es la idea principal detrás del concepto de quasi boundary triples utilizado en [16, 19, 17, 22].

A continuación, estudiamos las propiedades espectrales cualitativas del operador $H_{\epsilon,\mu}$. En particular, haremos un estudio detallado del espectro de $H_{\epsilon,\mu}$ cuando Σ satisface la hipótesis (2) en el caso crítico o no crítico. En primer lugar, mostramos un principio de Birman-Schwinger adaptado a nuestro contexto que vincula el espectro del operador de Dirac $\overline{H_{\epsilon,\mu}}$ en el hueco $(-m, m)$ con las propiedades espectrales de los operadores Λ^a_+. Este principio nos permitirá deducir, en particular, la existencia de valores propios para el operador $\overline{H_{\epsilon,\mu}}$ en el hueco $(-m, m)$. También mostramos una fórmula de Krein que vincula el resolvente del operador $\overline{H_{\epsilon,\mu}}$ con el del operador libre de Dirac, véase la Proposición 2.3.1 y el teorema 2.3.1 para más detalles. Con estas dos herramientas en la mano, y con la ayuda de los argumentos de compacidad y localización de algunos operadores no locales que desarrollamos en los lemas 2.3.2 y 2.3.3 damos en los teoremas 2.3.3 y 2.3.4 una caracterización completa del espectro esencial de $\overline{H_{\epsilon,\mu}}$ para cualquier combinación de las constantes de interacción cuando Σ satisface la segunda hipótesis. En particular, observamos que en el caso no crítico, y al contrario que en el caso de las superficies compactas, el espectro esencial emerge en el hueco $(-m, m)$, véase el teorema 2.3.3. En el caso crítico, mostramos que el espectro esencial $\overline{H_{\epsilon,\mu}}$ está dado por

$$\mathrm{Sp}_{\mathrm{ess}}(\overline{H_{\epsilon,\mu}}) = \big(-\infty, -m\big] \cup \Big\{-\frac{m\mu}{\epsilon}\Big\} \cup \big[m, +\infty\big),$$

lo que coincide con el resultado obtenido en [22].

La dificultad más importante que surge cuando se estudia el acoplamiento del operador de Dirac con las δ-interacciones es la regularidad de la superficie Σ que soporta este último. Como se observará en el capítulo 2, la regularidad C^2 de la superficie Σ es esencial para mostrar la autoadjunte del operador $H_{\epsilon,\mu}$. Así, el objetivo principal del capítulo 3 es generalizar los resultados obtenidos en el capítulo 2 al caso de superficies compactas no regulares para combinaciones de constantes de interacción no críticas, es decir, $\epsilon^2 - \mu^2 \neq 4$. Para ello, utilizamos técnicas de análisis armónico y teoría del potencial. En primer lugar, generalizamos los resultados obtenidos en el marco de las superficies regulares al marco de las superficies que coinciden localmente con la gráfica de una función Lipschitziana cuyas oscilaciones son nulas en promedio, es decir, $N \in L^\infty(\Sigma) \cap VMO(\Sigma)$. En este caso, nuestros principales resultados pueden resumirse a grandes rasgos como sigue:

- El operador $H_{\epsilon,\mu}$ es autoadjunto y $\mathrm{dom}(H_{\epsilon,\mu}) \subset H^{1/2}(\mathbb{R}^3 \setminus \Sigma)^4$.
- $\mathrm{Sp}_{\mathrm{ess}}(H_{\epsilon,\mu}) = (-\infty, -m] \cup [m, \infty)$.
- $\mathrm{Sp}_{\mathrm{disc}}(H_{\epsilon,\mu}) \cap (-m, m)$ es finito.

Además, destacamos la influencia de la regularidad de la superficie que soporta las interacciones delta en la regularidad de Sobolev del dominio del operador considerado en el caso de las superficies hölderianas. De hecho, en la sección **??**, después de haber estudiado las propiedades de regularización del operador $\{\alpha \cdot N, \mathscr{C}_\Sigma\}$ (ver lema 3.2.3) y del operador Φ así como el efecto de regularización del operador Λ_+, mostramos que

- Si Σ es de la clase $C^{1,\omega}$ con $\omega \leqslant 1/2$, entonces para todo $s < \omega$ tenemos

$$\mathrm{dom}(H_{\epsilon,\mu}) \subset \Big\{u + \Phi[g] : u \in H^1(\mathbb{R}^3)^4, g \in H^s(\Sigma)^4, u_{|\Sigma} = -\Lambda_+[g]\Big\} \subset H^{1/2+s}(\mathbb{R}^3 \setminus \Sigma)^4.$$

- Si Σ es de la clase $C^{1,\omega}$ con $\omega > 1/2$, entonces

$$\mathrm{dom}(H_{\epsilon,\mu}) = \Big\{u + \Phi[g] : u \in H^1(\mathbb{R}^3)^4, g \in H^{1/2}(\Sigma)^4, u_{|\Sigma} = -\Lambda_+[g]\Big\} \subset H^1(\mathbb{R}^3 \setminus \Sigma)^4.$$

Este resultado muestra claramente cómo la regularidad de la superficie Σ afecta a la regularidad de Sobolev de $\mathrm{dom}(H_{\epsilon,\mu})$.

En un segundo paso, consideramos el caso de las interacciones delta soportadas en superficies que satisfacen ciertas condiciones topológicas débiles. Más concretamente, estudiamos en la sección 3.2.3 las propiedades espectrales del operador de Dirac $H_{\epsilon,\mu}$ en el marco de las superficies uniformemente rectificables. Bajo ciertas condiciones sobre las constantes de acoplamiento, mostramos que el operador $H_{\epsilon,\mu}$ es autoadjunto y establecemos varias propiedades espectrales cualitativas en el caso lipschitziano. Más precisamente, suponemos que ϵ y μ satisfacen uno de los siguientes supuestos:

$$\text{(a)}\ 16\|W\|^2_{L^2(\Sigma)^2\to L^2(\Sigma)^2} < \epsilon^2 - \mu^2, \quad \text{(b)}\ \epsilon^2 - \mu^2 < 1/\|W\|^2_{L^2(\Sigma)^2\to L^2(\Sigma)^2},$$

donde W es la parte singular del operador de Cauchy $\mathscr{C}_S$, demostramos que $H_{ep,\mu}$ es autoadjunto. Si además suponemos que Σ es lipschitziano, entonces demostramos que las siguientes afirmaciones son ciertas:

- $\mathrm{Sp}_{\mathrm{ess}}(H_{\epsilon,\mu}) = (-\infty, -m] \cup [m, \infty)$.
- $\mathrm{Sp}_{\mathrm{disc}}(H_{\epsilon,\mu}) \cap (-m, m)$ es finito.
- $C_0 := \sup_{a\in[-m,m]} \|\mathscr{C}^a_\Sigma\| < \infty$. Además, $\mathrm{Sp}_{\mathrm{disc}}(H_{\epsilon,\mu}) \cap (-m, m) = \emptyset$ bien si $|\epsilon-\mu| < 1/C_0$ y $|\epsilon + \mu| < 1/C_0$, bien si $|\epsilon - \mu| > 4C_0$ y $|\epsilon + \mu| > 4C_0$.
- Si $\epsilon = 0$ y $\mu > 0$, entonces $H_{\epsilon,\mu}$ no tiene espectro discreto en el hueco $(-m, m)$.

Mencionamos que el capítulo 3 no sólo trata del estudio del operador de Dirac $H_{\epsilon,\mu}$, sino varios acoplamientos del operador de Dirac con combinaciones de potenciales singulares de tipo electrostático y magnético, así como el acoplamiento del operador de Dirac con potenciales singulares que implican al operador de Cauchy $\mathscr{C}^a_\Sigma$ para $a \in (-m, m)$. Además, derivamos varios modelos de operadores de Dirac que dan lugar al fenómeno de confinamiento.

En el capítulo 4, que es la segunda parte de esta tesis, nos interesa estudiar las propiedades pseudodiferenciales del análogo del operador de Dirichlet-Neumann para el operador de Dirac. En particular, estudiamos los operadores de Poincaré-Steklov (PS) asociados al operador de Dirac con la llamada condición de borde de MIT bag definida por

$$H_{\mathrm{MIT}}(m)\psi = H\psi, \quad \text{pour tout}\psi \in \mathrm{dom}(H_{\mathrm{MIT}}(m)) := \Big\{\psi \in H^1(\Omega)^4 : P_- t_\Sigma\psi = 0 \text{ sur } \Sigma\Big\}. \tag{0.0.22}$$

Aquí Ω es un abierto acotado de $\mathbb{R}^3$ cuya frontera Σ es regular, y $P_\pm := (I_4 \mp i\beta(\alpha \cdot n))/2$ son proyecciones a lo largo de la frontera Σ. Mencionamos que el operador $H_{\mathrm{MIT}}(m)$ es autoadjunto con un espectro discreto, y corresponde a la parte interna del operador de Dirac $H_{\epsilon,\mu}$ que actúa sobre Ω en el caso de confinamiento con parámetros $\mu = 2$ y $\epsilon = 0$ (ver también [7, 8, 90, 94] para una prueba directa de la auto-adjunción de $H_{\mathrm{MIT}}(m)$).

Más concretamente, consideramos el operador de Poincaré-Steklov $\mathscr{A}_m$ definido por

$$\mathscr{A}_m : P_- H^{1/2}(\Sigma)^4 \longrightarrow P_+ H^{1/2}(\Sigma)^4, \quad g \longmapsto \mathscr{A}_m(g) = P_+ t_\Sigma U_z(g), \tag{0.0.23}$$

donde para $z \in \rho(H_{\mathrm{MIT}}(m))$, $U_z(g) \in H^1(\Omega)^4$ es la solución única del siguiente problema elíptico:

$$\begin{cases} (H - z)U_z(g) = 0, & \text{en } \Omega, \\ P_- t_\Sigma U_z(g) = g, & \text{en } \Sigma. \end{cases}$$

En primer lugar, mostramos que para cualquier $z \in \rho(H)$ fijo y $m > 0$, el operador de Poincaré-Steklov $\mathscr{A}_m$ se ajusta bien al marco de los operadores pseudodiferenciales clásicos, y que

$$\mathscr{A}_m = S \cdot \left(\frac{\nabla_\Sigma \wedge n}{\sqrt{-\Delta_\Sigma}} \right) P_- \quad \mathrm{mod}\ Op\mathcal{S}^{-1}(\Sigma),$$

donde $S = i(\alpha \wedge \alpha)/2$ denota el momento angular de espín. La demostración de este resultado se basa esencialmente en el cálculo simbólico y en el hecho de que para $z \in \rho(H)$, obtenemos fácilmente una fórmula explícita para el operador $\mathscr{A}_m$ que implica al operador de Cauchy $\mathscr{C}_\mathcal{S}^z$, véase el teorema 4.3.1.

En un segundo paso, consideramos el caso de masas grandes $m > 0$, y nos interesa estudiar las propiedades de los operadores de Poincaré-Steklov desde el punto de vista de los operadores pseudodiferenciales semiclásicos con $1/m$ como parámetro semiclásico. Mencionamos que el estudio semiclásico de los operadores PS está motivado por la siguiente cuestión:

- Sea $M_0 > 0$ suficientemente grande, y sean $M \geqslant M_0$ y $z \in \rho(H_{\mathrm{MIT}}(m)) \cap \rho(H)$ fijos. Dados $f \in L^2(\mathbb{R}^3)^4$ y $U \in H^1(\mathbb{R}^3)^4$, ¿cuál es el problema de frontera en Ω cuyas soluciones se aproximan mucho a las de $(H + M\beta 1_{\mathbb{R}^3 \setminus \overline{O}} - z)U = f$?

Esta cuestión nos lleva al estudio espectral del operador de Dirac $H_M = H + M\beta 1_{\mathbb{R}^3\setminus\overline{\Omega}}$, donde $1_{\mathbb{R}^3\setminus\overline{\Omega}}$ es la función característica de $\mathbb{R}^3 \setminus \overline{\Omega}$. En efecto, la cuestión anterior, que puede verse como un problema de EDP, se reduce simplemente a un problema espectral para el operador H_M, a saber, obtener una fórmula explícita de su resolvente, y más precisamente una fórmula de tipo Krein que relacione el resolvente de H_M con el resolvente de un operador de referencia. Como se ha demostrado en [14] que el operador H_M converge en el sentido de la norma del resolvente al operador Hm cuando $M \to \infty$, esto hace que este último sea el candidato ideal para ser el operador de referencia. Así, para obtener esta fórmula de resolvente, resulta imprescindible la consideración de los operadores de Poincaré-Steklov desde el punto de vista de los operadores pseudodiferenciales semiclásicos. En esta dirección, mostramos en el teorema 4.4.1 que para cualquier $z \in \rho(H_{\mathrm{MIT}}(m))$ y $m > 0$ suficientemente grande, $\mathscr{A}_m$ es un operador $1/m$-pseudodiferencial de orden 0, y tenemos :

$$\mathscr{A}_m = S \cdot \left(\frac{\nabla_\Sigma \wedge n}{\sqrt{-\Delta_\Sigma + m^2} + m} \right) P_- \quad \mathrm{mod}\ \frac{1}{m} Op^{1/m}\mathcal{S}^{-1}(\Sigma).$$

Para demostrar este resultado, utilizamos las propiedades espectrales del operador de Dirac $H_{\mathrm{MIT}}(m)$ que mostramos en la sección 4.2, y que juegan un papel crucial en la demostración del resultado anterior, en particular las propiedades de regularización del resolvente de $H_{\mathrm{MIT}}(m)$, véase el teorema 4.2.2.

Utilizando las propiedades semiclásicas pseudodiferenciales de los operadores de Poincaré-Steklov, llegamos finalmente al resolvente de los operadores de Dirac H_M y $H_{\mathrm{MIT}}(m)$, véase el teorema 4.5.1 para la fórmula explícita. De este modo, obtenemos la respuesta a la pregunta que formulamos anteriormente. En efecto, como corolario de la fórmula del resolvente tenemos en el corolario 4.5.1 que existe un operador $1/M$-pseudodiferencial de orden 0, $\Xi_M^-(z)$, tal que la restricción de U, denotada por $U_{|\Omega}$, satisface el siguiente problema elíptico :

$$\begin{cases} (H - z)U_{|\Omega_i} = f & \text{en } \Omega, \\ \quad P_- t_\Sigma U_{|\Omega} = \Xi_M^-(z) P_+ t_\Sigma (H_{\mathrm{MIT}}(m) - z)^{-1}(f_{|\Omega}) & \text{en } \Sigma, \\ \quad P_+ t_\Sigma U_{|\Omega} = P_+ t_\Sigma (H_{\mathrm{MIT}}(m) - z)^{-1}(f_{|\Omega}) + \mathscr{A}_m P_- t_\Sigma U & \text{en } \Sigma, \end{cases}$$

Además, mostramos que el operador perturbado converge en el sentido de la norma resolvente al operador MIT bag y damos una estimación precisa de la tasa de convergencia, véase la proposición 4.5.1.

Chapter 1

Layer potentials associated with the Dirac operator

The purpose of this chapter is to fix some terminology that will be used throughout this thesis, and to present some tools that will be used in the following chapters.

We start first by setting notations, recalling some definitions and results from geometric measure theory, used in particular in Chapter 3. Subsequently, we recall the definition of some function spaces that are often used, in particular, we present some important properties of the Dirac-Sobolev space on Lipschitz domains. Then, we shall introduce and study some integral operators associated with the fundamental solution of the free Dirac operator, which will play an important role in the analysis of Dirac operators with δ-interactions.

1.1 Notation and Definitions

We use the following notations:

- For a Hilbert space $\mathfrak{h}$, we denote by $\mathscr{B}(\mathfrak{h})$ (respectively $\mathscr{K}(\mathfrak{h})$) the space of bounded (resp. compact), everywhere defined linear operators in $\mathfrak{h}$. If T is a closed operator in $\mathfrak{h}$ then its spectrum, essential spectrum, point spectrum and discrete spectrum are denoted by $\mathrm{Sp}(T)$, $\mathrm{Sp}_{\mathrm{ess}}(T)$, $\mathrm{Sp}_{\mathrm{pp}}(T)$ and $\mathrm{Sp}_{\mathrm{disc}}(T)$, respectively.

- For A, $B \in \mathscr{B}(\mathfrak{h})$, we denote by $[A, B]$ and $\{A, B\}$ the usual commutator and anticommutator brackets, respectively.

- We use the letter C (or c) to denote harmless positive constant, not necessarily the same at each occurrence.

- We write $A \lesssim B$ if there is $C > 0$ so that $A \leqslant CB$ and $A \lesssim_h B$ if the constant C depends on the parameter h.

- We use the notation $\mathbb{R}^3_\pm = \{x \in \mathbb{R}^3 : \pm x_3 > 0\}$ for the upper/lower half space. Also, the upper/lower complex half plane is denoted by $\mathbb{C}_\pm$.

- The square root $\sqrt{z}$ is fixed by the convention $\Im(z) > 0$ for $z \in \mathbb{C} \setminus [0, \infty)$.

- For $x = (x_1, \cdots, x_d) \in \mathbb{R}^d$, we let $|x|_\infty := \sup_{j \in 1, \cdots, d}\{|x_j|\}$ to be the l^∞ norm of x, and we denote by $|x| := |x|_2$ the standard Euclidean l^2 distance.

- For $\alpha = (\alpha_1, \cdots, \alpha_d) \in \mathbb{N}^d$ a vector of nonnegative integers, denote

$$\partial^\alpha = \frac{\partial^{|\alpha|}}{\partial_{x_1^{\alpha_1}} \cdots \partial_{x_1^{\alpha_d}}} \quad \text{with } |\alpha| = \sum_d^1 \alpha_j,$$

  and for a sufficiently smooth function u and $x \in \mathbb{R}^d$, denote

$$\partial^\alpha u = \frac{\partial^{|\alpha|} u}{\partial_{x_1^{\alpha_1}} \cdots \partial_{x_1^{\alpha_d}}} \quad \text{and } x^\alpha = x_1^{\alpha_1} \cdots x_d^{\alpha_d}.$$

- By $\mathscr{H}^2$ we denote the 2-dimensional Hausdorff measure, and we let $\mathrm{d}\sigma = \mathrm{d}\mathscr{H}^2|_{\mathrm{E}}$ to be the surface measure on a closed set $\mathrm{E} \subset \mathbb{R}^3$ of dimension 2.
- For $p, d \in \mathbb{N}^*$ and a closed subset $E \subset \mathbb{R}^d$, we always denote by $L^p(\mathbb{R}^d)$ and $L^p(E)$ the L^p-based Banach space with respect to the Lebesgue measure and the surface measure, respectively.
- We denote by $\operatorname{diam}(E)$ the diameter of E, that is $\operatorname{diam}(E) := \sup_{x,y \in E} |x - y|$.
- We denote by $B(x, r)$ the Euclidean ball of radius r centred at $x \in \mathbb{R}^3$.
- For an Ω open (proper) subset of $\mathbb{R}^3$, Ω^{c} denotes the complement of Ω.
- For a Borel set $B \subset \mathbb{R}^3$, we denote by 1_B the characteristic function of B, that is $1_B(x) = 1$ if $x \in B$ and $1_B(x) = 0$ if $x \notin B$.
- For a Borel set B of $\mathbb{R}^3$, the Lebesgue measure of B is denoted by $|B|$.
- For a Borel measure μ, and a Borel set B with $0 < \mu(B) < \infty$, we set

$$\fint_B U \mathrm{d}\mu := \mu(B)^{-1} \int_B U \mathrm{d}\mu,$$

  where U is any μ-integrable function on B.

Definition 1.1.1 (Ahlfors-David regular)**.** *We say that a set $E \subset \mathbb{R}^3$ is 2-dimensional Ahlfors-David regular, or simply ADR, if it is closed and there is some uniform constant C such that*

$$\frac{1}{C} r^2 \leqslant \mathscr{H}^2(B(x, r) \cap E) \leqslant C r^2, \quad \forall x \in E, r \in (0, \operatorname{diam}(E)). \tag{1.1.1}$$

Definition 1.1.2 (Uniformly rectifiable domains)**.** *We say that a compact set $E \subset \mathbb{R}^3$ is uniformly rectifiable provided that it is ADR and the following holds. There exist $\rho, M \in (0, \infty)$ (called the UR character of E) such that for each $x \in E$, $r \in (0, 1]$, there is a Lipschitz map $\phi : B_r \subset \mathbb{R}^2 \to \mathbb{R}^3$ (where B_r is a ball of radius r in $\mathbb{R}^2$) with Lipschitz constant $L_\phi \leqslant M$, such that*

$$\mathscr{H}^2(E \cap B(x, r) \cap \phi(B_r)) \geqslant \rho r^2. \tag{1.1.2}$$

A nonempty, proper and bounded open subset $\Omega \subset \mathbb{R}^3$ is called uniformly rectifiable, or simply UR, provided that $\partial\Omega$ is uniformly rectifiable and also $\mathscr{H}^2(\partial\Omega \setminus \partial_*\Omega) = 0$, where $\partial_*\Omega$ denotes the measure theoretic boundary of Ω, defined as

$$\partial_*\Omega := \left\{ x \in \partial\Omega : \limsup_{r \to 0} \frac{|B(x, r) \cap \Omega|}{r^3} > 0, \limsup_{r \to 0} \frac{|B(x, r) \cap \Omega^{\mathrm{c}}|}{r^3} > 0 \right\}.$$

Remark 1.1.1. *Notice that there are numerous characterizations of UR sets that are equivalent to the one given above. For our purposes, the most useful equivalent definition that one should keep in mind is as follows: If E is ADR, then E is UR if and only if the Riesz transform defined by*

$$g \in L^2(E) \to \mathscr{R}[g](x) = \lim_{\rho \searrow 0} \int_{|x-y|>\rho} \frac{x-y}{|x-y|^3} g(y) \mathrm{d}\sigma(y), \quad \text{for all } x \in E, \tag{1.1.3}$$

is bounded from $L^2(E)$ into itself, cf. [88].

Remark 1.1.2. *It is worth pointing out that, in principle, the measure theoretic boundary $\partial_*\Omega$ can be a much smaller than the topological $\partial\Omega$. In this sense, the condition $\mathcal{H}^2(\partial\Omega \setminus \partial_*\Omega) = 0$ in Definition 1.1.2 ensures that near points in boundary $\partial_*\Omega$ there is enough mass relative to the scale, both in Ω and Ω^{c}.*

Definition 1.1.3 (Lipschitz domains)**.** *We say a domain (connected open set) $\Omega \subset \mathbb{R}^d$ is γ-Lipschitz domain if for every $x \in \Omega$ there exists $r > 0$ and an isometric coordinate system with origin $x = x_0$ such that*

$$\{y \in \mathbb{R}^d : |x-y|_\infty < r\} \cap \Omega = \{y \in \mathbb{R}^d : |x-y|_\infty < r\} \cap \{(\tilde{y}, t) : \tilde{y} \in \mathbb{R}^{d-1},\, \phi(\tilde{y}) < t\},$$

for some Lipschitz function $\phi : \mathbb{R}^{d-1} \to \mathbb{R}$ with $\phi(x_0) = x_0$ and $\|\phi\|_\infty \leqslant \gamma$. We say a domain is a Lipschitz domain if it is a γ-Lipschitz domain for some $\gamma \geqslant 0$. We call a domain $\Omega \subset \mathbb{R}^d$ of the form

$$\Omega = \{(\tilde{y}, t) : \tilde{y} \in \mathbb{R}^{d-1},\, \phi(\tilde{y}) < t\},$$

for some Lipschitz function $\phi : \mathbb{R}^{d-1} \to \mathbb{R}$ with $\|\phi\|_\infty \leqslant \infty$ a Lipschitz graph domain.

Remark 1.1.3. *It is worth noting that, if $\phi : \mathbb{R}^{d-1} \to \mathbb{R}$ is a Lipschitz function, then Rademacher's therem entails that ϕ is Fréchet-differentiable almost everywhere with*

$$\|\nabla\phi\|_{L^\infty(\mathbb{R}^{d-1})} \leqslant L_\phi,$$

where L_ϕ is the Lipschitz constant of ϕ. In particular, if Ω is a Lipschitz graph domain (as in the definition above), then for $x = \phi(\tilde{x}) \in \partial\Omega$ the surface measure and the unit normal vector field are given by

$$\mathrm{d}\sigma(x) = \sqrt{1 + |\nabla\phi(\tilde{x})|^2}\mathrm{d}\tilde{x}, \quad N(x) = \frac{(-\nabla\phi(\tilde{x}), -1)}{\sqrt{1 + |\nabla\phi(\tilde{x})|^2}}.$$

Notice that when Ω is an ADR domain then the unit normal N is defined almost everywhere on $\partial_*\Omega$, and it is often referred to as the geometric measure theoretic outward unit normal to Ω, cf. [63].

Sometimes, a different smoothness condition will be needed, so we broaden the above definition as follows:

Definition 1.1.4. *For an integer $k \geqslant 1$, we say a domain $\Omega \subset \mathbb{R}^d$ is a C^k-smooth domain if the properties in the previous definition hold but with ϕ of class C^k and the L^∞ norm of all these ϕ and their first k derivatives are uniformly bounded. Likewise, for $\omega \in (0, 1]$, we define a $C^{k,\omega}$-smooth domain by adding the requirement that the kth order partial derivatives of ϕ be Hölder-continuous with exponent ω, i.e.,*

$$|\partial^\alpha\phi(\tilde{x}) - \partial^\alpha\phi(\tilde{y})| \lesssim |\tilde{x} - \tilde{y}|^\omega \quad \text{for all } \tilde{x}, \tilde{y} \in \mathbb{R}^{d-1} \text{ and } |\alpha| = k.$$

Finally, we say that Ω is a C^∞-smooth domain if it is C^k-smooth for any $k \in \mathbb{N}$.

Definition 1.1.5 (BMO and VMO)**.** *For an ADR set $E \subset \mathbb{R}^3$,* $\mathrm{BMO}(E, \mathrm{d}\sigma)$ *stands for the space of functions with bounded mean oscillation, relative to the surface measure* $\mathrm{d}\sigma$*. We denote by* $\mathrm{VMO}(E, \mathrm{d}\sigma)$ *the Sarason space of functions with vanishing mean oscillation on E, i.e., the closure of the set of bounded uniformly continuous functions defined on E in* $\mathrm{BMO}(E, \mathrm{d}\sigma)$*.*

Let us now assume that Ω is a UR domain with $\partial\Omega = \partial\overline{\Omega}$, and set

$$\Omega_+ = \Omega \text{ and } \Omega_- := \mathbb{R}^3 \setminus \overline{\Omega}. \tag{1.1.4}$$

Then, Ω_- is also a UR domain with the same ADR boundary as Ω_+ (cf. [63, Proposition 3.10]), which we denote by $\Sigma := \partial\Omega_+ = \partial\Omega_-$.

Definition 1.1.6. *Let $\Omega_\pm$ be as above. Fix $a > 0$ and let $x \in \Sigma$, then the nontangential approach regions of opening a at the point x are defined by*

$$\Gamma^{\Omega_\pm}(x) = \Gamma_a^{\Omega_\pm}(x) = \{y \in \Omega_\pm : |x - y| < (1 + a)\mathrm{dist}(y, \Sigma)\}. \tag{1.1.5}$$

If $x \in \Sigma$ and $U : \Omega_\pm \to \mathbb{C}^4$, then

$$U_\pm(x) = U|^{nt}_{\Omega_\pm}(x) := \lim_{\Gamma^{\Omega_\pm}(x) \ni y \longrightarrow x} U(y), \tag{1.1.6}$$

is the nontangential limit of U with respect to $\Omega_\pm$ at x. We also define the nontangential maximal function of U on Σ by

$$\mathcal{N}^{\Omega_\pm}[U](x) = \mathcal{N}_a^{\Omega_\pm}[U](x) = \sup\{|U(y)| : y \in \Gamma^{\Omega_\pm}(x)\}, \quad x \in \Sigma, \tag{1.1.7}$$

with the convention that $\mathcal{N}^{\Omega_\pm}[U](x) = 0$ when $\Gamma^{\Omega_\pm}(x) = \emptyset$. Given $g \in L^2(\Sigma)$, we define the Hardy-Littlewood maximal operator by

$$M^\Sigma g(x) = \sup_{r>0} ⨍_{B(x,r)\cap\Sigma} |g(y)| \mathrm{d}\sigma, \quad x \in \Sigma. \tag{1.1.8}$$

Then, by [45, p. 624], there is $C > 0$ such that

$$\|M^\Sigma g\|_{L^2(\Sigma)} \leqslant C\|g\|_{L^2(\Sigma)}, \quad \text{for all } g \in L^2(\Sigma). \tag{1.1.9}$$

1.2 Function spaces

1.2.1 Sobolev and Besov spaces

Sobolev spaces are fundamental in the study of partial differential equations. Since we are going to deal with partial differential operators, we shall present in this section several Sobolev and Besov spaces on Lipschitz domains (resp. on the boundary of Lipschitz domains). We refer to [1, 81] for comprehensive treatment of Sobolev spaces.

Sobolev on domains

Definition 1.2.1. *Let Ω be a non-empty open subset of $f\,\mathbb{R}^d$. For an integer $k \geqslant 0$ we let*

$$C^k(\Omega) = \{u : \Omega \to \mathbb{C} : \partial^\alpha u \text{ exists and is continuous on } \Omega \text{ for } |\alpha| \leqslant k\},$$

and we let $C^\infty(\Omega)$ denotes the usual space of indefinitely differentiable functions, i.e,

$$C^\infty(\Omega) = \bigcap_{k\geqslant 0} C^k(\Omega).$$

Similarly, we let

$$C_0^k(\Omega) = \{u \in C^k(\Omega) : \text{supp}(u) \subset K \subset\subset \Omega \textit{ for some compact set } K\},$$

and set

$$\mathscr{D}(\Omega) = C_0^\infty(\Omega) = \{u \in C^\infty(\Omega) : \text{supp}(u) \subset K \subset\subset \Omega \textit{ for some compact set } K\}.$$

Finally, we denote by $\mathscr{D}'(\Omega)$ the dual space of $\mathscr{D}(\Omega)$, i.e., the usual set of all distributions on Ω.

Definition 1.2.2 (Tempered distributions)**.** *For an integer $d \geqslant 1$, we let $\mathscr{S}(\mathbb{R}^d)$ be the Schwartz class of functions, i.e.,*

$$\mathscr{S}(\mathbb{R}^d) = \{u \in C^\infty(\mathbb{R}^d) : \sup_{x \in \mathbb{R}^d} |x^\alpha \partial^\beta u(x)| < \infty, \textit{ for all multi-indices } \alpha, \beta \in \mathbb{N}^d\}.$$

We denote by $\mathscr{S}'(\mathbb{R}^d)$ the dual space of $\mathscr{S}(\mathbb{R}^d)$, i.e., the space of tempered distributions.

Definition 1.2.3 (Fourier transform)**.** *For a function $f \in \mathscr{S}(\mathbb{R}^d)$, its Fourier transform is defined by*

$$\mathcal{F}[u](\xi) = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} e^{-ix\cdot\xi} u(x) \mathrm{d}x, \quad \forall \xi \in \mathbb{R}^d,$$

and its inverse Fourier transform is given by

$$\mathcal{F}^{-1}[u](x) = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} e^{i\xi\cdot x} u(\xi) \mathrm{d}\xi, \quad \forall x \in \mathbb{R}^d.$$

The Fourier transform defines a continuous linear operator from $\mathscr{S}(\mathbb{R}^d)$ into itself. By duality, we can also extend $\mathcal{F}$ to the space of tempered distributions $\mathscr{S}'(\mathbb{R}^d)$. In particular, the Fourier transform can be extended into an isometry in $L^2(\mathbb{R}^d)$.

Remark 1.2.1. *For $\overline{x} \in \mathbb{R}^{d-1}$ we will abbreviate the partial Fourier (resp. inverse Fourier) transform on the variable $\overline{x}$ with $\mathcal{F}_{\overline{x}}$ (resp. $\mathcal{F}_{\overline{x}}^{-1}$).*

Definition 1.2.4 (Sobolev space on $\mathbb{R}^d$)**.** *For $s \in \mathbb{R}$, we define the Sobolev space $H^s(\mathbb{R}^d)$ as follows:*

- *If $s = 0$, then $H^s(\mathbb{R}^d) = L^2(\mathbb{R}^d)$.*
- *If $s > 0$, then $H^s(\mathbb{R}^d) = \{u \in L^2(\mathbb{R}^d) : \int_{\mathbb{R}^d} (1 + |\xi|^2)^s |\mathcal{F}[u](\xi)|^2 \mathrm{d}\xi < \infty\}$, endowed with the norm*
$$\|f\|^2_{H^s(\mathbb{R}^d)} = \int_{\mathbb{R}^d} (1 + |\xi|^2)^s |\mathcal{F}[u](\xi)|^2 \mathrm{d}\xi, \quad \forall f \in H^s(\mathbb{R}^d).$$
- *If $s < 0$, then $H^s(\mathbb{R}^d)$ is defined as as the completion of $L^2(\mathbb{R}^d)$ with respect to the norm $\|\cdot\|_{H^s(\mathbb{R}^d)}$. Equivalently, $H^s(\mathbb{R}^d)$ can be viewed as an isometric realization of the dual space of $H^{-s}(\mathbb{R}^d)$.*

Definition 1.2.5 (Sobolev space on domains)**.** *Let Ω be a Lipschitz domain of $\mathbb{R}^d$ and let $k \in \mathbb{N}$. Then the Sobolev space $H^k(\Omega)$ of order k based on $L^2(\Omega)$ is defined by*

$$H^k(\Omega) = \{u \in L^2(\Omega) : \partial^\alpha u \in L^2(\Omega) \textit{ for } |\alpha| \leqslant k\},$$

endowed with the norm

$$\|u\|^2_{H^k(\Omega)} = \sum_{|\alpha|\leqslant k} \int_\Omega |\partial^\alpha u(x)|^2 \mathrm{d}x.$$

For $k=1$ we often use that

$$H^k(\Omega) = \{u \in L^2(\Omega) : \text{ there exists } \tilde{u} \in H^1(\mathbb{R}^d) \text{ such that } \tilde{u}|_\Omega = ui\},$$

endowed with the norm

$$\|u\|^2_{H^1(\Omega)} = \|u\|^2_{L^2(\Omega)} + \|\nabla u\|^2_{L^2(\Omega)},$$

and we let $H^1_0(\Omega)$ to be the closure of $C^\infty_0(\Omega)$ with respect to the above norm.
Now, for $0 < r < 1$ we define the semi-norms

$$\|u\|^2_{r,\Omega} = \int_\Omega \int_\Omega \frac{|u(x)-u(y)|^2}{|x-y|^{d+2r}} \mathrm{d}x\mathrm{d}y.$$

Then, for $s = k + r$ the Sobolev space of fractional order s is defined by

$$H^s(\Omega) = \{u \in H^k(\Omega) : \|\partial^\alpha u\|^2_{r,\Omega} < \infty \text{ for } |\alpha| = k\},$$

equiped with the norm

$$\|u\|^2_{H^s(\Omega)} = \|u\|^2_{H^k(\Omega)} + \sum_{|\alpha|=k} \|\partial^\alpha u\|^2_{r,\Omega}.$$

We recall that all the Sobolev spaces defined above are Hilbert spaces with respect to their norms.

Sobolev on the boundary

We next give the definition of Sobolev spaces on the boundary of Lipschitz domain. We also define the Besov space $B^2_{1/2}(\partial\Omega)$ when Ω is an a ADR domain, which is very important when dealing with δ-interactions supported on ADR surfaces. Recall that $L^2(\partial\Omega, \mathrm{d}\sigma) := L^2(\partial\Omega)$ denotes the usual L^2-space over $\partial\Omega$.

Definition 1.2.6. *Let Ω be a Lipschitz graph domain of $\mathbb{R}^d$, i.e.,*

$$\Omega = \{(\tilde{y}, t) : \tilde{y} \in \mathbb{R}^{d-1},\ \phi(\tilde{y}) < t\}.$$

For $g \in L^2(\partial\Omega)$, we define $g_\phi(\overline{x}) = g(\overline{x}, \nu\phi(\overline{x}))$ for $\overline{x} \in \mathbb{R}^{d-1}$. Then, for $s \in [0,1]$, the Sobolev space $H^s(\partial\Omega)$ of order s is defined by

$$H^s(\partial\Omega) := \{g \in L^2(\partial\Omega) : g_\phi \in H^s(\mathbb{R}^{d-1})\},$$

equipped with the scalar product

$$\langle g, f\rangle_{H^s(\partial\Omega)} = \langle g_\phi, f_\phi\rangle_{H^s(\mathbb{R}^{d-1})},$$

and we define $H^{-s}(\partial\Omega)$ as the completion of $L^2(\partial\Omega)$ with the following norm:

$$\|g\|_{H^{-s}(\partial\Omega)} := \|g_\phi \sqrt{1+|\nabla\phi|^2}\|_{H^{-s}(\mathbb{R}^{d-1})}, \text{ for all } s \in [0,1].$$

If Ω is a Lipschitz domain with a compact boundary $\partial\Omega$. Then, for $s \in [0,1]$, the Sobolev space $H^s(\partial\Omega)$ of order s is defined using local coordinates representation on the surface $\partial\Omega$, see [81] for example.

Notice that $H^{-s}(\partial\Omega)$ is a realization of the dual space of $H^s(\partial\Omega)$. That is,

$$\|g\|_{H^{-s}(\partial\Omega)^4} = \sup_{0\neq f\in H^s(\partial\Omega)} \frac{\langle g, f\rangle_{H^{-s}(\partial\Omega),H^s(\partial\Omega)}}{\|f\|_{H^s(\partial\Omega)^4}}.$$

see, e.g. [81].

When Ω is in the class $C^{1,\omega}$ with a compact boundary, $\omega \in (0,1)$, one can define equivalently the Sobolev space $H^s(\partial\Omega)^4$ as follows (see [67, Chapter 4] for example):

Definition 1.2.7. *Given $\omega \in (0,1)$ and assume that Ω is a bounded $C^{1,\omega}$-smooth domain with a compact boundary. Then, $g \in H^s(\partial\Omega)$ with $s \in (0,\omega)$, if and only if*

$$\|g\|^2_{H^s(\partial\Omega)^4} := \int_{\partial\Omega} |g(x)|^2 \mathrm{d}\sigma(x) + \int_{\partial\Omega}\int_{\partial\Omega} \frac{|g(x)-g(y)|^2}{|x-y|^{2(1+s)}} \mathrm{d}\sigma(y)\mathrm{d}\sigma(x) < \infty.$$

When studying δ-interaction supported on surface, we shall need to make sense of the restriction $U\restriction_{\partial\Omega}$ as an element of a Sobolev space on $\partial\Omega$ when U belongs to a Sobolev space on Ω or $\mathbb{R}^d$. Let us now recall some trace theorems that will be used in the rest of this thesis.

First, recall that if Ω is an non-empty open set of $\mathbb{R}^d$, then the mappings

$$\begin{aligned} t_{\partial\Omega} : \mathcal{D}(\overline{\Omega}) &\longrightarrow \mathcal{D}(\partial\Omega) \\ U &\longmapsto t_{\partial\Omega}U = U\restriction_{\partial\Omega}, \end{aligned}$$

$$\begin{aligned} t_{\partial\Omega} : \mathcal{D}(\mathbb{R}^d) &\longrightarrow \mathcal{D}(\partial\Omega) \\ U &\longmapsto t_{\partial\Omega}U = U\restriction_{\partial\Omega}, \end{aligned}$$

are well-defined and continuous.

Proposition 1.2.1. *Assume that Ω is a Lipschitz domain of $\mathbb{R}^d$. Then, the trace operator $t_{\partial\Omega} : \mathcal{D}(\overline{\Omega}) \longrightarrow \mathcal{D}(\partial\Omega)$ extend to a unique bounded linear operator $t_{\partial\Omega} : H^s(\Omega) \longrightarrow H^{s-1/2}(\partial\Omega)$ for all $s \in (1/2, 3/2)$, i.e.,*

$$\|t_{\partial\Omega}U\|_{H^{s-1/2}(\partial\Omega)} \lesssim \|U\|_{H^s(\Omega)}, \quad \forall U \in H^s(\Omega).$$

Moreover, if $s \in (1/2, 1]$, then $t_{\partial\Omega}$ has a bounded linear inverse operator $\mathcal{E}_\Omega : H^{s-1/2}(\partial\Omega) \longrightarrow H^s(\Omega)$, i.e.,

$$\|\mathcal{E}_\Omega[g]\|_{H^s(\Omega)} \lesssim \|g\|_{H^{s-1/2}(\partial\Omega)} \quad \textit{and}\ t_{\partial\Omega}\mathcal{E}_\Omega[g] = g \quad \forall g \in H^{s-1/2}(\partial\Omega).$$

For a function $u \in H^1(\mathbb{R}^d)$, with a slight abuse of terminology we will refer to $t_{\partial\Omega}u$ as the restriction of u on $\partial\Omega$ when Ω is Lipschitz. We shall also use a trace theorem for functions in the Sobolev space $H^1(\mathbb{R}^d)$ in the case of ADR surfaces. Assume that Ω is an ADR domains, then the Besov space $B^2_{1/2}(\partial\Omega)$ (see [73, Chapter V] for example), consists of all functions $g \in L^2(\partial\Omega)$ for which

$$\int\int_{|x-y|<1} \frac{|g(x)-g(y)|^2}{|x-y|^3} \mathrm{d}\sigma(y)\mathrm{d}\sigma(x) < \infty. \tag{1.2.1}$$

The Besov space is equipped with the norm

$$\|g\|^2_{B^2_{1/2}(\partial\Omega)} := \int_{\partial\Omega} |g(x)|^2 \mathrm{d}\sigma(x) + \int\int_{|x-y|<1} \frac{|g(x)-g(y)|^2}{|x-y|^3} \mathrm{d}\sigma(y)\mathrm{d}\sigma(x). \tag{1.2.2}$$

Given $U \in H^1(\mathbb{R}^d)$, set

$$T_{\partial\Omega} u(x) := \lim_{r \searrow 0} \fint_{B(x,r)} U(y)\mathrm{d}y, \tag{1.2.3}$$

at every point $x \in \partial\Omega$ where the limit exists. Then, we have the following trace theorem, for the proof we refer to [72, Theorem 1 and Example 1] and [73, Theorem 1, p.182].

Proposition 1.2.2. *Suppose that Ω is an ADR domain. Then the trace operator $t_{\partial\Omega} : \mathcal{D}(\mathbb{R}^d) \longrightarrow \mathcal{D}(\partial\Omega)$ extend to a bounded linear operator $T_{\partial\Omega}$ from $H^1(\mathbb{R}^d)$ to $B^2_{1/2}(\partial\Omega)$ (where T_Σ is given by (1.2.3)) with a bounded linear inverse operator $\mathcal{E}$ from $B^2_{1/2}(\partial\Omega)$ to $H^1(\mathbb{R}^d)$. In other words, $B^2_{1/2}(\partial\Omega)$ is the trace to $\partial\Omega$ of $H^1(\mathbb{R}^d)$ and $T_{\partial\Omega}\mathcal{E}$ is the identity operator.*

Remark 1.2.2. *For notational convenience, we use $t_{\partial\Omega}$ in the rest of the paper to denote the trace operator when $\partial\Omega$ is ADR, and we often use the fact that the trace operator $T_{\partial\Omega}$ coincide with $t_{\partial\Omega}$ when Ω is a Lipschitz domain (i.e., $H^{1/2}(\partial\Omega)$ is the trace to $\partial\Omega$ of $H^1(\mathbb{R}^d)$).*

1.2.2 The Dirac-Sobolev space

The aim of this part is to study the first order Sobolev space associated with the Dirac operator H on a Lipschitz domain $\Omega \subset \mathbb{R}^3$. The study of this space is crucial in the analysis of Dirac operators on domains with boundary condition, as well as shell interactions for Dirac operators. The results we are going to present here are well-known when Ω is a C^2-smooth domain with a compact boundary, and can be found in [90].

Throughout this subsection, unless stated otherwise, we assume that Ω is a Lipschitz domain, we let $\Sigma := \partial\Omega$ and we denote by N the outward unit normal to Ω.

Definition 1.2.8. *Let Ω be an open subset of $\mathbb{R}^3$. The first order Dirac-Sobolev space $H(\alpha, \Omega)$ is defined as follows:*

$$H(\alpha, \Omega) = \{\varphi \in L^2(\Omega)^4 : (\alpha \cdot \nabla)\varphi \in L^2(\Omega)^4\}, \tag{1.2.4}$$

equipped with the scalar product

$$\langle \varphi, \psi \rangle_{H(\alpha,\Omega)} = \langle \varphi, \psi \rangle_{L^2(\Omega)^4} + \langle (\alpha \cdot \nabla)\varphi, (\alpha \cdot \nabla)\psi \rangle_{L^2(\Omega)^4}, \quad \varphi, \psi \in H(\alpha, \Omega).$$

Here $(\alpha \cdot \nabla)\varphi$ is taken in the sense of distributions.

Remark 1.2.3. *Notice that if $\Omega = \mathbb{R}^3$, then $H(\alpha, \Omega)$ coincides with $H^1(\mathbb{R}^3)$. We also note that, since the multiplication by β is bounded in $L^2(\Omega)^4$, we have*

$$H(\alpha, \Omega) = \{\varphi \in L^2(\Omega)^4 : H\varphi \in L^2(\Omega)^4\}.$$

Let us now give some basic properties of this Dirac-Sobolev space. First, we recall the following consequence of the Green's formula.

Proposition 1.2.3. *Assume that Ω is a Lipschitz domain. Then, for all $\psi, \varphi \in H^1(\Omega)^4$ it holds that*

$$\langle (-i\alpha \cdot \nabla)\varphi, \psi \rangle_{L^2(\Omega)^4} - \langle \varphi, (-i\alpha \cdot \nabla)\psi \rangle_{L^2(\Omega)^4} = \langle (-i\alpha \cdot N) t_\Sigma \varphi, t_\Sigma \psi \rangle_{L^2(\Sigma)^4}.$$

Lemma 1.2.1. *Let Ω be a Lipschitz domain, then $(H(\alpha, \Omega), \langle \cdot, \cdot \rangle_{H(\alpha,\Omega)})$ is a Hilbert space and the following statement hold:*

(i) $C_0^\infty(\overline{\Omega})^4$ *is a dense subspace of* $H(\alpha,\Omega)$*. In particular,* $H^1(\Omega)^4$ *is dense in* $H(\alpha,\Omega)$ *and it holds that*

$$\|\psi\|_{H(\alpha,\Omega)} \lesssim \|\psi\|_{H^1(\Omega)^4} \quad \text{for all } \psi \in H^1(\Omega)^4.$$

(ii) Let $H_0(\alpha,\Omega)$ *be the completion of* $C_0^\infty(\Omega)^4$ *with respect to the norm* $\|\cdot\|_{H(\alpha,\Omega)}$*. Then,* $H_0(\alpha,\Omega)$ *coincides with* $H_0^1(\Omega)^4$*.*

Proof. Given a Cauchy sequence $(\psi_j)_{j\in\mathbb{N}} \subset H(\alpha,\Omega)$. Then, we have

$$\psi_j \xrightarrow[j\to\infty]{} \psi \in L^2(\Omega)^4 \quad \text{and} \quad (\alpha\cdot\nabla)\psi_j \xrightarrow[j\to\infty]{} \varphi \in L^2(\Omega)^4,$$

Since both $(\psi_j)_{j\in\mathbb{N}}$ and $((\alpha\cdot\nabla)\psi_j)_{j\in\mathbb{N}}$ are Cauchy sequence in $L^2(\Omega)^4$, and as $(\alpha\cdot\nabla)\psi = \lim_{j\to\infty}(\alpha\cdot\nabla)\psi_j = \varphi$ holds in $\mathscr{D}'(\Omega)^4$ and $\varphi \in L^2(\Omega)^4$, it follows that $\varphi = (\alpha\cdot\nabla)\psi$ in $L^2(\Omega)^4$. Therefore, $(H(\alpha,\Omega), \langle\cdot,\cdot\rangle_{H(\alpha,\Omega)})$ is a Hilbert space.

Since $C_0^\infty(\overline{\Omega})^4$ is dense in $H^1(\Omega)^4$, to prove (i) it suffices to show that $H^1(\Omega)^4$ is continuously embedded in $H(\alpha,\Omega)$. Let $\psi \in H^1(\Omega)^4$, then Hölder's inequality yields that

$$|(\alpha\cdot\nabla)\psi|^2 = \left|\sum_{j=1}^{3}(\alpha_j\partial_j)\psi\right|^2 \leqslant \left(\sum_{j=1}^{3}|(\alpha_j\partial_j)\psi|\right)^2 = 3\left(\sum_{j=1}^{3}|(\alpha_j\partial_j)\psi|^2\right) = 3|\nabla\psi|^2,$$

here we used that $|\alpha_j\psi| = |\psi|$. Hence we get

$$\|(\alpha\cdot\nabla)\psi\|_{L^2(\Omega)^4} = \left(\int_\Omega |(\alpha\cdot\nabla)\psi|^2\right)^{1/2} \leqslant 3^{1/2}\left(\int_\Omega |\nabla\psi|^2\right)^{1/2} = 3^{1/2}\|\nabla\psi\|_{L^2(\Omega)^4}.$$

Thus the inclusion $H^1(\Omega)^4 \subset H(\alpha,\Omega)$ is continuous and the inequality $\|\psi\|_{H(\alpha,\Omega)} \lesssim \|\psi\|_{H^1(\Omega)^4}$ holds for all $\psi \in H^1(\Omega)^4$, which proves (i).

Now, let us prove (ii). By definition, it is clear that $H_0^1(\Omega)^4 \subset H_0(\alpha,\Omega)$. To show the reverse inclusion, it is straightforward to see that

$$H_0(\alpha,\Omega) = \{\varphi \in L^2(\Omega)^4 : (\alpha\cdot\nabla)\varphi \in L^2(\Omega)^4 \text{ and } t_\Sigma\varphi = 0 \text{ on } \Sigma\}.$$

From this and the assertion (i) of this lemma, we easily get the inclusion $H_0(\alpha,\Omega) \subset H_0^1(\Omega)^4$, which completes the proof of (ii). □

Notice that if $\psi_1,\psi_2 \in H^1(\Omega)^4$ are such that $\|\psi_1-\psi_2\|_{H(\alpha,\Omega)} = 0$, then $\psi_1 = \psi_2$ in $L^2(\Omega)^4$, and thus $\psi_1 = \psi_2$ holds in $H^1(\Omega)^4$. As consequence of this and lemma 1.2.1 we have:

Corollary 1.2.1. *The following statements hold true:*

(i) The mapping $H^1(\Omega)^4 \ni \psi \longmapsto F(\psi) = \psi \in H(\alpha,\Omega)$ *is one-to-one and continuous.*

(ii) The mapping $H_0^1(\Omega)^4 \ni \psi \longmapsto F(\psi) = \psi \in H_0(\alpha,\Omega)$ *is continuous and bijective.*

The next proposition shows that the trace of a function $\psi \in H(\alpha,\Omega)$ belongs to $H^{-1/2}(\Sigma)^4$, and in particular, if $t_\Sigma\psi$ is in $H^{1/2}(\Sigma)^4$ then ψ is in $H^1(\Omega)^4$. The proof of this result follows the same lines as the one of [90, proposition 2.1], where the case of a C^2-smooth domain with a compact boundary is considered.

Proposition 1.2.4. *The following statements hold true:*

(i) *If Ω is a Lipschitz domain, then the operator $(\alpha \cdot N)t_\Sigma : H^1(\Omega)^4 \to L^2(\Sigma)^4$ extends into a continuous map $\widetilde{t_\Sigma} : H(\alpha,\Omega) \to H^{-1/2}(\Sigma)^4$, and we have*

$$\langle(-i\alpha\cdot\nabla)\psi,\varphi\rangle_{L^2(\Omega)^4} - \langle\psi,(-i\alpha\cdot\nabla)\varphi\rangle_{L^2(\Omega)^4} = \langle\widetilde{t_\Sigma}\psi, t_\Sigma\varphi\rangle_{H^{-1/2}(\Sigma)^4,H^{1/2}(\Sigma)^4}, \quad (1.2.5)$$

for all $\psi \in H(\alpha,\Omega)$ and $\varphi \in H^1(\Omega)^4$.

(ii) *if Ω is $C^{1,\omega}$-smooth domain, with $\omega \in (1/2,1)$, then the trace operator $t_\Sigma : H^1(\Omega)^4 \to H^{1/2}(\Sigma)^4$ has a unique extension to a bounded linear operator $t_\Sigma : H(\alpha,\Omega) \to H^{-1/2}(\Sigma)^4$, and we have*

$$\langle(-i\alpha\cdot\nabla)\psi,\varphi\rangle_{L^2(\Omega)^4} - \langle\psi,(-i\alpha\cdot\nabla)\varphi\rangle_{L^2(\Omega)^4} = \langle(-i\alpha\cdot N)t_\Sigma\psi, t_\Sigma\varphi\rangle_{H^{-1/2}(\Sigma)^4,H^{1/2}(\Sigma)^4}, \quad (1.2.6)$$

for all $\psi \in H(\alpha,\Omega)$ and $\varphi \in H^1(\Omega)^4$. In particular, for any $\psi \in H(\alpha,\Omega)$ satisfying $t_\Sigma\psi \in H^{1/2}(\Sigma)^4$, it holds that $\psi \in H^1(\Omega)^4$.

Proof. Fix $\psi \in H(\alpha,\Omega)$ and let $(\psi_j)_{j\in\mathbb{N}} \subset H^1(\Omega)^4$ be a sequence of functions that convergences to ψ in $H(\alpha,\Omega)$. Given an arbitrary function $g \in H^{1/2}(\Sigma)^4$ and let $\mathcal{E}_\Omega(g) \in H^1(\Omega)^4$, where $\mathcal{E}_\Omega$ is the extension operator from $H^{1/2}(\Sigma)^4$ to $H^1(\Omega)^4$ from Proposition 1.2.1. It follows from Proposition 1.2.3 that

$$\langle(-i\alpha\cdot\nabla)\psi_j,\mathcal{E}_\Omega(g)\rangle_{L^2(\Omega)^4} - \langle\psi_j,(-i\alpha\cdot\nabla)\mathcal{E}_\Omega(g)\rangle_{L^2(\Omega)^4} = \langle(-i\alpha\cdot N)t_\Sigma\psi, g\rangle_{L^2(\Sigma)^4}.$$

Hence, Cauchy-Schwarz inequality yields that

$$\begin{aligned}\left|\langle(\alpha\cdot N)t_\Sigma\psi_j, g\rangle_{L^2(\Sigma)^4}\right| &\leqslant \|(\alpha\cdot\nabla)\mathcal{E}_\Omega(g)\|_{L^2(\Omega)^4}\|\psi_j\|_{L^2(\Omega)^4} + \|\mathcal{E}_\Omega(g)\|_{L^2(\Omega)^4}\|(\alpha\cdot\nabla)\psi_j\|_{L^2(\Omega)^4}\\ &\leqslant \|\mathcal{E}_\Omega(g)\|_{H^1(\Omega)^4}\|\psi_j\|_{H(\alpha,\Omega)}.\end{aligned}$$

Now, applying the trace theorem (see Proposition 1.2.1) to the above inequality yields

$$\left|\langle(\alpha\cdot N)t_\Sigma\psi_j, g\rangle_{L^2(\Sigma)^4}\right| \lesssim \|g\|_{H^{1/2}(\Sigma)^4}\|\psi_j\|_{H(\alpha,\Omega)}.$$

Notice that for all $j \in \mathbb{N}$ we have $(\alpha\cdot N)t_\Sigma\psi_j \in L^2(\Sigma)^4$, and by definition it holds that

$$\begin{aligned}\|(\alpha\cdot N)t_\Sigma\psi_j\|_{H^{-1/2}(\Sigma)^4} &= \sup_{0\neq g\in H^{1/2}(\Sigma)} \frac{\left|\langle(\alpha\cdot N)t_\Sigma\psi_j, g\rangle_{H^{-1/2}(\Sigma)^4,H^{1/2}(\Sigma)}\right|}{\|f\|_{H^{1/2}(\Sigma)^4}}\\ &= \sup_{0\neq g\in H^{1/2}(\Sigma)} \frac{\left|\langle t_\Sigma\psi_j, (\alpha\cdot N)g\rangle_{L^2(\Sigma)}\right|}{\|f\|_{H^{1/2}(\Sigma)^4}} \lesssim \|\psi_j\|_{H(\alpha,\Omega)},\end{aligned}$$

because $(\alpha\cdot N) \in L^2(\Sigma)^4$. It follows from the above consideration that $((\alpha\cdot N)t_\Sigma\psi_j)_{j\in\mathbb{N}}$ is a Cauchy sequence of $H^{-1/2}(\Sigma)^4$. Consequently we get

$$(\alpha\cdot N)t_\Sigma\psi_j \xrightarrow[j\to\infty]{} f \in H^{-1/2}(\Sigma)^4,$$
$$\|f\|_{H^{-1/2}(\Sigma)^4} = \lim_{j\to\infty}\|(\alpha\cdot N)t_\Sigma\psi_j\|_{H^{-1/2}(\Sigma)^4} \lesssim \|\psi\|_{H(\alpha,\Omega)},$$

Since $H^1(\Omega)^4$ is a dense subspace of $H(\alpha,\Omega)$, it follows that the mapping $\widetilde{t_\Sigma} : H(\alpha,\Omega) \longrightarrow H^{-1/2}(\Sigma)^4$ defined by

$$\langle\widetilde{t_\Sigma}\psi, t_\Sigma\varphi\rangle_{H^{-1/2}(\Sigma)^4,H^{1/2}(\Sigma)^4} = \langle(-i\alpha\cdot\nabla)\psi,\varphi\rangle_{L^2(\Omega)^4} - \langle\psi,(-i\alpha\cdot\nabla)\varphi\rangle_{L^2(\Omega)^4}, \quad \forall\varphi \in H^1(\Omega)^4,$$

is a continuous extension of the mapping $(\alpha \cdot N)t_\Sigma : H^1(\Omega)^4 \to L^2(\Sigma)^4$. From this we have also the identity (1.2.5) and this proves (i).

Now we turn to the proof of (ii). Let $\omega \in (1/2, 1)$ and assume that Ω is $C^{1,\omega}$-smooth domain. Fix again $\psi \in H(\alpha, \Omega)$ and let $(\psi_j)_{j\in\mathbb{N}} \subset H^1(\Omega)^4$ be a sequence of functions that convergences to ψ in $H(\alpha, \Omega)$. Since, N is $C^{0,\omega}$-smooth and that $|(\alpha \cdot N(x))| = I$ holds for all $x \in \Sigma$, it follows that the multiplication operator by $(\alpha \cdot N)$ is bounded from $H^{1/2}(\Sigma)^4$ into itself. Therefore, following exactly the same arguments as in the proof of the statement (i) of this proposition, we get that $(t_\Sigma\psi_j)_{j\in\mathbb{N}}$ is a Cauchy sequence of $H^{-1/2}(\Sigma)^4$, and that

$$\|t_\Sigma\psi\|_{H^{-1/2}(\Sigma)^4} = \lim_{j\to\infty} \|t_\Sigma\psi_j\|_{H^{-1/2}(\Sigma)^4} \lesssim \|\psi\|_{H(\alpha,\Omega)}.$$

Thus, the trace operator extends into a continuous map $t_\Sigma : H(\alpha, \Omega) \to H^{-1/2}(\Sigma)^4$. As consequence, density arguments yields the Green's formula (1.2.5).

Finally, let $\psi \in H(\alpha, \Omega)$ be such that $t_\Sigma\psi \in H^{1/2}(\Sigma)^4$. Set $\tilde{\psi} = \psi - \mathcal{E}_\Omega(t_\Sigma\psi)$, then $\tilde{\psi} \in H_0^1(\Omega)^4$ holds by Corollary 1.2.1. Since, $\nabla\tilde{\psi}$, $\nabla\mathcal{E}_\Omega(t_\Sigma\psi) \in L^2(\Omega)^4$, it follows that $\nabla\psi \in L^2(\Omega)^4$ which yields that $\psi \in H^1(\Omega)^4$. This completes the proof of the proposition. □

We finish this part be recalling the following result concerning the trace of function in the Dirac-Sobolev space of order $1/2$, $H^{1/2}(\alpha, \Omega)^4$, it will be very useful when studying the point spectrum of Dirac operators with δ-interactions supported on compact Lipschitz surfaces. For the proof we refer to [24, Lemma 5.1].

Lemma 1.2.2. *Let Ω be a Lipschitz domain with a compact boundary Σ, and define the the Dirac-Sobolev space of order $1/2$ by*

$$H^{1/2}(\alpha, \Omega) = \{\varphi \in H^{1/2}(\Omega)^4 : H\varphi \in L^2(\Omega)^4\}.$$

Then, the trace operator $t_\Sigma : H^1(\Omega)^4 \to H^{1/2}(\Sigma)^4$ has a unique extension to a bounded linear operator $t_\Sigma : H^{1/2}(\alpha, \Omega) \to L^2(\Sigma)^4$

1.3 Integral operators associated with H, Hardy spaces and Calderón's decomposition

Boundary integral operators have played a key role in the study of many boundary value problems for partial differential equations that arise in various fields of mathematical physics, such as electromagnetism, elasticity and potential theory. They are namely involved as a tool for proving the existence of solutions as well as theirs construction via integral equation methods, cf. [52, 68, 69, 104].

To begin with, we give general results in the case of bounded uniformly rectifiable domains, which for our applications, is the most general framework that we can consider. Then, we consider the case of smooth domains, where there, we will be able to show some regularity results for these integral operators.

We first recall Schur's lemma for integral operators with a reproducing kernel. The proof is a standard application of Cauchy-Schwarz's inequality.

Theorem 1.3.1. *(Schur's test) Let $K(x, y)$ be a measurable function on a product space $(X, \Sigma, \mu) \times (Y, \Upsilon, \nu)$. Suppose that there are measurable functions $K_1(x, y)$, $K_2(x, y)$ such that*

$$|K(x, y)| \leqslant K_1(x, y)K_2(x, y),$$

and there are constants $C_1, C_2 > 0$ such that

$$\|K_1(x,\cdot)\|_{L^2(X,\mu)} \leqslant C_1, \quad \|K_2(\cdot,y)\|_{L^2(Y,\nu)} \leqslant C_2,$$

for μ-almost every x, respectively, ν-almost every y. Then the operator $T_K : L^2(X,\mu) \longrightarrow L^2(Y,\nu)$ defined by

$$T_K[f](x) := \int_Y K(x,y)f(y)\mathrm{d}\nu(y),$$

μ-almost every x and $f \in L^2(Y,\nu)$, is bounded with $\|T_K\|_{L^2(X,\mu)\longrightarrow L^2(Y,\nu)} \leqslant C_1C_2$.

Proof. Let $f \in L^2(Y,\nu)$, then applying Cauchy-Schwarz's inequality,

$$\begin{aligned} |T_K[f](x)| &= \int_Y |K(x,y)||f(y)|\mathrm{d}\nu(y) = \int_Y K_1(x,y)K_2(x,y)|f(y)|\mathrm{d}\nu(y) \\ &\leqslant \left(\int_Y K_1(x,y)^2\mathrm{d}\nu(y)\right)^{1/2}\left(\int_Y |K_2(x,y)f(y)|^2\mathrm{d}\nu(y)\right)^{1/2} \\ &\leqslant C_1^2\left(\int_Y |K_2(x,y)f(y)|^2\mathrm{d}\nu(y)\right)^{1/2} \end{aligned}$$

x almost every. Thus, integrating with respect to x and using Fubini's yields that

$$\begin{aligned} \int_X |T_K[f](x)|^2\mathrm{d}\mu(x) &\leqslant C_1^2\int_X\left(\int_Y |K_2(x,y)f(y)|^2\mathrm{d}\nu(y)\right)\mu(x) \\ &= C_1^2\int_Y\left(\int_X K_2(x,y)\mathrm{d}\mu(x)\right)f(y)|^2\mathrm{d}\nu(y) \quad \leqslant (C_1C_2)^2\left(\int_Y |f(y)|^2\mathrm{d}\nu(y)\right), \end{aligned}$$

finishing the proof of the theorem. □

The following lemma gives the fundamental solution of $(H-z)$.

Lemma 1.3.1. *For $z \in \rho(H)$, the fundamental solution of $(H-z)$ is given by*

$$\phi^z(x) = \frac{e^{i\sqrt{z^2-m^2}|x|}}{4\pi|x|}\left(z + m\beta + (1 - i\sqrt{z^2-m^2}|x|)i\alpha\cdot\frac{x}{|x|^2}\right), \quad \text{for all } x \in \mathbb{R}^3\setminus\{0\}. \tag{1.3.1}$$

Proof. Let $z \in \rho(H)$, and recall the algebraic identity $(H+z)(H+z) = \Delta + m^2 - z^2$. Since the fundamental solution of $(\Delta + m^2 - z^2)I_4$ is given by

$$\psi^z(x) = \frac{e^{i\sqrt{z^2-m^2}|x|}}{4\pi|x|}I_4, \quad \text{for } x \in \mathbb{R}^3. \tag{1.3.2}$$

Thus, $(H+z)\psi^z$ is the fundamental solution of $(H-z)$. Now, a simple computation shows that $(H+z)\psi^z(x) = \phi^z(x)$ for all $x \in \mathbb{R}^3\setminus\{0\}$, completing the proof. □

In the sequel, unless stated otherwise, we always assume that $\Omega \subset \mathbb{R}^3$ is a bounded UR domain with $\partial\Omega = \partial\overline{\Omega}$, or Ω is a graph Lipschitz domain, and we set

$$\Omega_+ = \Omega \text{ and } \Omega_- := \mathbb{R}^3\setminus\overline{\Omega}, \quad \Sigma = \partial\Omega. \tag{1.3.3}$$

Let us now introduce the families of integral operators we are interested in. For $z \in \rho(H)$ and $g \in L^2(\Sigma)^4$, we define the following operators

$$\begin{aligned} \Phi^z[g](x) &= \int_\Sigma \phi^z(x-y)g(y)\mathrm{d}\sigma(y), \qquad \text{for all } x \in \mathbb{R}^3, \\ \mathscr{C}^z_\Sigma[g](x) &= \lim_{\rho\searrow 0}\int_{|x-y|>\rho} \phi^z(x-y)g(y)\mathrm{d}\sigma(y), \qquad \text{for all } x \in \Sigma, \\ C^z_\pm[g](x) = \Phi^z|^{\mathrm{nt}}_{\Omega_\pm}[g](x) &= \lim_{\Gamma^{\Omega_\pm}(x)\ni y\longrightarrow x} \Phi^z[g](y), \qquad \text{for all } x \in \Sigma. \end{aligned} \tag{1.3.4}$$

Denote by $\tilde{\phi}$ the fundamental solution of the massless Dirac operator $-i\sigma\cdot\nabla$, that is

$$\tilde{\phi}(x) = i\sigma\cdot\frac{x}{|x|^3}, \qquad \text{for all } x \in \mathbb{R}^3\setminus\{0\}, \tag{1.3.5}$$

and we define the operator $\tilde{\Phi}: L^2(\Sigma)^2 \longrightarrow L^2(\mathbb{R}^3)^2$ as follows

$$\tilde{\Phi}[h](x) = \int_\Sigma \tilde{\phi}(x-y)h(y)\mathrm{d}\sigma(y), \quad \text{for all } x\in\mathbb{R}^3 \text{ and } \forall h \in L^2(\Sigma)^2.$$

Also, for $x \in \Sigma$ and $h \in L^2(\Sigma)^2$, we set

$$\begin{aligned} W_\pm[h](x) = \tilde{\Phi}|^{\mathrm{nt}}_{\Omega_\pm}[h](x) &= \lim_{\Gamma^{\Omega_\pm}(x)\ni y\longrightarrow x} \tilde{\Phi}[h](y), \\ W[h](x) &= \lim_{\rho\searrow 0}\int_{|x-y|>\rho} \tilde{\phi}(x-y)h(y)\mathrm{d}\sigma(y). \end{aligned} \tag{1.3.6}$$

Proposition 1.3.1. *For all $z \in \rho(H)$, the operators $\Phi^z : L^2(\Sigma)^4 \longrightarrow L^2(\mathbb{R}^3)^4$ and $\tilde{\Phi}$: $L^2(\Sigma)^2 \longrightarrow L^2(\mathbb{R}^3)^2$ are well defined and bounded.*

Proof. Fix $z\in\rho(H)$ and recall that $\mathrm{Im}(\sqrt{z^2-m^2})>0$. By definition of the fundamental solution ϕ^z, there is $\delta > 0$ such that

$$|\phi^z(x)| \lesssim e^{-\mathrm{Im}(\sqrt{z^2-m^2})|x|}, \text{ for all } |x| > 1/\delta, \tag{1.3.7}$$

$$|\phi^z(x)| \lesssim \frac{1}{|x|^2} \text{ for all } |x| < \delta. \tag{1.3.8}$$

Thus, $|\phi^z(x-y)| \leqslant K_1(x,y)K_2(x,y)$, with

$$K_1(x,y) = K_2(x,y) = \frac{e^{\frac{-\mathrm{Im}(\sqrt{z^2-m^2})|x-y|}{2}}}{|x-y|}, \quad x\in\mathbb{R}^3,\ y\in\Sigma.$$

Hence, the estimates (1.3.7) easily yield that

$$\sup_{y\in\Sigma}\int_{\mathbb{R}^3} K_j(x,y)^2\mathrm{d}x \lesssim \int_{\mathbb{R}^3}\frac{e^{\frac{-\mathrm{Im}(\sqrt{z^2-m^2})|x|}{2}}}{|x|}\mathrm{d}x < \infty,$$

and that

$$\sup_{x\in\mathbb{R}^3}\int_{\substack{|x-y|<R\\ y\in\Sigma}} K_j(x,y)^2\mathrm{d}\sigma(y) < \infty,$$

for all $R > 0$, as can be easily seen by decomposing the domain of integration in dyadic annuli and using the fact that σ is a 2-dimensional measure in $\mathbb{R}^3$. Hence we also have that

$$\sup_{x\in\mathbb{R}^3}\int_\Sigma K_j(x,y)^2 \mathrm{d}\sigma(y) < \infty,$$

and therefore theorem 1.3.1 yields that Φ^z is bounded from $L^2(\Sigma)^4$ to $L^2(\mathbb{R}^3)^4$.

The statement about the boundedness of $\tilde{\phi} : L^2(\Sigma)^2 \longrightarrow L^2(\mathbb{R}^3)^2$ is more delicate and needs sophisticated tools. The proof for the case of bounded UR domains can be found in [63, Section 3.3] and is based on the boundedness of the gradient of the Single layer. For the case of Lipschitz domain or the graph of Lipschitz domain, it is contained in [82, Proposition 5.2.8]. □

The following lemma gives us the relations between the operators defined above, and gathers their important properties. We mention that when Ω_+ is a bounded Lipschitz domain these results are well known, in this case we refer to [10, Lemma 3.3] for example. In the case of UR domains the lemma is somehow contained in [63], but for the convenience of the reader we give here the main ideas to establish it.

Lemma 1.3.2. *Let $z \in \rho(H)$ and suppose that Ω_+ is a bounded UR domain or a graph of Lipschitz domain. Let $\mathscr{C}^z_\Sigma$, $C^z_\pm$, $W_\pm$ and W be as above. Then $\mathscr{C}^z_\Sigma[g](x)$, $C^z_\pm[g](x)$, $W_\pm[h](x)$ and $W[h](x)$ exist for σ-a.e. $x \in \Sigma$, $\mathscr{C}^z_\Sigma$, $C^z_\pm \in \mathscr{B}(L^2(\Sigma)^4)$ and $W, W_\pm \in \mathscr{B}(L^2(\Sigma)^2)$. Furthermore, the following hold true:*

(i) $W_\pm = \mp\frac{i}{2}(\sigma\cdot N) + W$.

(ii) $C^z_\pm = \mp\frac{i}{2}(\alpha\cdot N) + \mathscr{C}^z_\Sigma$.

(iii) $((\sigma\cdot N)W)^2 = (W(\sigma\cdot N))^2 = -\frac{1}{4}I_2$.

(iv) $((\alpha\cdot N)\mathscr{C}^z_\Sigma)^2 = (\mathscr{C}^z_\Sigma(\alpha\cdot N))^2 = -\frac{1}{4}I_4$.

In particular, we have $\|W\| \geqslant \frac{1}{2}$ and $\|\mathscr{C}^z_\Sigma\| \geqslant \frac{1}{2}$.

Proof. We first give the proof in the case where Ω_+ is a bounded UR domain. Given $f \in L^2(\Sigma)$, thanks to [63, Proposition 3.30] we know that for each $j \in \{1,2,3\}$, the limit

$$\lim_{\rho\searrow 0}\int_{|x-y|>\rho}\frac{x_j-y_j}{4\pi|x-y|^3}f(y)\mathrm{d}\sigma(y), \tag{1.3.9}$$

exist at almost every $x \in \Sigma$. Moreover, it holds that

$$\lim_{\Gamma^{\Omega_\pm}(x)\ni w\longrightarrow x}\int\frac{w_j-y_j}{4\pi|w-y|^3}f(y)\mathrm{d}\sigma(y) = \mp\frac{1}{2}N_j(x)f(x) + \lim_{\rho\searrow 0}\int_{|x-y|>\rho}\frac{x_j-y_j}{4\pi|x-y|^3}f(y)\mathrm{d}\sigma(y). \tag{1.3.10}$$

Thus, working component by component it follows that $W_\pm[h](x)$ and $W[h](x)$ exist for σ-a.e. $x \in \Sigma$, and $W, W_\pm \in \mathscr{B}(L^2(\Sigma)^2)$. Item (i) follows by applying the jump relation (1.3.10) to the functions $\sigma_j h$, $j = 1,2,3$.

Now, we are going to show (ii) and complete the proof of the first statement. For that, fix $z \in \rho(H)$ and set

$$k(x) := \phi^z(x) - i\left(\alpha\cdot\frac{x}{|x|^3}\right), \quad \text{for all } x \in \mathbb{R}^3\setminus\{0\}. \tag{1.3.11}$$

Then there is a constant C such that $|k(\omega, y)| \leqslant C/|\omega - y|^{3/2} := \tilde{k}(\omega, y)$, for $\omega, y \in \overline{\Omega}_+$. Define

$$T[g](x) = \int_\Sigma \tilde{k}(x, y)g(y)\mathrm{d}\sigma(y). \tag{1.3.12}$$

Clearly, T is bounded in $L^2(\Sigma)^4$. Now, recall the definition of $\Gamma^{\Omega_\pm}(x)$ from (1.1.5). Let $x \in \Sigma$ and $\omega \in \Gamma^{\Omega_+}(x)$, then

$$\left|\int_{B(\omega,2|x-\omega|)\cap\Sigma} k(\omega, y)g(y)\mathrm{d}\sigma(y)\right| \leqslant \int_{B(\omega,2|x-\omega|)\cap\Sigma} C\left(\frac{1+a}{|x-\omega|}\right)^{3/2}|g(y)|\mathrm{d}\sigma(y). \tag{1.3.13}$$

Using the ADR property of Σ (more precisely, use the inequality $\mathscr{H}^2(B(x,r)\cap\Sigma) \leqslant Cr^2$), it follows that there is C_1 depending only on the ADR constant of Σ such that

$$\left|\int_{B(\omega,2|x-\omega|)\cap\Sigma} k(\omega, y)g(y)\mathrm{d}\sigma(y)\right| \leqslant C_1|x-\omega|^{1/2}M^\Sigma g(x), \tag{1.3.14}$$

where M^Σ is the Hardy-Littlewood maximal operator defined by (1.1.8). Now, let $y \in \Sigma \setminus B(x, 2|x-\omega|)$, then $|\omega - y| \leqslant 2|x-y|$, and thus $|k(\omega, y)| \leqslant \tilde{k}(\omega, y) \leqslant 2^3\tilde{k}(x, y)$. Therefore, we get

$$\left|\int_{\Sigma\setminus B(\omega,2|x-\omega|)} k(\omega, y)g(y)\mathrm{d}\sigma(y)\right| \leqslant 2^3T[|g|](x). \tag{1.3.15}$$

Thus, (1.3.14), (1.3.15) and the dominate convergence theorem yield that

$$\lim_{\Gamma^{\Omega_+}(x)\ni\omega\to x} \int_\Sigma k(\omega, y)g(y)\mathrm{d}\sigma(y) = \int_\Sigma k(x, y)g(y)\mathrm{d}\sigma(y), \tag{1.3.16}$$

holds for all $g \in L^2(\Sigma)^4$ and $\mathrm{d}\sigma\sigma$-a.e. $x \in \Sigma$. Similarly, one can show that

$$\lim_{\Gamma^{\Omega_-}(x)\ni\omega\to x} \int_\Sigma k(\omega, y)g(y)\mathrm{d}\sigma(y) = \int_\Sigma k(x, y)g(y)\mathrm{d}\sigma(y), \tag{1.3.17}$$

holds for all $g \in L^2(\Sigma)^4$ and for σ-a.e. $x \in \Sigma$. Thus, given any $g \in L^2(\Sigma)^4$, it follows from the above considerations and (1.3.11) that $\mathscr{C}^z_\Sigma[g](x)$ and $C^z_\pm[g](x)$ exist for σ-a.e. $x \in \Sigma$, and $\mathscr{C}^z_\Sigma$, $C^z_\pm \in \mathscr{B}(L^2(\Sigma)^4)$. Now, using (1.3.16), (1.3.17) and (i) (i.e working component by component) we easily get (ii).

Finally the proof of (iii) and (iv) is a relatively straightforward modification of the technique used in the proof of [10, Lemma 3.3](ii). Indeed, by [63, p. 2659] it follows that

$$\begin{aligned} \|\mathcal{N}^{\Omega_\pm}_a[\tilde{\Phi}[h]]\|_{L^2(\Sigma)^2} &\leqslant C\|h\|_{L^2(\Sigma)^2}, \\ \|\mathcal{N}^{\Omega_\pm}_a[\Phi^z[g]]\|_{L^2(\Sigma)^4} &\leqslant C\|g\|_{L^2(\Sigma)^4}, \end{aligned} \tag{1.3.18}$$

for some $C > 0$ depending only on a as well as the ADR and the UR constants of Σ. Now, observe that

$$(-i\sigma\cdot\nabla)\tilde{\Phi}[h] = 0 \text{ and } (H - z)\Phi^z[g] = 0 \text{ in } \Omega_\pm. \tag{1.3.19}$$

Then, by [63, Theorem 4.49] it holds that

$$\begin{aligned} \tilde{\Phi}[h] &= \int_\Sigma \tilde{\phi}(x-y)(\pm i\sigma\cdot N(y))h(y)\mathrm{d}\sigma(y), \quad x \in \Omega_\pm, \\ \Phi^z[g] &= \int_\Sigma \phi^z(x-y)(\pm i\alpha\cdot N(y))g(y)\mathrm{d}\sigma(y), \quad x \in \Omega_\pm. \end{aligned} \tag{1.3.20}$$

Although [63, Theorem 4.49] was stated in the case of tow-sided NTA domains with ADR boundaries (cf. Definition 1.3.1) it also holds for UR domains by the discussion on [63, p. 2758]. Now, given $x \in \Omega_+$, $h \in L^2(\Sigma)^2$ and $g \in L^2(\Sigma)^4$. Then, (i) (respectively (ii)) and (1.3.20) yield that

$$\begin{aligned} \tilde{\Phi}[(i\sigma \cdot N)h](x) &= \tilde{\Phi}[(i\sigma \cdot N)W_+(i\sigma \cdot N)h](x), \\ \Phi^z[(i\alpha \cdot N)g](x) &= \Phi^z[(i\alpha \cdot N)C^z_+(i\sigma \cdot N)g](x). \end{aligned} \tag{1.3.21}$$

Thus, taking the nontangential limit and using (i) yields that

$$\begin{aligned} \frac{1}{2} + W(i\sigma \cdot N) = W_+(i\sigma \cdot N) &= W_+(i\sigma \cdot N)W_+(i\sigma \cdot N) \\ &= \frac{1}{4} + W(i\sigma \cdot N) + (W(i\sigma \cdot N))^2. \end{aligned}$$

Thus, $-4(W(i\sigma \cdot N))^2 = I_4$, and hence $-4W(i\sigma \cdot N)W = -(i\sigma \cdot N)$ which yields that $-4((i\sigma \cdot N)W)^2 = I_4$. This proves the statements (iii). Similarly, (iv) follows by taking the nontangential limit in (1.3.21) using (ii). This completes the proof of the lemma when Ω_+ is a bounded UR domain.

Now assume that Ω_+ is a graph of Lipschitz domain. Then, the formulas (1.3.9) and (1.3.10) are still hold true by [82, Proposition 5.4.4] and [82, Theorem 5.4.7], respectively. Thus, one can adapt the above arguments in this case and get the claimed results, we omit the details. □

Remark 1.3.1. *Note that since $\phi^z(y-x)^* = \phi^{\overline{z}}(x-y)$, it follows that $(\mathscr{C}^z_\Sigma)^* = \mathscr{C}^{\overline{z}}_\Sigma$ in $L^2(\Sigma)^4$. In particular, $\mathscr{C}^z_\Sigma$ (W) is self-adjoint operators in $L^2(\Sigma)^4$ (respectively in $L^2(\Sigma)^2$), for all $z \in (-m, m)$.*

In order to understand better Lemma 1.3.2, we need to investigate the following class of domains.

Definition 1.3.1 (two-sided NTA domains)**.** *Following [68], we say that a nonempty, proper open set Ω of $\mathbb{R}^3$ is an NTA (non-tangentially accessible) domain if Ω satisfies both the two-sided Corkscrew and Harnack Chain conditions* (see [68],[63] or [61, Appendix] for the precise definition). Furthermore, we say that Ω is a two-sided NTA domain if both Ω and $\mathbb{R}^3 \setminus \overline{\Omega}$ are non-tangentially accessible domains.*

Assume that Ω_+ is a two-sided NTA domain with an ADR boundary† (which makes it a UR domain). Following [61], we define the Hardy spaces $\mathbb{H}^2_z(\Omega_\pm)^4$ by

$$\mathbb{H}^2_z(\Omega_+)^4 = \left\{u : \Omega_+ \to \mathbb{C}^4 : \mathcal{N}[u] \in L^2(\Sigma)^4 \text{ and } (H-z)u = 0\right\},$$

and

$$\begin{aligned} \mathbb{H}^2_z(\Omega_-)^4 = \{u : \Omega_- \to \mathbb{C}^4 : \mathcal{N}[u] \in &L^2(\Sigma)^4,\ (H-z)u = 0 \\ &\text{and } u(x) = \mathcal{O}(|x|^{-2}) \text{ as } |x| \to \infty\}. \end{aligned}$$

*Generally speaking, the Corkscrew condition is a quantitative, scale invariant version of openness, and the Harnack Chain condition is a scale invariant version of path connectedness.

†In the literature, a two-sided NTA domain whose boundary is ADR is often referred to as a 2-sided Chord arc domain.

Then, from (1.3.18) it follow that

$$\Phi^z \restriction_{\Omega_\pm} \in \mathbb{H}^2_z(\Omega_\pm)^4.$$

Now, the boundary Hardy spaces are defined as follows

$$\mathbb{H}^2_{z,\pm}(\Sigma)^4 = \left\{ u \restriction_\Sigma : u \in \mathbb{H}^2(\Omega_\pm)^4 \right\},$$

where the boundary trace is taken in a nontangential pointwise sense. Then, we have the following proposition is contained in [61, Subsection 2.3], but we give the proof for the sake of completeness.

Proposition 1.3.2. *Let $z \in \mathbb{C} \setminus ((-\infty, -m] \cup [m, \infty))$, then the following decomposition holds*

$$L^2(\Sigma)^4 = \mathbb{H}^2_{z,+}(\Sigma)^4 \oplus \mathbb{H}^2_{z,-}(\Sigma)^4,$$

Moreover, it holds that

$$\begin{aligned} \mathrm{Rn}\left(\frac{1}{2} + i\mathscr{C}^z_\Sigma(\alpha\cdot N)\right) &= \mathbb{H}^2_{z,+}(\Sigma)^4 = \mathrm{Kr}\left(-\frac{1}{2} + i\mathscr{C}^z_\Sigma(\alpha\cdot N)\right), \\ \mathrm{Rn}\left(-\frac{1}{2} + i\mathscr{C}^z_\Sigma(\alpha\cdot N)\right) &= \mathbb{H}^2_{z,-}(\Sigma)^4 = \mathrm{Kr}\left(\frac{1}{2} + i\mathscr{C}^z_\Sigma(\alpha\cdot N)\right). \end{aligned}$$

In other words, $\left(\frac{1}{2} \pm i\mathscr{C}^z_\Sigma(\alpha\cdot N)\right)$ is the Calderón's projector associated to $\mathbb{H}^2_{z,\pm}(\Sigma)^4$.

Proof. Since $\mathscr{C}^z_\Sigma$ is bounded invertible by Lemma 1.3.2, it follows that

$$\begin{aligned} \left(\pm\frac{1}{2} + i\mathscr{C}^z_\Sigma(\alpha\cdot N)\right)^2 &= \frac{1}{4} \pm i\mathscr{C}^z_\Sigma(\alpha\cdot N) - (\mathscr{C}^z_\Sigma(\alpha\cdot N))^2 \\ &= \left(\pm\frac{1}{2} + i\mathscr{C}^z_\Sigma(\alpha\cdot N)\right), \end{aligned}$$

proving that $\left(\frac{1}{2} \pm i\mathscr{C}^z_\Sigma(\alpha\cdot N)\right)$ are projectors, and hence

$$L^2(\Sigma)^4 = \mathrm{Rn}\left(\pm\frac{1}{2} + i\mathscr{C}^z_\Sigma(\alpha\cdot N)\right) \oplus \mathrm{Kr}\left(\pm\frac{1}{2} + i\mathscr{C}^z_\Sigma(\alpha\cdot N)\right).$$

Thus, to complete the proof of the proposition it suffices to show that

$$\mathbb{H}^2_{z,+}(\Sigma)^4 = \mathrm{Rn}\left(\frac{1}{2} + i\mathscr{C}^z_\Sigma(\alpha\cdot N)\right).$$

For this, note that by definition of the Hardy spaces $\mathbb{H}^2_z(\Omega_\pm)^4$, we know that for any $u \in \mathbb{H}^2_z(\Omega_+)^4$ there is $g \in L^2(\Sigma)^4$ such that $u_\pm = \Phi^z[i(\alpha\cdot N)g] \restriction_{\Omega_\pm}$. Thus, Lemma 1.3.2 (ii) yields that

$$u|^{\mathrm{nt}}_{\Omega_+} = \left(-\frac{i}{2} + \mathscr{C}^z_\Sigma\right)(i(\alpha\cdot N)g) = \left(\frac{1}{2} + i\mathscr{C}^z_\Sigma(\alpha\cdot N)\right) g.$$

This gives the inclusion $\mathbb{H}^2_{z,+}(\Sigma)^4 \subset \mathrm{Rn}\,(1/2 + i\mathscr{C}^z_\Sigma(\alpha\cdot N))$. Conversely, let $f \in L^2(\Sigma)^4$ and set $g = (1/2 + i\mathscr{C}^z_\Sigma(\alpha\cdot N))\, f$. Then $u = \Phi^z[i(\alpha\cdot N)g] \in \mathbb{H}^2_z(\Omega_+)^4$ and same the computation as above yields that $g = u|^{\mathrm{nt}}_{\Omega_+} \in \mathbb{H}^2_{z,+}(\Sigma)^4$, since $(1/2 + i\mathscr{C}^z_\Sigma(\alpha\cdot N))$ is a projector. Therefore, $\mathrm{Rn}\,(1/2 + i\mathscr{C}^z_\Sigma(\alpha\cdot N)) \subset \mathbb{H}^2_{z,+}(\Sigma)^4$, completing the proof of the proposition. □

Remark 1.3.2. *From the above proposition, we conclude that* $\mathscr{C}^z_\pm[i(\alpha\cdot N)g]\in\mathbb{H}^2_{z,\pm}(\Sigma)^4$*, for all* $g\in L^2(\Sigma)^4$*. Note that* $(1/2\pm i(\alpha\cdot N)\mathscr{C}^z_\Sigma)$ *are also projectors. This observation, is the main idea behind the Dirac operators considered in Section 3.3.*

In the sequel, we shall write Φ, $\mathscr{C}_\Sigma$ and $C_\pm$ instead of Φ^0, $\mathscr{C}^0_\Sigma$ and $C^0_\pm$, respectively. We next give some properties of the mapping Φ^z.

Lemma 1.3.3. *Let* Φ^z *be as in* (1.3.4) *with* $z\in\rho(H)$*, then*

(i) $(H-z)\Phi^z[g]=0$ *holds in* $\mathbb{R}^3\setminus\Sigma$ *for all* $g\in L^2(\Sigma)^4$*, and* $(\Phi^z)^*=t_\Sigma(H-\overline{z})^{-1}$*. Moreover,* $(\Phi^z)^*$ *is bounded surjective from* $L^2(\mathbb{R}^3)^4$ *to* $B^2_{1/2}(\Sigma)^4$ *if* Ω_+ *is a bounded UR domain, and to* $H^{1/2}(\Sigma)^4$ *if* Ω_+ *is a bounded Lipschitz domain or a graph of Lipschitz domain. In particular, it holds that*

$$\mathrm{Kr}((\Phi^z)^*)=\{u\in L^2(\mathbb{R}^3)^4:(H-\overline{z})^{-1}u\in H^1_0(\mathbb{R}^3\setminus\Sigma)^4\}. \tag{1.3.22}$$

(ii) For $u\in L^2(\mathbb{R}^3)^4$ *and* $g\in L^2(\Sigma)^4$ *it holds that*

$$\langle\Phi[g],u\rangle_{L^2(\mathbb{R}^3)^4}=\langle\psi,t_\Sigma(H^{-1}u)\rangle_{L^2(\Sigma)^4}$$

Proof. (i) Since ϕ^z is the fundamental solution of $(H-z)$ we immediately get that $(H-z)\Phi^z[g]=0$ in $\Omega_\pm$ for any $g\in L^2(\Sigma)^4$. Now, using that $\phi^z(x-y)^*=\phi^{\overline{z}}(y-x)$, a direct computation using Fubini's theorem yields that

$$\begin{aligned}\langle u,\Phi^z[g]\rangle_{L^2(\mathbb{R}^3)^4}&=\int_{\mathbb{R}^3}\left\langle u(x),\int_\Sigma\phi^z(x-y)g(y)\mathrm{d}\sigma(y)\right\rangle_{\mathbb{C}^4}\mathrm{d}x\\&=\int_{\mathbb{R}^3}\int_\Sigma\langle u(x),\phi^z(x-y)g(y)\rangle_{\mathbb{C}^4}\,\mathrm{d}\sigma(y)\mathrm{d}x\\&=\int_{\mathbb{R}^3}\int_\Sigma\left\langle\phi^{\overline{z}}(x-y)u(x),g(y)\right\rangle_{\mathbb{C}^4}\mathrm{d}\sigma(y)\mathrm{d}x\\&=\int_\Sigma\left\langle\int_{\mathbb{R}^3}\phi^{\overline{z}}(x-y)u(x)\mathrm{d}x,g(y)\right\rangle_{\mathbb{C}^4}\mathrm{d}\sigma(y)\\&=\langle t_\Sigma\left(\int_{\mathbb{R}^3}\phi^{\overline{z}}(y-x)u(x)\mathrm{d}x\right),g\rangle_{L^2(\Sigma)^4}\end{aligned}$$

Since for all $u\in L^2(\mathbb{R}^3)^4$ and all $x\in\mathbb{R}^3$ we have

$$(H-\overline{z})^{-1}u(x):=\int_{\mathbb{R}^3}\phi^{\overline{z}}(x-y)u(x)\mathrm{d}y,$$

it follows that

$$\langle u,\Phi^z[g]\rangle_{L^2(\mathbb{R}^3)^4}=\langle t_\Sigma(H-\overline{z})^{-1}u,g\rangle_{L^2(\Sigma)^4}$$

which means that that $(\Phi^z)^*=t_\Sigma(H-\overline{z})^{-1}$. Notice that $(H-\overline{z})^{-1}$ is bounded from $L^2(\mathbb{R}^3)^4$ to $H^1(\mathbb{R}^3)^4$ and t_Σ is surjective, thus the boundedness and the surjectivety of $(\Phi^z)^*$ from $L^2(\mathbb{R}^3)^4$ to $B^2_{1/2}(\Sigma)^4$ (resp. $H^{1/2}(\Sigma)^4$) in the case of UR domains (resp. Lipschitz domains) follows by Proposition 1.2.2 (resp. Proposition 1.2.1). Now, the formula (1.3.22) follows immediately from the formula $(\Phi^z)^*=t_\Sigma(H-\overline{z})^{-1}$, the fact that t_Σ is surjective and that $\mathrm{Kr}(t_\Sigma)=H^1_0(\mathbb{R}^3\setminus\Sigma)^4$, which completes the proof of (i). The assertion (ii) is a consequence of (i) and can also be proved exactly as in [10, Lemma 2.10.]. ◻

We finish this part be recalling the following result from [24, Lemma 5.2]. Recall the definition of the Dirac-Sobolev space $H^{1/2}(\alpha,\Omega_\pm)^4$ from Lemma 1.2.2.

Lemma 1.3.4. *Let Φ^z be as in (1.3.4) and assume that Ω_+ is a bounded Lipschitz domain. Then Φ^z is bounded from $L^2(\Sigma)^4$ to $H^{1/2}(\alpha,\Omega_+)^4 \oplus H^{1/2}(\alpha,\Omega_-)^4$. Moreover, the non-tangential limit in Lemma 1.3.2-*(ii) *coincides with the trace operator, that is*

$$t_\Sigma \Phi^z\big|_{\Omega_\pm} = C_\pm^z = \mp\frac{i}{2}(\alpha\cdot N) + \mathscr{C}_\Sigma^z.$$

1.3.1 The case of C^2-smooth domains

The main goal of this part is to establish some regularity results concerning the operators defined by (1.3.4) in the case of C^2-smooth domains, which will be crucial in the following chapters. We will use them to describe the domain of the adjoint of the Dirac operator with delta interactions supported on smooth surfaces. We mention that this results are well known in the case of bounded C^2-smooth domains, see, e.g., [16, 90, 19, 22].

Recall the definition of the Dirac-Sobolev space $H(\alpha,\Omega_\pm)$ from Subsection 1.2.2. Then, the following proposition gathers some properties of the Sobolev space $H(\alpha,\Omega_\pm)$ and of the integral operators Φ^z and $\mathscr{C}_\Sigma^z$.

Proposition 1.3.3. *Let $\omega\in(1/2,1)$ and assume that Ω_+ is a bounded $C^{1,\omega}$-smooth domains or the the graph of $C^{1,\omega}$-smooth function , i.e.,*

$$\Omega_+ = \{(\tilde{y},t) : \tilde{y}\in\mathbb{R}^{d-1},\ \phi(\tilde{y}) < t\},$$

with $\phi:\mathbb{R}^2\longrightarrow\mathbb{R}$ a $C^{1,\omega}$-smooth function. Let Φ^z and $\mathscr{C}_\pm^z$ be as in Lemma 1.3.2. Then, for all $z\in\rho(H)$ the following hold:

(i) The operator Φ^z is bounded from $H^{1/2}(\Sigma)^4$ to $H^1(\mathbb{R}^3\setminus\Sigma)^4$, and admits a continuous extension from $H^{-1/2}(\Sigma)^4$ to $H(\alpha,\Omega_+)\oplus H(\alpha,\Omega_-)$, which we still denote by Φ^z.

(ii) The operator $\mathscr{C}_\Sigma^z$ is bounded from $H^{1/2}(\Sigma)^4$ into itself, and admits a continuous extension $\tilde{\mathscr{C}}_\Sigma^z : H^{-1/2}(\Sigma)^4\to H^{-1/2}(\Sigma)^4$.

(iii) For any $g\in H^{1/2}(\Sigma)^4$ and $h\in H^{-1/2}(\Sigma)^4$ it holds that

$$\begin{aligned} t_\Sigma(\Phi^z[h]\restriction_{\Omega_\pm}) &= \left(\mp\frac{i}{2}(\alpha\cdot N)+\tilde{\mathscr{C}}_\Sigma^z\right)[h],\\ \langle\tilde{\mathscr{C}}_\Sigma^z[h],g\rangle_{H^{-1/2},H^{1/2}} &= \langle h,\mathscr{C}_\Sigma^{\overline{z}}[g]\rangle_{H^{-1/2},H^{1/2}}. \end{aligned} \tag{1.3.23}$$

(iv) For all $\varphi_\pm\in H(\alpha,\Omega_\pm)$ one has $\left(1/2\mp i\tilde{\mathscr{C}}_\Sigma^z(\alpha\cdot N)\right)t_\Sigma\varphi_\pm\in H^{1/2}(\Sigma)^4$.

Proof. Fix $\omega\in(1/2,1)$ and $z\in\rho(H)$. As a preliminary step, we establish the following result of general nature. Suppose that Ω_+ is a Lipschitz domain and consider the operator D_0 defined by

$$D_0\varphi = H\varphi,\quad \forall\varphi\in H_0^1(\mathbb{R}^3\setminus\Sigma)^4 =: \mathrm{dom}(D_0).$$

Then, using the properties of Sobolev spaces and the Green formulas from Proposition 1.2.3 and Proposition 1.2.4, it is easy to show that $(D_0,\mathrm{dom}(D_0))$ is densely defined, closed and symmetric, and that

$$D_0^*\varphi = H\varphi,\quad \forall\varphi\in\mathrm{dom}(D_0^*) = H(\alpha,\Omega_+)\oplus H(\alpha,\Omega_-)$$

Moreover, since $H^1(\Omega_\pm)^4$ is a dense subspace of $H(\alpha,\Omega_\pm)$ by Lemma 1.2.1, it easy follows that the operator $T = D_0^*\restriction H^1(\Omega_+)^4\oplus H^1(\Omega_-)^4$ is closable and that $\overline{T} = D_0^*$.

After this preamble, assume that Ω_+ is a bounded $C^{1,\omega}$-smooth domains or the the graph of $C^{1,\omega}$-smooth function. We are going to prove that Φ^z is bounded from $H^{1/2}(\Sigma)^4$ to $H^1(\mathbb{R}^3 \setminus \Sigma)^4$. Notice first that $\mathrm{Rn}(\Phi^z) = \mathrm{Kr}(T - z)$ holds for all $z \in \rho(H)$. Since $\mathrm{Kr}(T - z) \subset H^1(\mathbb{R}^3 \setminus \Sigma)^4$ it follows that $\Phi^z : H^{1/2}(\Sigma)^4 \longrightarrow H^1(\mathbb{R}^3 \setminus \Sigma)^4$ is everywhere defined. Now, given any subsequence $(g_j)_{j\in\mathbb{N}}$ such that

$$g_j \xrightarrow[j\to\infty]{} g \text{ in } H^{1/2}(\Sigma)^4, \quad \Phi^z[g_j] \xrightarrow[j\to\infty]{} h, \text{ in } H^1(\mathbb{R}^3 \setminus \Sigma)^4.$$

Then, the continuity of Φ^z from $L^2(\Sigma)^4$ to $L^2(\mathbb{R}^3)^4$ provided in Proposition 1.3.1 yields that $\Phi^z[g_j] \xrightarrow[j\to\infty]{} \Phi^z[g]$ in $L^2(\Sigma)^4$, and hence $\Phi^z[g] = h$ holds in $L^2(\mathbb{R}^3)^4$ and then in $H^1(\mathbb{R}^3 \setminus \Sigma)^4$. As $g \in H^{1/2}(\Sigma)^4$ we deduce that $\Phi^z : H^{1/2}(\Sigma)^4 \longrightarrow H^1(\mathbb{R}^3 \setminus \Sigma)^4$ is closed, and therefore bounded which prove the first statement of (i). To prove the second statement, recall the adjoint operator $(\Phi^z)^* : L^2(\mathbb{R}^3)^4 \longrightarrow H^{1/2}(\Sigma)^4$ from Proposition 1.3.3 and denote by $\widetilde{\Phi^z}$ it anti-dual, that is

$$\widetilde{\Phi^z} : H^{-1/2}(\Sigma)^4 \longrightarrow L^2(\mathbb{R}^3)^4.$$

Given $g \in L^2(\Sigma)^4$ and $u \in L^2(\mathbb{R}^3)^4$, then Proposition 1.3.3 yields that

$$\begin{aligned}\langle \Phi^z[g], u\rangle_{L^2(\mathbb{R}^3)^4} = \langle g, (\Phi^z)^* u\rangle_{L^2(\Sigma)^4} = \langle g, (\Phi^z)^* u\rangle_{H^{-1/2}(\Sigma)^4, H^{1/2}(\Sigma)^4} \\ \langle \widetilde{\Phi^z}[g], u\rangle_{L^2(\mathbb{R}^3)^4}.\end{aligned}$$

We deduce from this that $\widetilde{\Phi^z}$ is an extension of Φ^z. Hence, to complete the proof of (i) it suffices to prove that $\widetilde{\Phi^z}$ is bounded from $H^{-1/2}(\Sigma)^4$ to $H(\alpha, \Omega_+) \oplus H(\alpha, \Omega_-)$. For this, note that

$$\mathrm{Rn}(D_0 - \overline{z}) = \{u \in L^2(\mathbb{R}^3)^4 : (H - \overline{z})^{-1} u \in H^1_0(\mathbb{R}^3 \setminus \Sigma)^4\},$$

and hence $\mathrm{Rn}(D_0 - \overline{z}) = \mathrm{Kr}((\Phi^z)^*)$ holds by (1.3.22). Since $(\Phi^z)^* : L^2(\mathbb{R}^3)^4 \longrightarrow H^{1/2}(\Sigma)^4$ is closed, it follows from the closed range theorem that

$$\mathrm{Rn}(\widetilde{\Phi^z}) = (\mathrm{Kr}((\Phi^z)^*))^\perp = (\mathrm{Rn}(D_0 - \overline{z}))^\perp = \mathrm{Kr}(D_0^* - z),$$

is closed in $L^2(\mathbb{R}^3)^4$ which means that

$$\widetilde{\Phi^z} : H^{-1/2}(\Sigma)^4 \longrightarrow Kr(D_0^* - z) \subset H(\alpha, \Omega_+) \oplus H(\alpha, \Omega_-),$$

is bounded and bijective, which completes the proof of (i).

Let us move to the proof of (ii). Let $g \in H^{1/2}(\Sigma)^4$, then (i) yields $\Phi[g] \in H^1(\mathbb{R}^3 \setminus \Sigma)^4$. Since $t_\Sigma(\Phi^z|_{\Omega_\pm})[g]$ coincides with the nontangential limit $(\Phi^z[g])|^{nt}_{\Omega_\pm}$, by Lemma 1.3.2 we get that

$$\mathscr{C}^z_\Sigma[g] = \frac{1}{2}\left(t_\Sigma(\Phi^z|_{\Omega_+}) + t_\Sigma(\Phi^z|_{\Omega_-})\right)[g] \in H^{1/2}(\Sigma)^4.$$

Hence, $\mathscr{C}^z_\Sigma$ is bounded from $H^{1/2}(\Sigma)^4$ into itself. Consequently, using that $(\mathscr{C}^z_\Sigma)^* = \mathscr{C}^{\overline{z}}_\Sigma$, by duality we get the second statement statement of (ii). Finally, using (i) together with (ii), duality and density arguments we immediately get the assertions (iii).

The proof of (iv) follows exactly the same lines as the one [90, Proposition 2.7]. Indeed, fix $\varphi \in H(\alpha, \Omega_\pm)$ and let $(\varphi_j)_{j\in\mathbb{N}} \subset H^1(\Omega_\pm)^4$ be a sequence of functions that convergences to φ in $H(\alpha, \Omega_\pm)$. Given $g \in H^{1/2}(\Sigma)^4$ and fix $z \in \rho(H)$. Thanks to (i) we know that

$\Phi^{\overline{z}}[g] \in H^1(\Omega_+)^4 \oplus H^1(\Omega_-)^4$, thus the Greean's formula together with Lemma 1.3.2-(ii) yield that

$$\begin{aligned}\langle (H-z)\varphi_j, \Phi^{\overline{z}}[g]\rangle_{L^2(\Omega_\pm)^4} &= \langle \varphi, (H-\overline{z})\Phi^{\overline{z}}[g]\rangle_{L^2(\Omega_\pm)^4} + \langle \mp i(\alpha\cdot N)t_\Sigma\varphi_j, t_\Sigma\rangle_{L^2(\Sigma)^4} \\ &= \left\langle \mp i(\alpha\cdot N)t_\Sigma\varphi_j, \left(\mp\frac{i}{2}(\alpha\cdot N)+\mathscr{C}_\Sigma^z\right)[g]\right\rangle_{L^2(\Sigma)^4} \\ &= \langle (1/2 \mp i\mathscr{C}_\Sigma^z(\alpha\cdot N))\, t_\Sigma\varphi_j, g\rangle_{L^2(\Sigma)^4}.\end{aligned}$$

Thus (i) of this proposition yields that

$$\begin{aligned}\left|\left\langle g, \left(1/2 \mp i\tilde{\mathscr{C}}_\Sigma^z(\alpha\cdot N)\right) t_\Sigma\varphi_j\right\rangle_{L^2(\Sigma)^4}\right| &= \left|\langle (H-z)\varphi, \Phi^{\overline{z}}[g]\rangle_{L^2(\Omega_\pm)^4}\right| \\ &\lesssim \|g\|_{H^{-1/2}(\Sigma)^4}\|\varphi_j\|_{H(\alpha,\Omega_\pm)}.\end{aligned}$$

Since $H^{1/2}(\Sigma)^4$ is dense in $H^{-1/2}(\Sigma)^4$, $(1/2 \mp i\tilde{\mathscr{C}}_\Sigma^z(\alpha\cdot N))t_\Sigma\varphi_j \in H^{1/2}(\Sigma)^4$ for all $j\in\mathbb{N}$, it follows that $(1/2 \mp i\tilde{\mathscr{C}}_\Sigma^z(\alpha\cdot N))t_\Sigma\varphi_j$ defines a bounded linear form on $H^{-1/2}(\Sigma)^4$, and thus taking the limit $j \longrightarrow \infty$ yields that

$$\|\, (1/2 \mp i\mathscr{C}_\Sigma^z(\alpha\cdot N))\, t_\Sigma\varphi\|_{H^{1/2}(\Sigma)^4} \lesssim \|\varphi\|_{H(\alpha,\Omega_\pm)},$$

which means that $(1/2 \mp i\mathscr{C}_\Sigma^z(\alpha\cdot N))t_\Sigma\varphi \in H^{1/2}(\Sigma)^4$, finishing the proof of the proposition. □

Remark 1.3.3. *The proof above gives more, namely Φ^z is a bounded bijective operator from $H^{-1/2}(\Sigma)^4$ to $H(\alpha,\Omega_+)\oplus H(\alpha,\Omega_-)$.*

For $z\in\rho(H)$, recall that the trace of the single-layer operator associated with $(\Delta + m^2 - z^2)I_4$, denoted by S^z (and we simply write $S := S^0$ when $z=0$), has the integral representation

$$S^z[g](x) = \int_\Sigma \psi^z(x-y)g(y)\mathrm{d}\sigma(y), \qquad \text{for all } x\in\Sigma \text{ and } g\in L^2(\Sigma)^4. \tag{1.3.24}$$

where $\psi^z(x)$ is the fundamental solution of $(\Delta+m^2-z^2)I_4$ defined by (1.3.2).

In the rest of this section, we restrict ourselves to the following setting that we will consider in Chapter 2. We consider a surface $\Sigma\subset\mathbb{R}^3$ dividing the space into two regions $\Omega_\pm$, and we assume that it satisfies one of the hypotheses:

(H1) $\Sigma = \partial\Omega_+$ with Ω_+ a C^2-smooth bounded domain.

(H2) $\Sigma := \Sigma_\nu := \{(x_1,x_2,x_3)\in\mathbb{R}^3 : x_3 = \nu\phi(x_1,x_2)\}$, where $\nu\in\mathbb{R}_+$ and $\phi:\mathbb{R}^2\to\mathbb{R}$ is a C^2-smooth, compactly supported function. We denote by L_ϕ the Lipschitz constant of ϕ and by F we denote the flat part of Σ_ν i.e.

$$F := \{x = (x_1,x_2,\nu\phi(x_1,x_2))\in\Sigma_\nu : (x_1,x_2)\notin \mathrm{supp}(\phi)\}. \tag{1.3.25}$$

We parameterize Σ_ν by the mapping

$$\begin{cases}\tau:\mathbb{R}^2\longrightarrow\mathbb{R}^3\\ \quad\ \overline{x}\longmapsto(\overline{x},\nu\phi(\overline{x}))\end{cases} \tag{1.3.26}$$

For $x=(\overline{x},\nu\phi(\overline{x}))\in\Sigma_\nu$, we express the surface measure on Σ_ν via the formula $\mathrm{d}\sigma(x) = J_\nu(\overline{x})\mathrm{d}\overline{x}$, where J_ν is the Jacobian given by

$$J_\nu(\overline{x}) = \sqrt{1+\nu^2|\nabla\phi(\overline{x})|^2}. \tag{1.3.27}$$

The next result contains the main tools to prove the self-adjointness of Dirac operators with δ-interactions supported on surfaces satisfying (H1) or (H2). Recall that $\{A, B\} = AB + BA$ is the usual anticommutator bracket.

Lemma 1.3.5. *Let $z \in \rho(H)$, then the following hold:*

(i) The anticommutator $\{\beta, \mathscr{C}_\Sigma^z\}$ extends to a bounded operator from $H^{-1/2}(\Sigma)^4$ onto $H^{1/2}(\Sigma)^4$. In particular, if Σ satisfies (H1)*, then $\{\beta, \mathscr{C}_\Sigma^z\}$ is a compact operator in $L^2(\Sigma)^4$.*

(ii) The anticommutator $\{\alpha \cdot N, \mathscr{C}_\Sigma^z\}$ extends to a bounded operator from $H^{-1/2}(\Sigma)^4$ to $H^{1/2}(\Sigma)^4$. In particular, if Σ satisfies (H1)*, then $\{\alpha \cdot N, \mathscr{C}_\Sigma^z\}$ is a compact operator in $L^2(\Sigma)^4$.*

(iii) If Σ satisfies (H2)*, then $\{\alpha \cdot N, C_\Sigma\}$ is a compact operator in $L^2(\Sigma)^4$.*

Before going through the proof of Lemma 1.3.5, we introduce some suitable truncation functions that we often use in localization arguments when the surface Σ satisfies the assumption (H2).

Notation 1.3.1. *Fix $\nu > 0$ and suppose that Σ satisfies the assumption* (H2)*. We fix $R_2 > R_1 > 0$ such that $\Sigma_\nu \setminus F \subset B(0, R_1/2)$, where F is the flat part of Σ_ν given by* (1.3.25)*. We consider the C^∞-smooth and compactly supported functions $\chi_\nu : \Sigma_\nu \to \mathbb{R}$ and $\chi_0 : \Sigma_0 \to \mathbb{R}$, which satisfy*

$$\begin{aligned} \operatorname{supp}(\chi_\nu) \subset B(0, R_2) \cap \Sigma_\nu \quad &\textit{and } \chi_\nu(x) = 1 \textit{ for } x \in B(0, R_1) \cap \Sigma_\nu, \\ \operatorname{supp}(\chi_0) \subset B(0, R_2) \cap \Sigma_0 \quad &\textit{and } \chi_0(x) = 1 \textit{ for } x \in B(0, R_1) \cap \Sigma_0, \\ \chi_\nu(x) = \chi_0(x) \textit{ for } x \in C(0, R_1, R_2) \cap \Sigma_\nu &= C(0, R_1, R_2) \cap \Sigma_0, \end{aligned}$$

where $C(0, R_1, R_2)$ denotes the annulus $B(0, R_2) \setminus \overline{B(0, R_1)}$. We also denote by $\Xi : \mathbb{R}^3 \to \mathbb{R}$ a C^∞-smooth and compactly supported function, such that $\Xi(x) = 1$ for $x \in B(0, R_1)$ and $\Xi(x) = 0$ for $x \in \mathbb{R}^3 \setminus \overline{B(0, R_2)}$.

Remark 1.3.4. *Note that by definition, if $g \in H^{1/2}(\Sigma_\nu)^4$ and $f \in H^{1/2}(\Sigma_0)^4$ are such that $g = f$ on F, then it holds that*

$$(1 - \chi_\nu) g = (1 - \chi_0) f.$$

Proof of Lemma 1.3.5. Fix $z \in \rho(H)$, we are going to prove item (i). For this, observe that by the anticommuation relations of the Dirac matrices we have

$$\beta \phi^z(x - y) + \phi^z(x - y)\beta = 2 \frac{e^{i\sqrt{z^2 - m^2}|x - y|}}{4\pi |x - y|} (z\beta + m I_4),$$

and thus

$$\{\beta, \mathscr{C}_\Sigma^z\}[g](x) = 2(z\beta + m I_4) S^z[g](x), \quad \forall g \in L^2(\Sigma)^4.$$

Hence, by [81, Theorem 6.11] (see also [82] for example) we know that S^z is bounded from $L^2(\Sigma)^4$ to $H^1(\Sigma)^4$. Thus, $\{\beta, \mathscr{C}_\Sigma^z\}$ is bounded from $L^2(\Sigma)^4$ to $H^1(\Sigma)^4$, and hence the first statement of (i) follows by duality and interpolation arguments. Since the embedding $H^{1/2}(\Sigma)^4 \hookrightarrow L^2(\Sigma)^4$ is compact when Σ satisfies (H1), we then get that $\{\beta, \mathscr{C}_\Sigma^z\}$ is a compact operator in $L^2(\Sigma)^4$, finishing the proof of (i).

Proof of (ii)**: the case of** (H1)**.** The proof of this statement is similar to that of [90, Proposition 2.8] where the case $z = 0$ was proved, and follows essentially from the fact the kernel of $\{\alpha\cdot N, \mathscr{C}^z_\Sigma\}$ is not singular. Indeed, let $x\in\Sigma$ and $y\in\mathbb{R}^3$, then a straightforward computation using the anticommutation relations of the Dirac matrices yields that

$$(\alpha\cdot N(x))(\alpha\cdot y) = -(\alpha\cdot y)(\alpha\cdot N(x)) + 2(N(x)\cdot y)I_4. \tag{1.3.28}$$

Recall the definition of ψ^z from (1.3.2), then it follows from (1.3.28) that

$$\begin{aligned}(\alpha\cdot N(x))\phi^z(y) =& -\phi^z(y)(\alpha\cdot N(x)) - \frac{e^{i\sqrt{z^2-m^2}|y|}}{2i\pi|y|^3}(1-i\sqrt{z^2-m^2}|y|)(N(x)\cdot y)I_4 &(1.3.29)\\ &+2z(\alpha\cdot N(x))\psi^z(y). &(1.3.30)\end{aligned}$$

Note that there are constants C_1 and C_2 such that, for all $x,y\in\Sigma$, it holds that

$$|N(x)-N(y)|\leqslant C_1|x-y| \quad \text{and} \quad |N(x)\cdot(x-y)|\leqslant C_2|x-y|^2,$$

this can be proved in the same way as in Proposition 4.4.5 below, see also [53, Lemma 3.15]. Using this, for $g\in L^2(\Sigma)^4$, we get that

$$\begin{aligned}\{\alpha\cdot N, \mathscr{C}^z_\Sigma\}[g](x) &= \int_\Sigma K_z(x,y)g(y)\mathrm{d}\sigma(y) + 2z(\alpha\cdot N(x))S^z[g](x)\\ &:= T_{z,1}[g](x) + T_{z,2}[g](x),\end{aligned} \tag{1.3.31}$$

where the kernel K_z is given by

$$\begin{aligned}K_z(x,y) =& \phi^z(x-y)(\alpha\cdot(N(y)-N(x)) &(1.3.32)\\ &- \frac{e^{i\sqrt{z^2-m^2}|x-y|}}{2i\pi|x-y|^3}(1-i\sqrt{z^2-m^2}|x-y|)(N(x)\cdot(x-y))I_4. &(1.3.33)\end{aligned}$$

Since Σ is C^2-smooth, it follows immediately from (i) that $T_{z,2}$ is bounded from $H^{-1/2}(\Sigma)^4$ to $H^{1/2}(\Sigma)^4$. Hence, it remains to prove that $T_{z,1}$ is bounded from $H^{-1/2}(\Sigma)^4$ to $H^{1/2}(\Sigma)^4$. For this, recall that $|\phi^z(x-y)| = \mathcal{O}(|x-y|)^{-2})$ when $|x-y|\to 0$, thus (1.3.29) and (1.3.32) implies that $|K_z(x,y)|\leqslant \mathcal{O}(|x-y|^{-1})$ when $|x-y|\to 0$. Therefore, K_z is a pseudo-homogeneous kernel of class -1 in the sense of [89, §4.3.3] , and thus [89, Theorem 4.4.2] yields $T_{z,1}$ is bounded from $L^2(\Sigma)^4$ to $H^1(\Sigma)^4$. Hence, by duality and interpolation arguments it follows that $T_{z,1}$ extends continuously to a bounded from $H^{-1/2}(\Sigma)^4$ to $H^{1/2}(\Sigma)^4$. Thus, $\{\beta, \mathscr{C}^z_\Sigma\}$ is bounded from $H^{-1/2}(\Sigma)^4$ to $H^{1/2}(\Sigma)^4$, and hence compact in $L^2(\Sigma)^4$.

Proof of (ii)**: the case of** (H2)**.** Now, assume that Σ satisfies (H2) and recall that F denotes the flat part of $\Sigma=\Sigma_\nu$. Notice that

$$N(y)-N(x) = 0 = N(x)\cdot(x-y) \quad \text{if } x,y\in F.$$

Therefore the kernel $K_z(x,y)$ vanishes for all $x,y\in F$, and from the above considerations it holds that $|K_z(x,y)|\leqslant C|x-y|^{-1}$ when $|x-y|\to 0$. Let $R_2>R_1>0$ and χ_ν be as in Notation 1.3.1. Since $K_z(x,y)$ vanishes for all $x,y\in F$, it follows that $(1-\chi_\nu)T_{z,1}(1-\chi_\nu)=0$. Thereby, $T_{z,1}$ can be written as follows

$$T_{z,1} = \chi_\nu T_{z,1}\chi_\nu + \chi_\nu T_{z,1}(1-\chi_\nu) + (1-\chi_\nu)T_{z,1}\chi_\nu := T_1+T_2+T_3. \tag{1.3.34}$$

Again, T_1 can be extended to a bounded operators from $H^{-1/2}(\Sigma)^4$ to $H^{1/2}(\Sigma)^4$ in the same way as in the case of the assumption (H1). Now we are going to show that T_2 is bounded from $H^{-1/2}(\Sigma)^4$ into $H^{1/2}(\Sigma)^4$, the proof for T_3 is similar. For this, we first observe that T_2

vanishes identically for $x \notin \Sigma \cap B(0, R_1/2)$, and it can be written for $x \in \Sigma \cap B(0, R_1/2)$ as follows:

$$T_2[g](x) = \int_{y \in \Sigma \setminus B(0,R_1)\cap\Sigma} K_z(x,y)(1-\chi_\nu)(y)g(y)\mathrm{d}\sigma(y).$$

which means that T_2 is not singular. Indeed, this follows from the definition of the cut-off function χ_ν and the fact that the kernel $K_z(x, y)$ vanishes for $x, y \in (B(0, R_1) \cap \Sigma) \setminus (B(0, R_1/2) \cap \Sigma) \subset F$.

Next, recall the definitions of τ and J_ν from (3.1.6) and (1.3.27). Since the mapping $(\mathscr{J}_\nu g)(\tilde{x}) = J_\nu^{1/2}(\tilde{x})g(\tau(\tilde{x}))$ is an isometric isomorphism from $L^2(\Sigma)^4$ into $L^2(\mathbb{R}^2)^4$. If we let $V = \{\tilde{x} \in \mathbb{R}^2 : \tau(\tilde{x}) \in \Sigma \cap B(0, R_1/2)\}$, then it is not difficult to check that $\mathscr{J}_\nu T_2 \mathscr{J}_\nu^{-1} = \tilde{T}_2$, where $\tilde{T}_2 : L^2(\mathbb{R}^2)^4 \to L^2(\mathbb{R}^2)^4$ is defined, for $\tilde{x} \in V$, by

$$\tilde{T}_2[f](\tilde{x}) = \int_{\substack{\tilde{y}\in\mathbb{R}^2 \\ \tau(\tilde{y})\in\Sigma\setminus B(0,R_1)\cap\Sigma}} J_\nu^{1/2}(\tilde{x})K_z(\tau(\tilde{x}),\tau(\tilde{y}))(1-\chi_\nu(\tau(\tilde{y})))J_\nu^{1/2}(\tilde{y})f(\tilde{y})d\tilde{y},$$

and $\tilde{T}_2[f](\tilde{x}) = 0$ for $\tilde{x} \in \mathbb{R}^2 \setminus \overline{V}$. Since N is C^1-smooth, it is clear that the mapping $V \ni \tilde{x} \to K_z(\tau(\tilde{x}), \tau(\tilde{y}))$ is C^1-smooth for all $\tilde{y} \in \mathbb{R}^2$, and the mapping $\mathbb{R}^2 \setminus \overline{V} \ni \tilde{y} \to K_z(\tau(\tilde{x}), \tau(\tilde{y}))(1 - \chi_\nu(\tau(\tilde{y})))$ is C^∞-smooth for all $\tilde{x} \in V$, since $N(\tau(\tilde{y}))$ is constant in this case. From this, it follows that $\tilde{T}_2[f]$ is differentiable on V and it holds that

$$\begin{aligned}
\partial_{\overline{x}}(\tilde{T}_2[f])(\tilde{x}) = &\int_{\substack{\tilde{y}\in\mathbb{R}^2 \\ \tau(\tilde{y})\in\Sigma\setminus B(0,R_2)\cap\Sigma}} (\partial_{\overline{x}}J_\nu^{1/2})(\tilde{x})K_z(\tau(\tilde{x}),\tau(\tilde{y}))(1-\chi_\nu(\tau(\tilde{y})))J_\nu^{1/2}(\tilde{y})f(\tilde{y})d\tilde{y} \\
&+ \int_{\substack{\tilde{y}\in\mathbb{R}^2 \\ \tau(\tilde{y})\in\Sigma\setminus B(0,R_2)\cap\Sigma}} J_\nu^{1/2}(\tilde{x})\left(\partial_{\overline{x}}K_z(\tau(\tilde{x}),\tau(\tilde{y})\right)(1-\chi_\nu(\tau(\tilde{y})))J_\nu^{1/2}(\tilde{y})f(\tilde{y})d\tilde{y} \\
&:=(T_{2,1}[f])(\overline{x}) + (T_{2,2}[f])(\overline{x}).
\end{aligned}$$

Since $(\partial_{\overline{x}}J_\nu^{1/2})$ is bounded, it is easy to see that $T_{2,1}$ is bounded from $L^2(\mathbb{R}^2)^4$ into itself. Now, observe that $|\tilde{x} - \tilde{y}|^2 \leqslant |\tau(\tilde{x}) - \tau(\tilde{y})|^2$ holds for $\tilde{x}, \tilde{y} \in \mathbb{R}^2$, using this we see that

$$|J_\nu^{1/2}(\tilde{x})\left(\partial_{\overline{x}}K_z(\tau(\tilde{x}),\tau(\tilde{y})\right)(1-\chi_\nu(\tau(\tilde{y})))J_\nu^{1/2}(\tilde{y})| \leqslant K_1(\tilde{x},\tilde{y})K_2(\tilde{x},\tilde{y}),$$

where $K_1(\tilde{x}, \tilde{y}) = |\tilde{x} - \tilde{y}|^{-2}$ and $K_2(\tilde{x}, \tilde{y}) = e^{-\mathrm{Im}\sqrt{z^2-m^2}|\tilde{x}-\tilde{y}|}/|\tilde{x} - \tilde{y}|$. Note that

$$\sup_{\overline{x}\in V} \int_{\substack{\tilde{y}\in\mathbb{R}^2 \\ \tau(\tilde{y})\in\Sigma\setminus B(0,R_1)\cap\Sigma}} |K_1(\tilde{x},\tilde{y})|^2 d\tilde{y} < \infty, \qquad \sup_{\substack{\tilde{y}\in\mathbb{R}^2 \\ \tau(\tilde{y})\in\Sigma\setminus B(0,R_1)\cap\Sigma}} \int_{\tilde{x}\in V} |K_2(\tilde{x},\tilde{y})|^2 d\overline{x} < \infty.$$

Hence, the Schur test from Theorem 1.3.1 yields that $T_{2,2}$ is bounded from $L^2(\mathbb{R}^2)^4$ into itself. Thus T_2 is bounded from $L^2(\Sigma)^4$ to $H^1(\Sigma)^4$, and by duality and interpolation arguments it can be continuously extended to a bounded operator from $H^{-1/2}(\Sigma)^4$ to $H^{1/2}(\Sigma)^4$. Therefore $\{\alpha \cdot N, \mathscr{C}_\Sigma^z\}$ extends to a bounded operator from $H^{-1/2}(\Sigma)^4$ to $H^{1/2}(\Sigma)^4$. The second statement is a direct consequence of the Sobolev injection, and this completes the proof of (ii).

Now we turn to the proof of (iii). Assume that Σ satisfies (H2), then from (ii) we know that the operator $\{\alpha \cdot N, C_\Sigma\}$ coincides with $T_{z,1}$ for $z = 0$, and it is bounded from $H^{-1/2}(\Sigma)^4$ to $H^{1/2}(\Sigma)^4$. Hence, $\{\alpha \cdot N, C_\Sigma\}$ is compact on $L^2(\Sigma)^4$ by the decomposition (1.3.34) and the compactness of the Sobolev embedding $\chi_\nu H^{1/2}(\Sigma)^4 \hookrightarrow L^2(\Sigma)^4$. This finishes the proof of the lemma. □

Remark 1.3.5. *Actually the above result is not surprising since the integral kernels associated to the anticommutators* $\{\alpha \cdot N, \mathscr{C}_\Sigma^z\}$ *and* $\{\beta, \mathscr{C}_\Sigma^z\}$ *behave locally like* $|x-y|^{-1}$*, when* $|x-y|$ *tends to zero. Moreover, the anticommutators are actually bounded from* $L^2(\Sigma)^4$ *to* $H^1(\Sigma)^4$*, and since* Σ *is* C^2*-smooth, by interpolation arguments we get that* $\{\alpha \cdot N, \mathscr{C}_\Sigma^z\}$, $\{\beta, \mathscr{C}_\Sigma^z\}$: $H^{s-1}(\Sigma)^4 \to H^s(\Sigma)^4$ *are bounded operators for any* $s \in [0,1]$.

Chapter 2

On the Dirac operator with δ-interactions supported on smooth surfaces

The results presented in this chapter have been the subject of the paper [29].

2.1 Introduction

The purpose of this chapter is to study spectral properties of the families of Dirac operators defined formally by

$$\begin{aligned} H_\kappa &:= H + (\epsilon I_4 + \mu\beta + \eta(\alpha\cdot N))\delta_{\partial\Omega}, \quad \kappa := (\epsilon,\mu,\eta)\in\mathbb{R}^3, \\ H_{\zeta,\upsilon} &:= H + \left(-i\zeta\gamma_5 + i\upsilon\beta\,(\alpha\cdot N)\right)\delta_{\partial\Omega}, \quad (\zeta,\upsilon)\in\mathbb{R}^2, \end{aligned} \tag{2.1.1}$$

in the Hilbert space $L^2(\mathbb{R}^3)^4$ when $\Sigma\subset\mathbb{R}^3$ is a smooth surface. Here $\gamma_5 := \alpha_1\alpha_2\alpha_3$ denotes the so-called chirality matrix, and satisfies the algebraic properties

$$\gamma_5 = \begin{pmatrix} 0 & I_2 \\ I_2 & 0 \end{pmatrix}, \quad \gamma_5\beta = -\beta\gamma_5 \text{ and } \gamma_5(\alpha\cdot x) = (\alpha\cdot x)\gamma_5,\ \forall x\in\mathbb{R}^3. \tag{2.1.2}$$

We shall consider throughout this chapter surfaces $\Sigma\subset\mathbb{R}^3$ satisfying either the assumption (H1) or the assumption (H2).

Let us now describe the structure of this chapter. We first focus on the study of the Dirac operator H_κ. In the next section, we give the rigorous definition of the Hamiltonian H_κ and we developed a strategy to prove its self-adjointness when Σ satisfies the first and second assumptions, the main result being Theorem 2.2.1. Section 2.3 is devoted to the spectral study of H_κ. There, we focus on the case where Ω is a locally deformed half-space and we give a complete description of the essential spectrum of H_κ, for the non-critical and critical combinations of coupling constants in Theorem 2.3.3 and Theorem 2.3.4, respectively. Finally, in Section 2.4, we adapt the arguments developed in Sections 2.2 and 2.3 to study the spectral properties of the Dirac operator $H_{\zeta,\upsilon}$, for all possible combinations of interaction strengths. The main results in this section are Theorem 2.4.1 and Theorem 2.4.2.

2.2 Self-adjointness of H_κ

In this section, we study the self-adjointness of the Dirac operator H_κ. In our setting, it will be seen that the special value $\epsilon^2 - \mu^2 - \eta^2 = 4$ plays a critical role in the analysis of the spectral properties of H_κ. Before stating the main result of this part, some notations are needed. Recall the definition of the operators Φ^z, $\mathscr{C}_\Sigma^z$ and $C_\pm^z$ from (1.3.4).

Notation 2.2.1. *For $\kappa = (\epsilon, \mu, \eta) \in \mathbb{R}^3$, we set*

$$\operatorname{sgn}(\kappa) := \epsilon^2 - \mu^2 - \eta^2. \tag{2.2.1}$$

If $\operatorname{sgn}(\kappa) \neq 0$, then for $z \in \rho(H)$ we define the operators $\Lambda_\pm^z$ as follows:

$$\Lambda_\pm^z = \frac{1}{\operatorname{sgn}(\kappa)}(\epsilon I_4 \mp (\mu\beta + \eta(\alpha \cdot N))) \pm \mathscr{C}_\Sigma^z, \quad \forall z \in \mathbb{C} \setminus ((-\infty, -m] \cup [m, \infty)).$$

Since $(\alpha \cdot N)$ is C^1-smooth and symmetric, thanks to the properties of Cauchy operator $\mathscr{C}_\Sigma^z$ from Lemma 1.3.2 and Proposition 1.3.3, it easily follows that $\Lambda_\pm^z$ are bounded (and self-adjoint for $z \in (-m, m)$) from $L^2(\Sigma)^4$ onto itself, and bounded from $H^{1/2}(\Sigma)^4$ onto itself.

In the sequel, we shall write Φ, $\mathscr{C}_\Sigma$, $C_\pm$ and $\Lambda_\pm$ instead of Φ^0, $\mathscr{C}_\Sigma^0$, $C_\pm^0$ and $\Lambda_\pm^0$, respectively. Now we are in position to give the first definition of the Dirac Hamiltonian with δ-interactions supported on Σ, the main object of the present paper.

Definition 2.2.1. *Let $\kappa = (\epsilon, \mu, \eta) \in \mathbb{R}^3$ be such that $\operatorname{sgn}(\kappa) \neq 0$. The Dirac operator coupled with a combination of electrostatic, Lorentz scalar and normal vector field δ-shell interactions of strength ϵ, μ and η respectively, is the operator $H_\kappa = H + V_\kappa$, acting in $L^2(\mathbb{R}^3)^4$ and defined on the domain*

$$\operatorname{dom}(H_\kappa) = \left\{ u + \Phi[g] : u \in H^1(\mathbb{R}^3)^4, g \in L^2(\Sigma)^4, t_\Sigma u = -\Lambda_+[g] \right\},$$

where

$$V_\kappa(\varphi) = \frac{1}{2}(\epsilon I_4 + \mu\beta + \eta(\alpha \cdot N)))(\varphi_+ + \varphi_-)\delta_\Sigma,$$

with $\varphi_\pm = t_\Sigma u + C_\pm[g]$. Hence, H_κ acts in the sense of distributions as $H_\kappa(\varphi) = Hu$, for all $\varphi = u + \Phi[g] \in \operatorname{dom}(H_\kappa)$.

In what follows we denote by $\widetilde{\Lambda}_\pm^z$ the continuous extension of $\Lambda_\pm^z$ defined from $H^{-1/2}(\Sigma)^4$ into itself. Now we can state the first main theorem of this chapter. The rest of this part will be devoted to the proof of this result.

Theorem 2.2.1. *Let H_κ be as in Definition 2.2.1. Then, the following statements hold true:*

(i) If $\operatorname{sgn}(\kappa) \neq 4$, then H_κ is self-adjoint and we have

$$\operatorname{dom}(H_\kappa) = \left\{ u + \Phi[g] : u \in H^1(\mathbb{R}^3)^4, g \in H^{1/2}(\Sigma)^4, t_\Sigma u = -\Lambda_+[g] \right\}.$$

(ii) If $\operatorname{sgn}(\kappa) = 4$, then H_κ is essentially self-adjoint and we have

$$\operatorname{dom}(\overline{H_\kappa}) = \left\{ u + \Phi[g] : u \in H^1(\mathbb{R}^3)^4, g \in H^{-1/2}(\Sigma)^4, t_\Sigma u = -\widetilde{\Lambda}_+[g] \right\}.$$

Proposition 2.2.1. *Let H_κ be as in Definition 2.2.1, then H_κ is closable.*

Proof. Since any symmetric operator on a Hilbert space with dense domain of definition always admits a closure, to prove the proposition it suffices to show the following:

(i) $\mathrm{dom}(H_\kappa)$ is dense in $L^2(\mathbb{R}^3)^4$.

(ii) H_κ is symmetric on $\mathrm{dom}(H_\kappa)$.

First, observe that $C_0^\infty(\mathbb{R}^3\backslash\Sigma)^4 \subset \mathrm{dom}(H_\kappa) \subset L^2(\mathbb{R}^3)^4$. since $C_0^\infty(\mathbb{R}^3\backslash\Sigma)^4$ is a dense subspace of $L^2(\mathbb{R}^3)^4$ we then get (i). Now we are going to prove (ii). For this, let $\varphi, \psi \in \mathrm{dom}(H_\kappa)$ with $\varphi = u + \Phi[g]$ and $\psi = v + \Phi[h]$, then we have

$$\begin{aligned}\langle H_\kappa\varphi, \psi\rangle_{L^2(\mathbb{R}^3)^4} - \langle \varphi, H_\kappa\psi\rangle_{L^2(\mathbb{R}^3)^4} &= \langle Hu, v + \Phi[h]\rangle_{L^2(\mathbb{R}^3)^4} - \langle u + \Phi[g], Hv\rangle_{L^2(\mathbb{R}^3)^4}\\ &= \langle Hu, \Phi[h]\rangle_{L^2(\mathbb{R}^3)^4} - \langle \Phi[g], Hv\rangle_{L^2(\mathbb{R}^3)^4}\\ &= \langle t_\Sigma u, h\rangle_{L^2(\Sigma)^4} - \langle g, t_\Sigma v\rangle_{L^2(\Sigma)^4},\end{aligned}$$

where in the last equality Lemma 1.3.3 was used. Now, the self-adjointness of Λ_+ together with the conditions $t_\Sigma u = -\Lambda_+[g]$ and $t_\Sigma v = -\Lambda_+[h]$ yield that

$$\langle H_\kappa\varphi, \psi\rangle_{L^2(\mathbb{R}^3)^4} - \langle \varphi, H_\kappa\psi\rangle_{L^2(\mathbb{R}^3)^4} = \langle -\Lambda_+[g], h\rangle_{L^2(\Sigma)^4} - \langle g, -\Lambda_+[h]\rangle_{L^2(\Sigma)^4} = 0, \tag{2.2.2}$$

which means that H_κ is symmetric on $\mathrm{dom}(H_\kappa)$, and this concludes the proof. □

The following proposition gives a description of the domain of the adjoint operator H_κ^*.

Proposition 2.2.2. *Let H_κ be as in Definition 2.2.1. Then we have*

$$\mathrm{dom}(H_\kappa^*) = \left\{u + \Phi[g] : u \in H^1(\mathbb{R}^3)^4, g \in H^{-1/2}(\Sigma)^4, t_\Sigma u = -\widetilde{\Lambda}_+[g]\right\}. \tag{2.2.3}$$

Proof. Let D be the set on the right-hand side of (2.2.3). First we prove the inclusion $D \subset \mathrm{dom}(H_\kappa^*)$. Given $\varphi := v + \Phi[h] \in D$ and $\psi = u + \Phi[g] \in \mathrm{dom}(H_\kappa)$, then

$$\begin{aligned}\langle \varphi, H_\kappa\psi\rangle_{L^2(\mathbb{R}^3)^4} &= \langle Hv, u\rangle_{L^2(\mathbb{R}^3)^4} + \langle \Phi[h], Hu\rangle_{L^2(\mathbb{R}^3)^4} = \langle Hv, u\rangle_{L^2(\mathbb{R}^3)^4} + \langle h, t_\Sigma u\rangle_{H^{-1/2},H^{1/2}}\\ &= \langle Hv, u\rangle_{L^2(\mathbb{R}^3)^4} + \langle h, -\Lambda_+[g]\rangle_{H^{-1/2},H^{1/2}} = \langle Hv, u\rangle_{L^2(\mathbb{R}^3)^4} + \langle t_\Sigma v, g\rangle_{H^{-1/2},H^{1/2}}\\ &= \langle Hv, \psi\rangle_{L^2(\mathbb{R}^3)^4}.\end{aligned}$$

Which yields $\varphi \subset \mathrm{dom}(H_\kappa^*)$ and thus $D \subset \mathrm{dom}(H_\kappa^*)$.

Now we prove the inclusion $\mathrm{dom}(H_\kappa^*) \subset D$. Fix $\varphi \in \mathrm{dom}(H_\kappa^*)$, we first show that there exist functions $v \in H^1(\mathbb{R}^3)^4$ and $h \in H^{-1/2}(\Sigma)^4$ uniquely determined by φ such that $\varphi = v + \Phi[h]$. For that, let $\psi = (\psi_+, \psi_-) \in \mathscr{D}(\Omega_+)^4 \oplus \mathscr{D}(\Omega_-)^4$, then by definition there is $U = (U_+, U_-) \in L^2(\mathbb{R}^3)^4$ such that

$$\begin{aligned}\langle H\varphi, \psi\rangle_{\mathscr{D}'(\mathbb{R}^3)^4,\mathscr{D}(\mathbb{R}^3)^4} &= \langle \varphi, H\psi\rangle_{\mathscr{D}'(\mathbb{R}^3)^4,\mathscr{D}(\mathbb{R}^3)^4} = \langle \varphi_+, H\psi_+\rangle_{L^2(\Omega_+)^4} + \langle \varphi_-, H\psi_-\rangle_{L^2(\Omega_-)^4}\\ &= \langle U_+, \psi_+\rangle_{L^2(\Omega_+)^4} + \langle U_-, \psi_-\rangle_{L^2(\Omega_-)^4} = \langle U, \psi\rangle_{L^2(\mathbb{R}^3)^4}\end{aligned}$$

Thus we obtain $H\varphi_\pm = U_\pm$ in $\mathscr{D}'(\Omega_\pm)^4$ and then in $L^2(\Omega_\pm)^4$. From this we conclude that $\varphi \in H(\alpha, \Omega_+) \oplus H(\alpha, \Omega_-)$. Set

$$h = i(\alpha \cdot N)(t_\Sigma\varphi_+ - t_\Sigma\varphi_-) \ \text{ and } \ v = \varphi - \Phi[h]. \tag{2.2.4}$$

As $t_\Sigma\varphi_\pm \in H^{-1/2}(\Sigma)^4$ holds by Proposition 1.3.3, it follows that $h \in H^{-1/2}(\Sigma)^4$ and $v \in H(\alpha, \Omega_+) \oplus H(\alpha, \Omega_-)$. Moreover, a simple computation yields that

$$t_\Sigma(v \restriction_{\Omega_\pm}) = \left(\frac{1}{2} - i\widetilde{\mathscr{C}}_\Sigma(\alpha \cdot N)\right) t_\Sigma\varphi_+ + \left(\frac{1}{2} + i\widetilde{\mathscr{C}}_\Sigma(\alpha \cdot N)\right) t_\Sigma\varphi_-.$$

Thanks to Proposition 1.3.3-(iv) we know that $t_\Sigma v \in H^{1/2}(\Sigma)^4$, which yields that $v \in H^1(\mathbb{R}^3)^4$ and justifies the decomposition $\varphi = v + \Phi[h]$. Since $\varphi \in \mathrm{dom}(H_\kappa^*) \cap H(\alpha, \Omega_+) \oplus H(\alpha, \Omega_-)$ it follows that

$$\begin{aligned} 0 &= \langle(-i\alpha\cdot N)t_\Sigma\varphi_+, t_\Sigma\psi_+\rangle_{H^{-1/2},H^{1/2}} - \langle(-i\alpha\cdot N)t_\Sigma\varphi_-, t_\Sigma\psi_-\rangle_{H^{-1/2},H^{1/2}} \\ &= \langle t_\Sigma v, g\rangle_{L^2(\Sigma)^4} - \langle h, t_\Sigma u\rangle_{H^{-1/2},H^{1/2}}, \end{aligned} \tag{2.2.5}$$

for all $\psi = u + \Phi[g] \in \mathrm{dom}(H_\kappa) \cap H^1(\Omega_+)^4 \oplus H^1(\Omega_-)^4$. Indeed, using the Green's formula (1.2.6) we easily get

$$\begin{aligned} \langle\varphi, H_\kappa\psi\rangle_{L^2(\mathbb{R}^3)^4} =& \langle\varphi_+, H\psi_+\rangle_{L^2(\Omega_+)^4} + \langle\varphi_-, H\psi_-\rangle_{L^2(\Omega_-)^4} \\ =& \langle H\varphi_+, \psi_+\rangle_{L^2(\Omega_+)^4} + \langle H\varphi_-, \psi_-\rangle_{L^2(\Omega_-)^4} \\ &- \langle(-i\alpha\cdot N)t_\Sigma\varphi_+, t_\Sigma\psi_+\rangle_{H^{-1/2},H^{1/2}} + \langle(-i\alpha\cdot N)t_\Sigma\varphi_-, t_\Sigma\psi_-\rangle_{H^{-1/2},H^{1/2}}. \end{aligned}$$

Therefore, (2.2.5) follows from the above computations, the definition of the adjoint operator and (1.3.23).

Let $g \in H^{1/2}(\Sigma)^4$ and set $u = E(-\Lambda_+[g]) \in H^1(\mathbb{R}^3)^4$, where E is the extension operator. Since $u + \Phi[g] \in \mathrm{dom}(H_\kappa)$, by (2.2.5) we obtain

$$\langle t_\Sigma v, g\rangle_{L^2(\Sigma)^4} - \langle h, t_\Sigma u\rangle_{H^{-1/2},H^{1/2}} = \langle t_\Sigma v + \widetilde{\Lambda}_+[h], g\rangle_{H^{-1/2},H^{1/2}} = 0, \tag{2.2.6}$$

where the condition $t_\Sigma u = -\Lambda_+[g]$ was used in the last step. Since (2.2.6) holds for all $g \in H^{1/2}(\Sigma)^4$, we conclude that $t_\Sigma v = -\widetilde{\Lambda}_+[h]$ holds in $H^{-1/2}(\Sigma)^4$ and then in $H^{1/2}(\Sigma)^4$. Consequently, we get the inclusion $\mathrm{dom}(H_\kappa^*) \subset D$, which completes the proof of the proposition. □

We are now in position to prove Theorem 2.2.1.

Proof of Theorem 2.2.1 (i) Let $z \in \rho(H)$ and let $\kappa \in \mathbb{R}^3$ be such that $\mathrm{sgn}(\kappa) \notin \{0, 4\}$ (where $\mathrm{sgn}(\kappa)$ is given by (2.2.1)). Using the definition of $\widetilde{\Lambda}^z_\pm$ and Lemma 1.3.2-(iv), a simple computation gives

$$\begin{aligned} \widetilde{\Lambda}^z_\pm\widetilde{\Lambda}^z_\mp &= \frac{1}{\mathrm{sgn}(\kappa)} - (\widetilde{\mathscr{C}}^z_\Sigma)^2 + \frac{\mu}{\mathrm{sgn}(\kappa)}\{\beta, \widetilde{\mathscr{C}}^z_\Sigma\} + \frac{\eta}{\mathrm{sgn}(\kappa)}\{\alpha\cdot N, \widetilde{\mathscr{C}}^z_\Sigma\} \\ &= \frac{1}{\mathrm{sgn}(\kappa)} - \frac{1}{4} - \mathscr{C}^z_\Sigma(\alpha\cdot N)\{\alpha\cdot N, \widetilde{\mathscr{C}}^z_\Sigma\} + \frac{\mu}{\mathrm{sgn}(\kappa)}\{\beta, \widetilde{\mathscr{C}}^z_\Sigma\} + \frac{\eta}{\mathrm{sgn}(\kappa)}\{\alpha\cdot N, \widetilde{\mathscr{C}}^z_\Sigma\}. \end{aligned} \tag{2.2.7}$$

Thus, if $g \in H^{-1/2}(\Sigma)^4$ is such that $\widetilde{\Lambda}^z_+[g] \in H^{1/2}(\Sigma)^4$, then from (2.2.7) we see that

$$g = \frac{4(\mathrm{sgn}(\kappa))}{4 - \mathrm{sgn}(\kappa)}\left(\Lambda^z_-\widetilde{\Lambda}^z_+ + \mathscr{C}^z_\Sigma(\alpha\cdot N)\{\alpha\cdot N, \widetilde{\mathscr{C}}^z_\Sigma\} - \frac{\mu}{\mathrm{sgn}(\kappa)}\{\beta, \widetilde{\mathscr{C}}^z_\Sigma\} - \frac{\eta}{\mathrm{sgn}(\kappa)}\{\alpha\cdot N, \widetilde{\mathscr{C}}^z_\Sigma\}\right)[g].$$

Therefore, Lemma 1.3.5 yields that $g \in H^{1/2}(\Sigma)^4$. Consequently, given any $\varphi = u + \Phi[g] \in \mathrm{dom}(H_\kappa^*)$, since $g \in H^{-1/2}(\Sigma)^4$ and $t_\Sigma u = \widetilde{\Lambda}_+[g] \in H^{1/2}(\Sigma)^4$, we deduce that $g \in H^{1/2}(\Sigma)^4$. Thus, $\mathrm{dom}(H_\kappa^*) = \mathrm{dom}(H_\kappa)$ and it holds that

$$\mathrm{dom}(H_\kappa) = \left\{u + \Phi[g] : u \in H^1(\mathbb{R}^3)^4, g \in H^{1/2}(\Sigma)^4, t_\Sigma u = -\Lambda_+[g]\right\}.$$

This finishes the proof of (i).

(ii) Fix $\kappa \in \mathbb{R}^3$ such that $\mathrm{sgn}(\kappa) = 4$. Since H_κ is closable by Proposition 2.2.1, it follows that $\overline{H_\kappa} \subset H_\kappa^*$. Let us prove the other inclusion, for this given $\varphi = u + \Phi[g] \in \mathrm{dom}(H_\kappa^*)$ and let $(h_j)_{j\in\mathbb{N}} \subset H^{1/2}(\Sigma)^4$ be a sequence of functions that converges to g in $H^{-1/2}(\Sigma)^4$. Set

$$g_j := g + \frac{2}{\epsilon}\widetilde{\Lambda}_-[h_j - g], \quad \forall j \in \mathbb{N}. \tag{2.2.8}$$

Then $(g_j)_{j\in\mathbb{N}}, (\Lambda_+[g_j])_{j\in\mathbb{N}} \subset H^{1/2}(\Sigma)^4$, and it holds that

$$g_j \xrightarrow[j\to\infty]{} g \text{ in } H^{-1/2}(\Sigma)^4, \quad \Lambda_+[g_j] \xrightarrow[j\to\infty]{} \widetilde{\Lambda}_+[g], \text{ in } H^{1/2}(\Sigma)^4. \tag{2.2.9}$$

Indeed, note that $\widetilde{\Lambda}_+ + \widetilde{\Lambda}_- = \epsilon/2$, thus one can write g_j as follows

$$g_j = \frac{2}{\epsilon}(\widetilde{\Lambda}_+[g] + \widetilde{\Lambda}_-[h_j]).$$

Using this, (2.2.9) easily follows since $\widetilde{\Lambda}_\pm\widetilde{\Lambda}_\mp$ are bounded from $H^{-1/2}(\Sigma)^4$ to $H^{1/2}(\Sigma)^4$ by Lemma 1.3.5 and (2.2.7). Now for $j \in \mathbb{N}$, we define $\varphi_j := u_j + \Phi[g_j]$, where

$$u_j = u - v_j \quad \text{and} \quad v_j = \mathscr{E}\left(\frac{2}{\epsilon}\widetilde{\Lambda}_+\widetilde{\Lambda}_-[h_j - g]\right),$$

where $\mathscr{E}$ is the extension operator from $H^{1/2}(\Sigma)^4$ to $H^1(\mathbb{R}^3)^4$. Clearly, $u_j \in H^1(\mathbb{R}^3)^4$ and $t_\Sigma u_j = -\Lambda_+[g_j] \in H^{1/2}(\Sigma)^4$, which means that $(\varphi_j)_{j\in\mathbb{N}} \subset \mathrm{dom}(H_\kappa)$. Moreover, since $(h_j)_{j\in\mathbb{N}}$ (resp. $(g_j)_{j\in\mathbb{N}}$) converges to g in $H^{-1/2}(\Sigma)^4$ as $j \longrightarrow \infty$, using the continuity of $\widetilde{\Lambda}_\pm\widetilde{\Lambda}_\mp$ from $H^{-1/2}(\Sigma)^4$ to $H^{1/2}(\Sigma)^4$, it follows that

$$(\varphi_j, H_\kappa\varphi_j) \xrightarrow[j\to\infty]{} (\varphi, H_\kappa^*\varphi) \quad \text{in } L^2(\mathbb{R}^3)^4.$$

Therefore $H_\kappa^* \subset \overline{H_\kappa}$ and the Theorem is proved. □

Remark 2.2.1. *It is worthwhile to mention that, in view of* (2.2.4)*, the functions u and g in $\varphi = u + \Phi[g] \in \mathrm{dom}(\overline{H_\kappa})$ are uniquely determined by φ. Moreover, by Proposition 1.3.3-*(iv) *we have that $(\Phi^z - \Phi)[g] \in H^1(\mathbb{R}^3)^4$. Consequently, for any $z \in \rho(\overline{H_\kappa}) \cap \rho(H)$ and $\varphi = u+\Phi[g] \in \mathrm{dom}(\overline{H_\kappa})$, there exist uniquely determined functions $v \in H^1(\mathbb{R}^3)^4$ and $g \in H^{1/2}(\Sigma)^4$ (resp. $g \in H^{-1/2}(\Sigma)^4$ when $\mathrm{sgn}(\kappa) = 4$) such that $\varphi = v + \Phi^z[g]$ and $(\overline{H_\kappa} - z)\varphi = (H - z)v$ (just write $\varphi = u - (\Phi^z - \Phi)[g] + \Phi^z[g]$).*

In the following, we explain how to define the Dirac operator $\overline{H_\kappa}$ via a transmission condition. Let $\varphi = u+\Phi[g] \in \mathrm{dom}(\overline{H_\kappa})$ and set $\varphi_\pm := \varphi\restriction_{\Omega_\pm}$. It is clear that $\varphi_\pm, (\alpha\cdot\nabla)\varphi_\pm \in L^2(\Omega_\pm)^4$. Now, we define $\delta_\Sigma\varphi$ as the distribution

$$\langle\delta_\Sigma\varphi, \psi\rangle_{\mathscr{D}'(\mathbb{R}^3)^4,\mathscr{D}(\mathbb{R}^3)^4} := \frac{1}{2}\int_\Sigma \langle t_\Sigma\varphi_+ + t_\Sigma\varphi_-, \psi\rangle_{\mathbb{C}^4} \mathrm{d}\sigma(x), \quad \text{for all } \psi \in \mathscr{D}(\mathbb{R}^3)^4.$$

Therefore, a computation in the sense of distributions yields

$$\begin{aligned}\overline{H_\kappa}\varphi =&(-i\alpha\cdot\nabla + m\beta)\varphi + \frac{1}{2}(\epsilon I_4 + \mu\beta + \eta(\alpha\cdot N))(t_\Sigma\varphi_+ + t_\Sigma\varphi_-)\delta_\Sigma,\\ =&(-i\alpha\cdot\nabla + m\beta)\varphi_+ \oplus (-i\alpha\cdot\nabla + m\beta)\varphi_- + i\alpha\cdot N(t_\Sigma\varphi_+ - t_\Sigma\varphi_-)\delta_\Sigma\\ &+ \frac{1}{2}(\epsilon I_4 + \mu\beta + \eta(\alpha\cdot N))(t_\Sigma\varphi_+ + t_\Sigma\varphi_-)\delta_\Sigma.\end{aligned}$$

Using the Plemelj-Sokhotski jump formula (see Lemma 1.3.2), a computation shows that

$$\frac{1}{2}(\epsilon I_4 + \mu\beta + \eta(\alpha\cdot N))(t_\Sigma\varphi_+ + t_\Sigma\varphi_-)\delta_\Sigma + i\alpha\cdot N(t_\Sigma\varphi_+ - t_\Sigma\varphi_-)\delta_\Sigma = 0, \tag{2.2.10}$$

holds in $H^{-1/2}(\Sigma)^4$. Since $(-i\alpha\cdot\nabla + m\beta)\varphi_+ \oplus (-i\alpha\cdot\nabla + m\beta)\varphi_- \in L^2(\mathbb{R}^3)^4$, given $\varphi = (\varphi_+, \varphi_-) \in L^2(\mathbb{R}^3)^4$ such that $(\alpha\cdot\nabla)\varphi_\pm \in L^2(\Omega_\pm)^4$ and satisfying (2.2.10), it holds that $\overline{H_\kappa}\varphi \in L^2(\mathbb{R}^3)^4$. In particular, this leads to the following definition:

Definition 2.2.2. *Let $\kappa = (\epsilon, \mu, \eta) \in \mathbb{R}^3$ be such that $\operatorname{sgn}(\kappa) \neq 0$ and $m > 0$. The self-adjoint Dirac operator coupled with a combination of electrostatic, Lorentz scalar and normal vector field δ-shell interactions of strength ϵ, μ and η respectively, is the operator $\overline{H_\kappa}$ defined on the domain*

$$\operatorname{dom}(\overline{H_\kappa}) = \{\varphi = (\varphi_+, \varphi_-) \in L^2(\Omega_+)^4 \oplus L^2(\Omega_-)^4 : (\alpha\cdot\nabla)\varphi_\pm \in L^2(\Omega_\pm)^4 \text{ and (2.2.10) holds in } H^{-1/2}(\Sigma)^4\},$$

and acts in the sense of distributions as $\overline{H_\kappa}(\varphi) = (H\varphi_+) \oplus (H\varphi_-)$, for all $\varphi \in \operatorname{dom}(\overline{H_\kappa})$.

Remark 2.2.2. *Assume that $\operatorname{sgn}(\kappa) \neq 0, 4$. Since the operator Φ is bounded from $H^{1/2}(\Sigma)^4$ to $H^1(\mathbb{R}^3\setminus\Sigma)^4$, it holds that $\varphi_\pm := \varphi|_{\Omega_\pm} \in H^1(\Omega_\pm)^4$. Moreover, following the same arguments as above, we conclude that the transmission condition (2.2.10) holds actually in $H^{1/2}(\Sigma)^4$. Therefore, it follows that*

$$\operatorname{dom}(H_\kappa) = \left\{\varphi = (\varphi_+, \varphi_-) \in H^1(\Omega_+)^4 \oplus H^1(\Omega_-)^4 : \text{(2.2.10) holds in } H^{1/2}(\Sigma)^4\right\}.$$

Let us make some comments on the technique developed here. Note that the condition on Σ of being C^2-smooth is minimal to prove the self-adjointness of $\overline{H_\kappa}$ when $\operatorname{sgn}(\kappa) = 4$. Indeed, the main ingredient that we have used is the continuity of $\Lambda_\pm\Lambda_\mp$ from $H^{-1/2}(\Sigma)^4$ to $H^{1/2}(\Sigma)^4$, or equivalently, the continuity of the anticommutators $\{\beta, \mathscr{C}_\Sigma\}$ and $\{\alpha\cdot N, \mathscr{C}_\Sigma\}$. Since $\{\beta, \mathscr{C}_\Sigma\}$ involves the trace of the single-layer potential, we can always extend it to a bounded operator from $H^{-1/2}(\Sigma)$ to $H^{1/2}(\Sigma)$, even if Σ is Lipschitz. However, $\{\alpha\cdot N, \mathscr{C}_\Sigma\}$ involves the principal value of the double-layer potential, its adjoint and the commutascrtors $[N_k, R_j]$, where R_j are the Riesz transforms (see Lemma 3.2.1), and it is well known that the C^2 regularity is minimal to extend continuously these operators from $H^{-1/2}(\Sigma)$ to $H^{1/2}(\Sigma)$. However, if $\operatorname{sgn}(\kappa) \neq 0, 4$ and Ω_+ is a bounded $C^{1,\gamma}$-smooth domain, for some $\gamma \in (1/2, 1)$, then one can manage to prove the self-adjointness of H_κ using the technique developed in this part, see Chapter 3 for more details.

2.2.1 On the Dirac Operator with Electrostatic and Lorentz scalar δ-Shell interactions

We discuss in this part the self-adjointness of the Dirac operator H_κ in the case $\eta = 0$, and we denote it by $H_{\epsilon,\mu}$. This operator is known as the Dirac operator with electrostatic and Lorentz scalar δ-shell interactions, cf. [11],[17],[22]. If $|\epsilon| \neq |\mu|$, from Theorem 2.2.1 we get immediately the following result.

Proposition 2.2.3. *Given $\epsilon, \mu \in \mathbb{R}\setminus\{0\}$ such that $|\epsilon| \neq |\mu|$, and define the operators $\Lambda_\pm$ as follows*

$$\Lambda_\pm = \frac{1}{\epsilon^2 - \mu^2}(\epsilon I_4 \mp \mu\beta) \pm C_\Sigma.$$

Then, the following hold:

(i) If $\epsilon^2 - \mu^2 \neq 4$, then $H_{\epsilon,\mu}$ is self-adjoint and we have

$$\mathrm{dom}(H_{\epsilon,\mu}) = \left\{ u + \Phi[g] : u \in H^1(\mathbb{R}^3)^4, g \in H^{1/2}(\Sigma)^4, t_\Sigma u = -\Lambda_+[g] \right\}.$$

(ii) If $\epsilon^2 - \mu^2 = 4$, then $H_{\epsilon,\mu}$ is essentially self-adjoint and we have

$$\mathrm{dom}(\overline{H_{\epsilon,\mu}}) = \left\{ u + \Phi[g] : u \in H^1(\mathbb{R}^3)^4, g \in H^{-1/2}(\Sigma)^4, t_\Sigma u = -\widetilde{\Lambda}_+[g] \right\}.$$

Next we turn to the special case $\mu = \pm\epsilon$. Set $P_\pm = (I_4 \pm \beta)/2$, then $H_{\epsilon,\mu}$ is formally given by

$$H_{\epsilon,\pm\epsilon} = H + P_\pm V_{\epsilon,\pm\epsilon} = -i\alpha \cdot \nabla + m\beta + 2\epsilon P_\pm \delta_\Sigma.$$

Define

$$\begin{aligned} \Lambda_+ &= P_+ \left(1/2\epsilon + C_\Sigma\right) P_+ \text{ and } \ \Lambda_- = P_+ \left(1/2\epsilon - C_\Sigma\right) P_+, \quad \text{if } \mu = \epsilon, \\ \Lambda_+ &= P_- \left(1/2\epsilon + C_\Sigma\right) P_- \text{ and } \ \Lambda_- = P_- \left(1/2\epsilon - C_\Sigma\right) P_-, \quad \text{if } \mu = -\epsilon, \end{aligned} \tag{2.2.11}$$

Clearly, $\Lambda_\pm$ are bounded and self-adjoint from $P_\pm L^2(\Sigma)^4$ onto itself (resp. from $P_\pm H^{1/2}(\Sigma)^4$ into itself). To define $H_{\epsilon,\pm\epsilon}$ as in Definition 2.2.1 (i.e., $H_{\epsilon,\pm\epsilon}\varphi = Hu$ holds in the sense of distributions for $\varphi = u + \Phi[g]$, with $u \in H^1(\mathbb{R}^3)^4$ and $g \in H^{1/2}(\Sigma)^4$), we shall take $g \in P_\pm H^{1/2}(\Sigma)^4$ and assume the condition $P_\pm t_\Sigma u = -P_\pm \Lambda_+[g]$. Indeed, if we take

$$\mathrm{dom}(H_{\epsilon,\pm\epsilon}) = \left\{ u + \Phi[g] : u \in H^1(\mathbb{R}^3)^4, g \in P_\pm L^2(\Sigma)^4 \text{ and } P_\pm t_\Sigma u = -P_\pm \Lambda_+[g] \right\}, \tag{2.2.12}$$

Then, in a similar way as in Proposition 2.2.1 and Proposition 2.2.2, one can check that $(H_{\epsilon,\pm\epsilon}, \mathrm{dom}(H_{\epsilon,\pm\epsilon}))$ is closable and its adjoint is defined on the domain

$$\mathrm{dom}(H^*_{\epsilon,\pm\epsilon}) = \left\{ u + \Phi[g] : u \in H^1(\mathbb{R}^3)^4, g \in P_\pm H^{-1/2}(\Sigma)^4, P_\pm t_\Sigma u = -P_\pm \widetilde{\Lambda}_+[g] \right\}, \tag{2.2.13}$$

where $\widetilde{\Lambda}_\pm$ denotes the bounded extension of $\Lambda_\pm$ from $P_\pm H^{-1/2}(\Sigma)^4$ into itself, and we obtain in this case the analogue of Theorem 2.2.1, which is as follows:

Proposition 2.2.4. *Assume that $\epsilon \neq 0$, then $(H_{\epsilon,\pm\epsilon}, \mathrm{dom}(H_{\epsilon,\pm\epsilon}))$ is self-adjoint and we have*

$$\mathrm{dom}(H_{\epsilon,\pm\epsilon}) = \left\{ u + \Phi[g] : u \in H^1(\mathbb{R}^3)^4, g \in P_\pm H^{1/2}(\Sigma)^4, P_\pm t_\Sigma u = -P_\pm \Lambda_+[g] \right\}.$$

Proof. We show the result only for the case $\mu = \epsilon$, since the case $\mu = -\epsilon$ can be treated analogously. Fix $\epsilon \neq 0$ and let $\widetilde{\Lambda}_\pm$ be as in (2.2.11). Using the relations $P_\pm \alpha_j = P_\mp \alpha_j$ and $P_\pm \beta = \beta P_\pm$, a simple computation yields

$$\widetilde{\Lambda}_- \widetilde{\Lambda}_+ = \frac{1}{4\epsilon^2} P_+ - P_+ \widetilde{C_\Sigma} P_+ \widetilde{C_\Sigma} P_+ = \frac{1}{4\epsilon^2} P_+ - m^2 (S)^2 P_+, \tag{2.2.14}$$

where S is given by (1.3.24). Recall that SP_+ is bounded from $P_+ H^{-1/2}(\Sigma)^4$ into $P_+ H^{1/2}(\Sigma)^4$. Since Λ_- is bounded from $P_+ H^{1/2}(\Sigma)^4$ onto itself, it follows from (2.2.14) that if $g \in P_+ H^{-1/2}(\Sigma)^4$ and $\widetilde{\Lambda}_+[g] \in P_+ H^{1/2}(\Sigma)^4$, then $g \in P_+ H^{1/2}(\Sigma)^4$. Which yields that $\mathrm{dom}(H_{\epsilon,\epsilon}) = \mathrm{dom}(H^*_{\epsilon,\epsilon})$ and the proposition is proved. $\square$

2.2.2 The operators $\Lambda^a_\pm$

Let $a \in (-m, m)$ and let $\Lambda^a_\pm$ be as in the Notation 2.2.1. From the proof of Theorem 2.2.1, it is evident that the study of the self-adjointness character of H_κ is related to the spectral properties of Λ_+. The goal of this part is to establish the connection between H_κ and Λ_+. For this, we introduce the Laplace-Beltrami operators Δ_Σ on Σ and we define the operator $L := (c - \Delta_\Sigma)I_4$ with $c \gg 1$ (we assume here that c is big enough if Σ satisfies (H2), so that c is not in the spectrum of Δ_Σ and there is $\gamma > 0$ such that $(-\Delta_\Sigma + c - \gamma)$ is strictly positive). It is well known that $L^{\pm 1/4}$ is a bijective operator from $H^{\pm 1/2}(\Sigma)^4$ onto $L^2(\Sigma)^4$. Hence, one can write the domain of H_κ as follows:

$$\mathrm{dom}(H_\kappa) = \left\{ u + \Phi L^{1/4}[g] : u \in H^1(\mathbb{R}^3)^4, g \in H^{1/2}(\Sigma)^4 \text{ and } L^{1/4} t_\Sigma u = -L^{1/4}\Lambda_+ L^{1/4}[g] \right\},$$

which leads us to define the following unbounded operators

$$\mathscr{L}^a_\pm := L^{1/4}\Lambda^a_\pm L^{1/4} \quad \text{with} \quad \mathrm{dom}(\mathscr{L}^a_\pm) = \left\{ g \in H^{1/2}(\Sigma)^4 : \Lambda^a_\pm L^{1/4}[g] \in H^{1/2}(\Sigma)^4 \right\}. \tag{2.2.15}$$

In the following lemma, we study the self-adjointness character of $\mathscr{L}^a_\pm$, which will clarify the relation between H_κ and $\Lambda^a_\pm$.

Lemma 2.2.1. *Let $\kappa \in \mathbb{R}^3$ be such that $\mathrm{sgn}(\kappa) \neq 0$, and let $\mathscr{L}^a_\pm$ be as in (2.2.15). The following hold:*

(i) If $\mathrm{sgn}(\kappa) \neq 4$, then $\mathscr{L}^a_\pm$ is self-adjoint with $\mathrm{dom}(\mathscr{L}^a_\pm) = H^1(\Sigma)^4$.

(ii) If $\mathrm{sgn}(\kappa) = 4$, then $\mathscr{L}^a_\pm$ is essentially self-adjoint and we have

$$\mathrm{dom}(\overline{\mathscr{L}^a_\pm}) = \left\{ g \in L^2(\Sigma)^4 : \widetilde{\Lambda}^a_\pm L^{1/4}[g] \in H^{1/2}(\Sigma)^4 \right\}.$$

Proof. Since $L^{1/4}$ and C^a_Σ are self-adjoint operators on $L^2(\Sigma)^4$, it follows that $\mathscr{L}^a_\pm$ is symmetric. Moreover, we have $C^\infty(\Sigma)^4 \subset \mathrm{dom}(\mathscr{L}^a_\pm) \subset L^2(\Sigma)^4$, which yields that $\mathrm{dom}(\mathscr{L}^a_\pm)$ is a dense subspace of $L^2(\Sigma)^4$, therefore $\mathscr{L}^a_\pm$ is closable. Let $h \in \mathrm{dom}(\mathscr{L}^{a*}_\pm)$ and let $g \in C^\infty(\Sigma)^4$. By Proposition 1.3.3 we have

$$\langle h, \mathscr{L}^a_\pm[g]\rangle_{L^2(\Sigma)^4} = \langle L^{1/4}h, \Lambda^a_\pm L^{1/4}[g]\rangle_{H^{-1/2},H^{1/2}} = \langle \widetilde{\Lambda}^a_\pm L^{1/4}h, L^{1/4}[g]\rangle_{H^{-1/2},H^{1/2}}.$$

As $h \in \mathrm{dom}(\mathscr{L}^{a*}_\pm)$, there is $f \in L^2(\Sigma)^4$ such that

$$\langle f, g\rangle_{L^2(\Sigma)^4} = \langle h, \mathscr{L}^a_\pm[g]\rangle_{L^2(\Sigma)^4} = \langle \widetilde{\Lambda}^a_\pm L^{1/4}h, L^{1/4}[g]\rangle_{H^{-1/2},H^{1/2}}.$$

Hence, for all $g \in C^\infty(\Sigma)^4$, we get

$$\langle L^{-1/4}[f], L^{1/4}g\rangle_{H^{-1/2},H^{1/2}} = \langle \widetilde{\Lambda}^a_\pm L^{1/4}h, L^{1/4}[g]\rangle_{H^{-1/2},H^{1/2}},$$

which implies that $\widetilde{\Lambda}^a_\pm L^{1/4}[h] = L^{-1/4}[f]$ holds in $H^{-1/2}(\Sigma)^4$ and then in $H^{1/2}(\Sigma)^4$. Therefore $\widetilde{\Lambda}^a_\pm L^{1/4}[h] \in H^{1/2}(\Sigma)^4$, and we have the inclusion

$$\mathrm{dom}(\mathscr{L}^{a*}_\pm) \subset \left\{ g \in L^2(\Sigma)^4 : \widetilde{\Lambda^a_\pm} L^{1/4}[g] \in H^{1/2}(\Sigma)^4 \right\}.$$

Now, one can easily check the other inclusion and we thus get the equality. Hence, item (i) is an immediate consequence of Lemma 1.3.5 and (2.2.7). To prove the second item, it is sufficient to show that $\mathscr{L}_{\pm}^{a*} \subset \overline{\mathscr{L}_{\pm}^{a}}$. For this, one can take the sequence of functions defined by (3.3.24) (just switch the roles of $\widetilde{\Lambda}_{\pm}^{a}$ and $\widetilde{\Lambda}_{\mp}^{a}$) and use the fact that $\widetilde{\Lambda}_{\pm}^{a}\widetilde{\Lambda}_{\mp}^{a}$ are continuous from $H^{-1/2}(\Sigma)^4$ to $H^{1/2}(\Sigma)^4$, we omit the details. This finishes the proof of the lemma. □

Note that, for any $\psi = u + \Phi[g] \in \mathrm{dom}(H_\kappa)$ and $\varphi = v + \Phi[h] \in \mathrm{dom}(H_\kappa^*)$, it holds that

$$\langle H_\kappa^* \varphi, \psi\rangle_{L^2(\mathbb{R}^3)^4} - \langle \varphi, H_\kappa \psi\rangle_{L^2(\mathbb{R}^3)^4} = \langle -\widetilde{\Lambda}_+[h], g\rangle_{H^{-1/2},H^{1/2}} - \langle h, -\Lambda_+[g]\rangle_{H^{-1/2},H^{1/2}}. \tag{2.2.16}$$

Taking into account the above lemma, from (2.2.2) and (2.2.16) it easily follows that:

$$H_\kappa \text{ is (essentially) self-adjoint } \Longleftrightarrow \mathscr{L}_+ \text{ is (essentially) self-adjoint.} \tag{2.2.17}$$

As mentioned in the introduction, the operator $\mathscr{L}_+$ appears in this form when we study the self-adjoint extension of H_κ from the point of view of the boundary triples theory (see [19] and [22]; for a more general view of the theory we refer to [18] and [35] for example). Indeed, denote by $S := H \upharpoonright H_0^1(\mathbb{R}^3 \setminus \Sigma)^4$, and define the operator

$$T\varphi = Hu, \quad \text{for } \varphi = u + \Phi[g] \in \mathrm{dom}(T) = \{u + \Phi[g] : u \in H^1(\mathbb{R}^3)^4, g \in L^2(\Sigma)^4\},$$

Next, we define the linear mappings $\Gamma_1, \Gamma_2 : \mathrm{dom}(T) \longrightarrow L^2(\Sigma)^4$ by

$$\Gamma_1(\varphi) = g \quad \text{and} \quad \Gamma_2(\varphi) = t_\Sigma u + C_\Sigma[g].$$

Then, $\{L^2(\Sigma)^4, \Gamma_1, \Gamma_2\}$ is a quasi-boundary triples for $\overline{T} = S^*$ (see e.g., [19, Theorem 4.1]), where

$$\mathrm{dom}(\overline{T}) = \{u + \Phi[g] : u \in H^1(\mathbb{R}^3)^4, g \in H^{-1/2}(\Sigma)^4\} = H(\alpha, \Omega_+) \oplus H(\alpha, \Omega_-),$$

and $\overline{T}\varphi = Hu$ (in the sense of distributions) and the space $H(\alpha, \Omega_\pm)$ has been defined in (1.2.4). Moreover, if we define the mappings $\widetilde{\Gamma}_1 : \mathrm{dom}(\overline{T}) \longrightarrow H^{-1/2}(\Sigma)^4$ and $\widetilde{\Gamma}_2 : \mathrm{dom}(\overline{T}) \longrightarrow H^{1/2}(\Sigma)^4$ by

$$\widetilde{\Gamma}_1(\varphi) = g \quad \text{and} \quad \widetilde{\Gamma}_2(\varphi) = t_\Sigma u,$$

then $L^{-1/4}\widetilde{\Gamma}_1, L^{1/4}\widetilde{\Gamma}_2 : \mathrm{dom}(\overline{T}) \longrightarrow L^2(\Sigma)^4$ are well-defined and bounded, and that

$$\{L^2(\Sigma)^4, L^{-1/4}\widetilde{\Gamma}_1, L^{1/4}\widetilde{\Gamma}_2\}$$

is an ordinary boundary triple for $\overline{T} = S^*$. Now it is easy to check that

$$H_\kappa = T \upharpoonright \mathrm{Kr}((\epsilon I_4 + \mu\beta + \eta(\alpha\cdot N))\Gamma_2 + \Gamma_1) \text{ and } H_\kappa^* = \overline{T} \upharpoonright \mathrm{Kr}(L^{1/4}\widetilde{\Gamma}_2 + \mathscr{L}_+^* L^{-1/4}\widetilde{\Gamma}_1).$$

Thus, after transforming the quasi-boundary triples to an ordinary boundary triples (see e.g., [19, Theorem 4.5]), we get the equivalence (2.2.17), see, e.g., [19, Corollary 2.8].

2.3 Spectral properties

In this section, we examine the spectral properties of the operator H_κ. First, we give a necessary condition for the existence of the point spectrum in the gap $(-m, m)$ and a Krein-type resolvent formula. More precisely, recall that $\mathrm{sgn}(\kappa)$ is defined in (2.2.1), then we have the following.

Proposition 2.3.1. *Let H_κ be as in Definition 2.2.1 and let $(\Phi^z)^*$ be the adjoint of Φ^z from Lemma 1.3.3. If $\mathrm{sgn}(\kappa) = 4$, then the following hold:*

(i) Given $a \in (-m, m)$, then one has $\mathrm{Kr}(\overline{H_\kappa} - a) \neq \{0\} \iff \mathrm{Kr}(\widetilde{\Lambda}_+^a) \neq \{0\}$ (Birman-Schwinger principle) and $\mathrm{Kr}(\overline{H_\kappa} - a) = \{\Phi^a[g] : g \in \mathrm{Kr}(\widetilde{\Lambda}_+^a)\}$.

(ii) For all $z \in \mathbb{C} \setminus \mathbb{R}$, the operator $\widetilde{\Lambda}_+^z$ takes the space $\{g \in H^{-1/2}(\Sigma)^4 : \widetilde{\Lambda}_+^z[g] \in H^{1/2}(\Sigma)^4\}$ bijectively to $H^{1/2}(\Sigma)^4$. In particular, $\widetilde{\Lambda}_+^z$ admits a bounded inverse from $H^{1/2}(\Sigma)^4$ to $H^{-1/2}(\Sigma)^4$, and we have

$$(\overline{H_\kappa} - z)^{-1} = (H - z)^{-1} - \Phi^z(\widetilde{\Lambda}_+^z)^{-1}(\Phi^{\overline{z}})^*. \tag{2.3.1}$$

If $\mathrm{sgn}(\kappa) \neq 0, 4$ and $z \in \mathbb{C} \setminus \mathbb{R}$, then Λ_+^z is bounded invertible from $H^{1/2}(\Sigma)^4$ to $H^{1/2}(\Sigma)^4$ and the above statements hold true with $\Lambda_+^\bullet$ instead of $\widetilde{\Lambda}_+^\bullet$. In particular ,

$$(H_\kappa - z)^{-1} = (H - z)^{-1} - \Phi^z(\Lambda_+^z)^{-1}(\Phi^{\overline{z}})^*.$$

Proof. We prove the statements for $\mathrm{sgn}(\kappa) = 4$, the case $\mathrm{sgn}(\kappa) \neq 0, 4$ follows the same lines.

(i) Let us prove the implication $(\Rightarrow)$ and the inclusion $\mathrm{Kr}(\overline{H_\kappa} - a) \subset \{\Phi^a[g] : g \in \mathrm{Kr}(\widetilde{\Lambda}_+^a)\}$. Let $a \in (-m, m)$ and assume that there is a nonzero $\varphi = u + \Phi[g] \in \mathrm{dom}(\overline{H_\kappa})$ such that $\overline{H_\kappa}\varphi = a\varphi$. First observe that $\widetilde{\Lambda}_+^a - \widetilde{\Lambda}_+ = \widetilde{C_\Sigma^a} - \widetilde{C_\Sigma}$. Now, using the definition of $\overline{H_\kappa}$, we then get

$$Hu = a\varphi = a(u + \Phi[g]). \tag{2.3.2}$$

From this we deduce that $(H - a)Hu = ag\delta_\Sigma$ holds in $\mathscr{D}'(\mathbb{R}^3)^4$, and therefore

$$Hu = a\Phi^a[g]. \tag{2.3.3}$$

From this, it is clear that if $a = 0$ then $u = 0$. Therefore, $\varphi = \Phi[g] \neq 0$ (with $g \neq 0$, as otherwise φ would be zero) and $g \in \mathrm{Kr}(\widetilde{\Lambda}_+)$, which yields that $\mathrm{Kr}(\overline{H_\kappa}) \subset \{\Phi[g] : g \in \mathrm{Kr}(\widetilde{\Lambda}_+)\}$. Now assume that $a \neq 0$, then from (2.3.2) and (2.3.3) it follows that $u = (\Phi^a - \Phi)[g]$. Since $\varphi = u + \Phi[g] \in \mathrm{dom}(\overline{H_\kappa})$, it holds that $t_\Sigma u = -\widetilde{\Lambda}_+[g]$, and by Proposition 1.3.3(iii) we also get that $t_\Sigma u = (\widetilde{C_\Sigma^a} - \widetilde{C_\Sigma})[g] = -\widetilde{\Lambda}_+[g]$. Hence, we obtain that $0 \neq g \in \mathrm{Kr}(\widetilde{\Lambda}_+^a)$ and $\varphi = \Phi^a[g]$, therefore $\mathrm{Kr}(\overline{H_\kappa} - a) \subset \{\Phi^a[g] : g \in \mathrm{Kr}(\widetilde{\Lambda}_+^a)\}$.

Conversely, let $a \in (-m, m)$ be such that $\widetilde{\Lambda}_+^a[g] = 0$, for a nonzero $g \in H^{-1/2}(\Sigma)^4$. Then, it is clear that $\varphi = \Phi[g] \in \mathrm{dom}(\overline{H_\kappa})$ and we have $0 \neq \varphi \in \mathrm{Kr}(\overline{H_\kappa})$ when $a = 0$, which gives the result in this case. Now suppose that $a \neq 0$, let $u = aH^{-1}\Phi^a[g] \in H^1(\mathbb{R}^3)^4$ and set $\varphi = u + \Phi[g]$. Then $Hu = a\Phi^a[g]$ and $(H - a)u = a\Phi[g]$ in $\mathscr{D}'(\mathbb{R}^3)^4$, this amounts to saying that $\overline{H_\kappa}\varphi = Hu = a(u + \Phi[g]) = a\varphi$ and $u = \Phi^a[g] - \Phi[g]$. Furthermore, we can easily see that $t_\Sigma u = (\widetilde{C_\Sigma^a} - \widetilde{C_\Sigma})[g] = -\widetilde{\Lambda}_+[g]$. Summing up, we have proved that $\varphi = \Phi^a[g] \in \mathrm{dom}(\overline{H_\kappa})$ and $\overline{H_\kappa}\varphi = a\varphi$, which yields that $\varphi \in \mathrm{Kr}(\overline{H_\kappa} - a)$. This ends the proof of (i).

(ii) Fix $z \in \mathbb{C} \setminus \mathbb{R}$ and set $\mathcal{G} = \{g \in H^{-1/2}(\Sigma)^4 : \widetilde{\Lambda}_+^z[g] \in H^{1/2}(\Sigma)^4\}$. Since $\overline{H_\kappa}$ is self-adjoint it follows that $(\overline{H_\kappa} - z)^{-1}$ is well-defined and bounded. Moreover, using the same arguments as in the proof of (i), one can see that $\mathrm{Kr}(\widetilde{\Lambda}_+^z) = \{0\}$, as otherwise z would be a non-real eigenvalue of $\overline{H_\kappa}$. Now we are going to prove that $\widetilde{\Lambda}_+^z$ admits a bounded inverse from $H^{1/2}(\Sigma)^4$ to $H^{-1/2}(\Sigma)^4$ and to show the identity (2.3.1). For this, let $u \in L^2(\mathbb{R}^3)^4$ and set $\varphi := (\overline{H_\kappa} - z)^{-1}u \in \mathrm{dom}(\overline{H_\kappa})$. Thanks to Remark 2.2.1, we know that there are unique functions $v \in H^1(\mathbb{R}^3)^4$ and $g \in H^{-1/2}(\Sigma)^4$ such that $\varphi = v + \Phi^z[g]$. Moreover one has $(\overline{H_\kappa} - z)\varphi = (H - z)v$, and thus $v = (H - z)^{-1}u$, which means actually that $\varphi = (H - z)^{-1}u + \Phi^z[g]$. Next, observe that

$$i\alpha \cdot N(t_\Sigma\varphi_+ - t_\Sigma\varphi_-) = g \quad \text{and} \quad \frac{1}{2}(t_\Sigma\varphi_+ + t_\Sigma\varphi_-) = (H - z)^{-1}u \restriction_\Sigma + \widetilde{\mathscr{C}_\Sigma^z}[g].$$

Using that $(H-z)^{-1}u\restriction_{\Sigma} = (\Phi^{\overline{z}})^* u$ and the transmission condition (2.2.10), we obtain that $\widetilde{\Lambda}_+^z[g] = -(\Phi^{\overline{z}})^* u \in H^{1/2}(\Sigma)^4$. Since this is true for all $u \in L^2(\mathbb{R}^3)^4$, $\mathrm{Rn}((\Phi^{\overline{z}})^*) = H^{1/2}(\Sigma)^4$ and $\mathrm{Kr}(\widetilde{\Lambda}_+^z) = \{0\}$, it follows that the mapping

$$\widetilde{\Lambda}_+^z : \{g \in H^{-1/2}(\Sigma)^4 : u + \Phi^z[g] \in \mathrm{dom}(\overline{H_\kappa}) \text{ for some } u \in H^1(\mathbb{R}^3)^4\} \to H^{1/2}(\Sigma)^4$$

is well-defined and bijective, and that

$$\{g \in H^{-1/2}(\Sigma)^4 : u + \Phi^z[g] \in \mathrm{dom}(\overline{H_\kappa}) \text{ for some } u \in H^1(\mathbb{R}^3)^4\} \subset \mathcal{G}.$$

Now, given $g \in \mathcal{G}$, then as simple computation shows that the function $\varphi = E(\widetilde{\Lambda}_+^z[g]) + \Phi^z[g]$ fulfils the transmission condition (2.2.10), and that

$$\begin{aligned} H(\varphi\restriction_{\Omega_\pm}) &= HE_{\Omega_\pm}(\widetilde{\Lambda}_+^z[g]) + z(\Phi^z[g]\restriction_{\Omega_\pm}) + (H-z)(\Phi^z[g]\restriction_{\Omega_\pm}) \\ &= HE_{\Omega_\pm}(\widetilde{\Lambda}_+^z[g]) + z(\Phi^z[g]\restriction_{\Omega_\pm}) \in L^2(\Omega_\pm)^4, \end{aligned}$$

which implies that $\varphi \in \mathrm{dom}(\overline{H_\kappa})$ and proves the inclusion

$$\mathcal{G} \subset \{g \in H^{-1/2}(\Sigma)^4 : u + \Phi^z[g] \in \mathrm{dom}(\overline{H_\kappa}) \text{ for some } u \in H^1(\mathbb{R}^3)^4\}.$$

From the above considerations we deduce that the mapping $\widetilde{\Lambda}_+^z : \mathcal{G} \to H^{1/2}(\Sigma)^4$ is well-defined and bijective, which proves the first statement of (ii). Since the inverse $(\widetilde{\Lambda}_+^z)^{-1} : H^{1/2}(\Sigma)^4 \to \mathcal{G}$ is everywhere defined and $\widetilde{\Lambda}_+^z$ is injective, to complete the proof of (ii) it suffices to show that $\widetilde{\Lambda}_+^z : \mathcal{G} \to H^{1/2}(\Sigma)^4$ it is closed. So, suppose that $(g_j)_{j\in\mathbb{N}} \subset \mathcal{G}$ is a sequence of function such that

$$g_j \xrightarrow[j\to\infty]{} g \in H^{-1/2}(\Sigma)^4 \quad \text{and} \quad \widetilde{\Lambda}_+^z[g_j] \xrightarrow[j\to\infty]{} h \in H^{1/2}(\Sigma)^4.$$

Since, $\widetilde{\Lambda}_+^z$ is bounded from $H^{-1/2}(\Sigma)^4$ into itself, it follows that $\widetilde{\Lambda}_+^z[g_j] \xrightarrow[j\to\infty]{} \widetilde{\Lambda}_+^z[g] = h$ in $H^{-1/2}(\Sigma)^4$. Thus, $\widetilde{\Lambda}_+^z[g] = h$ in $H^{1/2}(\Sigma)^4$ which implies that $\widetilde{\Lambda}_+^z : \mathcal{G} \to H^{1/2}(\Sigma)^4$ is closed. Therefore, $(\widetilde{\Lambda}_+^z)^{-1} : H^{1/2}(\Sigma)^4 \to \mathcal{G}$ is everywhere defined and closed, and hence bounded. Consequently, we get that the operator $\widetilde{\Lambda}_+^z$ admits a bounded inverse $(\widetilde{\Lambda}_+^z)^{-1}$ from $H^{1/2}(\Sigma)^4$ to $H^{-1/2}(\Sigma)^4$. Summing up, we have proved that

$$(\overline{H_\kappa} - z)^{-1} u = (H-z)^{-1} u - \Phi^z[(\widetilde{\Lambda}_+^z)^{-1}(\Phi^{\overline{z}})^* u],$$

holds for all $u \in L^2(\mathbb{R}^3)^4$, which proves the identity (2.3.1) and completes the proof of the proposition. □

Remark 2.3.1. *A careful inspection of the argument used above reveals that* $\dim\mathrm{Kr}(\overline{H_\kappa} - a)$ *is equal to* $\dim\mathrm{Kr}(\widetilde{\Lambda}_+^a)$*, since* Φ^z *is injective. Moreover, item* (ii) *holds true for all* $z \in \rho(\overline{H_\kappa}) \cap \rho(H)$*.*

The following lemma refines and reformulates Proposition 2.3.1 in terms of the operator $\overline{\mathcal{L}_+^a}$ introduced in Subsection 2.2.2, and will be a key tool in the analysis of the spectrum of $\overline{H_\kappa}$ when $\mathrm{sgn}(\kappa) = 4$.

Theorem 2.3.1. *Let* $\overline{\mathcal{L}_+^a}$ *be the self-adjoint operator in Lemma 2.2.1, and let* H_κ *be as in Definition 2.2.1. For* $z \in \mathbb{C} \setminus \mathbb{R}$ *we define the operator* $\overline{\mathcal{L}_+^z} = L^{1/4}\widetilde{\Lambda}_+^z L^{1/4}$ *with* $L^{1/4}$ *as in Subsection 2.2.2. Then the following hold true:*

(i) For all $a \in (-m, m)$, one has

$$a \in \mathrm{Sp_p}(\overline{H_\kappa}) \Longleftrightarrow 0 \in \mathrm{Sp_p}(\overline{\mathscr{L}_+^a}), \tag{2.3.4}$$
$$a \in \mathrm{Sp_{disc}}(\overline{H_\kappa}) \Longleftrightarrow 0 \in \mathrm{Sp_{disc}}(\overline{\mathscr{L}_+^a}), \tag{2.3.5}$$
$$a \in \mathrm{Sp_{ess}}(\overline{H_\kappa}) \Longleftrightarrow 0 \in \mathrm{Sp_{ess}}(\overline{\mathscr{L}_+^a}). \tag{2.3.6}$$

(ii) Let $z \in \rho(\overline{H_\kappa}) \cap \rho(H)$ and assume that $\mathrm{sgn}(\kappa) = 4$. Then, the operator $\overline{\mathscr{L}_+^z}$ is bounded from $L^2(\Sigma)^4$ to $H^{-1}(\Sigma)^4$ and admits a bounded inverse from $L^2(\Sigma)^4$ to $L^2(\Sigma)^4$ for $z \in \mathbb{C} \setminus \mathbb{R}$, and admits a bounded inverse from $L^2(\Sigma)^4$ to $\mathrm{dom}(\overline{\mathscr{L}_+^z})$ for $z \in (-m, m)$. Moreover, it holds that

$$(\overline{H_\kappa} - z)^{-1} = (H - z)^{-1} - \Phi^z L^{\frac{1}{4}} \left(\overline{\mathscr{L}_+^z}\right)^{-1} L^{\frac{1}{4}} (\Phi^{\overline{z}})^*.$$

Before going through the proof of Theorem 2.3.1 we establish the following lemma.

Lemma 2.3.1. *Let $z_1, z_2 \in \rho(H)$ and let $\overline{\mathscr{L}_+^{z_j}}$ be as in Theorem 2.3.1, then*

$$\overline{\mathscr{L}_+^{z_1}} - \overline{\mathscr{L}_+^{z_2}} = (z_1 - z_2) L^{\frac{1}{4}} (\Phi^{\overline{z_2}})^* \Phi^{z_1} L^{\frac{1}{4}}, \tag{2.3.7}$$

In particular, for $a \in (-m, m)$ and $r_0 < \mathrm{dist}(a, \mathrm{Sp}(H) \cup \mathrm{Sp}(\overline{H_\kappa}) \setminus \{a\})$, one has an expansion of the form

$$\overline{\mathscr{L}_+^z} = \overline{\mathscr{L}_+^a} + (z - a) L^{\frac{1}{4}} (\Phi^a)^* \Phi^a L^{\frac{1}{4}} + (z - a)^2 \mathscr{R}(z), \tag{2.3.8}$$

for any z such that $0 < |z - a| < r_0$, where $\mathscr{R}$ is holomorphic in a neighbourhood of a.

Proof. Fix $z_1, z_2 \in \rho(H)$, recall the first resolvent identity

$$(H - \overline{z_1})^{-1} = -(H - \overline{z_2})^{-1} + (\overline{z_1} - \overline{z_2})(\Phi^{\overline{z_1}})^* (H - \overline{z_2})^{-1},$$

By definition of the mapping $(\Phi^{z_j})^*$, we have that

$$\begin{aligned}(\Phi^{z_1})^* - (\Phi^{z_2})^* &= t_\Sigma[(H - \overline{z_1})^{-1} - (H - \overline{z_2})^{-1}] = (\overline{z_1} - \overline{z_2}) t_\Sigma[(H - \overline{z_1})^{-1} (H - \overline{z_2})^{-1}] \\ &= (\overline{z_1} - \overline{z_2})(\Phi^{z_1})^* (H - \overline{z_2})^{-1},\end{aligned} \tag{2.3.9}$$

where the first resolvent identity was used in the second equality. Since Φ^{z_k} is the adjoint of $(\Phi^{z_k})^*$, taking the adjoint in (2.3.9) yields that

$$\Phi^{z_1} - \Phi^{z_2} = (z_1 - z_2)(H - z_2)^{-1} \Phi^{z_1} \tag{2.3.10}$$

Since $\widetilde{\Lambda}_+^{z_1} - \widetilde{\Lambda}_+^{z_2} = t_\Sigma(\Phi^{z_1} - \Phi^{z_2})$ holds by Proposition 1.3.3, taking the trace in (2.3.10) and multiplying by $L^{\frac{1}{4}}$ yields the formula (2.3.7). Notice that (2.3.7) implies that

$$\frac{d}{dz} \overline{\mathscr{L}_+^z} = L^{\frac{1}{4}} (\Phi^{\overline{z}})^* \Phi^z L^{\frac{1}{4}}, \quad \forall z \in \rho(H).$$

Using this and the fact that $\mathscr{C}_\Sigma^z$ is holomorphic for all $z \in \rho(H)$, we get the last statement of the lemma. ☐

In particular, for $a \in (-m,m)$ and $r_0 < \mathrm{dist}(a, \mathrm{Sp}(H) \cup \mathrm{Sp}(\overline{H_\kappa}) \setminus \{a\})$, one has an expansion of the form

$$\overline{\mathscr{L}_+^z} = \overline{\mathscr{L}_+^a} + (z-a)L^{\frac{1}{4}}(\Phi^{\overline{a}})^*\Phi^a L^{\frac{1}{4}} + (z-a)^2\mathscr{R}(z), \tag{2.3.11}$$

for any z such that $0 < |z-a| < r_0$, where $\mathscr{R}$ is holomorphic in a neighbourhood of a. As $L^{\frac{1}{4}}(\Phi^{\overline{a}})^*\Phi^a L^{\frac{1}{4}}$ is a bounded, positive definite and self-adjoint operator in $L^2(\Sigma)^4$

Proof of Theorem 2.3.1. We will prove the statements for $\mathrm{sgn}(\kappa) = 4$, the case $\mathrm{sgn}(\kappa) \notin \{0,4\}$ follows in the same way.

Proof of (ii). We note first that, for $z \in \mathbb{C} \setminus \mathbb{R}$, the statement follows from the definition of $\overline{\mathscr{L}_+^z}$, the fact that $L^{\frac{1}{4}} : H^s(\Sigma)^4 \to H^{s-1/2}(\Sigma)^4$ is bijective and continuous for any $s \in [-1/2, 1]$, Proposition 2.3.1-(ii) and Remark 2.3.1. Note that the case $z \in (-m,m)$ follows in the same way, since $\overline{\mathscr{L}_+^z}$ is self-adjoint and $\mathrm{dom}(\overline{\mathscr{L}_+^z}) = L^{\frac{1}{4}}\mathscr{G}$, where the set $\mathscr{G}$ is defined as in the proof of Proposition 2.3.1-(ii).

Proof of (ii). Fix $a \in (-m,m)$, then by definition it holds that : 0 is an eigenvalue of $\overline{\mathscr{L}_+^a}$ if and only if $\mathrm{Kr}(\widetilde{\Lambda}_+^a) \neq \{0\}$, and that $\dim\mathrm{Kr}(\overline{\mathscr{L}_+^a}) = \dim\mathrm{Kr}(\widetilde{\Lambda}_+^a)$. Thus, Proposition 2.3.1-(i) together with Remark 2.3.1 yield that 0 is an eigenvalue of $\overline{\mathscr{L}_+^a}$ if and only if a is an eigenvalue of $\overline{H_\kappa}$, and that

$$\mathrm{Kr}(\overline{H_\kappa} - a) = \{\Phi^a L^{\frac{1}{4}}[g] : g \in \mathrm{Kr}(\overline{\mathscr{L}_+^a})\}, \quad \dim\mathrm{Kr}(\overline{H_\kappa} - a)) = \dim\mathrm{Kr}(\overline{\mathscr{L}_+^a}). \tag{2.3.12}$$

This gives in particular the equivalence (2.3.4).

Thanks to (2.3.4) and (2.3.12), to show the equivalence (2.3.5) it is sufficient to prove that

$$a \in (-m,m) \text{ is an isolated point of } \mathrm{Sp}(\overline{H_\kappa}) \Longleftrightarrow 0 \text{ is an isolated point of } \mathrm{Sp}(\overline{\mathscr{L}_+^a}). \tag{2.3.13}$$

Let us prove the implication ($\Longleftarrow$). Assume that $a \in (-m,m)$ and $0 \in \mathrm{Sp}_{\mathrm{disc}}(\overline{\mathscr{L}_+^a})$. Define the operators

$$B_a = \overline{\mathscr{L}_+^a} \upharpoonright (\mathrm{Kr}(\overline{\mathscr{L}_+^a})^\perp \cap \mathrm{dom}(\overline{\mathscr{L}_+^a})), \quad A_a = (\overline{H_\kappa} - a) \upharpoonright (\mathrm{Kr}(\overline{H_\kappa} - a)^\perp \cap \mathrm{dom}(\overline{H_\kappa})). \tag{2.3.14}$$

Thanks [60, Theorem 6.7.], we know that B_a has a bounded inverse $(B_a)^{-1}$. Thus, the operator

$$(A_a)^{-1} = (H-a)^{-1} - \Phi^a L^{\frac{1}{4}}(B_a)^{-1}L^{\frac{1}{4}}(\Phi^{\overline{a}})^*,$$

is everywhere defined and bounded from $L^2(\mathbb{R}^3)^4$ to $\mathrm{dom}(\overline{H_\kappa})$. Moreover, from (2.3.12) and the definition of A_a and B_a it follows that $(A_a)^{-1} : L^2(\mathbb{R}^3)^4 \longrightarrow (\mathrm{Kr}(\overline{H_\kappa} - a)^\perp \cap \mathrm{dom}(\overline{H_\kappa}))$ is bounded and that $A_a(A_a)^{-1}f = f$ for all $f \in L^2(\mathbb{R}^3)^4$. Therefore, A_a has a bounded inverse, which means that using (2.3.11) and following exactly the same arguments as in the proof of [35, Theorem 3.2.] we obtain that $(\overline{H_\kappa} - a) \upharpoonright (\mathrm{Kr}(\overline{H_\kappa} - a)^\perp \cap \mathrm{dom}(\overline{H_\kappa}))$ has a bounded inverse. Thus, [60, Theorem 6.7.] yields that a is an isolated point of $\mathrm{Sp}(\overline{H_\kappa})$, and thus $a \in \mathrm{Sp}_{\mathrm{disc}}(\overline{H_\kappa})$.

The proof of the implication ($\Longrightarrow$) follows exactly the same lines as in [35, Theorem 3.2.]. Suppose that $a \in (-m,m) \cap \mathrm{Sp}_{\mathrm{disc}}(\overline{H_\kappa})$, then there is $r_0 > 0$ such that for all $z \in B(a,r_0)\setminus\{a\} \subset \rho(\overline{H_\kappa})$, the resolvent $(\overline{H_\kappa} - z)^{-1}$ is holomorphic and $(\overline{H_\kappa} - a)^{-1}$ is meromorphic. Thanks to the resolvent formula from (ii) and the holomorphic properties of Φ^z and $(\Phi^z)^*$, it follows that $(\overline{\mathscr{L}_+^a})^{-1}$ is meromorphic and the mapping $B(a,r_0) \setminus \{a\} \ni z \longmapsto (\overline{\mathscr{L}_+^z})^{-1}$ is holomorphic, and thus the inverse $(\overline{\mathscr{L}_+^z})^{-1}$ exist and is bounded for all $z \in B(a, r_0) \setminus \{a\}$. Using this and the formula (2.3.11) from Lemma 2.3.1, we can choose $0 < r_1 < r_0$ small enough such that for $0 < |z - a| < r_1$, the operator

$$\overline{\mathscr{L}_+^a} + (z-a)L^{\frac{1}{4}}(\Phi^a)^*\Phi^a L^{\frac{1}{4}},$$

has a bounded inverse. As $\mathscr{P}(a) := L^{\frac{1}{4}}(\Phi^{\overline{a}})^*\Phi^a L^{\frac{1}{4}}$ is a bounded, positive definite and self-adjoint operator in $L^2(\Sigma)^4$, we have

$$\overline{\mathscr{L}_+^a} + (z-a)L^{\frac{1}{4}}(\Phi^a)^*\Phi^a L^{\frac{1}{4}} = \mathscr{P}(a)^{1/2}(\mathscr{P}(a)^{-1/2}\overline{\mathscr{L}_+^a}\mathscr{P}(a)^{-1/2} + (z-a)I_4)\mathscr{P}(a)^{1/2}.$$

Since this true for all z such that $0 < |z - a| < r_1$, using the properties of $\mathscr{P}(a)$ we deduce that

$$\mathscr{P}(a)^{-1/2}\overline{\mathscr{L}_+^a}\mathscr{P}(a)^{-1/2} + (z-a)I_4,$$

has a bounded inverse, and thus 0 is an isolated point of $\mathrm{Sp}(\mathscr{P}(a)^{-1/2}\overline{\mathscr{L}_+^a}\mathscr{P}(a)^{-1/2})$. Therefore, [35, Lemma 3.1] yields that 0 is an isolated point of $\mathrm{Sp}(\overline{\mathscr{L}_+^a})$, finishing the proof of (2.3.13) and the equivalence (2.3.5).

Finally, thanks to (2.3.5) and the self-adjointness of $\overline{\mathscr{L}_+^a}$ for $a \in (-m, m)$, to show the equivalence (2.3.6) is suffices to prove that

$$a \in \rho(\overline{H_\kappa}) \cap (-m, m) \Longleftrightarrow 0 \in \rho(\overline{\mathscr{L}_+^a}). \tag{2.3.15}$$

Let $a \in \rho(\overline{H_\kappa}) \cap (-m, m)$, then (2.3.12) implies that $\mathrm{Kr}(\overline{\mathscr{L}_+^a}) = \{0\}$. On the other hand, from (ii) and the proof of Proposition 2.3.1-(ii) we know that $\mathrm{Rn}(\overline{\mathscr{L}_+^a}) = L^2(\Sigma)^4$ and that $\overline{\mathscr{L}_+^a}$ admits a bounded inverse from $L^2(\Sigma)^4$ to $\mathrm{dom}(\overline{\mathscr{L}_+^a})$. Since $\overline{\mathscr{L}_+^a}$ is self-adjoint in $L^2(\Sigma)^4$ by Lemma 2.2.1, it follows that $\overline{\mathscr{L}_+^a}$ is invertible from $L^2(\Sigma)^4$ to $\mathrm{dom}(\overline{\mathscr{L}_+^a})$, and hence $0 \in \rho(\overline{\mathscr{L}_+^a})$. Conversely, if $a \in (-m, m)$ and $0 \in \rho(\overline{\mathscr{L}_+^a})$, then $(\overline{\mathscr{L}_+^a})^{-1}$ is bounded from $L^2(\Sigma)^4$ to $\mathrm{dom}(\overline{\mathscr{L}_+^a}) \subset L^2(\Sigma)^4$. Using the properties of Φ^a and Lemma 1.3.2, it is straightforward to check that

$$\begin{aligned} &g := (H-a)^{-1}f - \Phi^a L^{\frac{1}{4}}\left(\overline{\mathscr{L}_+^a}\right)^{-1} L^{\frac{1}{4}}(\Phi^{\overline{a}})^* f \in \mathrm{dom}(\overline{H_\kappa}), \\ &(\overline{H_\kappa} - a)g = f, \end{aligned}$$

hold for any $f \in L^2(\mathbb{R}^3)^4$. From this it follows that $(\overline{H_\kappa} - a)$ admits a bounded inverse from $L^2(\mathbb{R}^3)^4$ to $\mathrm{dom}(\overline{H_\kappa})$ and that $\mathrm{Rn}(\overline{H_\kappa} - a) = L^2(\mathbb{R}^3)^4$. Since $\mathrm{Kr}(\overline{H_\kappa} - a) = \{0\}$ holds by (2.3.12), we get that $(\overline{H_\kappa} - a)$ is boundedly invertible from $L^2(\mathbb{R}^3)^4$ to $\mathrm{dom}(\overline{H_\kappa})$, which implies that $a \in \rho(\overline{H_\kappa})$. This proves the equivalence (2.3.15) and completes the proof of the lemma. □

2.3.1 Non-critical case

This part deals with the basic spectral properties of H_κ when $\kappa = (\epsilon, \mu, 0)$ (i.e., $\eta = 0$) and $\mathrm{sgn}(\kappa) \neq 0, 4$. We first discus the basic spectral properties for surfaces satisfying the assumption (H1), which are mainly known for the Dirac operator coupled with a combination of electrostatic and Lorentz scalar δ-interactions (i.e $\eta = 0$), see e.g., [17]. Then, we address the case of surfaces satisfying the hypothesis (H2).

Theorem 2.3.2. *Let $\kappa \in \mathbb{R}^3$ be such that $\mathrm{sgn}(\kappa) \neq 0, 4$, and suppose that Σ satisfies* (H1). *The following statements hold true:*

(i) $\mathrm{Sp}_{\mathrm{ess}}(H_\kappa) = (-\infty, -m] \cup [m, +\infty)$.

(ii) $\mathrm{Sp}_{\mathrm{disc}}(H_\kappa) \cap (-m, m)$ *is finite.*

proof. (i) Since Σ is compact and $(\Phi^{\overline{z}})^*$ is bounded from $L(\mathbb{R}^3)^4$ to $H^{1/2}(\Sigma)^4$, and $H^{1/2}(\Sigma)^4$ is compactly embedded in $L^2(\Sigma)^4$, thanks to the boundedness properties of the operators Φ^z and $(\Lambda_+^z)^{-1}$ we get that $\Phi^z(\Lambda_+^z)^{-1}(\Phi^{\overline{z}})^*$ is a compact operator in $L(\mathbb{R}^3)^4$. As $\mathrm{Sp}_{\mathrm{ess}}(H) = (-\infty, -m] \cup [m, +\infty)$, and

$$(H_\kappa - z)^{-1} - (H - z)^{-1} = -\Phi^z(\Lambda_+^z)^{-1}(\Phi^{\overline{z}})^*,$$

holds by Proposition 2.3.1. By Weyl's theorem we deduce that $\mathrm{Sp}_{\mathrm{ess}}(H_\kappa) = \mathrm{Sp}_{\mathrm{ess}}(H)$, and this proves the assertion (i).

(ii) As H_κ is self-adjoint, in order to prove the statement it is sufficient to show that the square operator $(H_\kappa)^2$ has at most finitely many eigenvalues in $(-\infty, m^2)$. To this end, let $\mathfrak{Q}$ be the quadratic form associated to $(H_\kappa)^2$ with domain $\mathrm{dom}(H_\kappa)$, then following the idea of [22, Proposition 3.9] (see also [66, 17]) we will construct a closed quadratic form $\widetilde{\mathfrak{Q}}$ such that its associated self-adjoint operator has at most finitely many eigenvalues in $(-\infty, m^2)$, $\mathrm{dom}(\mathfrak{Q}) \subset \mathrm{dom}(\widetilde{\mathfrak{Q}})$ and $\widetilde{\mathfrak{Q}}[\varphi] \leqslant \mathfrak{Q}[\varphi]$ holds for all $\varphi \in \mathrm{dom}(\mathfrak{Q})$ (i.e., $\mathfrak{Q}$ is minorated by $\widetilde{\mathfrak{Q}}$ in the sense of closed quadratic forms).

We first note that $\mathfrak{Q}$ is closed because H_κ is self-adjoint, and thanks to Proposition 1.2.3, for all $\varphi \in \mathrm{dom}(H_\kappa)$ we have

$$\begin{aligned}
\|H_\kappa \varphi\|^2_{L^2(\mathbb{R}^3)^4} =& \|(-i\alpha \cdot \nabla + m\beta)\varphi_+\|^2_{L^2(\Omega_+)^4} + \|(\alpha \cdot \nabla + m\beta)\varphi_-\|^2_{L^2(\Omega_-)^4} \\
=& \|(\alpha \cdot \nabla)\varphi_+\|^2_{L^2(\Omega_+)^4} + \|(\alpha \cdot \nabla)\varphi_-\|^2_{L^2(\Omega_-)^4} + m^2\|\varphi\|^2_{L^2(\mathbb{R}^3)^4} \\
&+ \langle(-i\alpha \cdot N)t_\Sigma\varphi_+, m\beta t_\Sigma\varphi_+\rangle_{L^2(\Sigma)^4} - \langle(-i\alpha \cdot N)t_\Sigma\varphi_-, m\beta t_\Sigma\varphi_-\rangle_{L^2(\Sigma)^4} \\
=& \mathfrak{Q}[\varphi]
\end{aligned}$$

Now we are going to construct the closed form $\widetilde{\mathfrak{Q}}$. Let $r_1 > r_0 > 0$ be such that Σ is strictly contained in the ball $B(0, r_0)$, and let $f_0, f_1 \in C^\infty(\mathbb{R}^3; [0, 1])$ such that

$$f_0^2 + f_1^2 = 1, \quad f_0 = 1 \text{ in } B(0, r_0), \quad f_1 = 1 \text{ in } \mathbb{R}^3 \setminus \overline{B(0, r_1)}. \tag{2.3.16}$$

Clearly, we have

$$\begin{aligned}
f_0 = 0 \text{ in } \mathbb{R}^3 \setminus \overline{B(0, r_1)} \ \text{ and } \ f_1 = 0 \text{ in } B(0, r_0), \\
\mathrm{supp}(\nabla(f_j)^2) \subset C(0, r_0, r_1) \ \text{ and } \ \nabla(f_0)^2 = -\nabla(f_1)^2 \text{ in } C(0, r_0, r_1),
\end{aligned} \tag{2.3.17}$$

where $C(0, r_0, r_1)$ is the annulus $B(0, r_1) \setminus \overline{B(0, r_0)}$. Now, it is straightforward to check that

$$f_j\varphi \in \mathrm{dom}(H_\kappa), \quad H_\kappa(f_j\varphi) = f_j H_\kappa\varphi - i\alpha \cdot (\nabla f_j)\varphi, \tag{2.3.18}$$

for all $\varphi \in \mathrm{dom}(H_\kappa)$. Notice also that, since $f_1 = 0$ in $B(0, r_0)$, and $\Sigma \subset B(0, r_0)$ it holds that

$$f_1\varphi \in H_0^1(\overline{\Omega_-})^4 \text{ for all } \varphi \in \mathrm{dom}(H_\kappa). \tag{2.3.19}$$

Fix $\varphi \in \mathrm{dom}(H_\kappa)$ and $j \in \{0, 1\}$, then

$$\begin{aligned}
\mathfrak{Q}[f_j\varphi] =& \|H(f_j\varphi)\|^2_{L^2(\Omega_+)^4} + \|H(f_j\varphi)\|^2_{L^2(\Omega_-)^4} \\
=& \langle f_j H_\varphi - i\alpha \cdot (\nabla f_j)\varphi, f_j H\varphi - i\alpha \cdot (\nabla f_j)\varphi\rangle_{L^2(\Omega_+)^4} \\
&+ \langle f_j H_\varphi - i\alpha \cdot (\nabla f_j)\varphi, f_j H\varphi - i\alpha \cdot (\nabla f_j)\varphi\rangle_{L^2(\Omega_+)^4} =: I_j^{\Omega_+} + I_j^{\Omega_-}.
\end{aligned}$$

Using that $|\alpha\cdot(\nabla f_j)\varphi|^2=|\nabla f_j|^2|\varphi|^2$, we get that

$$\begin{aligned}I_j^{\Omega_\pm}=&\langle f_j^2H\varphi,H\varphi\rangle_{L^2(\Omega_\pm)^4}+\langle|\nabla f_j|\varphi,\varphi\rangle_{L^2(\Omega_\pm)^4}+2\mathrm{Re}\langle f_jH\varphi,-i\alpha\cdot(\nabla f_j)\varphi\rangle_{L^2(\Omega_+)^4}\\ =&\langle f_j^2H\varphi,H\varphi\rangle_{L^2(\Omega_\pm)^4}+\langle|\nabla f_j|\varphi,\varphi\rangle_{L^2(\Omega_\pm)^4}+\mathrm{Re}\langle H\varphi,-i\alpha\cdot(\nabla f_j^2)\varphi\rangle_{L^2(\Omega_+)^4}.\end{aligned}$$

Using that $\nabla(f_0)^2=-\nabla(f_1)^2$ (see (2.3.17)), we deduce that

$$\begin{aligned}\mathcal{Q}[f_0\varphi]+\mathcal{Q}[f_1\varphi]=&\langle(f_0^2+f_1^2)H\varphi,H\varphi\rangle_{L^2(\Omega_+)^4}+\langle(f_0^2+f_1^2)H\varphi,H\varphi\rangle_{L^2(\Omega_-)^4}\\ &+\langle(|\nabla f_0|+|\nabla f_1|)\varphi,\varphi\rangle_{L^2(\mathbb{R}^3)^4}.\end{aligned}$$

As $f_0^2+f_1^2=1$, it follows that

$$\begin{aligned}\mathcal{Q}[f_0\varphi]+\mathcal{Q}[f_1\varphi]=&\|H\varphi\|^2_{L^2(\Omega_+)^4}+\|H\varphi\|^2_{L^2(\Omega_-)^4}+\langle(|\nabla f_0|+|\nabla f_1|)\varphi,\varphi\rangle_{L^2(\mathbb{R}^3)^4}\\ =&\|H_\kappa\varphi\|^2_{L^2(\mathbb{R}^3)^4}+\langle(|\nabla f_0|+|\nabla f_1|)\varphi,\varphi\rangle_{L^2(\mathbb{R}^3)^4}\\ =&\mathcal{Q}[\varphi]+\langle(|\nabla f_0|+|\nabla f_1|)\varphi,\varphi\rangle_{L^2(\mathbb{R}^3)^4}.\end{aligned}$$

Therefore

$$\mathcal{Q}[\varphi]=\mathcal{Q}[f_0\varphi]+\mathcal{Q}[f_1\varphi]-\langle(|\nabla f_0|+|\nabla f_1|)\varphi,\varphi\rangle_{L^2(\mathbb{R}^3)^4},$$

using $f_0^2+f_1^2=1$, the above equality becomes

$$\mathcal{Q}[\varphi]=\Big(\mathcal{Q}[f_0\varphi]-\langle V(f_0\varphi),(f_0\varphi)\rangle_{L^2(\mathbb{R}^3)^4}\Big)+\Big(\mathcal{Q}[f_1\varphi]-\langle V(f_1\varphi),(f_1\varphi)\rangle_{L^2(\mathbb{R}^3)^4}\Big)$$

where $V:=(|\nabla f_0|+|\nabla f_1|)$.

Next, notice that for all $\psi\in\mathrm{dom}(H_\kappa)\cap H_0^1(\mathbb{R}^3\setminus\overline{B(0,r_0)})^4$, we have that

$$\begin{aligned}\mathcal{Q}[\psi]=&\|(\alpha\cdot\nabla)\psi\|^2_{L^2(\Omega_-\setminus\overline{B(0,r_0)})^4}+m^2\|\psi\|^2_{L^2(\Omega_-\setminus\overline{B(0,r_0)})^4}\\ =&\|\nabla\psi\|^2_{L^2(\Omega_-\setminus\overline{B(0,r_0)}))^4}+m^2\|\psi\|^2_{L^2(\Omega_-\setminus\overline{B(0,r_0)})^4}\end{aligned}$$

Now, thanks to (2.3.19), the above considerations lead us to define the sesquilinear forms

$$\begin{cases}\mathrm{dom}(\mathcal{Q}_1):=H^1(\mathbb{R}^3\setminus\overline{B(0,r_1)})^4\\ \mathcal{Q}_1[\psi]:=\|\nabla\psi\|^2_{L^2(\mathbb{R}^3\setminus\overline{B(0,r_1)})^4}+m^2\|\psi\|^2_{L^2(\mathbb{R}^3\setminus\overline{B(0,r_1)})^4},\end{cases}$$

$$\begin{cases}\mathrm{dom}(\mathcal{Q}_2):=\{\psi\in H^1(C(0,r_0,r_1))^4:\psi=0\text{ on }\partial B(0,r_0)\},\\ \mathcal{Q}_2[\psi]:=\|\nabla\psi\|^2_{L^2(C(0,r_0,r_1))^4}+m^2\|\psi\|^2_{L^2(C(0,r_0,r_1))^4}-\langle V\psi,\psi\rangle_{L^2(C(0,r_0,r_1))^4},\end{cases}$$

$$\begin{cases}\mathrm{dom}(\mathcal{Q}_3):=\{\psi\in\mathrm{dom}(H_\kappa):\mathrm{supp}(\psi)\subset\overline{B(0,r_1)}\},\\ \mathcal{Q}_3[\psi]:=\mathcal{Q}[\psi]-\langle V\psi,\psi\rangle_{L^2(C(0,r_0,r_1))^4},\end{cases}$$

It is clear that $\mathcal{Q}_j[\psi]\geqslant C\|\psi\|^2$ for $j\in\{1,2,3\}$, thus $\mathcal{Q}_j$ is semibounded from below, which actually means that $\mathcal{Q}_j$ is a closed quadratic form. Therefore, the quadratic form

$$\widetilde{\mathcal{Q}}=\mathcal{Q}_1\oplus\mathcal{Q}_2\oplus\mathcal{Q}_3$$

is a closed. Now, it is straightforward to check that $\mathrm{dom}(\mathcal{Q})\subset\mathrm{dom}(\widetilde{\mathcal{Q}})$ and $\widetilde{\mathcal{Q}}[\varphi]\leqslant\mathcal{Q}[\varphi]$ holds for all $\varphi\in\mathrm{dom}(\mathcal{Q})$, which actually means that $\mathcal{Q}$ is minorated by $\widetilde{\mathcal{Q}}$ in the sense of closed quadratic forms. Therefore, if we denote by H_j and H_j the operators associated with $\mathcal{Q}_j$ and $\mathcal{Q}_{\text{ext}}$, respectively, then the min-max principle yields that

$$\mathrm{Sp}_{\mathrm{disc}}(H_1 \oplus H_2 \oplus H_3) \cap (-\infty, m^2) \text{ is finite} \Longrightarrow \mathrm{Sp}_{\mathrm{disc}}((H_\kappa)^2) \cap (-\infty, m^2) \text{ is finite}$$
$$\Longleftrightarrow \mathrm{Sp}_{\mathrm{disc}}(H_\kappa) \cap (-m, m) \text{ is finite}$$

Since the injections $\mathrm{dom}(\mathcal{Q}_2) \hookrightarrow L^2(C(0,r_0,r_1))^4$ $\mathrm{dom}(\mathcal{Q}_3) \hookrightarrow L^2(B(0,r_1))^4$ are compact, we conclude that the operator $(H_2, \mathrm{dom}(\mathcal{Q}_2))$ and $(H_3, \mathrm{dom}(\mathcal{Q}_3))$ have compact resolvent. Therefore, H_2 and H_3 have a finite purely discrete spectrum in $(-\infty, m^2)$. Now, note that for all $\psi \in \mathrm{dom}(\mathcal{Q}_1)$ we have

$$\|H_1\psi\|^2_{L^2(\mathbb{R}^3\setminus\overline{B(0,r_1)})^4} = \|\nabla\psi\|^2_{L^2(\mathbb{R}^3\setminus\overline{B(0,r_1)})^4} + m^2\|\psi\|^2_{L^2(\mathbb{R}^3\setminus\overline{B(0,r_1)})^4} \geqslant m^2\|\psi\|^2_{L^2(\mathbb{R}^3\setminus\overline{B(0,r_1)})^4}$$

Thus $\mathrm{Sp}_{\mathrm{disc}}(H_1) \cap (-\infty, m^2) = \emptyset$. Therefore, $\mathrm{Sp}_{\mathrm{disc}}(H_1 \oplus H_2) \oplus H_3) \cap (-\infty, m^2)$ is finite, which implies that $\mathrm{Sp}_{\mathrm{disc}}(H_\kappa) \cap (-m, m)$ is finite. This finishes the proof of the theorem. □

Remark 2.3.2. *It is worth noting that the crucial ingredient in the proof of Theorem* (2.3.2)(ii) *is the Sobolev regularity of* $\mathrm{dom}(H_\kappa)$. *In particular, if* Σ *is less regular (say Lipschitz) and as far as* H_κ *is self-adjoint,* $\mathrm{dom}(H_\kappa) \subset H^s(\mathbb{R}^3 \setminus \Sigma)^4$ *for some* $s > 0$, *and* $t_\Sigma\varphi_\pm \in L^2(\Sigma)^4$ *holds for all* $\varphi = (\varphi_+, \varphi_-) \in \mathrm{dom}(H_\kappa)$, *then Theorem* (2.3.2)(ii) *remains valid.*

In the rest of this section, we focus on the spectral properties of H_κ when Σ satisfies the assumption (H2). In order to avoid ambiguities we use the following notations:

Notation 2.3.1. *For all* $\nu \geqslant 0$, *we denote by* $\overline{H^\nu_\kappa}$ *(respectively* Φ^z_ν, $\widetilde{\Lambda}^z_{+,\nu}$ *and* $(\Phi^{\overline{z}}_\nu)^*$*) the operator* $\overline{H_\kappa}$ *(respectively* Φ^z, $\widetilde{\Lambda}^z_+$ *and* $(\Phi^{\overline{z}})^*$*) whenever* $\Sigma = \Sigma_\nu$, *i.e* Σ *satisfies* (H2), *and we write* $\overline{H_k}$ *(respectively* Φ^z, $\widetilde{\Lambda}^z_+$ *and* $(\Phi^{\overline{z}})^*$*) instead of* $\overline{H^0_\kappa}$ *(respectively* Φ^z_0, $\widetilde{\Lambda}^z_{+,0}$ *and* $(\Phi^{\overline{z}}_0)^*$*), i.e., when* $\nu = 0$.

The following theorem gives us a complete description of the essential spectrum of H_κ when Σ satisfies (H2) and $\eta = 0$.

Theorem 2.3.3. *Let* $\kappa \in \mathbb{R}^2 \times \{0\}$ *be such that* $\mathrm{sgn}(\kappa) = \epsilon^2 - \mu^2 \neq 0, 4$, *and suppose that* Σ *satisfies* (H2) *with* $\nu \geqslant 0$. *Set*

$$a_\pm = m\frac{-16\epsilon\mu \pm (\mathrm{sgn}(\kappa)-4)^2\sqrt{\frac{(\mathrm{sgn}(\kappa)+4)^2}{(\mathrm{sgn}(\kappa)-4)^2}}}{(\mathrm{sgn}(\kappa)-4)^2 + 16\epsilon^2}, \quad a^* = -m\frac{-16\epsilon\mu}{(\mathrm{sgn}(\kappa)-4)^2 + 16\epsilon^2}. \tag{2.3.20}$$

The following hold:

(i) If $\epsilon^2 - \mu^2 > 4$, *then*

$$\mathrm{Sp}_{\mathrm{ess}}(H^\nu_\kappa) = \begin{cases} (-\infty, -m] \cup [a_+, +\infty), & \text{for } \epsilon > 0 \text{ and } \mu \in \mathbb{R}, \\ (-\infty, a_-] \cup [m, +\infty), & \text{for } \epsilon < 0 \text{ and } \mu \in \mathbb{R}. \end{cases}$$

(ii) If $0 < \epsilon^2 - \mu^2 < 4$, *then*

$$\mathrm{Sp}_{\mathrm{ess}}(H^\nu_\kappa) = \begin{cases} (-\infty, a_-] \cup [m, +\infty), & \text{for } \epsilon > 0 \text{ and } \mu \in \mathbb{R}, \\ (-\infty, -m] \cup [a_+, +\infty), & \text{for } \epsilon < 0 \text{ and } \mu \in \mathbb{R}. \end{cases}$$

(iii) If $-4 < \epsilon^2 - \mu^2 < 0$*, then*

$$\mathrm{Sp}_{\mathrm{ess}}(H^\nu_\kappa) = \begin{cases} (-\infty, -m] \cup [m, +\infty), & \text{for } \mu > 0 \text{ and } \epsilon \in \mathbb{R}, \\ (-\infty, a_-] \cup [a_+, +\infty), & \text{for } \mu < 0 \text{ and } \epsilon \in \mathbb{R}. \end{cases}$$

(iv) If $\epsilon^2 - \mu^2 = -4$*, then*

$$\mathrm{Sp}_{\mathrm{ess}}(H^\nu_\kappa) = \begin{cases} (-\infty, -m] \cup [m, +\infty), & \text{for } \mu > 0 \text{ and } \epsilon \in \mathbb{R}, \\ (-\infty, a^*] \cup [m, +\infty), & \text{for } \mu < 0 \text{ and } \epsilon > 0, \\ (-\infty, -m] \cup [a^*, +\infty), & \text{for } \mu < 0 \text{ and } \epsilon < 0, \\ \mathbb{R}, & \text{for } \mu = -2 \text{ and } \epsilon = 0. \end{cases}$$

(v) If $\epsilon^2 - \mu^2 < -4$*, then*

$$\mathrm{Sp}_{\mathrm{ess}}(H^\nu_\kappa) = \begin{cases} (-\infty, -m] \cup [m, +\infty), & \text{for } \mu > 0 \text{ and } \epsilon \in \mathbb{R}, \\ (-\infty, a_-] \cup [a_+, +\infty), & \text{for } \mu < 0 \text{ and } \epsilon \in \mathbb{R}. \end{cases}$$

Furthermore, we have $\mathrm{Sp}(H_\kappa) = \mathrm{Sp}_{\mathrm{ess}}(H_\kappa)$.

Remark 2.3.3. *Note that a similar statement can be formulated when* $\eta \neq 0$*, in that case we have*

$$a_\pm = m \frac{-16\epsilon\mu \pm (\mathrm{sgn}(\kappa) - 4)^2 \sqrt{\frac{(\mathrm{sgn}(\kappa)+4)^2 + 16\eta^2}{(\mathrm{sgn}(\kappa)-4)^2}}}{(\mathrm{sgn}(\kappa) - 4)^2 + 16\epsilon^2}.$$

The statements (i) *and* (ii) *still hold true, and for* $\mathrm{sgn}(\kappa) < 0$ *several cases should be taken into account, so for the sake of readability we chose not to write it here.*

Tp prove Theorem 2.3.3 for $\nu > 0$ we will use the following compactness result, which will be used in the localization arguments.

Lemma 2.3.2. *Fix* $\nu > 0$ *and* $z \in \mathbb{C} \setminus \mathbb{R}$*, and let* $\mathscr{T} : L^2(\mathbb{R}^3)^4 \to L^2(\mathbb{R}^3)^4$ *be the operator defined, for every* $f \in L^2(\mathbb{R}^3)^4$*, by*

$$\begin{aligned} \mathscr{T}[f](x) = \Big(& (1 - \Xi)\Phi^z_\nu (1 - \chi_\nu)(\Lambda^z_{+,\nu})^{-1}(1 - \chi_\nu)(\Phi^{\bar{z}}_\nu)^* \\ & - (1 - \Xi)\Phi^z (1 - \chi_0)(\Lambda^z_+)^{-1}(1 - \chi_0)(\Phi^{\bar{z}})^* \Big)[f](x). \end{aligned} \tag{2.3.21}$$

with χ_0*,* χ_ν *and* Ξ *as in Notation 1.3.1. Then* $\mathscr{T}$ *is compact in* $L^2(\mathbb{R}^3)^4$.

Proof. Let $\nu > 0$ and $z \in \mathbb{C} \setminus \mathbb{R}$ be fixed, and note that from definition of the mapping $(\Phi^{\bar{z}}_\nu)^*$ and Remark 1.3.4 it follows that

$$(1 - \chi_\nu)(\Phi^{\bar{z}}_\nu)^*[f] = (1 - \chi_0)(\Phi^{\bar{z}})^*[f], \quad \forall f \in L^2(\mathbb{R}^3)^4,$$

holds in $H^{1/2}(\Sigma_\nu \cap \mathrm{supp}(1 - \chi_\nu))^4 = H^{1/2}(\Sigma_0 \cap \mathrm{supp}(1 - \chi_0))^4$, and can be regarded as an equality in the sense of functions in $H^{1/2}(\Sigma_\nu)^4$ and in $H^{1/2}(\Sigma_0)^4$. Similarly, if g is such that $\mathrm{supp}(g) \subseteq \mathrm{supp}(1 - \chi_0)$, we can consider g as a function in $H^{1/2}(\Sigma_\nu)^4$ and also as a function in $H^{1/2}(\Sigma_0)^4$, and we have the equalities

$$\begin{aligned}(1-\Xi)\Phi^z_\nu g =&(1-\Xi)\Phi^z g,\\ (1-\chi_\nu)\Lambda^z_{+,\nu}(1-\chi_\nu)g =&(1-\chi_0)\Lambda^z_{+,0}(1-\chi_0)g.\end{aligned}$$

With this interpretation in mind, we can then write $\mathscr{T}$ as follows

$$\begin{aligned}\mathscr{T}[f](x) =&(1-\Xi)\Phi^z\Big((1-\chi_\nu)(\Lambda^z_{+,\nu})^{-1}(1-\chi_\nu)-(1-\chi_0)(\Lambda^z_{+})^{-1}(1-\chi_0)\Big)(\Phi^{\overline{z}})^*[f](x)\\ :=&(1-\Xi)\Phi^z T_\nu(\Phi^{\overline{z}})^*[f](x)\end{aligned}$$

T_ν is considered as an operator from $L^2(\Sigma_0)^4$ into itself. Now, we are going to show that $T_\nu(\Phi^{\overline{z}})^*$ is compact from $L^2(\mathbb{R}^3)^4$ into $L^2(\Sigma_0)^4$. Set $F=(1-\chi_\nu)(\Phi^{\overline{z}}_\nu)^*[f]=(1-\chi_0)(\Phi^{\overline{z}})^*[f]$ for $f\in L^2(\mathbb{R}^3)^4$, then

$$\begin{aligned}\Lambda^z_+(1-\chi_\nu)(\Lambda^z_{+,\nu})^{-1}F &= \chi_0\Lambda^z_+(1-\chi_\nu)(\Lambda^z_{+,\nu})^{-1}F+(1-\chi_0)\Lambda^z_+(1-\chi_\nu)(\Lambda^z_{+,\nu})^{-1}F\\ &= \chi_0\Lambda^z_+(1-\chi_\nu)(\Lambda^z_{+,\nu})^{-1}F+(1-\chi_\nu)\Lambda^z_{+,\nu}(1-\chi_\nu)(\Lambda^z_{+,\nu})^{-1}F\\ &= \chi_0\Lambda^z_+(1-\chi_\nu)(\Lambda^z_{+,\nu})^{-1}F+(1-\chi_0)F-(1-\chi_\nu)\Lambda^z_{+,\nu}\chi_\nu(\Lambda^z_{+,\nu})^{-1}F.\end{aligned}$$

Thus we get

$$\begin{aligned}(1-\chi_\nu)(\Lambda^z_{+,\nu})^{-1}F =&(1-\chi_0)(\Lambda^z_{+})^{-1}F+[\chi_0,(\Lambda^z_+)^{-1}]F+(\Lambda^z_+)^{-1}\chi_0\Lambda^z_+(1-\chi_\nu)(\Lambda^z_{+,\nu})^{-1}F\\ &-(\Lambda^z_+)^{-1}(1-\chi_\nu)\Lambda^z_{+,\nu}\chi_\nu(\Lambda^z_{+,\nu})^{-1}F.\end{aligned}$$

Using the compactness of the embedding $\chi_\bullet H^{1/2}(\Sigma_\bullet)^4\hookrightarrow L^2(\Sigma_\bullet)^4$ for $\bullet=0,\,\nu$, it follows that $T_\nu(\Phi^{\overline{z}})^*$ is compact from $L^2(\mathbb{R}^3)^4$ into $L^2(\Sigma_0)^4$. Since $(1-\Xi)\Phi^z$ is bounded from $L^2(\Sigma_0)^4$ into $L^2(\mathbb{R}^3)^4$, we then get that $\mathscr{T}$ is compact in $L^2(\mathbb{R}^3)^4$. □

We can now establish Theorem 2.3.3.

Proof of Theorem 2.3.3. We first prove assertions (i) – (v) when $\nu=0$, we then use compactness arguments and Proposition 2.3.1(ii) to get the result when $\nu>0$. To this end and for the convenience of the reader we divide the proof in three steps.

Step 1. We analyze the spectrum of H_κ in the gap $(-m,m)$. For this, let $a\in(-m,m)$ and set

$$\Gamma_{\pm m,\pm a}(\xi)=[\alpha\cdot(\xi_1,\xi_2,0)\pm m\beta\pm a]\,.$$

Since the α_j's anticommute with β, a simple computation shows that

$$\begin{aligned}(\Gamma_{m,a}(\xi))^2 &= |\xi|^2+m^2-a^2+2a\Gamma_{m,a}(\xi),\\ \Gamma_{-m,-a}(\xi)\Gamma_{m,a}(\xi) &= |\xi|^2+m^2-a^2-2m\beta\Gamma_{m,a}(\xi),\\ \Gamma_{m,-a}(\xi)\Gamma_{m,a}(\xi) &= |\xi|^2+m^2-a^2.\end{aligned}\tag{2.3.22}$$

Using the Fourier-Plancherel operator it is not hard to prove that Λ^a_+ is unitarily equivalent to the following multiplication operator:

$$\Pi^a_+:=\frac{1}{\mathrm{sgn}(\kappa)}(\epsilon I_4-\mu\beta-\eta(\alpha\cdot N))+\frac{1}{2\sqrt{|\xi|^2+m^2-a^2}}\Gamma_{m,a}(\xi).$$

Moreover, taking into account the properties (2.3.22), a simple computation shows that Π^a_+ is invertible and its inverse is given explicitly by

$$(\Pi^a_+)^{-1}=C^{-1}\left(1+\frac{\epsilon a+\mu m}{\sqrt{|\xi|^2+m^2-a^2}}-\frac{(\epsilon+\mu\beta+\eta(\alpha\cdot N))}{2\sqrt{|\xi|^2+m^2-a^2}}\Gamma_{m,a}(\xi)\right)(\epsilon+\mu\beta+\eta(\alpha\cdot N)),\tag{2.3.23}$$

if and only if $C \neq 0$ for all $\xi \in \mathbb{R}^2$, where C is given by

$$C = \frac{4 - \operatorname{sgn}(\kappa)}{4} + \frac{\epsilon a + \mu m}{\sqrt{|\xi|^2 + m^2 - a^2}}.$$

Since $\operatorname{sgn}(\kappa) \neq 4$, it follows that $-m\mu/\epsilon \notin \operatorname{Sp}(H_\kappa)$, for all $\epsilon \neq 0$. In the following, we always assume that $a \neq -m\mu/\epsilon$ when $\epsilon \neq 0$, and we look for the values of a for which we have $C = 0$. Note that

$$C = 0 \Longleftrightarrow \sqrt{|\xi|^2 + m^2 - a^2} = \frac{4(\epsilon a + \mu m)}{\operatorname{sgn}(\kappa) - 4}.$$

Thus, $C = 0$ for some $|\xi| \in \mathbb{R}_+$, only if

$$\frac{4(\epsilon a + \mu m)}{\operatorname{sgn}(\kappa) - 4} > 0. \tag{2.3.24}$$

Assume that (2.3.24) holds true, then $C = 0$ if and only if $|\xi|^2 = P(a)$, where the polynomial $P(a)$ is given by

$$P(a) = \frac{(\operatorname{sgn}(\kappa) - 4)^2 + 16\epsilon^2}{(\operatorname{sgn}(\kappa) - 4)^2} a^2 + \frac{32\epsilon\mu m}{(\operatorname{sgn}(\kappa) - 4)^2} a - \frac{(\operatorname{sgn}(\kappa) - 4)^2 - 16\mu^2}{(\operatorname{sgn}(\kappa) - 4)^2} m^2.$$

Recall a_+, a_- and a^* from (2.3.20), then a_+ and a_- are the zeros of $P(a)$ when $\epsilon^2 - \mu^2 \neq -4$, and a^* is a double root of $P(a)$ when $\epsilon^2 - \mu^2 = -4$. Thus $P(a) \geqslant 0$ if and only if $a \geqslant a_+$ or $a \leqslant a_-$. In the remainder of the proof we deal with assertion (i), the other assertions follow in the same way. Assume that $\epsilon^2 - \mu^2 > 4$, then

$$a_\pm = m\frac{-16\epsilon\mu \pm (\operatorname{sgn}(\kappa) - 4)(\operatorname{sgn}(\kappa) + 4)}{(\operatorname{sgn}(\kappa) - 4)^2 + 16\epsilon^2} \quad \text{and} \quad -m < a_- < a_+ < m.$$

As $\operatorname{sgn}(\kappa) > 4$, it follows that the condition (2.3.24) is equivalent to

$$a > -\frac{\mu m}{\epsilon} \text{ if } \epsilon > 0 \quad \text{or} \quad a < -\frac{\mu m}{\epsilon} \text{ if } \epsilon < 0.$$

Now using the fact that $\epsilon^2 > \mu^2$, a simple computation yields

$$a_+ > -\frac{\mu m}{\epsilon} \text{ and } a_- < -\frac{\mu m}{\epsilon}.$$

Hence, if $\epsilon > 0$ (resp. $\epsilon < 0$) then for all $a \geqslant a_+$ (resp. $a \leqslant a_-$) we have $P(a) \geqslant 0$ and the condition (2.3.24) holds true. Consequently, the set of ξ for which $C = 0$ is given by the circle $\{\xi : |\xi| = \sqrt{P(a)}\}$, and in that case 0 is in the essential spectrum of Λ_+^a. Therefore we conclude by Proposition 2.3.1 that

$$(a_+, m) \subset \operatorname{Sp}_{\text{ess}}(H_\kappa) \text{ and } (-m, a_+) \subset \rho(H_\kappa), \text{ for } \epsilon > 0$$
$$(-m, a_-) \subset \operatorname{Sp}_{\text{ess}}(H_\kappa) \text{ and } (a_-, m) \subset \rho(H_\kappa), \text{ for } \epsilon < 0.$$

Step 2. Now we prove the inclusion $(-\infty, -m) \cup (m, +\infty) \subset \operatorname{Sp}_{\text{ess}}(H_\kappa)$, for this we construct a singular sequence for H_κ and a. Fix $a \in (-\infty, -m) \cup (m, \infty)$ and define

$$\varphi : \begin{cases} \mathbb{R}^3 \longrightarrow \mathbb{C}^4 \\ (\overline{x}, x_3) \longmapsto \left(\frac{\xi_1 - i\xi_2}{a - m}, 0, 0, 1\right)^t e^{i\overline{x}\cdot\xi}, \end{cases}$$

here $\xi = (\xi_1, \xi_2)$ and $|\xi|^2 = a^2 - m^2$. Observe that we have $(-i\alpha\cdot\nabla + m\beta - a)\varphi = 0$. Let $R > 0$, $\chi \in C_0^\infty(\mathbb{R}^2, \mathbb{R})$ and $\theta \in C_0^\infty([0,\infty[, \mathbb{R})$ such that

$$\theta(r) = \begin{cases} 1 & \text{for } r \in [2R, 3R], \\ 0 & \text{for } r \in [0, R]. \end{cases}$$

For $n \in \mathbb{N}^\star$, we define the sequences of functions

$$\begin{aligned} \varphi_{+,n}(\overline{x}, x_3) &= n^{-\frac{3}{2}}\varphi(\overline{x}, x_3)\chi(\overline{x}/n)\theta(x_3/n) \quad \text{for } x_3 > 0, \\ \varphi_{-,n}(\overline{x}, x_3) &= n^{-\frac{3}{2}}\varphi(\overline{x}, x_3)\chi(\overline{x}/n)\theta(-x_3/n) \quad \text{for } x_3 < 0. \end{aligned} \tag{2.3.25}$$

It is clear that $\varphi_{\pm,n} \in H^1(\Omega_\pm)$ and $t_\Sigma\varphi_{\pm,n} = 0$, thus $\varphi_n := (\varphi_{+,n}, \varphi_{-,n}) \in \mathrm{dom}(H_\kappa)$. Moreover, $(\varphi_n)_{n\in\mathbb{N}^\star}$ converges weakly to zero and we have

$$\|\varphi_n\|^2_{L^2(\mathbb{R}^3)^4} = \|\varphi_{+,n}\|^2_{L^2(\Omega_+)^4} + \|\varphi_{-,n}\|^2_{L^2(\Omega_-)^4} = \frac{2a}{a-m}\|\chi\|^2_{L^2(\mathbb{R}^2)}\|\theta\|^2_{L^2(\mathbb{R}_+)} > 0,$$

and

$$\begin{aligned} \|\left(-i\alpha\cdot\nabla + m\beta - a\right)\varphi_n\|^2_{L^2(\mathbb{R}^3)^4} =& \|\left(-i\alpha\cdot\nabla + m\beta - a\right)\varphi_{+,n}\|^2_{L^2(\Omega_+)^4} \\ &+ \|\left(-i\alpha\cdot\nabla + m\beta - a\right)\varphi_{-,n}\|^2_{L^2(\Omega_-)^4} \\ &\leqslant \frac{4a}{n^2(a-m)}\Big(\|\nabla\eta\|^2_{L^2(\mathbb{R}^2)}\|\theta\|^2_{L^2(\mathbb{R}_+)} + \|\chi\|^2_{L^2(\mathbb{R}^2)}\|\theta'\|^2_{L^2(\mathbb{R}_+)}\Big). \end{aligned}$$

Thus, we get

$$\frac{\|\left(-i\alpha\cdot\nabla + m\beta - a\right)\varphi_n\|_{L^2(\mathbb{R}^3)^4}}{\|\varphi_n\|_{L^2(\mathbb{R}^3)^4}} \xrightarrow[n\to\infty]{} 0.$$

From this and *Step 1*, we deduce that

$$\begin{aligned} &(-\infty, -m) \cup (a_+, m) \cup (m, \infty) \subset \mathrm{Sp}_{\mathrm{ess}}(H_\kappa) \subset \mathrm{Sp}(H_\kappa) \subset (-\infty, -m] \cup [a_+, \infty), \text{ for } \epsilon > 0, \\ &(-\infty, -m) \cup (-m, a_-) \cup (m, \infty) \subset \mathrm{Sp}_{\mathrm{ess}}(H_\kappa) \subset \mathrm{Sp}(H_\kappa) \subset (-\infty, a_-] \cup [m, \infty), \text{ for } \epsilon < 0. \end{aligned}$$

Since the spectrum of a self-adjoint operator is closed, the end-points also belong to the spectrum, and hence for $\epsilon^2 - \mu^2 > 4$, we get

$$\mathrm{Sp}(H_\kappa) = \mathrm{Sp}_{\mathrm{ess}}(H_\kappa) = \begin{cases} (-\infty, -m] \cup [a_+, +\infty), & \text{for } \epsilon > 0 \text{ and } \mu \in \mathbb{R}, \\ (-\infty, a_-] \cup [m, +\infty), & \text{for } \epsilon < 0 \text{ and } \mu \in \mathbb{R}, \end{cases}$$

which proves the result when $\nu = 0$.

Step 3. Assume that $\nu > 0$, and recall the definitions of χ_0, χ_ν and Ξ from Notation 1.3.1. We are going to show the equality $\mathrm{Sp}_{\mathrm{ess}}(H^\nu_\kappa) = \mathrm{Sp}_{\mathrm{ess}}(H_\kappa)$. For this, fix $z \in \mathbb{C}\setminus\mathbb{R}$ and let $\mathcal{T} : L^2(\mathbb{R}^3)^4 \to L^2(\mathbb{R}^3)^4$ be the bounded operator defined by

$$\mathcal{T} = \Phi^z_\nu(\Lambda^z_{+,\nu})^{-1}(\Phi^{\overline{z}}_\nu)^* - \Phi^z(\Lambda^z_+)^{-1}(\Phi^{\overline{z}})^*.$$

Then $\mathcal{T}$ is a compact operator in $L^2(\mathbb{R}^3)^4$. Indeed, note that $\mathcal{T}$ can be written as follows:

$$\begin{aligned} \mathcal{T} =& \Phi^z_\nu(\Lambda^z_{+,\nu})^{-1}\chi_\nu(\Phi^{\overline{z}}_\nu)^* - \Phi^z(\Lambda^z_+)^{-1}\chi_0(\Phi^{\overline{z}})^* \\ &+ \Big[\Phi^z_\nu\chi_\nu(\Lambda^z_{+,\nu})^{-1}(1-\chi_\nu)(\Phi^{\overline{z}}_\nu)^* - \Phi^z\chi_0(\Lambda^z_+)^{-1}(1-\chi_0)(\Phi^{\overline{z}})^*\Big] \\ &+ \Big[\Phi^z_\nu(1-\chi_\nu)(\Lambda^z_{+,\nu})^{-1}(1-\chi_\nu)(\Phi^{\overline{z}}_\nu)^* - \Phi^z(1-\chi_0)(\Lambda^z_+)^{-1}(1-\chi_0)(\Phi^{\overline{z}})^*\Big] \\ &:= \mathcal{T}_1 + \mathcal{T}_2 + \mathcal{T}_3 + \mathcal{T}_4 \end{aligned}$$

Since χ_ν and χ_0 are smooth and compactly supported, it follows that the Sobolev injection $\chi_\bullet H^{1/2}(\Sigma_\bullet)^4 \hookrightarrow L^2(\Sigma_\bullet)^4$ is compact, where $\bullet = 0, \nu$. As $(\Phi_\nu^{\bar{z}})^* = (H-z)^{-1}\upharpoonright_{\Sigma_\nu}$ is bounded from $L^2(\mathbb{R}^3)^4$ to $H^{1/2}(\Sigma_\nu)^4$ and $(\Lambda_{+,\nu}^z)^{-1}$ is bounded from $H^{1/2}(\Sigma_\nu)^4$ into itself, for all $\nu \geqslant 0$, we get that $\mathcal{T}_1$, $\mathcal{T}_2$ and $\mathcal{T}_3$ are compact operators on $L^2(\mathbb{R}^3)^4$. As before, localizing with respect to the function Ξ and using the compactness of the Sobolev embedding, we see that $\mathcal{T}_4 = \mathcal{T}_5 + \mathscr{T}$, where $\mathcal{T}_5$ is a compact operator in $L^2(\mathbb{R}^3)^4$, and $\mathscr{T}$ is as in (2.3.21). From this and Lemma 2.3.2 we deduce that $\mathcal{T}$ is a compact operator in $L^2(\mathbb{R}^3)^4$. Hence by Proposition 2.3.1 it follows that $\mathcal{T} = (H_\kappa^\nu - z)^{-1} - (H_\kappa - z)^{-1}$ is a compact operator in $L^2(\mathbb{R}^3)^4$. Therefore, by Weyl's theorem we conclude that H_κ^ν has the same essential spectrum as H_κ. This finishes the proof of the theorem. □

As mentioned in the introduction, in [51] the Schrödinger operator with δ-interactions (i.e. the coupling $\Delta + \epsilon\delta_\Sigma$ in $\mathbb{R}^3$) was considered for a surface Σ satisfying the assumption (H2). There the authors showed that for a fixed ϵ (such that $\mathrm{Sp}_{\mathrm{disc}}(\Delta + \epsilon\delta_\Sigma) \neq \emptyset$) the discrete spectrum of $\Delta + \epsilon\delta_\Sigma$ consists of exactly one simple eigenvalue for all sufficiently small $\nu > 0$. Moreover, an asymptotic of this eigenvalue has been proved in terms of ϵ, ν and ϕ. Thus, it would be interesting to investigate such a problem for the couplings $H + \epsilon\delta_\Sigma$ and $H + \beta\delta_\Sigma$, and see if results of this type are valid.

2.3.2 Critical case

From now, we assume that $\mathrm{sgn}(\kappa) = 4$. The goal of this subsection is to prove the following result.

Theorem 2.3.4. *Let $\kappa = (\epsilon, \mu, \eta) \in \mathbb{R}^3$ be such that $\mathrm{sgn}(\kappa) = 4$ and let $\overline{H_\kappa}$ be as in Theorem 2.2.1. If Σ satisfies (H2), then for all $\nu \geqslant 0$ it holds that*

$$\mathrm{Sp}_{\mathrm{ess}}(\overline{H_\kappa^\nu}) = \big(-\infty, -m\big] \cup \left\{-\frac{m\mu}{\epsilon}\right\} \cup \big[m, +\infty\big), \tag{2.3.26}$$

and the equality $\mathrm{Sp}(\overline{H_\kappa^0}) = \mathrm{Sp}_{\mathrm{ess}}(\overline{H_\kappa^0})$ holds true (i.e. when $\nu = 0$).

A few comments are in order. Note that $\epsilon^2 > \mu^2$, thus the point $-m\mu/\epsilon$ belongs to the gap $(-m, m)$. Moreover, one can imagine that the operator $\overline{H_\kappa}$ is unitarily equivalent to $\overline{H_{\epsilon_1,\mu_1}}$, for some $\epsilon_1, \mu_1 \in \mathbb{R}$, such that $\epsilon_1^2 - \mu_1^2 = 4$ and $\epsilon_1/\epsilon = \mu_1/\mu$. Indeed, in [78] and [41] it has been shown that the potential $\eta(\alpha \cdot N)\delta_\Sigma$ can always be absorbed as a change of gauge. So the existence of such a unitary transformation is not excluded. Another way to understand Theorem 2.3.4 comes from the way in which we have presented the operator H_κ. In fact, in this chapter we introduced the operator H_κ as the perturbation of the coupling $H + (\epsilon I_4 + \mu\beta)\delta_\Sigma$ with the singular potential $\eta(\alpha \cdot N)\delta_\Sigma$. However, the right way is to say that H_κ is the perturbation of $H + \eta(\alpha \cdot N))\delta_\Sigma$ with the singular potential $(\epsilon I_4 + \mu\beta)\delta_\Sigma$, since as we will see in Chapter 3, for all $\eta \in \mathbb{R}$, the operator $H + \eta(\alpha \cdot N)\delta_\Sigma$ is self-adjoint (even if Σ is Lipschitz) and $\mathrm{Sp}(H + \eta(\alpha \cdot N)\delta_\Sigma) = \big(-\infty, -m\big] \cup \big[m, +\infty\big)$.

From Theorem 2.3.4 we get a simple way to describe functions belonging to the domain of $\overline{H_\kappa}$ when $\Sigma = \Sigma_0$, i.e. $\nu = 0$. Indeed, we have the following result.

Corollary 2.3.1. *Assume that $\Sigma := \Sigma_0$ and let $\overline{H_\kappa}$ be as above. The following hold:*

(i) If $\mu \neq 0$, then

$$\mathrm{dom}(\overline{H_\kappa}) = \left\{u + \Phi[-\widetilde{\Lambda}_+^{-1}[t_\Sigma u]] : u \in H^1(\mathbb{R}^3)^4\right\}.$$

(ii) If $\mu = 0$, then $\mathrm{dom}(\overline{H_\kappa}) = \mathrm{dom}(H_\kappa) + \Phi[\mathrm{Kr}(\widetilde{\Lambda}_+)]$.

Proof. The assertion (i) is a direct consequence of Theorem 2.3.4 and Proposition 2.3.1. The assertion (ii) follows exactly as in [10, Proposition 3.10]. □

The main properties of the operators $\overline{\mathscr{L}^a_\pm}$ which are relevant for us to prove Theorem 2.3.4 are collected in the following proposition.

Proposition 2.3.2. *Let $\kappa = (\epsilon, \mu, \eta) \in \mathbb{R}^3$ be such that $\mathrm{sgn}(\kappa) \neq 0$ and let $\mathscr{L}^a_{\pm,\kappa} := \mathscr{L}^a_\pm$ be as in Lemma 2.2.1. Then, for all $a \in (-m, m)$, it holds that*

$$0 \in \mathrm{Sp}_\bullet(\overline{\mathscr{L}^a_{+,\kappa}}) \Longleftrightarrow 0 \in \mathrm{Sp}_\bullet(\overline{\mathscr{L}^{-a}_{+,\widetilde{\kappa}}}) \Longleftrightarrow 0 \in \mathrm{Sp}_\bullet(\overline{\mathscr{L}^{-a}_{-,\kappa}}),$$

where $\widetilde{\kappa} = (-\epsilon, \mu, -\eta)$ and $\bullet \in \{\mathrm{ess}, \mathrm{disc}\}$. In particular, $a \in \mathrm{Sp}(\overline{H_\kappa})$ if and only if $-a \in \mathrm{Sp}(\overline{H_{\widetilde{\kappa}}})$.

Proof. Fix $\kappa = (\epsilon, \mu, \eta) \in \mathbb{R}^3$ such that $\mathrm{sgn}(\kappa) \neq 0$. Following [17, Proposition 4.2], for $f \in L^2(\Sigma)^4$ we define

$$\mathscr{C}(f) = i\beta\alpha_2\overline{f}^{\mathrm{c}}, \quad T(f) = \gamma_5\beta f, \tag{2.3.27}$$

γ_5 is the chirality matrix defined by (2.1.2), and $\overline{f}^{\mathrm{c}}$ is the complex conjugate of f. Remark that $\overline{\alpha_2}^{\mathrm{c}} = -\alpha_2$, using this and the properties of γ_5 given by (2.1.2), it easily follows that $\mathscr{C}^2(f) = f$ and $T^2(f) = -f$. Moreover, a simple computation using the anticommutation relations of Dirac matrices yields that

$$\Lambda^{\pm a}_{\pm,\kappa}[T(f)] = T(\Lambda^{\mp a}_{\mp,\kappa}[f]), \qquad \Lambda^a_{+,\kappa}[\mathscr{C}(f)] = -\mathscr{C}(\Lambda^{-a}_{+,\widetilde{\kappa}}[f]), \quad \Lambda^{-a}_{+,\widetilde{\kappa}}[\mathscr{C}(f)] = -\mathscr{C}(\Lambda^a_{+,\kappa}[f]). \tag{2.3.28}$$

Fix $a \in (-m, m)$ and assume that $0 \in \mathrm{Sp}_{\mathrm{ess}}(\overline{\mathscr{L}^a_+})$. Then, there exists a sequence of functions $(g_j)_{j\in\mathbb{N}} \subset \mathrm{dom}(\overline{\mathscr{L}^a_+}) \subset L^2(\Sigma)^4$, such that $||g_j||_{\mathrm{L}^2(\Sigma)^4} = 1$, $(g_j)_{j\in\mathbb{N}}$ converges weakly to 0 and $\left|\left|\overline{\mathscr{L}^a_{+,\kappa}} g_j\right|\right|_{\mathrm{L}^2(\Sigma)^4} \xrightarrow[j\to\infty]{} 0$. Hence, if we set $f_j = \mathscr{C}(g_j)$ and $h_j = T(g_j)$, then it is clear that $(f_j)_{j\in\mathbb{N}}$ and $(h_j)_{j\in\mathbb{N}}$ converge weakly to zero and we have

$$||h_j||_{\mathrm{L}^2(\Sigma)^4} = ||f_j||_{\mathrm{L}^2(\Sigma)^4} = 1, \quad f_j \in \mathrm{dom}(\overline{\mathscr{L}^{-a}_{+,\widetilde{\kappa}}}) \text{ and } h_j \in \mathrm{dom}(\overline{\mathscr{L}^{-a}_{-,\kappa}}), \quad \forall j \in \mathbb{N}.$$

Now using (2.3.28) it follows that

$$\left|\left|\overline{\mathscr{L}^{-a}_{+,\widetilde{\kappa}}}[f_j]\right|\right|_{\mathrm{L}^2(\Sigma)^4} = \left|\left|\overline{\mathscr{L}^{-a}_{-,\kappa}}[h_j]\right|\right|_{\mathrm{L}^2(\Sigma)^4} = \left|\left|\overline{\mathscr{L}^a_{+,\kappa}}[g_j]\right|\right|_{\mathrm{L}^2(\Sigma)^4}.$$

Therefore $0 \in \mathrm{Sp}(\overline{\mathscr{L}^{-a}_{+,\widetilde{\kappa}}})$ and $0 \in \mathrm{Sp}(\overline{\mathscr{L}^{-a}_{-,\kappa}})$. The reverse implications follow in the same way. Now that $0 \in \mathrm{Sp}_{\mathrm{disc}}(\overline{\mathscr{L}^a_+}) \Longleftrightarrow 0 \in \mathrm{Sp}_{\mathrm{disc}}(\overline{\mathscr{L}^{-a}_{+,\widetilde{\kappa}}}) \Longleftrightarrow 0 \in \mathrm{Sp}_{\mathrm{disc}}(\overline{\mathscr{L}^{-a}_{-,\kappa}})$ is a direct consequence of (2.3.28), and this finishes the proof of the first statement. The last statement is a direct consequence of the first one and Theorem 2.3.1. This completes the proof. □

Proposition 2.3.3. *Let $a \in (-m, m)$ and let $\overline{\mathscr{L}^a_\pm}$ be as in Lemma 2.2.1. Assume that $\nu = 0$, then it holds that*

$$0 \in \mathrm{Sp}(\overline{\mathscr{L}^a_+}) \Longleftrightarrow a = -\frac{m\mu}{\epsilon} \quad \text{and} \quad 0 \in \mathrm{Sp}(\overline{\mathscr{L}^a_-}) \Longleftrightarrow a = \frac{m\mu}{\epsilon}.$$

Moreover, 0 is an isolated eigenvalue of $\overline{\mathscr{L}_+^{-m\mu/\epsilon}}$ and $\overline{\mathscr{L}_-^{m\mu/\epsilon}}$ with infinite multiplicity.

Proof. Given $a \in (-m, m)$, once the claimed statement is shown for $\overline{\mathscr{L}^a_+}$, by Proposition 2.3.2 we get the result for $\overline{\mathscr{L}^a_-}$. As in (the proof of) Theorem 2.3.3, on the Fourier side, if we let $\langle \xi \rangle := (1 + |\xi|^2)^{1/2}$ then one can check that $\overline{\mathscr{L}^a_+}$ is unitary equivalent to the following multiplication operator:

$$\widetilde{\Pi^a_+} := \langle \xi \rangle \left(\frac{1}{\operatorname{sgn}(\kappa)}(\epsilon I_4 - (\mu\beta + \eta(\alpha \cdot N))) + \frac{1}{2\sqrt{|\xi|^2 + m^2 - a^2}} \Gamma_{m,a}(\xi) \right).$$

Since $\operatorname{sgn}(\kappa) = 4$, from (2.3.23) it follows that $\widetilde{\Pi^a_+}$ is invertible for all $a \neq -m\mu/\epsilon$, and we have

$$(\widetilde{\Pi^a_+})^{-1} = \frac{1}{\langle \xi \rangle} \left(1 + \frac{\sqrt{|\xi|^2 + m^2 - a^2}}{\epsilon a + \mu m} - \frac{(\epsilon + (\mu\beta + \eta(\alpha \cdot N)))}{2(\epsilon a + \mu m)} \Gamma_{m,a}(\xi) \right) (\epsilon + (\mu\beta + \eta(\alpha \cdot N))).$$

Furthermore it holds that

$$\frac{1}{\langle \xi \rangle} \widetilde{\Pi^a_+} \left(1 - \frac{(\epsilon + \mu\beta + \eta(\alpha \cdot N))}{2\sqrt{|\xi|^2 + m^2 - a^2}} \Gamma_{m,a}(\xi) \right) = 0, \text{ for } a = -\frac{m\mu}{\epsilon}.$$

From this, it follows that 0 is an eigenvalue of the operators $\overline{\mathscr{L}^{-m\mu/\epsilon}_+}$ with infinite multiplicity, and thereby $0 \in \operatorname{Sp}_{\text{ess}}(\overline{\mathscr{L}^{-m\mu/\epsilon}_+})$. Thus, we conclude that $0 \in \operatorname{Sp}(\overline{\mathscr{L}^a_+})$ if and only if $a\epsilon = -m\mu$. Now we turn to prove the last statement for the operator $\overline{\mathscr{L}^{-m\mu/\epsilon}_+}$, similar arguments give the result for $\overline{\mathscr{L}^{m\mu/\epsilon}_-}$. A simple computation yields

$$\det(\widetilde{\Pi^a_+} - \theta) = \left[\theta \Big(\theta - \underbrace{\langle \xi \rangle \Big(\frac{a}{\sqrt{|\xi|^2 + m^2 - a^2}} + \frac{\epsilon}{2} \Big)}_{\theta_1(|\xi|)} \Big) \right]^2,$$

where $\det(\widetilde{\Pi^a_+} - \theta)$ is the determinant of $(\widetilde{\Pi^a_+} - \theta)$. By studying the variations of the non-trivial root θ_1 for $a = -m\mu/\epsilon$, we obtain that

$$\operatorname{Sp}(\overline{\mathscr{L}^{-m\mu/\epsilon}_+}) = \{0\} \cup \theta_1([0, \infty)) = \{0\} \cup \left[\frac{\epsilon}{2} - \frac{\mu}{\sqrt{\epsilon^2 - \mu^2}}, \infty \right] \quad \text{if } \epsilon > 0,$$
$$\operatorname{Sp}(\overline{\mathscr{L}^{-m\mu/\epsilon}_+}) = \theta_1([0, \infty)) \cup \{0\} = \left[-\infty, \frac{\epsilon}{2} + \frac{\mu}{\sqrt{\epsilon^2 - \mu^2}} \right] \cup \{0\} \quad \text{if } \epsilon < 0.$$

Since $\operatorname{sgn}(\kappa) = \epsilon^2 - \mu^2 - \eta^2 = 4$, it follows that

$$\frac{\epsilon}{2} - \frac{\mu}{\sqrt{\epsilon^2 - \mu^2}} = \frac{\sqrt{\mu^2 + \eta^2 + 4}}{2} - \frac{\mu}{\sqrt{\eta^2 + 4}} > 0, \quad \text{for } \epsilon > 0,$$
$$\frac{\epsilon}{2} - \frac{\mu}{\sqrt{\epsilon^2 - \mu^2}} = -\frac{\sqrt{\mu^2 + \eta^2 + 4}}{2} + \frac{\mu}{\sqrt{\eta^2 + 4}} < 0, \quad \text{for } \epsilon < 0.$$

From this we get that 0 is an isolated eigenvalue of $\overline{\mathscr{L}^{-m\mu/\epsilon}_+}$ with infinite multiplicity, and this completes the proof of the proposition. □

Remark 2.3.4. *The reader should not confuse the unbounded operator* $\mathscr{L}^{-m\mu/\epsilon}_+$ *with the original operator* $\Lambda^{-m\mu/\epsilon}_+$, *which is indeed a bounded operator on* $L^2(\Sigma)^4$ *with closed range.*

In the following lemma, we establish compactness results concerning the nonlocal operators $L_\nu^{\frac{1}{4}} := L^{\frac{1}{4}}$, $\nu \geqslant 0$, defined in Subsection 2.2.2, they will be crucial in the proof of Theorem 2.3.4. In the proof we use the same interpretation as in Lemma 2.3.2 with χ_0 and χ_ν as in Notation 1.3.1. We also recall the unitary transformation $\mathscr{J}_\nu : L^2(\Sigma_\nu)^4 \to L^2(\Sigma_0)^4 \simeq L^2(\mathbb{R}^2)^4$, defined for $g \in L^2(\Sigma_\nu)^4$, by $(\mathscr{J}_\nu g)(\tilde{x}) = J_\nu^{1/2}(\tilde{x}) g(\tau(\tilde{x}))$ (with τ and J_ν as in (3.1.6) and (1.3.27), respectively).

Lemma 2.3.3. *Let $\nu > 0$, then*

$$\mathcal{M}_1 = \left((1-\chi_\nu) L_\nu^{\frac{1}{4}} \mathscr{J}_\nu^{-1} - (1-\chi_0) L_0^{\frac{1}{4}}\right)(1-\chi_0) : L^2(\mathbb{R}^2)^4 \to H^{-1}(\mathbb{R}^2)^4,$$
$$\mathcal{M}_2 = (1-\chi_0)\left(\mathscr{J}_\nu L_\nu^{\frac{1}{4}}(1-\chi_\nu) - L_0^{\frac{1}{4}}(1-\chi_0)\right) : H^1(\mathbb{R}^2)^4 \to L^2(\mathbb{R}^2)^4,$$

are compact operators.

proof. We give the proof for the operator $\mathcal{M}_1$, the statement for the operator $\mathcal{M}_2$ can be verified in the same way. For this, we first establish a similar property for the resolvents and their negative powers. Let $g \in L^2(\mathbb{R}^2)^4$ and set $G = (1-\chi_0)g$. We note that from the definition of the cutoff functions it holds that

$$(1-\chi_\nu) L_\nu^1 \mathscr{J}_\nu^{-1} G - (1-\chi_0) L_0^1 G = 0. \tag{2.3.29}$$

Then, as in the proof of Lemma 2.3.2, we can transmit the above equality, modulo compact operator, to the resolvents as well. Indeed, given $z \in \rho(L_\nu^1) \cap \rho(L_0^1)$, then using (2.3.29) we get that

$$(L_0^1 - z)(1-\chi_\nu)(L_\nu^1 - z)^{-1} \mathscr{J}_\nu^{-1} G = (1-\chi_0) G + \mathscr{L}_1 G, \tag{2.3.30}$$

where $\mathscr{L}_1$ is given by

$$\mathscr{L}_1 G = \left(\chi_0 (L_0^1 - z)(1-\chi_\nu) - (1-\chi_\nu)(L_\nu^1 - z)\chi_\nu\right)(L_\nu^1 - z)^{-1} \mathscr{J}_\nu^{-1} G.$$

It is clear that $\mathscr{L}_1$ is bounded from $L^2(\mathbb{R}^2)^4$ into itself, and as it contains the cutoff functions χ_0 and χ_ν, the compactness of the embedding $\chi_\nu H^s(\Sigma_\nu)^4 \hookrightarrow H^{s-1/2}(\Sigma_\nu)^4$ implies that $\mathscr{L}_1$ is compact from $L^2(\mathbb{R}^2)^4$ to $H^{-1/2}(\mathbb{R}^2)^4$. Note that from (2.3.30) we have

$$(1-\chi_\nu)(L_\nu^1 - z)^{-1} \mathscr{J}_\nu^{-1} G - (1-\chi_0)(L_0^1 - z)^{-1} G = [\chi_0, (L_0^1 - z)^{-1}] G + (L_0^1 - z)^{-1} \mathscr{L}_1 G, \tag{2.3.31}$$

and since $(L_\nu^1 - z)^{-1}$ is bounded from $L^2(\Sigma_\nu)^4$ to $H^2(\Sigma_\nu)^4$, using the compactness property of $\mathscr{L}_1$ and the compactness of the Sobolev embedding we get that

$$\left((1-\chi_\nu)(L_\nu^1 - z)^{-1} \mathscr{J}_\nu^{-1} - (1-\chi_0)(L_0^1 - z)^{-1}\right)(1-\chi_0) : L^2(\mathbb{R}^2)^4 \to H^{3/2}(\mathbb{R}^2)^4,$$

is a compact operator. Next, we use the functional calculus to transmit the above property for the operators $L_\nu^{-\frac{3}{4}}$ and $L_0^{-\frac{3}{4}}$. Recall that we have chosen c so that $(L_\nu^1 - \gamma) = (-\Delta_\Sigma + c - \gamma)$ is a positive operator for some $\gamma > 0$ (see the beginning of Subsection 2.2.2). Thus, $(L_\nu^1 - z)^{-1}$ is well-defined for any $z \in \mathbb{C} \setminus [\gamma, \infty)$. Moreover, for $0 < \theta < \pi/2$ and $\gamma > \gamma' > 0$, we can define $L_\nu^{-\frac{3}{4}}$ by the Cauchy formula (see, e.g., [96, Chap III, §3])

$$L_\nu^{-\frac{3}{4}} = \frac{i}{2\pi} \int_{\mathscr{L}_{\theta,\gamma'}} z^{-\frac{3}{4}} (L_\nu^1 - z)^{-1} \mathrm{d}z,$$

where for $\omega \in \mathbb{C}$ such that $\mathrm{Re}(\omega) < 0$, z^ω is the determination of the power function defined on $\mathbb{C} \setminus (-\infty, 0]$, and the integration is along the contour $\mathscr{Z}_{\theta,\gamma'}$ defined by

$$\mathscr{Z}_{\theta,\gamma'} := \{z \in \mathbb{C} : |z| \geqslant \gamma' \text{ and } |\mathrm{Arg}(z)| = \theta\} \cup \{z \in \mathbb{C} : |z| = \gamma' \text{ and } |\mathrm{Arg}(z)| \leqslant \theta\}.$$

From the Cauchy formula and the identity 2.3.31 we obtain that

$$\begin{aligned}(1-\chi_\nu)L_\nu^{-\frac{3}{4}}\mathscr{J}_\nu^{-1}(1-\chi_0) =& \frac{i}{2\pi}\int_{\mathscr{Z}_{\theta,\gamma'}} z^{-\frac{3}{4}}(1-\chi_\nu)(L_\nu^1 - z)^{-1}\mathscr{J}_\nu^{-1}(1-\chi_0)\mathrm{d}z \\ =& \frac{i}{2\pi}\int_{\mathscr{Z}_{\theta,\gamma'}} z^{-\frac{3}{4}}(1-\chi_0)(L_0^1 - z)^{-1}(1-\chi_0)\mathrm{d}z + \mathscr{L}_2 \\ =& (1-\chi_0)L_0^{-\frac{3}{4}}(1-\chi_0) + \mathscr{L}_2,\end{aligned}$$

with

$$\mathscr{L}_2 := \frac{i}{2\pi}\int_{\mathscr{Z}_{\theta,\gamma'}} z^{-\frac{3}{4}}\left([\chi_0, (L_0^1 - z)^{-1}] + (L_0^1 - z)^{-1}\mathscr{L}_1\right)\mathrm{d}z.$$

Since $L_\nu^{-\frac{3}{4}}$ is bounded from $L^2(\Sigma_\nu)^4$ to $H^{3/2}(\Sigma_\nu)^4$, thanks to the cutoff functions and the properties of $\mathscr{L}_1$, we have that $\mathscr{L}_2$ is compact from $L^2(\mathbb{R}^2)^4$ to $H^1(\mathbb{R}^2)^4$. Therefore, the operator

$$\left((1-\chi_\nu)L_\nu^{-\frac{3}{4}}\mathscr{J}_\nu^{-1} - (1-\chi_0)L_0^{-\frac{3}{4}}\right)(1-\chi_0) = \mathscr{L}_2 \tag{2.3.32}$$

is a compact from $L^2(\mathbb{R}^2)^4$ to $H^1(\mathbb{R}^2)^4$. Now we are able to prove the statement for $\mathcal{M}_1$. Indeed, localizing with respect to χ_0 and χ_ν, and using the property of the power of the resolvents (i.e., (2.3.31) and (2.3.32)), we get that

$$\begin{aligned}(1-\chi_\nu)L_\nu^{\frac{1}{4}}\mathscr{J}_\nu^{-1}G =& L_0^1 L_0^{-1}(1-\chi_\nu)L_\nu^{\frac{1}{4}}\mathscr{J}_\nu^{-1}G = L_0^1(1-\chi_\nu)L_\nu^{-1}(1-\chi_\nu)L_\nu^{\frac{1}{4}}\mathscr{J}_\nu^{-1}G + J_1G \\ =& L_0^1(1-\chi_\nu)L_\nu^{-\frac{3}{4}}\mathscr{J}_\nu^{-1}G + \sum_{k=1}^{2} J_kG = L_0^1(1-\chi_0)L_0^{-\frac{3}{4}}G + \sum_{k=1}^{3} J_kG \\ =& (1-\chi_0)L_0^{\frac{1}{4}}G + \sum_{k=1}^{4} J_kG,\end{aligned}$$

where for $1 \leqslant k \leqslant 4$, J_k is bounded from $L^2(\mathbb{R}^2)^4$ to $H^{-1/2}(\mathbb{R}^2)^4$ and involves the cutoff functions χ_0 and χ_ν, and hence J_k is compact from $L^2(\mathbb{R}^2)^4$ to $H^{-1}(\mathbb{R}^2)^4$ by the compactness of the injection $\chi_\nu H^{-1/2}(\Sigma_\nu)^4 \hookrightarrow H^{-1}(\Sigma_\nu)^4$. Therefore, $\mathcal{M}_1 : L^2(\mathbb{R}^2)^4 \to H^{-1}(\mathbb{R}^2)^4$ is compact, and this completes the proof. □

We are now in a position to give the proof of our main result in this subsection. To avoid ambiguity, in the proof we use the labels S_ν^z and $\widetilde{\Lambda}_{\pm,\nu}^z$ to denote the trace of the single layer given by (1.3.24) and the operator $\widetilde{\Lambda}_\pm^z$, respectively.

Proof of Theorem 2.3.4. Assume that Σ satisfies (H2) and fix $\nu \geqslant 0$. The result will follow from the following statements:

(a) $(-\infty, -m) \cup (m, +\infty) \subset \mathrm{Sp}_{\mathrm{ess}}(\overline{H_\kappa^\nu})$.

(b) $\{-m\mu/\epsilon\} \in \mathrm{Sp}_{\mathrm{ess}}(\overline{H_\kappa^\nu})$ and $\{m\mu/\epsilon\} \notin \mathrm{Sp}_{\mathrm{ess}}(\overline{H_\kappa^\nu})$.

(c) $\mathrm{Sp}_{\mathrm{ess}}(\overline{H_\kappa^\nu}) \cap [(-m, m) \setminus \{-m\mu/\epsilon, m\mu/\epsilon\}] = \emptyset$.

Proof of (a)**.** Given $a \in (-\infty,-m)\cup(m,\infty)$ and let $(\varphi_n)_{n\in\mathbb{N}}$ be the sequence of functions defined by (2.3.25) with $R = 2\sup\{|x| : x \in \Sigma_\nu \setminus \overline{F}\}$. By construction, it is clear that $(\varphi_n)_{n\in\mathbb{N}}$ is a singular sequence for $\overline{H^\nu_\kappa}$ and a. Thus, we get the inclusion $(-\infty,-m)\cup(m,+\infty) \subset \mathrm{Sp_{ess}}(\overline{H^\nu_\kappa})$, which yields (a).

Proof of (b)**.** From Proposition 2.3.3 and Theorem 2.3.1, we know that item (b) holds true for $\nu = 0$. Next, assume that $\nu > 0$, we are going to prove that $\{-m\mu/\epsilon\} \in \mathrm{Sp_{ess}}(\overline{H^\nu_\kappa})$ and the same arguments yield that $\{m\mu/\epsilon\} \notin \mathrm{Sp_{ess}}(\overline{H^\nu_\kappa})$. To this end, we argue by contradiction and we split the proof into two steps. Set $\lambda = -m\mu/\epsilon$ and suppose that $\lambda \notin \mathrm{Sp_{ess}}(\overline{H^\nu_\kappa})$, then by Theorem 2.3.1 and Proposition 2.3.2 it follows that $0 \notin \mathrm{Sp_{ess}}(\overline{\mathscr{L}^\lambda_{+,\nu}})$ and $0 \notin \mathrm{Sp_{ess}}(\overline{\mathscr{L}^{-\lambda}_{-,\nu}})$. In the next two steps we will introduce an auxiliary operator which will allow us to obtain a contradiction to fact that $0 \notin \mathrm{Sp_{ess}}(\overline{\mathscr{L}^\lambda_{+,\nu}})$.

Step 1. We set $B_\nu := \widetilde{\Lambda}^\lambda_{+,\nu}\widetilde{\Lambda}^{-\lambda}_{-,\nu}$, $D_\nu := \Lambda^{-\lambda}_{-,\nu}\Lambda^\lambda_{+,\nu}$, and we consider the operator $\Upsilon^\lambda_\nu : L^2(\Sigma_\nu)^4 \longrightarrow L^2(\Sigma_\nu)^4$ defined by:

$$\Upsilon^\lambda_\nu := L_\nu^{\frac14} D_\nu B_\nu L_\nu^{\frac14} = L_\nu^{\frac14}(\Lambda^{-\lambda}_{-,\nu}\Lambda^\lambda_{+,\nu})(\widetilde{\Lambda}^\lambda_{+,\nu}\widetilde{\Lambda}^{-\lambda}_{-,\nu})L_\nu^{\frac14}.$$

From the definitions of ϕ^z and ψ^z (see (1.3.1) and (1.3.2)), it is clear that $\psi^{-\lambda} = \psi^\lambda$, and that

$$\phi^{-\lambda}(x) = \phi^\lambda(x) - 2\lambda\psi^\lambda, \quad \text{for all } x \in \mathbb{R}^3 \setminus \{0\}.$$

Using this, we get that

$$B_\nu = \widetilde{\Lambda}^\lambda_{+,\nu}\widetilde{\Lambda}^\lambda_{-,\nu} + 2\lambda\Lambda^\lambda_{+,\nu}S^\lambda_\nu, \quad D_\nu = \Lambda^\lambda_{-,\nu}\Lambda^\lambda_{+,\nu} + 2\lambda S^\lambda_\nu\Lambda^\lambda_{+,\nu}. \tag{2.3.33}$$

Since $L_\nu^{\frac14} : H^s(\Sigma)^4 \to H^{s-1/2}(\Sigma)^4$ is bijective and continuous for any $s \in [-1/2, 1]$, using (2.3.33), (2.2.7) and Lemma 1.3.5 it easily follows that Υ^λ_ν is a bounded, self-adjoint operator on $L^2(\Sigma_\nu)^4$. Note that by hypothesis and the definition of Υ^λ_ν it holds that $0 \notin \mathrm{Sp_{ess}}(\Upsilon^\lambda_\nu)$.

Step 2. We now show that $0 \in \mathrm{Sp_{ess}}(\overline{\mathscr{L}^\lambda_{+,0}})$ implies that $0 \in \mathrm{Sp_{ess}}(\Upsilon^\lambda_\nu)$, which is a contradiction to the fact that $0 \notin \mathrm{Sp_{ess}}(\Upsilon^\lambda_\nu)$, and hence $\lambda \notin \mathrm{Sp_{ess}}(\overline{H^\nu_\kappa})$ can not be true. For this, we are going to prove that

$$\mathscr{J}_\nu\Upsilon^\lambda_\nu\mathscr{J}_\nu^{-1} - \Upsilon^\lambda_0 : L^2(\mathbb{R}^2)^4 \to L^2(\mathbb{R}^2)^4,$$

is a compact operator. Indeed, since $\widetilde{\Lambda}^\lambda_{+,\nu}\widetilde{\Lambda}^\lambda_{-,\nu} = \widetilde{\Lambda}^\lambda_{-,\nu}\widetilde{\Lambda}^\lambda_{+,\nu}$ and $S^\lambda_\nu : H^{s-1}(\Sigma_\nu)^4 \to H^s(\Sigma_\nu)^4$ is bounded for any $s \in [0,1]$, it follows from (2.3.33) that

$$\begin{aligned}\mathscr{J}_\nu\Upsilon^\lambda_\nu\mathscr{J}_\nu^{-1} &= \mathscr{J}_\nu L_\nu^{\frac14}\left(\Lambda^\lambda_{-,\nu}\Lambda^\lambda_{+,\nu}\right)\left(\widetilde{\Lambda}^\lambda_{+,\nu}\widetilde{\Lambda}^\lambda_{-,\nu}\right)L_\nu^{\frac14}\mathscr{J}_\nu^{-1} + (2\lambda)^2\,\mathscr{J}_\nu L_\nu^{\frac14}S^\lambda_\nu\left(\widetilde{\Lambda}^\lambda_{+,\nu}\right)^2 S^\lambda_\nu L_\nu^{\frac14}\mathscr{J}_\nu^{-1}\\ &\quad + 2\lambda\,\mathscr{J}_\nu L_\nu^{\frac14}\{\widetilde{\Lambda}^\lambda_{+,\nu}\widetilde{\Lambda}^\lambda_{-,\nu}\widetilde{\Lambda}^\lambda_{+,\nu}, S^\lambda\}L_\nu^{\frac14}\mathscr{J}_\nu^{-1} := \mathcal{T}_{1,\nu} + \mathcal{T}_{2,\nu} + \mathcal{T}_{3,\nu}.\end{aligned} \tag{2.3.34}$$

Now, we set $\widetilde{\mathcal{T}}_{j,\nu} = \mathcal{T}_{j,\nu} - \mathcal{T}_{j,0}$ for $j \in \{1,2,3\}$. To avoid repetitions, in what follows we only show that $\widetilde{\mathcal{T}}_{1,\nu}$ is a compact operator, since the same arguments yield that $\widetilde{\mathcal{T}}_{2,\nu}$ and $\widetilde{\mathcal{T}}_{3,\nu}$ are compact operators. For this, we are going to use localization arguments as in the second step. Note first that since $\mathrm{sgn}(\kappa) = 4$, from (2.2.7) and the proof of Lemma 1.3.5 it follows that

$$\begin{aligned}\widetilde{\Lambda}^\lambda_{+,\nu}\widetilde{\Lambda}^\lambda_{-,\nu} &= -C^\lambda_{\Sigma_\nu}(\alpha\cdot N)\{\alpha\cdot N, \widetilde{\mathscr{C}}^\lambda_{\Sigma_\nu}\} + \frac{\mu}{4}\{\beta, \widetilde{\mathscr{C}}^\lambda_{\Sigma_\nu}\} + \frac{\eta}{4}\{\alpha\cdot N, \widetilde{\mathscr{C}}^\lambda_{\Sigma_\nu}\}\\ &= \left(-C^\lambda_{\Sigma_\nu}(\alpha\cdot N) + \frac{\eta}{4}\right)T_{\lambda,\nu} + \left(-2\lambda C^\lambda_{\Sigma_\nu} + \frac{\mu}{4}(\lambda\beta + mI_4) + \frac{\lambda\eta}{2}(\alpha\cdot N)\right)S^\lambda_\nu,\end{aligned}$$

where $T_{\lambda,\nu}$ correspond to the integral operator $T_{z,1}$ given by (1.3.31). Using this it follows that $\mathscr{T}_{1,\nu} = K_{1,\nu} + K_{2,\nu} + K_{3,\nu}$, where $K_{j,\nu}$ are given by

$$K_{1,\nu} = \mathscr{J}_\nu L_\nu^{\frac{1}{4}} \left(\left(-C_{\Sigma_\nu}^\lambda (\alpha \cdot N) + \frac{\eta}{4} \right) T_{\lambda,\nu} \right)^2 L_\nu^{\frac{1}{4}} \mathscr{J}_\nu^{-1},$$

$$K_{2,\nu} = \mathscr{J}_\nu L_\nu^{\frac{1}{4}} \left\{ \left(-C_{\Sigma_\nu}^\lambda (\alpha \cdot N) + \frac{\eta}{4} \right) T_{\lambda,\nu}, \left(-2\lambda C_{\Sigma_\nu}^\lambda + \frac{\mu}{4}(\lambda\beta + mI_4) + \frac{\lambda\eta}{2}(\alpha \cdot N) \right) S_\nu^\lambda \right\} L_\nu^{\frac{1}{4}} \mathscr{J}_\nu^{-1},$$

$$K_{3,\nu} = \mathscr{J}_\nu L_\nu^{\frac{1}{4}} \left(\left(-2\lambda C_{\Sigma_\nu}^\lambda + \frac{\mu}{4}(\lambda\beta + mI_4) + \frac{\lambda\eta}{2}(\alpha \cdot N) \right) S_\nu^\lambda \right)^2 L_\nu^{\frac{1}{4}} \mathscr{J}_\nu^{-1}.$$

By definition we know that $(1 - \chi_\nu)T_{\lambda,\nu}(1 - \chi_\nu) = 0$ and $T_{\lambda,0} = 0$ (i.e. when $\Sigma = \mathbb{R}^2 \times \{0\}$). From this we get that $K_{1,\nu} = \Gamma_{1,\nu}\Gamma_{2,\nu}$, with

$$\Gamma_{1,\nu} = \mathscr{J}_\nu L_\nu^{\frac{1}{4}} \left(-C_{\Sigma_\nu}^\lambda (\alpha \cdot N) + \frac{\eta}{4} \right) T_{\lambda,\nu} \left(-C_{\Sigma_\nu}^\lambda (\alpha \cdot N) + \frac{\eta}{4} \right),$$
$$\Gamma_{2,\nu} = (\chi_\nu T_{\lambda,\nu}\chi_\nu + \chi_\nu T_{\lambda,\nu}(1 - \chi_\nu) + (1 - \chi_\nu)T_{\lambda,\nu}\chi_\nu)\, L_\nu^{\frac{1}{4}} \mathscr{J}_\nu^{-1},$$

and that

$$\mathscr{T}_{1,0} = L_0^{\frac{1}{4}} \left(\left(-2\lambda C_{\Sigma_0}^\lambda + \frac{\mu}{4}(\lambda\beta + mI_4) + \frac{\lambda\eta}{2}(\alpha \cdot N) \right) S_0^\lambda \right)^2 L_0^{\frac{1}{4}}.$$

By Remark 1.3.5 we know that $T_{\lambda,\nu} : H^{s-1}(\Sigma_\nu)^4 \to H^s(\Sigma_\nu)^4$ is bounded for any $s \in [0, 1]$, thus $\Gamma_{1,\nu} : L^2(\mathbb{R}^2)^4 \to H^{1/2}(\Sigma_\nu)^4$ and $\Gamma_{2,\nu} : H^{1/2}(\Sigma_\nu)^4 \to H^1(\mathbb{R}^2)^4$ are well-defined and bounded. Consequently, using the compactness of the Sobolev embedding $\chi_\nu H^s(\Sigma_\nu)^4 \hookrightarrow H^{s-1/2}(\Sigma_\nu)^4$ we get that $K_{1,\nu} : L^2(\mathbb{R}^2)^4 \to L^2(\mathbb{R}^2)^4$ is a compact operator. Similarly, one can check that $K_{2,\nu}$ is a compact operator on $L^2(\mathbb{R}^2)^4$.

At this stage, we have shown that $\widetilde{\mathscr{T}}_{1,\nu} = \mathscr{T}_{1,\nu} - \mathscr{T}_{1,0} = K_{3,\nu} - \mathscr{T}_{1,0} + \widetilde{K}_\nu$, where $\widetilde{K}_\nu$ is compact in $L^2(\mathbb{R}^2)^4$. Hence, to show the claim of the current step it remains to prove that $K_{3,\nu} - \mathscr{T}_{1,0}$ is compact on $L^2(\mathbb{R}^2)^4$. For this, observe that

$$(1 - \chi_\nu)C_{\Sigma_\nu}^\lambda (1 - \chi_\nu) = (1 - \chi_0)C_{\Sigma_0}^\lambda (1 - \chi_0),$$
$$(1 - \chi_\nu)S_\nu^\lambda (1 - \chi_\nu) = (1 - \chi_0)S_0^\lambda (1 - \chi_0),$$

hold by Remark 1.3.4. Thus, localizing with respect to χ_0 and χ_ν and combining the above observation with the compactness of Sobolev injections and the properties of the operators $\mathcal{M}_k$ from Lemma 2.3.3, it follows that $K_{3,\nu} - \mathscr{T}_{1,0}$ is compact in $L^2(\mathbb{R}^2)^4$. Therefore, $\mathscr{J}_\nu \Upsilon_\nu^{-m\mu/\epsilon} \mathscr{J}_\nu^{-1} - \Upsilon_0^{-m\mu/\epsilon}$ is compact in $L^2(\mathbb{R}^2)^4$. Since $0 \in \mathrm{Sp}_{\mathrm{ess}}\left(\Upsilon_0^{-m\mu/\epsilon}\right)$ because $0 \in \mathrm{Sp}_{\mathrm{ess}}\left(\overline{\mathscr{L}_{+,0}^{-m\mu/\epsilon}}\right)$ and $0 \in \mathrm{Sp}_{\mathrm{ess}}\left(\overline{\mathscr{L}_{-,0}^{m\mu/\epsilon}}\right)$ by Proposition 2.3.3, it follows from Weyl's theorem that $0 \in \mathrm{Sp}_{\mathrm{ess}}\left(\Upsilon_\nu^{-m\mu/\epsilon}\right)$. Therefore, $0 \in \mathrm{Sp}_{\mathrm{ess}}(\overline{\mathscr{L}_{+,\nu}^{-m\mu/\epsilon}})$ which implies that $-m\mu/\epsilon \in \mathrm{Sp}_{\mathrm{ess}}(\overline{H_\kappa^\nu})$, and this proves (b).

We now show (c), so assume that $a \in (-m, m) \setminus \{-m\mu/\epsilon, m\mu/\epsilon\}$. We introduce the operator $G_\nu^a : L^2(\Sigma_\nu)^4 \longrightarrow L^2(\Sigma_\nu)^4$ defined by $G_\nu^a := L_\nu^{\frac{1}{4}}(\Lambda_{-,\nu}^a \Lambda_{+,\nu}^a)(\widetilde{\Lambda}_{-,\nu}^a \widetilde{\Lambda}_{+,\nu}^a)L_\nu^{\frac{1}{4}}$. Using that $\widetilde{\Lambda}_{-,\nu}^a \widetilde{\Lambda}_{+,\nu}^a = \widetilde{\Lambda}_{+,\nu}^a \widetilde{\Lambda}_{-,\nu}^a$, it follows that G_ν^a is bounded and self-adjoint in $L^2(\Sigma_\nu)^4$. Moreover, by definition it holds that

$$0 \in \mathrm{Sp}_{\mathrm{ess}}(\overline{\mathscr{L}_{\pm,\nu}^a}) \Longrightarrow 0 \in \mathrm{Sp}_{\mathrm{ess}}(G_\nu^a). \tag{2.3.35}$$

Since $L_\nu^{\frac{1}{4}}$ is an isomorphism, it follows from Proposition 2.3.3 that $\widetilde{\Lambda}_{+,0}^a$ and $\widetilde{\Lambda}_{-,0}^a$ are bounded, invertible operators for all $a \in (-m, m) \setminus \{-m\mu/\epsilon, m\mu/\epsilon\}$, and that $0 \in \mathrm{Sp}_{\mathrm{ess}}(G_0^a)$ if and only if $a = \mp m\mu/\epsilon$. Next, we claim that, if $a \neq \mp m\mu/\epsilon$ then $0 \notin \mathrm{Sp}_{\mathrm{ess}}(G_\nu^a)$. To see this, note that $\mathscr{J}_\nu G_\nu^a \mathscr{J}_\nu^{-1}$ coincides with the operator $\mathcal{T}_{1,\nu}$ defined by (2.3.34), for $\lambda = a$. Thus, the same arguments as those used in the proof of (b) show that $\mathscr{J}_\nu G_\nu^a \mathscr{J}_\nu^{-1} - G_0^a$ is a compact operator in $L^2(\mathbb{R}^2)^4$. Consequently, Weyl's theorem yields that $\mathrm{Sp}_{\mathrm{ess}}(G_\nu^a) = \mathrm{Sp}_{\mathrm{ess}}(G_0^a)$, and this proves the result asserted. Using this, it follows from (2.3.35) that, if $a \neq \mp m\mu/\epsilon$ then $0 \notin \mathrm{Sp}_{\mathrm{ess}}(\overline{\mathscr{L}_{\pm,\nu}^a})$. Therefore, Theorem 2.3.1 yields that $\mathrm{Sp}_{\mathrm{ess}}(\overline{H_\kappa^\nu}) \cap [(-m, m) \setminus \{-m\mu/\epsilon, m\mu/\epsilon\}] = \emptyset$, which proves (c).

Summing up, from (a) and (b) we obtain that $(-\infty, -m) \cup \{-m\mu/\epsilon\} \cup (m, +\infty) \subset \mathrm{Sp}_{\mathrm{ess}}(\overline{H_\kappa^\nu})$. From (b) and (c) we get the inclusion $\mathrm{Sp}_{\mathrm{ess}}(\overline{H_\kappa^\nu}) \subset (-\infty, -m] \cup \{-m\mu/\epsilon\} \cup [m, +\infty)$. Since the essential spectrum of a self-adjoint operator is closed, we get then the equality (2.3.26). This completes the proof of the theorem. $\square$

Actually in the case $\Sigma = \mathbb{R}^2 \times \{0\}$, one can check directly using the separation of variables that $a = -m\mu/\epsilon$ is an eigenvalue of $\overline{H_\kappa}$ with infinite multiplicity. Indeed, let $a = -m\mu/\epsilon$ and $\varphi \in \mathrm{dom}(\overline{H_\kappa})$ such that:

$$(\overline{H_\kappa} - a)\varphi = 0, \quad \text{in } L^2(\mathbb{R}^3)^4. \tag{2.3.36}$$

A simple computation yields the following relations

$$\begin{aligned}
\left[\frac{1}{2}(\epsilon I_4 - \mu\beta + \eta\alpha_3) + i\alpha_3\right]\left[\frac{1}{2}(\epsilon I_4 + \mu\beta - \eta\alpha_3) - i\alpha_3\right] &= (2 - i\eta)I_4,\\
\left[\frac{1}{2}(\epsilon I_4 - \mu\beta + \eta\alpha_3) + i\alpha_3\right]\left[\frac{1}{2}(\epsilon I_4 + \mu\beta - \eta\alpha_3) + i\alpha_3\right] &= i\alpha_3(\epsilon + \mu\beta).
\end{aligned} \tag{2.3.37}$$

Hence, using the relation (2.3.37) and the Definition 2.2.2, another way of stating (2.3.36) is to say:

$$\begin{cases} (H - a)\varphi = 0 \quad \text{for all } x_3 \neq 0,\\ (2 - i\eta)t_\Sigma\varphi_+ = -i\alpha_3(\epsilon + \mu\beta)t_\Sigma\varphi_- \quad \text{for } x_3 = 0. \end{cases} \tag{2.3.38}$$

Since $(H + a)(H - a) = (-\Delta + m^2 - a^2)I_4$, one gets that φ is also solution to the following equation

$$(-\Delta + m^2 - a^2)I_4\varphi = 0, \quad \text{for all } x_3 \neq 0$$

Thus, applying Fourier-Plancherel operator on $\overline{x} = (x_1, x_2)$, we get that

$$\mathscr{F}_{\overline{x}}[\varphi](\xi, x_3) = \begin{cases} e^{-x_3\sqrt{|\xi|^2+m^2-a^2}}\mathscr{F}_{\overline{x}}[\psi_+](\xi) & \text{for } x_3 > 0,\\ e^{x_3\sqrt{|\xi|^2+m^2-a^2}}\mathscr{F}_{\overline{x}}[\psi_-](\xi) & \text{for } x_3 < 0, \end{cases}$$

for some $\psi_\pm \in H^{\frac{1}{2}}(\mathbb{R}^2)$. Since $(H + a)\varphi = 2a\varphi$, by applying the inverse Fourier-Plancherel operator, we obtain that

$$\varphi(\overline{x}, x_3) = \begin{cases} \dfrac{1}{2\pi}\displaystyle\int_{\mathbb{R}^2} e^{i\overline{x}\cdot\xi}e^{-x_3\sqrt{|\xi|^2+m^2-a^2}}\Gamma_i(\xi)\mathscr{F}_{\overline{x}}[\psi_+](\xi)\mathrm{d}\xi & \text{for } x_3 > 0,\\ \dfrac{1}{2\pi}\displaystyle\int_{\mathbb{R}^2} e^{i\overline{x}\cdot\xi}e^{x_3\sqrt{|\xi|^2+m^2-a^2}}\Gamma_{-i}\mathscr{F}_{\overline{x}}[\psi_-](\xi)\mathrm{d}\xi & \text{for } x_3 < 0, \end{cases}$$

where $\Gamma_{\pm i}(\xi) = \left[\alpha \cdot (\xi_1, \xi_2, \pm i\sqrt{|\xi|^2 + m^2 - a^2}) + m\beta + a\right]$. From this, it is clear that

$$\varphi_\pm, (\alpha \cdot \nabla)\varphi_\pm \in L^2(\Omega_\pm).$$

Now, if we set

$$\psi_- = -\frac{\eta - i2}{\epsilon^2-\mu^2}(\epsilon+\mu\beta)\alpha_3\psi_+,$$

then we get

$$(2-i\eta)\Gamma_{+i}(\xi)\mathscr{F}_{\overline{x}}\left[\psi_+\right](\xi) = -i\alpha_3(\epsilon I_4-\mu\beta)\Gamma_{-i}(\xi)\mathscr{F}_{\overline{x}}\left[\psi_-\right](\xi).$$

which means that (φ_+,φ_-) satisfies the transmission condition from (2.3.38) . From this considerations it follows that for all $\psi \in H^{\frac{1}{2}}(\mathbb{R}^2)$ the function

$$\varphi(\overline{x},x_3) = \begin{cases} \dfrac{1}{2\pi}\displaystyle\int_{\mathbb{R}^2} e^{i\overline{x}\cdot\xi}e^{-x_3\sqrt{|\xi|^2+m^2-a^2}}\Gamma_i(\xi)\mathscr{F}_{\overline{x}}\left[\psi_+\right](\xi) & \text{for } x_3>0,\\ \dfrac{-i}{4\pi}\displaystyle\int_{\mathbb{R}^2} e^{i\overline{x}\cdot\xi}e^{x_3\sqrt{|\xi|^2+m^2-a^2}}\Gamma_{-i}(\lambda-\mu\beta)\alpha_3\mathscr{F}_{\overline{x}}\left[\psi_+\right](\xi) & \text{for } x_3<0, \end{cases}$$

is an eigenvector associated to the eigenvalue $a=-m\mu/\epsilon$.

2.4 Quantum confinement induced by Dirac operators with anomalous magnetic δ-shell interactions

The main goal of this section is to derive a new model of Dirac operators with δ-shell interactions which generate confinement. Let us explain how to derive this model. Using the unit $c=\hbar=1$, where c is the speed of light and $\hbar$ is the Planck's constant, the Dirac operator for a charge e in an external electromagnetic field (ϕ_{el},A) is given by:

$$H(e) = \alpha\cdot(-i\nabla - eA(t,x)) + m\beta + e\phi_{el}(t,x)I_4,$$

see [103] for example. Recall that the electric and magnetic field strengths are

$$E(t,x) = -\nabla\phi_{el}(t,x) - \frac{\partial A(t,x)}{\partial t}, \quad B(t,x) = \nabla\times A(t,x),$$

where $\partial/\partial t$ denotes the partial derivative with respect to time $t\in\mathbb{R}$. In this case, the anomalous magnetic potential is given by:

$$V(t,x) = \upsilon\left(i\beta(\alpha\cdot E(t,x)) - \frac{1}{4}\beta((\alpha\times\alpha)\cdot B(t,x))\right),$$

here $(\alpha\wedge\alpha)/4 = -i\gamma_5\alpha/2$ is the spin angular momentum, γ_5 is the chirality matrix defined by (2.1.2), and the coupling constant υ is the magnitude of the anomalous potential. Now, if we put $\phi_{el}(t,x)=|x|$ and $A(t,x)=0$, we then obtain

$$V(x) = i\upsilon\beta\left(\alpha\cdot\frac{x}{|x|}\right).$$

Next, given $R>0$, if $x\in\mathbb{S}^2_R=\{x\in\mathbb{R}^3 : |x|=R\}$, then $x/|x|$ coincide with the normal vector field $N(x)$. Thus we get

$$V_\upsilon(x) := i\upsilon\beta(\alpha\cdot N(x)), \quad \forall x\in\mathbb{S}^2_R.$$

Given a surface $\Sigma\subset\mathbb{R}^3$ satisfying the assumption (H1) or (H2), we can now consider the following Dirac operator

$$H+V_\upsilon = H + i\upsilon\beta(\alpha\cdot N)\delta_\Sigma, \quad \upsilon\in\mathbb{R}.$$

and called it Dirac operator with anomalous magnetic δ-shell interactions of strength υ. We mention that the bidimensional analogue of $H + V_\upsilon$ was also introduced and studied in [41]. However, instead of deriving the potential V_υ as we have done here, they rigorously proved that the two-dimensional analog of V_υ can be approximated by regular shrinking potentials of magnetic type, and thus they justified the fact that V_υ is a "magnetic" δ-shell interactions. In this direction we mention that similar results on the approximation of electrostatic and Lorentz scalar δ-interactions have been proved in [79, 80].

Remark 2.4.1. *If one choose a time independent magnetic field $A(x)$ so that $B(x) = x/|x|$ and put $\phi_{el}(t,x) = 0$ for all $t \in \mathbb{R}$, we then get the δ-potential $V_{\widetilde{\upsilon}} = i\widetilde{\upsilon}\beta\gamma_5(\alpha \cdot N)\delta_\Sigma$. Note that in dimension 2, the potential $V_{\widetilde{\upsilon}}$ coincides with the electrostatic δ-potential, and in dimension 3 it gives rise to a different δ-potential. The spectral properties of $(H + V_{\widetilde{\upsilon}})$ will be discussed in details in Chapter 3.*

Now, for $\zeta \in \mathbb{R}$, we define the potential $V_\zeta = \zeta\gamma_5\delta_\Sigma$. To our knowledge, the potential V_ζ seems to have no physical interpretation, but mathematically it has the same properties as the electrostatic potential if $\zeta = \pm 2$; cf. Remark 2.4.2.

Unless otherwise stated, in this section we assume that Σ satisfies the assumption (H1), and we consider the Dirac operator $H_{\zeta,\upsilon}$, which is formally given by

$$H_{\zeta,\upsilon} = H + V_{\zeta,\upsilon} = H + (\zeta\gamma_5 + i\upsilon\beta(\alpha\cdot N))\,\delta_\Sigma, \quad \zeta, \upsilon \in \mathbb{R}.$$

Compared to the operators studied before, the operator $H_{\zeta,\upsilon}$ is very different. Due to the presence of an anomalous magnetic potential, several properties of commutativity are no longer true in this case. Moreover, $H_{0,\upsilon}$ (i.e. $\zeta = 0$) has the particularity of combining two important phenomena that we have already seen. As indicated in the introduction, the Dirac operator $(H_{0,\pm 2}, \mathrm{dom}(H_{0,\pm 2}))$ is essentially self-adjoint and Σ becomes impenetrable; see Theorem 2.4.2 below.

Given $z \in \mathbb{C} \setminus ((-\infty, -m] \cup [m, \infty))$, we define the operators $\Lambda_\pm^z$ as follows:

$$\Lambda_\pm^z = \frac{1}{\zeta^2 + \upsilon^2}(\zeta\gamma_5 + i\upsilon\beta(\alpha\cdot N)) \pm \mathscr{C}_\Sigma^z.$$

Since $i\beta(\alpha \cdot N)$ is C^1-smooth and symmetric, it follows that $\Lambda_\pm^z$ are bounded from $L^2(\Sigma)^4$ onto itself (resp. from $H^{1/2}(\Sigma)^4$ onto itself). Moreover, $\Lambda_\pm^z$ are self-adjoint on $L^2(\Sigma)^4$, for all $z \in (-m, m)$.

Now, using the same notations as in Section 2.1, the Dirac operator $H_{\zeta,\upsilon}$ (acting in $L^2(\mathbb{R}^3)^4$) is defined on the domain

$$\mathrm{dom}(H_{\zeta,\upsilon}) = \left\{ u + \Phi[g] : u \in H^1(\mathbb{R}^3)^4, g \in L^2(\Sigma)^4, t_\Sigma u = -\Lambda_+[g] \right\},$$

and the potential $V_{\zeta,\upsilon}$ acts as follows

$$V_{\zeta,\upsilon}(\varphi) = \frac{1}{2}(\zeta\gamma_5 + i\upsilon\beta(\alpha\cdot N))(\varphi_+ + \varphi_-)\delta_\Sigma,$$

with $\varphi_\pm = t_\Sigma u + C_\pm[g]$. Thus, $H_{\zeta,\upsilon}$ acts in the sense of distributions as $H_{\zeta,\upsilon}(\varphi) = Hu$, for all $\varphi = u + \Phi[g] \in \mathrm{dom}(H_{\zeta,\upsilon})$.

We remind the reader that $\widetilde{\Lambda}_\pm^z$ denotes the continuous extension of $\Lambda_\pm^z$ defined from $H^{-1/2}(\Sigma)^4$ onto itself. Using the same method as in Section 2.2, one can show that $H_{\zeta,\upsilon}$ is closable and the domain of the adjoint is given by

$$\mathrm{dom}(H_{\zeta,\upsilon}^*) = \left\{ u + \Phi[g] : u \in H^1(\mathbb{R}^3)^4, g \in H^{-1/2}(\Sigma)^4, t_\Sigma u = -\widetilde{\Lambda}_+[g] \right\}.$$

In the following, we briefly discuss the basic spectral properties of $H_{\zeta,\upsilon}$ in the non-critical case, i.e. $\zeta^2 + \upsilon^2 \neq 4$. The following theorem gathers the most important properties of $H_{\zeta,\upsilon}$.

Theorem 2.4.1. *Let $(\zeta, \upsilon) \in \mathbb{R}^2$ be such that $\zeta^2 + \upsilon^2 \neq 0, 4$. Then $H_{\zeta,\upsilon}$ is self adjoint and we have*

$$\mathrm{dom}(H_{\zeta,\upsilon}) = \left\{u + \Phi(g) : u \in H^1(\mathbb{R}^3)^4, g \in H^{1/2}(\Sigma)^4, t_\Sigma u = -\Lambda_+[g]\right\} \subset H^1(\mathbb{R}^3 \setminus \Sigma)^4.$$

Moreover, the following statements hold true:

(i) Given $a \in (-m, m)$, then $\mathrm{Kr}(H_{\zeta,\upsilon} - a) \neq \{0\} \iff \mathrm{Kr}(\Lambda_+^a) \neq \{0\}$.

(ii) For all $z \in \rho(H_{\zeta,\upsilon}) \cap \rho(H)$, it holds that

$$(H_{\zeta,\upsilon} - z)^{-1} = (H - z)^{-1} - \Phi^z (\Lambda_+^z)^{-1} (\Phi^{\bar{z}})^*.$$

Furthermore, if Σ satisfies (H1), *then*

(iii) $\mathrm{Sp}_{\mathrm{ess}}(H_{\zeta,\upsilon}) = (-\infty, -m] \cup [m, +\infty)$.

(iv) $\mathrm{Sp}_{\mathrm{disc}}(H_{\zeta,\upsilon}) \cap (-m, m)$ *is finite.*

Proof. Recall that $[A, B] = AB - BA$ denotes the usual commutator bracket. Suppose that $\zeta^2 + \upsilon^2 \neq 0, 4$ and fix $z \in \mathbb{C} \setminus ((-\infty, -m] \cup [m, \infty))$, then a simple computation yields

$$\Lambda_\mp^z \Lambda_\pm^z = \frac{1}{\zeta^2 + \upsilon^2} - \frac{1}{4} - \mathscr{C}_\Sigma^z (\alpha \cdot N)\{\alpha \cdot N, \mathscr{C}_\Sigma^z\} \pm \frac{\zeta}{\zeta^2 + \upsilon^2}[\gamma_5, \mathscr{C}_\Sigma^z] \pm \frac{i\upsilon}{\zeta^2 + \upsilon^2}[\beta(\alpha \cdot N), \mathscr{C}_\Sigma^z].$$

Using the anticommuations relations of the Dirac matrices and the properties of γ_5 given by (2.1.2), we easily get that

$$[\gamma_5, \mathscr{C}_\Sigma^z] = 2m\gamma_5 \beta S^z, \quad [\beta(\alpha \cdot N), \mathscr{C}_\Sigma^z] = \beta\{\alpha \cdot N, \mathscr{C}_\Sigma^z\} - \{\beta, \mathscr{C}_\Sigma^z\}(\alpha \cdot N).$$

Thus, Lemma 1.3.5 implies that $\Lambda_\mp^z \Lambda_\pm^z$ extends to a bounded operator from $H^{-1/2}(\Sigma)^4$ to $H^{1/2}(\Sigma)^4$. Therefore, the same method as in the proof of Theorem 2.2.1 yields that

$$\mathrm{dom}(H_{\zeta,\upsilon}^*) = \mathrm{dom}(H_{\zeta,\upsilon}) = \left\{u + \Phi[g] : u \in H^1(\mathbb{R}^3)^4, g \in H^{1/2}(\Sigma)^4, t_\Sigma u = -\Lambda_+[g]\right\}.$$

Therefore, $H_{\zeta,\upsilon}$ is self-adjoint and $\mathrm{dom}(H_{\zeta,\upsilon}) \subset H^1(\mathbb{R}^3 \setminus \Sigma)^4$. Assertions (i) and (ii) can be proved as in Proposition 2.3.1.

Now assume that Σ satisfies (H1). Then, $\Phi^z(\Lambda_+^z)^{-1}(\Phi^{\bar{z}})^*$ is a compact operator in $L(\mathbb{R}^3)^4$ and $\mathrm{Sp}_{\mathrm{ess}}(H) = (-\infty, -m] \cup [m, +\infty)$, and thus the assertion (iii) follows immediately from (ii) and Weyl's theorem. Finally, assertion (iv) is a consequence of the Sobolev injection. Indeed, one can easily adapt the proof of Theorem 2.3.2 and show that $\mathrm{Sp}_{\mathrm{disc}}(H_{\zeta,\upsilon}) \cap (-m, m)$ is finite. We omit the details. □

In the following theorem, we discuss the self-adjointness of $H_{\zeta,\upsilon}$ in the critical case, i.e. $\zeta^2 + \upsilon^2 = 4$. We mention that the assertions (a) and (c) have already been proved in [65], where the author studied the inner part of $H_{0,\pm 2}$ acting on Ω_+, known as the Dirac operator with zig-zag boundary conditions, we refer to [41] for the two-dimensional case.

Theorem 2.4.2. *Let $(\zeta, \upsilon) \in \mathbb{R}^2$ be such that $\zeta^2 + \upsilon^2 = 4$, then $H_{\zeta,\upsilon}$ is essentially self -adjoint and we have*

$$\mathrm{dom}(\overline{H_{\zeta,\upsilon}}) = \left\{u + \Phi[g] : u \in H^1(\mathbb{R}^3)^4, g \in H^{-1/2}(\Sigma)^4, t_\Sigma u = -\widetilde{\Lambda}_+[g]\right\}. \tag{2.4.1}$$

Moreover, the following assertions hold true:

(i) $a \in \mathrm{Sp}(\overline{H_{\zeta,\upsilon}}) \Longleftrightarrow -a \in \mathrm{Sp}(\overline{H_{-\zeta,\upsilon}})$.

(ii) *For all* $z \in \rho(H) \cap \rho(\overline{H_{\zeta,\upsilon}})r$, *the operator* $\widetilde{\Lambda}_+^z$ *takes the space* $\{g \in H^{-1/2}(\Sigma)^4 : \widetilde{\Lambda}_+^z[g] \in H^{1/2}(\Sigma)^4\}$ *bijectively to* $H^{1/2}(\Sigma)^4$. *In particular,* $\widetilde{\Lambda}_+^z$ *admits a bounded inverse from* $H^{1/2}(\Sigma)^4$ *to* $H^{-1/2}(\Sigma)^4$, *and we have*

$$(\overline{H_{\zeta,\upsilon}} - z)^{-1} = (H - z)^{-1} - \Phi^z(\widetilde{\Lambda}_+^z)^{-1}(\Phi^{\overline{z}})^*.$$

(iii) *If* $\zeta = 0$, *then* Σ *becomes impenetrable and it holds that*

$$\overline{H_{0,\upsilon}} = H_\upsilon^{\Omega_+} \oplus H_\upsilon^{\Omega_-} = (-i\alpha\cdot\nabla + m\beta) \oplus (-i\alpha\cdot\nabla + m\beta)\,, \tag{2.4.2}$$

where $H_\upsilon^{\Omega_\pm}$ *are the self-adjoint Dirac operators defined on*

$$\mathrm{dom}(H_\upsilon^{\Omega_\pm}) = \Big\{\varphi_\pm \in L^2(\Omega_\pm)^4 : (\alpha\cdot\nabla)\varphi_\pm \in L^2(\Omega_\pm)^4 \text{ and } P_{\mp,\upsilon}t_\Sigma\varphi_\pm = 0\Big\}\,,$$

where the boundary condition has to be understood as an equality in $H^{-1/2}(\Sigma)^4$, *and* $P_{\pm,\upsilon}$ *are the projectors defined by*

$$P_{\pm,\upsilon} = \frac{1}{2}\left(I_4 \pm \frac{\upsilon}{2}\beta\right). \tag{2.4.3}$$

Furthermore, we have

(a) $-m$ *and* m *are eigenvalues of* $\overline{H_{0,\upsilon}}$ *with infinite multiplicities.*

(b) $\mathrm{Sp}(\overline{H_{0,\upsilon}}) = (-\infty, -m] \cup [m, +\infty)$.

(c) *if* Σ *satisfies* (H1) *and* $\{\lambda_j\}_{j\in\mathbb{N}^*}$ *is the sequence of eigenvalues of the Dirichlet Laplacian* $(-\Delta)$ *in* Ω_+, *counted with their multiplicities. Then, for all* $j \in \mathbb{N}^*$, $\lambda_j^\pm(m) = \pm\sqrt{m^2 + \lambda_j}$ *is an embedded eigenvalue of* $\overline{H_{0,\upsilon}}$ *with finite multiplicity.*

Proof. Let us show the first statement. The proof is a relatively straightforward modification of the technique used in the proof of Theorem 2.2.1. Indeed, as $H_{\zeta,\upsilon}$ is closable the only thing left to prove is the inclusion $H_{\zeta,\upsilon}^* \subset \overline{H_{\zeta,\upsilon}}$. For this, let $\varphi = u + \Phi[g] \in \mathrm{dom}(H_{\zeta,\upsilon}^*)$ and let $(h_j)_{j\in\mathbb{N}} \subset H^{1/2}(\Sigma)^4$ be a sequence of functions that converges to g in $H^{-1/2}(\Sigma)^4$. Set

$$g_j := \frac{1}{2}\left(\zeta\gamma_5 + i\upsilon\beta(\alpha\cdot N)\right)\left(\widetilde{\Lambda}_+[g] + \Lambda_-[h_j]\right), \quad \forall j \in \mathbb{N}.$$

Clearly, $(g_j)_{j\in\mathbb{N}} \subset H^{1/2}(\Sigma)^4$. Since Λ_+ is bounded from $H^{1/2}(\Sigma)^4$ onto itself, we then get that $(\Lambda_+[g_j])_{j\in\mathbb{N}} \subset H^{1/2}(\Sigma)^4$. Now, remark that

$$-\frac{1}{2}\left(\zeta\gamma_5 + i\upsilon\beta(\alpha\cdot N)\right)\widetilde{\Lambda}_-[g] = -g + \frac{1}{2}\left(\zeta\gamma_5 + i\upsilon\beta(\alpha\cdot N)\right)\widetilde{\Lambda}_+[g].$$

Using this, we obtain that

$$g_j := g - \frac{1}{2}\left(\zeta\gamma_5 + i\upsilon\beta(\alpha\cdot N)\right)\widetilde{\Lambda}_-[h_j - g], \quad \forall j \in \mathbb{N}.$$

As $\widetilde{\Lambda}_-$ is bounded from $H^{-1/2}(\Sigma)^4$ onto itself, it follows that $g_j \xrightarrow[j\to\infty]{} g$ in $H^{-1/2}(\Sigma)^4$. Moreover, we have

$$\widetilde{\Lambda}_+[g_j - g] = -\frac{1}{2}\widetilde{\Lambda}_+\left(\zeta\gamma_5 + i\upsilon\beta(\alpha\cdot N)\right)\widetilde{\Lambda}_-[g - h_j] = \left(\widetilde{\Lambda}_+\widetilde{\Lambda}_-\widetilde{\Lambda}_- + \Lambda_+\widetilde{\Lambda}_+\widetilde{\Lambda}_-\right)[h_j - g]. \tag{2.4.4}$$

From the proof of Theorem 2.4.1 we know that

$$\widetilde{\Lambda}_{\mp}\widetilde{\Lambda}_{\pm} = -\widetilde{\mathscr{C}}_{\Sigma}(\alpha\cdot N)\{\alpha\cdot N,\widetilde{\mathscr{C}}_{\Sigma}\} \pm \frac{m\zeta}{2}\gamma_5\beta S \pm \frac{iv}{4}\Big(\beta\{\alpha\cdot N,\widetilde{\mathscr{C}}_{\Sigma}\} - \{\beta,\widetilde{\mathscr{C}}_{\Sigma}\}(\alpha\cdot N)\Big). \quad (2.4.5)$$

Thus, it follows from Lemma 1.3.5 that $\widetilde{\Lambda}_{\pm}\widetilde{\Lambda}_{\mp}$ are bounded from $H^{-1/2}(\Sigma)^4$ to $H^{1/2}(\Sigma)^4$. Therefore, (2.4.4) yields that

$$\Lambda_+[g_j] \xrightarrow[j\to\infty]{} \widetilde{\Lambda}_+[g], \text{ in } H^{1/2}(\Sigma)^4.$$

Let

$$v_j = \mathcal{E}\left(\frac{1}{2}\widetilde{\Lambda}_+\left(\zeta\gamma_5 + iv\beta(\alpha\cdot N)\right)\widetilde{\Lambda}_-[h_j - g]\right) \in H^1(\mathbb{R}^3)^4, \quad \forall j \in \mathbb{N},$$

and define $\varphi_j := u_j + \Phi[g_j]$, where $u_j = u - v_j$. It is clear that $u_j \in H^1(\mathbb{R}^3)^4$ and $t_\Sigma u_j = -\Lambda_+[g_j] \in H^{1/2}(\Sigma)^4$, hence $(\varphi_j)_{j\in\mathbb{N}} \subset \mathrm{dom}(H_{\zeta,v})$. Moreover, since $(h_j)_{j\in\mathbb{N}}$ (resp $(g_j)_{j\in\mathbb{N}}$) converges to g in $H^{-1/2}(\Sigma)^4$ as $j \longrightarrow \infty$, using the continuity of $\widetilde{\Lambda}_{\pm}\widetilde{\Lambda}_{\mp}$ it follows that

$$(\varphi_j, H_{\zeta,v}\varphi_j) \xrightarrow[j\to\infty]{} (\varphi, H^*_{\zeta,v}\varphi) \text{ in } L^2(\mathbb{R}^3)^4.$$

Therefore $H^*_{\zeta,v} \subset \overline{H_{\zeta,\mu}}$ and hence $\overline{H_{\zeta,v}}$ is self-adjoint and $\mathrm{dom}(\overline{H_{\zeta,v}})$ is given by (2.4.1), and this finishes the proof of the first statement.
In order to continue the proof of the theorem we use the definition of $\mathrm{dom}(\overline{H_{\zeta,v}})$ with transmission condition. As in Definition 2.2.2, using the Plemelj-Sokhotski formula, one can show that $\overline{H_{\zeta,v}}$ acts in the sense of distributions as

$$\overline{H_{\zeta,v}}\varphi = \left(-i\nabla\cdot\alpha + m\beta\right)\varphi_+ \oplus \left(-i\nabla\cdot\alpha + m\beta\right)\varphi_-,$$

for $\varphi = (\varphi_+,\varphi_-) \in L^2(\mathbb{R}^3)^4$ such that $(\alpha\cdot\nabla)\varphi_\pm \in L^2(\Omega_\pm)^4$ and satisfies the following transmission condition in $H^{-1/2}(\Sigma)^4$:

$$\left(\frac{1}{2}(\zeta\gamma_5 + iv\beta(\alpha\cdot N)) + i(\alpha\cdot N)\right)t_\Sigma\varphi_+ = -\left(\frac{1}{2}(\zeta\gamma_5 + iv\beta(\alpha\cdot N)) - i(\alpha\cdot N)\right)t_\Sigma\varphi_-.$$

Now, let us show item (i), for this recall the operator C defined in (2.3.27). Then, a trivial computation yields that

$$\varphi \in \mathrm{dom}(\overline{H_{\zeta,v}}) \Longleftrightarrow C[\varphi] \in \mathrm{dom}(\overline{H_{-\zeta,v}}).$$

Since for all $u \in L^2(\mathbb{R}^3)^4$, we have

$$C[(-i\alpha\cdot\nabla + m\beta)u] = -(-i\alpha\cdot\nabla + m\beta)C[u],$$

it follows that a belongs to $\mathrm{Sp}(\overline{H_{\zeta,v}})$ if and only if $-a$ belongs to $\mathrm{Sp}(\overline{H_{-\zeta,v}})$, which yields (i).
Item (ii) follows in the same way as Proposition 2.3.1. To prove item (iii), observe that

$$\mathrm{dom}(\overline{H_{0,v}}) = \Big\{\varphi = (\varphi_+,\varphi_-) \in L^2(\Omega_+)^4 \oplus L^2(\Omega_-)^4 : (\alpha\cdot\nabla)\varphi_\pm \in L^2(\Omega_\pm)^4 \text{ and}$$
$$i(\alpha\cdot N)P_{-,v}t_\Sigma\varphi_+ = i(\alpha\cdot N)P_{+,v}t_\Sigma\varphi_-\Big\},$$

where $P_{\pm,v}$ are the projectors given by (2.4.3). From this we deduce that a function $\varphi = (\varphi_+,\varphi_-) \in L^2(\Omega_+)^4 \oplus L^2(\Omega_-)^4$ with $(\alpha\cdot\nabla)\varphi_\pm \in L^2(\Omega_\pm)^4$ belongs to $\mathrm{dom}(\overline{H_{0,v}})$ if and only if $P_{\mp,\upsilon} t_\Sigma \varphi_\pm = 0$ holds in $H^{-1/2}(\Sigma)^4$. Therefore, Σ becomes impenetrable and the decomposition (2.4.2) holds true.

In the rest of the proof we assume that $\upsilon = 2$, the case $\upsilon = -2$ can be recovered by the same arguments. Let us show the assertion (a). To do this, we first show that $-m$ is an eigenvalue of $H_2^{\Omega_+}$ with infinite multiplicity, and hence of $\overline{H_{0,2}}$. Observe that, for any $\varphi = (\varphi_1, \varphi_2)^\top \in \mathrm{dom}(H_2^{\Omega_+})$, we have $\varphi_1 \in H_0^1(\Omega_+)^2$ and $(\sigma \cdot \nabla)\varphi_2 \in L^2(\Omega_+)^2$. Let $\psi \in C^2(\Omega_+)^2$ be a harmonic function with respect to $\sigma \cdot \nabla$ (i.e. $(\sigma \cdot \nabla)\psi = 0$ in Ω_+) and set $\varphi = (0, \psi)^\top$.Clearly $\varphi \in \mathrm{dom}(H_2^{\Omega_+})$, and we have that

$$(H_2^{\Omega_+} + m)\varphi = \begin{pmatrix} -i(\sigma \cdot \nabla)\psi \\ 0 \end{pmatrix} + m \begin{pmatrix} 2 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ \psi \end{pmatrix} = 0.$$

Since the set of harmonic functions with respect to $(\sigma \cdot \nabla)$ is infinite dimensional, we get that $-m$ is an eigenvalue of $\overline{H_{0,2}}$ with infinite multiplicity. By (i) we also get that m is an eigenvalue of $\overline{H_{0,2}}$ with infinite multiplicity, which proves the assertion (a).

Now we are going to prove (b) and (c), for this purpose, we consider the following Dirac operators

$$D_2^{\Omega_\pm}\psi = (-i\alpha \cdot \nabla + m\beta)\,\psi, \quad \psi \in \mathrm{dom}(D_2^{\Omega_\pm}) = \left\{\varphi_\pm \in H^1(\Omega_\pm)^4 : P_{\mp,2} t_\Sigma \varphi_\pm = 0\right\}.$$

Then, one can easily verify that $D_2^{\Omega_\pm}$ are symmetric and closable operators. Moreover, it holds that $\overline{D_2^{\Omega_\pm}} = H_2^{\Omega_\pm}$. Indeed, denote by $\mathfrak{Q}_2^{\Omega_\pm}$ the quadratic form associated to $(D_2^{\Omega_\pm})^2$. Given $\varphi \in \mathrm{dom}(D_2^{\Omega_\pm})$, using the Green's formula and the boundary conditions, it easily follows that:

$$\mathfrak{Q}_2^{\Omega_\pm}[\varphi] = \|(\alpha \cdot \nabla)\varphi\|^2_{L^2(\Omega_\pm)^4} + m^2 \|\varphi\|^2_{L^2(\Omega_\pm)^4}. \tag{2.4.6}$$

Hence, we get $\mathfrak{Q}_2^{\Omega_\pm}[\varphi] \geqslant m^2 \|\varphi\|^2_{L^2(\Omega_\pm)^4}$. Thus $(D_2^{\Omega_\pm})^2$ is lower semi-bounded. Therefore, by [50, Theorem 6.3.2] it follows that $(H_2^{\Omega_\pm})^2$ is the Friedrich's extension of $(D_2^{\Omega_\pm})^2$ and it holds that

$$\mathrm{Sp}(H_2^{\Omega_\pm}) \subset (-\infty, -m] \cup [m, +\infty).$$

From this we see that if Σ satisfies (H2), then $\mathrm{Sp}(\overline{H_{0,\upsilon}}) \subset (-\infty, -m] \cup [m, +\infty)$. Since similar arguments as those of the proof of Theorem 2.3.4 yield the inclusion $(-\infty, -m) \cup (m, +\infty) \subset \mathrm{Sp}(\overline{H_{0,\upsilon}})$, we then the statement (b) in this case.

In the rest of the proof we assume that Σ satisfies (H1). Let $(-\Delta^{\Omega_\pm})$ be the Dirichlet realization of $(-\Delta)$ in $\Omega_\pm$, with domain $H^2(\Omega_\pm) \cap H_0^1(\Omega_\pm)$. Using Weyl's theorem and the fact that $H_0^1(\Omega_+)$ is compactly embedded in $L^2(\Omega_+)$, it is not hard to show that

$$\begin{aligned} &\mathrm{Sp}(-\Delta^{\Omega_-} + m^2) = [m^2, +\infty), \\ &\mathrm{Sp}(-\Delta^{\Omega_+} + m^2) = \mathrm{Sp}_{\mathrm{disc}}(-\Delta^{\Omega_+} + m^2) = \{m^2 + \lambda_j, j \in \mathbb{N}\}, \end{aligned} \tag{2.4.7}$$

with $\lambda_j > 0$ for all $j \in \mathbb{N}$, and $\lambda_j \longrightarrow \infty$ as $j \longrightarrow \infty$. Using the boundary condition, we see that

$$\varphi = \begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix} \in \mathrm{dom}(D_2^{\Omega_+}) \Longrightarrow \varphi_2 \in H_0^1(\Omega_+)^2, \quad \varphi = \begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix} \in \mathrm{dom}(D_2^{\Omega_-}) \Longrightarrow \varphi_1 \in H_0^1(\Omega_-)^2. \tag{2.4.8}$$

We denote by $\widetilde{\mathfrak{Q}}^{\Omega_\pm}$ the quadratic form associated to $(-\Delta^{\Omega_\pm} + m^2)I_2$, that is

$$\widetilde{\mathfrak{Q}}^{\Omega_\pm}[u] = \|\nabla u\|^2_{L^2(\Omega_\pm)^2} + m^2\|u\|^2_{L^2(\Omega_\pm)^2}, \quad \forall u \in H^1_0(\Omega_\pm)^2.$$

Note that, for every $u \in H^2(\Omega_\pm)^2 \cap H^1_0(\Omega_\pm)^2$, it holds that

$$\begin{aligned}\|(\sigma\cdot\nabla)u\|^2_{L^2(\Omega_\pm)^2} &= \langle u, -\Delta u\rangle_{L^2(\Omega_\pm)^2} \pm \langle(\sigma\cdot N)t_\Sigma u, t_\Sigma(\sigma\cdot\nabla)u\rangle_{H^{1/2}(\Sigma)^2} \\ &= \|\nabla u\|^2_{L^2(\Omega_\pm)^2} \pm \langle(t_\Sigma u, (N\cdot\nabla)t_\Sigma u\rangle_{H^{1/2}(\Sigma)^2} = \|\nabla u\|^2_{L^2(\Omega_\pm)^2}.\end{aligned}$$

By density, it also holds for all $u \in H^1_0(\Omega_\pm)^2$. Using this and (2.4.8), it follows from (2.4.6) that

$$\begin{aligned}\mathfrak{Q}_2^{\Omega_+}[\varphi] &= \|(\sigma\cdot\nabla)\varphi_1\|^2_{L^2(\Omega_+)^2} + m^2\|\varphi_1\|^2_{L^2(\Omega_+)^2} + \widetilde{\mathfrak{Q}}^{\Omega_+}[\varphi_2], \quad \forall\varphi \in \mathrm{dom}(D_2^{\Omega_+}),\\ \mathfrak{Q}_2^{\Omega_-}[\varphi] &= \|(\sigma\cdot\nabla)\varphi_2\|^2_{L^2(\Omega_-)^2} + m^2\|\varphi_2\|^2_{L^2(\Omega_-)^2} + \widetilde{\mathfrak{Q}}^{\Omega_-}[\varphi_1], \quad \forall\varphi \in \mathrm{dom}(D_2^{\Omega_-}).\end{aligned}$$

Thus, (2.4.7) together with assertion (i) yield that $\lambda_j^\pm(m) = \pm\sqrt{m^2+\lambda_j}$ is an eigenvalue of $\overline{H_{0,2}}$ with finite multiplicity, and that

$$\mathrm{Sp}(\overline{H_{0,2}}) = (-\infty, -m] \cup [m, +\infty),$$

which yields (b) and (c) for Σ satisfying (H1), and achieves the proof of theorem. □

We finish this Chapter by pointing out the following remark and its consequence.

Remark 2.4.2. *Let $\zeta = \pm 2$ and let $\overline{H_{\zeta,0}}$ be as in Theorem 2.4.2. Given $(\varphi_+, \varphi_-) \in \mathrm{dom}(\overline{H_{\zeta,0}})$, we write $\varphi_\pm = (\varphi_{\pm,1}, \varphi_{\pm,2})^\top$. Then, one can write the transmission condition as follows:*

$$t_\Sigma\varphi_{+,1} = \frac{i\zeta}{2}(\sigma\cdot N)t_\Sigma\varphi_{-,2}, \quad t_\Sigma\varphi_{+,2} = \frac{i\zeta}{2}(\sigma\cdot N)t_\Sigma\varphi_{-,1}.$$

Thus, we deduce that $\overline{H_{\zeta,0}}$ coincide with the Dirac operator coupled with the electrostatic δ-interactions of strength $-\zeta$. Hence, in this sense, one can consider the potential V_ζ as an electrostatic potential for $\zeta = \pm 2$.

As a direct consequence of Theorem 2.3.4 and Remark 2.4.2 we have:

Corollary 2.4.1. *Let $\overline{H_{\zeta,\upsilon}}$ be as in Theorem 2.4.2. If $\zeta = \pm 2$ and $\upsilon = 0$, then*

$$\mathrm{Sp}_{\mathrm{ess}}(\overline{H_{\zeta,\upsilon}}) = \big(-\infty, -m\big] \cup \{0\} \cup \big[m, +\infty\big).$$

Chapter 3

Analysis of Dirac operators with δ-interactions supported on the boundaries of rough domains

The results presented in this chapter have been the subject of the paper [30].

Throughout this chapter, unless stated otherwise, we always assume that $\Omega \subset \mathbb{R}^3$ is a bounded UR domain (see Definition 1.1.2) with $\partial\Omega = \partial\overline{\Omega}$, and we set

$$\Omega_+ = \Omega \;\text{ and }\; \Omega_- := \mathbb{R}^3 \setminus \overline{\Omega}, \quad \Sigma = \partial\Omega. \tag{3.0.1}$$

Our main goal in this chapter is to investigate the spectral properties of Dirac operators of the form $H_{a,\tau} = H + A_{a,\tau}\delta_\Sigma$, where $A_{a,\tau}$ is a bounded invertible, self-adjoint operator in $L^2(\Sigma)^4$, depending on parameters $(a,\tau) \in \mathbb{R}\times\mathbb{R}^n$, $n \geqslant 1$. We investigate the self-adjointness and the related spectral properties of $H_{a,\tau}$, such as the phenomenon of confinement and the Sobolev regularity of the domain in different situations. More precisely, the structure of the chapter is as follows. Sections 3.1 and 3.2 are the heart of the chapter and contain our most important contributions. In Section 3.1, we provide the necessary materials to tackle all the problems related to the self-adjointness, the confinement phenomenon and the characterization of the (essential/discrete) spectrum of the operator H_τ. To be precise, it contains Theorem 3.1.2 about the self-adjointness in the critical case, a general criterion on the perturbed Dirac operator H_τ to induce the confinement phenomenon (see Propositions 3.1.3 and 3.1.4) and the proof of the Birman-Schwinger principle and the Krein-resolvent formula in the Lipschitz case (see Proposition 3.1.1).

Section 3.2, is divided into four subsections as follows. Subsection 3.2.1, is devoted to the study of the Dirac operator H_κ (which has already been studied in Chapter 2)

$$H_\kappa = H + V_\kappa = H + (\epsilon I_4 + \mu\beta + \eta(\alpha\cdot N))\delta_\Sigma, \quad \kappa := (\epsilon,\mu,\eta) \in \mathbb{R}^3,$$

when Ω is a Lipschitz domain with a normal in VMO. In there, we explore the connection between the geometric properties of the domain Ω and the compactness of the anticommuatator $\{\alpha\cdot N, \mathscr{C}_\Sigma\}$, and we give the spectral properties of H_κ for non-critical parameters, the main results being Theorem 3.2.1 and Theorem 3.2.2. Subsequently, in subsection 3.2.2, we prove Theorem 3.2.3 about the Sobolev regularity of $\mathrm{dom}(H_\kappa)$, in the case of Hölder's domains $C^{1,\omega}$. After this, we consider in subsection 3.2.3 the couplings $(H + V_\epsilon + V_\mu)$ and $(H + V_\eta)$, in the case of UR domains. The main results in this subsection are Theorem 3.2.4 and Theorem 3.2.5 and their consequences regarding the confinement phenomenon.

Being interested by the question of confinement and self-adjointness of Dirac operators with boundary conditions, we introduce and study in subsection 3.2.4 the spectral properties of the new Dirac operators

$$H_{\tilde{\mu}} = H + V_{\tilde{v}} = H + i\tilde{\mu}\gamma_5\beta\delta_\Sigma, \quad \tilde{\mu} \in \mathbb{R},$$
$$H_{\tilde{v}} = H + V_{\tilde{v}} = H + i\tilde{v}\gamma_5\beta(\alpha\cdot N)\delta_\Sigma, \quad \tilde{v} \in \mathbb{R}.$$

Namely, we show that $H_{\tilde{\mu}}$ ($H_{\tilde{v}}$) shares almost the same properties as the Dirac operator coupled with the Lorentz scalar (respectively the anomalous magnetic) δ-interactions, and in particular, it generates the confinement when $\tilde{\mu} = \pm 2$ (respectively $\tilde{v} = \pm 2$), cf. Propositions 3.2.7 and 3.2.9. In the same spirit, being motivated by the natural way that the Calderón's projector appears in our analysis (see Proposition 1.3.2), we consider in Section 3.3 the families of Dirac operators with δ-interactions defined by:

$$(-m, m) \ni a \longmapsto H_{a,\lambda} = H + \lambda\mathscr{C}^a\delta_\Sigma, \quad \lambda \in \mathbb{R}\setminus\{0\},$$
$$(-m, m) \ni a \longmapsto H_{a,\lambda'} = H + \lambda'(\alpha\cdot N)\mathscr{C}^a_\Sigma(\alpha\cdot N)\delta_\Sigma, \quad \lambda' \in \mathbb{R}\setminus\{0\},$$

where $\mathscr{C}^a_\Sigma$ is the Cauchy operator associated with $(H-a)$. There, we prove that $H_{a,\lambda}$ and $H_{a,\lambda'}$ induce the confinement, and that the boundary conditions of the resulting Dirac operator are exactly given by the Calderón's projector or its adjoint.

3.1 Self-adjointness and confinement: critical and non-critical case

In this section, we gather the main tools to tackle the different problems that we are going to consider. Before going any further, let us define the general form of the operators we are interested on and explain the philosophy of our technique.

Let $A_\tau : L^2(\Sigma)^4 \longrightarrow L^2(\Sigma)^4$ be a bounded invertible, and self-adjoint operator depending on a parameter $\tau \in \mathbb{R}^n$ with $n \in \mathbb{N}^*$. We assume that the inverse of A_τ is given explicitly by

$$A_\tau^{-1} = \frac{1}{\operatorname{sgn}(\tau)}\widetilde{A}_\tau, \tag{3.1.1}$$

where $\operatorname{sgn}(\tau)$ is a real number, defined by $\operatorname{sgn}(\tau)I_4 = \widetilde{A}_\tau A_\tau = A_\tau\widetilde{A}_\tau$. Except for some special situations, we always deal with the case $\operatorname{sgn}(\tau) \neq 0$. For the case $\operatorname{sgn}(\tau) = 0$ we need to slightly modify our definition to handle such a situation.

Next, we define the operators $\Lambda^z_{\tau,\pm}$ as follows:

$$\Lambda^z_{\tau,\pm} = A_\tau^{-1} \pm \mathscr{C}^z_\Sigma, \quad \forall z \in \mathbb{C}\setminus((-\infty,-m]\cup[m,\infty)). \tag{3.1.2}$$

Clearly, $\Lambda^z_{\tau,\pm}$ are bounded (and self-adjoint for $z \in (-m, m)$) from $L^2(\Sigma)^4$ onto itself. In the sequel, we shall write Φ, $\mathscr{C}_\Sigma$, $C_\pm$ and $\Lambda_{\tau,\pm}$ instead of Φ^0, $\mathscr{C}^0_\Sigma$, $C^0_\pm$ and $\Lambda^0_{\tau,\pm}$.

Now, we define the perturbed Dirac operator H_τ acting in $L^2(\mathbb{R}^3)^4$, by

$$H_\tau = H + V_\tau = H + A_\tau\delta_\Sigma, \tag{3.1.3}$$

on the domain

$$\operatorname{dom}(H_\tau) = \left\{\varphi = u + \Phi[g] : u \in H^1(\mathbb{R}^3)^4, g \in L^2(\Sigma)^4, t_\Sigma u = -\Lambda_{\tau,+}[g]\right\}, \tag{3.1.4}$$

where

$$V_\tau(\varphi) = \frac{1}{2}A_\tau(\varphi_+ + \varphi_-)\delta_\Sigma \quad \text{and} \quad \varphi_\pm = t_\Sigma u + \Phi|^{\mathrm{nt}}_{\Omega_\pm}[g]. \tag{3.1.5}$$

Notice that H_τ is well defined and acts in the sense of distributions as $H_\tau(\varphi) = H(u)$, for all $\varphi = u + \Phi[g] \in \mathrm{dom}(H_\tau)$. Indeed, thanks to Proposition 1.2.2, we know that for any $u \in H^1(\mathbb{R}^3)^4$, $t_\Sigma u$ is well defined and belongs to the Besov space $B^2_{1/2}(\Sigma)^4$. Next, recall that the mapping $\Phi : L^2(\Sigma)^4 \longrightarrow L^2(\mathbb{R}^3)^4$ is well-defined and bounded by Proposition 1.3.1, moreover, by Lemma 1.3.2 we also know that $\Phi|^{\mathrm{nt}}_{\Omega_\pm}$ exists and is bounded in $L^2(\Sigma)^4$. Thus, for all $\varphi = u + \Phi[g] \in \mathrm{dom}(H_\tau)$ we have

$$\begin{aligned} V_\tau(\varphi) =& \frac{1}{2}A_\tau(\varphi_+ + \varphi_-)\delta_\Sigma = \frac{1}{2}A_\tau(t_\Sigma u + \Phi|^{\mathrm{nt}}_{\Omega_\pm}[g] \\ =& A_\tau(t_\Sigma u + \mathscr{C}_\Sigma[g]) = A_\tau(-\Lambda_{\tau,+} + \mathscr{C}_\Sigma)[g] = -(A_\tau)(A_\tau^{-1})[g] = -g, \end{aligned}$$

and since $H_\tau(\varphi) = Hu + g\sigma + V_\tau(\varphi)$ holds in the sense of distributions, from the above computation we see that $H_\tau(\varphi) = Hu \in L^2(\mathbb{R}^3)^4$. Finally, let $u, v \in H^1(\mathbb{R}^3)^4$ and $g, h \in L^2(\Sigma)^4$, then

$$Hu + g\sigma = H(u + \Phi[g]) = H(u + \Phi[g]) = Hv + h\sigma.$$

Since σ is 2-dimensional, and thus, the Lebesgue measure in $\mathbb{R}^3$ and σ are mutually singular, it follows that $g = h$ in $L^2(\Sigma)^4$ and $H(u - v) = 0$ in $L^2(\mathbb{R}^3)^4$. Since H is self-adjoint in $H^1(\mathbb{R}^3)^4$, we also get that $u = v$. Thus, if $u, v \in H^1(\mathbb{R}^3)^4$ and $g, h \in L^2(\Sigma)^4$ are such that $u + \Phi[g] = v + \Phi[h]$, then $u = v$ and $g = h$, and therefore, H_τ is well defined.

As we have seen in Chapter 2, for some particular values of $\mathrm{sgn}(\tau)$, two interesting phenomena appear in the spectral study of the Dirac operator H_τ. The first one is the confinement phenomenon, assuming that H_τ is essentially self-adjoint, from the mathematical point of view this means that for any datum $\varphi_0 \in \mathrm{dom}(\overline{H_\tau})$ with support in $\Omega_\pm$, the unique solution $\varphi \in C^1(\mathbb{R}, L^2(\mathbb{R}^3)^4)$ of the following Cauchy problem

$$\begin{cases} i\partial_t\varphi(t,x) = \overline{H_\tau}\varphi(t,x), \\ \quad \varphi(0,x) = \varphi_0(x), \end{cases} \tag{3.1.6}$$

remains for all times supported in $\Omega_\pm$. More concretely, if we let

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

Then $\overline{H_\tau}$ decouples as follows

$$\overline{H_\tau} = H_\tau^{\Omega_+} \oplus H_\tau^{\Omega_-}, \tag{3.1.7}$$

where $H_\tau^{\Omega_\pm}$ are self-adjoint Dirac operators acting in $\Omega_\pm$ with some boundary conditions. Moreover, the propagator satisfies

$$e^{-it\overline{H}_\tau} = e^{-itH_\tau^{\Omega_+}} \oplus e^{-itH_\tau^{\Omega_-}}.$$

In this chapter, we always use the characterization (3.1.7), and we say that $\overline{H}_\tau$ (or V_τ) generates confinement or equivalently Σ is impenetrable.

The second one is called critical combinations of the coupling constants, it results in the loss of the Sobolev regularity of functions in the domain of H_τ for smooth domain Ω_+, i.e $\mathrm{dom}(\overline{H_\tau}) \not\subset H^s(\mathbb{R}^3 \setminus \Sigma)^4$, for all $s > 0$. To our knowledge, there is no fixed definition for such a case, because the spectral study of H_τ depends significantly on the smoothness of the domain Ω_+. As we have pointed out in Chapter 2, it seems that the C^2-smoothness condition on Ω_+ is necessary to prove the self-adjointness in $L^2(\mathbb{R}^3)^4$ of H_τ in such a case. Thus, for our applications we fix the definition of the critical combinations of the coupling constants as follows:

Definition 3.1.1 (Critical parameters)**.** *Let Ω_+ be a bounded C^2-smooth domain and let H_τ be as in (3.1.4). We say that the parameter $\tau \in \mathbb{R}^n$, $n \in \mathbb{N}^*$, is critical if $\Lambda_{\tau,+} \in \mathcal{K}(L^2(\Sigma)^4)$ or $\Lambda_{\tau,\mp}\Lambda_{\tau,\pm} \in \mathcal{K}(L^2(\Sigma)^4)$.*

In what follows, we shall use the phrase *"characteristics of the model"*, or simply *"characteristics of the potential"*, to refer to the above phenomena.

3.1.1 Non-critical parameters

As already mentioned in the introduction, the self-adjointness (in the non-critical case) of the Dirac operator H_τ will be derived using the main result of [10]. Notice that the way [10, Theorem 2.11(iii)] was stated does not take into account the case of UR domains, but can extend to this case without any difficulty. However, for the sake of completeness and for the convenience of the reader, we give here the proof of this result which reads as follows.

Theorem 3.1.1. *Suppose that Ω_+ is a UR domain, and let H_τ and $\Lambda_{\tau,+}$ be as above. If $\Lambda_{\tau,+}$ is a Fredholm operator, then $(H_\tau, \mathrm{dom}(H_\tau))$ is self-adjoint.*

Proof. We first prove that $(H_\tau, \mathrm{dom}(H_\tau))$ is closable. For this, note that $C_0^\infty(\mathbb{R}^3 \setminus \Sigma)^4 \subset \mathrm{dom}(H_\tau) \subset L^2(\mathbb{R}^3)^4$, and since $C_0^\infty(\mathbb{R}^3 \setminus \Sigma)^4$ is a dense subspace of $L^2(\mathbb{R}^3)^4$ it follows that $\mathrm{dom}(H_\tau)$ is a dense subspace of $L^2(\mathbb{R}^3)^4$. We next show that H_τ is symmetric on $\mathrm{dom}(H_\tau)$. So, let $\varphi, \psi \in \mathrm{dom}(H_\tau)$ with $\varphi = u + \Phi[g]$ and $\psi = v + \Phi[h]$, then we have

$$\begin{aligned}\langle H_\tau\varphi, \psi\rangle_{L^2(\mathbb{R}^3)^4} - \langle \varphi, H_\tau\psi\rangle_{L^2(\mathbb{R}^3)^4} &= \langle Hu, v + \Phi[h]\rangle_{L^2(\mathbb{R}^3)^4} - \langle u + \Phi[g], Hv\rangle_{L^2(\mathbb{R}^3)^4}\\ &= \langle Hu, v\rangle_{L^2(\mathbb{R}^3)^4} - \langle u+, Hv\rangle_{L^2(\mathbb{R}^3)^4} + \langle Hu, \Phi[h]\rangle_{L^2(\mathbb{R}^3)^4} - \langle \Phi[g], Hv\rangle_{L^2(\mathbb{R}^3)^4}\\ &= \langle Hu, \Phi[h]\rangle_{L^2(\mathbb{R}^3)^4} - \langle \Phi[g], Hv\rangle_{L^2(\mathbb{R}^3)^4}.\end{aligned}$$

Thanks to Lemma 1.3.3 we have that

$$\begin{aligned}\langle Hu, \Phi[h]\rangle_{L^2(\mathbb{R}^3)^4} - \langle \Phi[g], Hv\rangle_{L^2(\mathbb{R}^3)^4} &= \langle \Phi^* Hu, h\rangle_{L^2(\Sigma)^4} - \langle g, \Phi^* Hv\rangle_{L^2(\Sigma)^4}\\ &= \langle t_\Sigma(H^{-1}H)u, h\rangle_{L^2(\Sigma)^4} - \langle g, t_\Sigma(H^{-1}H)v\rangle_{L^2(\Sigma)^4}\\ &= \langle t_\Sigma u, h\rangle_{L^2(\Sigma)^4} - \langle g, t_\Sigma v\rangle_{L^2(\Sigma)^4},\end{aligned}$$

Thus, using the self-adjointness of $\Lambda_{\tau,+}$, the fact that $t_\Sigma u = -\Lambda_{\tau,+}[g]$ and $t_\Sigma v = -\Lambda_{+,\tau}[h]$, we obtain

$$\langle H_\tau\varphi, \psi\rangle_{L^2(\mathbb{R}^3)^4} - \langle \varphi, H_\tau\psi\rangle_{L^2(\mathbb{R}^3)^4} = \langle -\Lambda_{\tau,+}[g], h\rangle_{L^2(\Sigma)^4} - \langle g, -\Lambda_{\tau,+}[h]\rangle_{L^2(\Sigma)^4} = 0,$$

which actually means that H_τ is symmetric on $\mathrm{dom}(H_\tau)$, and hence, $(H_\tau, \mathrm{dom}(H_\tau))$ is closable. Thus, to prove the self-adjointness of $(H_\tau, \mathrm{dom}(H_\tau))$ it suffices to show the inclusions $H_\tau^* \subset H_\tau$. To this end, we claim that for any $\psi \in \mathrm{dom}(H_\tau^*)$ there is a sequence of functions $(h_j)_{j\in\mathbb{N}} \subset \mathrm{Kr}(\Lambda_{\tau,+})$ such that

$$\psi = \lim_{j\to\infty} (H^{-1}H_\tau^*\psi - \Phi[t_\Sigma H^{-1}H_\tau^*\psi] + \Phi[h_j]) \text{ in } L^2(\mathbb{R}^3)^4.$$

Notice that once this claim is shown we then get $H_\tau^* \subset H_\tau$. Indeed, since $\Lambda_{\tau,+}$ is Fredholm it follows that $\{\Phi[g] : g \in \mathrm{Kr}(\Lambda_{\tau,+})\}$ is closed in $L^2(\mathbb{R}^3)^4$, and hence, there is $h \in \mathrm{Kr}(\Lambda_{\epsilon,+})$ such that

$$\Phi[h_j] \xrightarrow[j\to\infty]{} \Phi[h] \ \text{ in } \ L^2(\mathbb{R}^3)^4.$$

Since $\Phi[h_j], \Phi[h] \in \mathrm{dom}(H_\tau)$, if we set $\psi_j = (H^{-1}H_\tau^*\psi - \Phi[t_\Sigma H^{-1}H_\tau^*\psi] + \Phi[h_j])$, then it is clear that $\psi_j \in \mathrm{dom}(H_\tau)$ and that $H_\tau\psi_j = H_\tau^*\psi$ for all $j \in \mathbb{N}$. Therefore, we get

$$(\psi_j, H_\tau\psi_j) \xrightarrow[j\to\infty]{} (\psi, H_\tau^*\psi) \ \text{ in } \ L^2(\mathbb{R}^3)^4,$$

which actually proves the inclusion $H_\tau^* \subset H_\tau$.

Let us now show the claim, so let $(\psi, G) \in \mathcal{G}(H_\tau^*)$, then we have

$$\langle H_\tau\varphi, \psi\rangle_{L^2(\mathbb{R}^3)^4} = \langle \varphi, G\rangle_{L^2(\mathbb{R}^3)^4}, \quad \forall \varphi = u + \Phi[g] \in \mathrm{dom}(H_\tau).$$

Since $H^{-1}G \in H^1(\mathbb{R}^3)^4$, using that $\Lambda_{\tau,+}$ is Fredholm it follows that $t_\Sigma H^{-1}G = h + \Lambda_{\tau,+}[f]$, with $h \in \mathrm{Kr}(\Lambda_{\tau,+})$. Clearly, $\Phi[h] \in \mathrm{dom}(H_\tau)$ and $H_\tau\Phi[h] = 0$, and thus we get

$$0 = \langle H_\tau\Phi[h], \psi\rangle_{L^2(\mathbb{R}^3)^4} = \langle \Phi[h], G\rangle_{L^2(\mathbb{R}^3)^4} = \langle h, t_\Sigma H^{-1}G\rangle_{L^2(\Sigma)^4},$$

where in the last equalities Lemma 1.3.3 was used. As $t_\Sigma H^{-1}G = h + \Lambda_{\tau,+}[f]$ and $\Lambda_{\tau,+}[h] = 0$, it follows from the self-adjointness of $\Lambda_{\tau,+}$ that

$$0 = \langle h, t_\Sigma H^{-1}G\rangle_{L^2(\Sigma)^4} = \langle h, h\rangle_{L^2(\Sigma)^4}.$$

From this, we conclude that $P_+ t_\Sigma H^{-1}G = \Lambda_{\epsilon,+}[f]$. Hence, combining Lemma 1.3.3 with the previous conclusion yield that

$$\begin{aligned}
\langle Hu, \psi\rangle_{L^2(\mathbb{R}^3)^4} = \langle u + \Phi[g], G\rangle_{L^2(\mathbb{R}^3)^4} &= \langle Hu, H^{-1}G\rangle_{L^2(\mathbb{R}^3)^4} + \langle g, t_\Sigma H^{-1}G\rangle_{L^2(\Sigma)^4} \\
&= \langle Hu, H^{-1}G\rangle_{L^2(\mathbb{R}^3)^4} + \langle g, \Lambda_{\tau,+}[f]\rangle_{L^2(\Sigma)^4} \\
&= \langle Hu, H^{-1}G\rangle_{L^2(\mathbb{R}^3)^4} - \langle t_\Sigma u, f\rangle_{L^2(\Sigma)^4},
\end{aligned}$$

From this it follows that $\langle Hu, \psi\rangle_{L^2(\mathbb{R}^3)^4} = \langle Hu, H^{-1}G - \Phi[f]\rangle_{L^2(\mathbb{R}^3)^4}$. Hence, we get

$$\langle Hu, \psi - (H^{-1}G - \Phi[f])\rangle_{L^2(\mathbb{R}^3)^4} = 0 \quad \text{for all } u \in H^1(\mathbb{R}^3)^4 \text{ such that } t_\Sigma u \in \mathrm{Rn}(\Lambda_{\tau,+}).$$

As $\Lambda_{\tau,+}$ is Fredholm and self-adjoint, using Lemma 1.3.3 we obtain that:

$$t_\Sigma u \in \mathrm{Rn}(\Lambda_{\tau,+}) \iff 0 = \langle t_\Sigma u, h\rangle_\Sigma = \langle Hu, \Phi[h]\rangle_{L^2(\mathbb{R}^3)^4} \ \text{ for all } \ h \in \mathrm{Kr}(\Lambda_{\tau,+}),$$

which entails that

$$\psi - H^{-1}G + \Phi[f] \in \{\Phi[g] : g \in \mathrm{Kr}(\Lambda_{\tau,+})\}.$$

Thus, for all $(\psi, G) \in \mathcal{G}(H_\tau^*)$, there exist $(h_j)_{j\in\mathbb{N}} \subset \mathrm{Kr}(\Lambda_{\tau,+})$ and $f \in \mathrm{Rn}(\Lambda_{\tau,+})$ such that the following hold:

$$\begin{gathered}
\lim_{j\to\infty} \Phi[h_j] = \Phi[h] \in \mathrm{dom}(H_\tau) \text{ with } h \in \mathrm{Kr}(\Lambda_{\tau,+}), \\
\psi = \lim_{j\to\infty} (H^{-1}G - \Phi[f] + \Phi[h_j]) = H^{-1}G - \Phi[f] + \Phi[h] \ \text{ in } L^2(\mathbb{R}^3)^4.
\end{gathered}$$

This proves the claim and completes the proof the theorem. □

To study the spectral properties of H_τ (for non-critical parameter) we shall restrict ourselves to the case of Lipschitz domains. The following proposition gives us a criterion for the existence of eigenvalues in the gap $(-m, m)$, and a Krein-type resolvent formula for H_τ.

Proposition 3.1.1. *Let H_τ be as in (3.1.4) with a non-critical parameter $\tau \in \mathbb{R}^n$. The following hold:*

(i) Given $z \in (-m, m)$, then $\mathrm{Kr}(H_\tau - z) \neq \{0\} \Longleftrightarrow \mathrm{Kr}(\Lambda^z_{\tau,+}) \neq \{0\}$.

(ii) Let $z \in \mathbb{C} \setminus \mathbb{R}$ and assume that $\Lambda^z_{\tau,+}$ is Fredholm. Then $\Lambda^z_{\tau,+}$ is invertible in $L^2(\Sigma)^4$ and it holds that

$$(H_\tau - z)^{-1}(v) = (H - z)^{-1}(v) - \Phi^z(\Lambda^z_{\tau,+})^{-1} t_\Sigma (H - z)^{-1}(v), \quad \forall\, v \in L^2(\mathbb{R}^3)^4. \tag{3.1.8}$$

In particular, we have

$$\mathrm{Sp}_{\mathrm{ess}}(H_\tau) = (-\infty, -m] \cup [m, +\infty). \tag{3.1.9}$$

(iii) $\mathrm{Sp}_{\mathrm{disc}}(H_\kappa) \cap (-m, m)$ is finite.

Proof. The proof of item (i) follows exactly in the same way as in Proposition 2.3.1. Let us show (ii). Fix $z \in \mathbb{C} \setminus \mathbb{R}$ and suppose that $\Lambda^z_{\tau,+}$ is Fredholm. Then, from (i) and the fact that H_τ is self-adjoint it is clear that $\mathrm{Kr}(\Lambda^z_{\tau,+}) = 0$ and $\mathrm{Rn}(\Lambda^z_{\tau,+}) = L^2(\Sigma)^4$, as otherwise z will be a non-real eigenvalue of H_τ. Hence, we conclude that $\Lambda^z_{\tau,+} : L^2(\Sigma)^4 \longrightarrow L^2(\Sigma)^4$ is bijective and thus (3.1.8) makes sense. Now given $v \in L^2(\mathbb{R}^3)^4$, we set

$$\varphi = (H - z)^{-1}(v) - \Phi^z(\Lambda^z_{\tau,+})^{-1} t_\Sigma (H - z)^{-1}(v).$$

To prove item (ii), it remains to show that $\varphi \in \mathrm{dom}(H_\tau)$. For this, remark that $\varphi = u + \Phi[g]$ where

$$\begin{aligned} u =& (H - z)^{-1}(v) - (\Phi^z - \Phi)(\Lambda^z_{\tau,+})^{-1} t_\Sigma (H - z)^{-1}(v), \\ g =& -(\Lambda^z_{\tau,+})^{-1} t_\Sigma (H - z)^{-1}(v). \end{aligned}$$

Notice that $(\Lambda^z_{\tau,+})^{-1} t_\Sigma (H - z)^{-1}$ is bounded from $L^2(\mathbb{R}^3)^4$ to $L^2(\Sigma)^4$ and $(H - z)u = v + z\Phi[g] \in L^2(\mathbb{R}^3)^4$. Consequently, we get that $g \in L^2(\Sigma)^4$ and $u \in H^1(\mathbb{R}^3)^4$. Moreover, using Lemma 1.3.2(ii) we obtain

$$\begin{aligned} t_\Sigma u &= \Big(t_\Sigma (H - z)^{-1} - (\mathscr{C}^z_\Sigma - \mathscr{C}_\Sigma)(\Lambda^z_{\tau,+})^{-1} t_\Sigma (H - z)^{-1}\Big)(v) \\ &= \Big(t_\Sigma (H - z)^{-1} - (\Lambda^z_{\tau,+} - \Lambda_{\tau,+})(\Lambda^z_{\tau,+})^{-1} t_\Sigma (H - z)^{-1}\Big)[v] = -\Lambda_{\tau,+}[g]. \end{aligned}$$

Thus $\varphi \in \mathrm{dom}(H_\tau)$, which yields (ii). Since the Sobolev embedding $H^{1/2}(\Sigma)^4 \hookrightarrow L^2(\Sigma)^4$ is compact, it follows that $\Phi^z(\Lambda^z_{\tau,+})^{-1} t_\Sigma (H - z)^{-1} \in \mathscr{K}(L^2(\mathbb{R}^3)^4)$. Therefore, we deduce by Weyl's theorem that $\mathrm{Sp}_{\mathrm{ess}}(H_\tau)$ is given by (3.1.9).

Finally, by Lemma 1.3.4 we know $\mathrm{dom}(H_\tau) \subset H^{1/2}(\alpha, \Omega_+) \oplus H^{1/2}(\alpha, \Omega_-)$. Hence, thanks to Remark 2.3.2, the assertion (iii) follows in the same way as in Theorem 2.3.2. This completes the proof of the proposition. □

3.1.2 Critical parameters

To avoid repetitions, in this part we explain our strategy to prove the self-adjointness of H_τ in the critical case, which is a generalization of the technique developed in Chapter 2. Here we assume that Ω_+ is a bounded C^2-smooth domain. All the problems that we are going to consider share the following properties when the parameter τ is critical:

(P1) A_τ and $\widetilde{A}_\tau$ admit continuous extensions from $H^{-1/2}(\Sigma)^4$ into itself, which we still denote by A_τ and $\widetilde{A}_\tau$. Moreover, $\mathrm{sgn}(\tau) I_4 = \widetilde{A}_\tau A_\tau = A_\tau \widetilde{A}_\tau$, holds in $H^{-1/2}(\Sigma)^4$.

(P2) The operator $\widetilde{\Lambda}^z_{\tau,\pm} A_\tau \widetilde{\Lambda}^z_{\tau,\mp}$ is bounded from $H^{-1/2}(\Sigma)^4$ to $H^{1/2}(\Sigma)^4$, where $\widetilde{\Lambda}^z_{\tau,\pm}$ is the continuous extension of $\Lambda^z_{\tau,\pm}$ defined from $H^{-1/2}(\Sigma)^4$ onto itself.

Now, following the same arguments as in Section 2.2, one can easily show that H_τ is closable. Moreover, the adjoint operator H_τ^* acts in the sense of distributions as $H_\tau^*(u+\Phi[g]) = H(u)$, on the domains

$$\mathrm{dom}(H_\tau^*) = \left\{\varphi = u + \Phi[g] : u \in H^1(\mathbb{R}^3)^4, g \in H^{-1/2}(\Sigma)^4, t_\Sigma u = -\widetilde{\Lambda}_{\tau,+}[g]\right\}. \tag{3.1.10}$$

Then we have the following theorem.

Theorem 3.1.2. *Let H_τ be as in (3.1.4) with a critical parameter $\tau \in \mathbb{R}^n$. If (P1) and (P2) hold, then H_τ is essentially self-adjoint and we have*

$$\mathrm{dom}(\overline{H_\tau}) = \left\{\varphi = u + \Phi[g] : u \in H^1(\mathbb{R}^3)^4, g \in H^{-1/2}(\Sigma)^4, t_\Sigma u = -\widetilde{\Lambda}_{\tau,+}[g]\right\}. \tag{3.1.11}$$

Before going through the proof of Theorem 3.1.2, a few remarks are in order. Note that for $u + \Phi[g] \in \mathrm{dom}(\overline{H_\tau})$ the equality $t_\Sigma u = -\widetilde{\Lambda}_{\tau,+}[g]$ should be read as a transmission condition (see Proposition 3.1.2 below), and we stress that this does not necessarily imply that $\widetilde{\Lambda}_{\tau,+}$ regularizes from $H^{-1/2}(\Sigma)^4$ to $H^{1/2}(\Sigma)^4$, nor that g belongs to $H^{1/2}(\Sigma)^4$. We mention that the assumption (P2) allows us to guarantee the inclusion $H_\tau^* \subset \overline{H_\tau}$. As in Chapter 2, once A_τ is given one can usually prove that there exist $g \in H^{-1/2}(\Sigma)^4$ and $u \in H^1(\mathbb{R}^3)^4$, such that $u + \Phi[g] \in \mathrm{dom}(\overline{H_\tau})$, leading to loss of regularity (i.e., $\Phi[g] \notin H^s(\mathbb{R}^3 \setminus \Sigma)^4$ for all $s > 0$), and therefore $\mathrm{dom}(\overline{H_\tau}) \not\subset \mathrm{dom}(H_\tau)$, see, e.g., [10, 19, 22, 41, 90].

Proof of Theorem 3.1.2 Since H_τ is closable, it is sufficient to show the inclusion $H_\tau^* \subset \overline{H_\tau}$. To this end, fix $\varphi = u + \Phi[g] \in \mathrm{dom}(H_\tau^*)$ and let $(h_j)_{j\in\mathbb{N}} \subset H^{1/2}(\Sigma)^4$ be a sequence of functions that converges to g in $H^{-1/2}(\Sigma)^4$. Set

$$g_j := g + A_\tau \widetilde{\Lambda}_{\tau,-}[h_j - g], \quad \forall j \in \mathbb{N}. \tag{3.1.12}$$

Then

$$\begin{aligned} (g_j)_{j\in\mathbb{N}} \subset H^{1/2}(\Sigma)^4 \ \text{ and } \ g_j \xrightarrow[j\to\infty]{} g \text{ in } H^{-1/2}(\Sigma)^4, \\ (\Lambda_{\tau,+}[g_j])_{j\in\mathbb{N}} \subset H^{1/2}(\Sigma)^4 \ \text{ and } \ \Lambda_{\tau,+}[g_j] \xrightarrow[j\to\infty]{} \widetilde{\Lambda}_{\tau,+}[g], \text{ in } H^{1/2}(\Sigma)^4. \end{aligned} \tag{3.1.13}$$

Indeed, observe that

$$-A_\tau \widetilde{\Lambda}_{\tau,-}[g] = -A_\tau \left(\frac{1}{\mathrm{sgn}(\tau)} \widetilde{A}_\tau - \mathscr{C}_\Sigma\right)[g] = -g + A_\tau \widetilde{\Lambda}_{\tau,+}[g]. \tag{3.1.14}$$

where the property (P1) was used in the last equality. Hence, we obtain that

$$\begin{aligned} g_j &:= A_\tau \left(\widetilde{\Lambda}_{\tau,+}[g] + \Lambda_{\tau,-}[h_j]\right), \\ \widetilde{\Lambda}_{\tau,+}[g_j - g] &= \widetilde{\Lambda}_{\tau,+} A_\tau \widetilde{\Lambda}_{\tau,-}[h_j - g]. \end{aligned}$$

Therefore, (3.1.13) follows by (3.1.12), the continuity of $\Lambda_{\tau,-}$ in $H^{1/2}(\Sigma)^4$, and the property (P2). Now, define

$$v_j = \mathcal{E}\left(\widetilde{\Lambda}_{\tau,+} A_\tau \widetilde{\Lambda}_{\tau,-}[h_j - g]\right), \text{ for all } j \in \mathbb{N}. \tag{3.1.15}$$

Clearly, $v_j \in H^1(\mathbb{R}^3)^4$ and $v_j \xrightarrow[j\to\infty]{} 0$ in $H^1(\mathbb{R}^3)^4$. Now set $\varphi_j := u_j + \Phi[g_j]$, where $u_j = u - v_j$, for all $j \in \mathbb{N}$. Note that

$$t_\Sigma u_j = t_\Sigma u - \widetilde{\Lambda}_{\tau,+} A_\tau \widetilde{\Lambda}_{\tau,-}[h_j - g] = -\widetilde{\Lambda}_{\tau,+}[g_j] + (t_\Sigma u + \widetilde{\Lambda}_{\tau,+}[g]) = -\Lambda_{\tau,+}[g_j].$$

Thus, $t_\Sigma u_j = -\Lambda_{\tau,+}[g_j]$ holds in $H^{1/2}(\Sigma)^4$, which means that $(\varphi_j)_{j\in\mathbb{N}} \subset \mathrm{dom}(H_\tau)$. Using that $H_\tau(\varphi_j) = H(u) - H(v_j)$, and the fact that $(g_j)_{j\in\mathbb{N}}$ converges to g in $H^{-1/2}(\Sigma)^4$ when $j \longrightarrow \infty$, we obtain that

$$(\varphi_j, H_\tau \varphi_j) \xrightarrow[j\to\infty]{} (\varphi, H_\tau^* \varphi) \text{ in } L^2(\mathbb{R}^3)^4 \times L^2(\mathbb{R}^3)^4, \tag{3.1.16}$$

which proves the inclusion $H_\tau^* \subset \overline{H_\tau}$, and this concludes the proof of the theorem. □

Remark 3.1.1. *Notice that if* $0 \neq g \in H^{-1/2}(\Sigma)^4 \setminus L^2(\Sigma)^4$ *is such that* $A_\tau \widetilde{\Lambda}_{\tau,-}[g] \notin L^2(\Sigma)^4$, *then* $\mathrm{dom}(\overline{H_\tau}) \not\subset \mathrm{dom}(H_\tau)$. *Indeed, if we set*

$$\varphi = \frac{1}{2}\mathcal{E}\left(\widetilde{\Lambda}_{\tau,+} A_\tau \widetilde{\Lambda}_{\tau,-}[g]\right) - \Phi[A_\tau \widetilde{\Lambda}_{\tau,-}[g]]. \tag{3.1.17}$$

Then, it is clear that $\varphi \notin \mathrm{dom}(H_\tau)$ *and* $\varphi \in \mathrm{dom}(\overline{H_\tau})$.

To make the boundary conditions in (3.1.11) clearer, the next proposition gives us another way to define the Dirac operator $\overline{H_\tau}$.

Proposition 3.1.2. *Let* $\overline{H_\tau}$ *be as in Theorem 3.1.2. Then we have*

$$\mathrm{dom}(\overline{H_\tau}) = \Big\{(\varphi_+, \varphi_-) \in L^2(\Omega_+)^4 \oplus L^2(\Omega_-)^4 : (\alpha\cdot\nabla)\varphi_\pm \in L^2(\Omega_\pm)^4 \text{ and } \left(\frac{1}{2} + iA_\tau^{-1}(\alpha\cdot N)\right) t_\Sigma \varphi_+ = -\left(\frac{1}{2} + iA_\tau^{-1}(\alpha\cdot N)\right) t_\Sigma \varphi_- \Big\},$$

where the transmission condition holds in $H^{-1/2}(\Sigma)^4$.

Proof. Given $\varphi = (u + \Phi[g]) \in \mathrm{dom}(\overline{H_\tau})$, set $\varphi_\pm := \varphi|_{\Omega_\pm}$. Then, a simple computation in the sense of distributions shows that

$$\begin{aligned}\overline{H_\tau}(\varphi) =& (-i\alpha\cdot\nabla + m\beta)\varphi + \frac{1}{2}A_\tau(t_\Sigma\varphi_+ + t_\Sigma\varphi_-)\delta_\Sigma, \\ =& (-i\alpha\cdot\nabla + m\beta)\varphi_+ \oplus (-i\alpha\cdot\nabla + m\beta)\varphi_- + i\alpha\cdot N(t_\Sigma\varphi_+ - t_\Sigma\varphi_-)\delta_\Sigma \\ &+ \frac{1}{2}A_\tau(t_\Sigma\varphi_+ + t_\Sigma\varphi_-)\delta_\Sigma.\end{aligned}$$

Thus, the proposition follows from this, the definition of $\widetilde{\Lambda}_{\tau,+}$ and Proposition 1.3.3. □

3.1.3 On the confinement

In this part, we briefly discuss the case where the operator H_τ generates confinement. In such a case we shall always restrict ourselves to Lipschitz domains. We mention that, for some Dirac operators (for example the coupling of the free Dirac operator with the Lorentz scalar δ-potential), one can prove that they generate the confinement for UR domains, provided that $B^2_{1/2}(\Sigma)$ is the trace to $H^1(\Omega_\pm)^4$. For instance this is possible if Ω_+ is a two-sided NTA domain with an ADR boundary by combing Proposition 1.2.2 with Jones's results [71, Theorem 1 and Theorem 2], for more details we refer to [59]. As we have observed in Section 2.4 (see also [41] for the two-dimensional case) the anomalous magnetic δ-potential generates confinement with a critical parameter. So, here we are going to show how to deal with both situations, i.e., confinement with critical or non-critical parameters.

Recall the definition of $\mathrm{dom}(H_\tau)$ from (3.1.4). Let $\Phi_{\Omega_\pm} : L^2(\Sigma)^4 \longrightarrow L^2(\Omega_\pm)^4$ be the operators defined by $\Phi_{\Omega_\pm}[g](x) = \Phi[g](x)$, for $g \in L^2(\Sigma)^4$ and $x \in \Omega_\pm$. Given any $\varphi = (u + \Phi[g]) \in \mathrm{dom}(H_\tau)$, we set

$$\varphi_\pm := \varphi|_{\Omega_\pm} = u|_{\Omega_\pm} + \Phi_{\Omega_\pm}[g]. \tag{3.1.18}$$

For simplicity, we denote by $\lim_{\mathrm{nt}} \varphi_\pm$ the nontangential limit of $\varphi_\pm$. By definition it holds that

$$\begin{aligned} t_\Sigma u = -\Lambda_{\tau,+}[g] &\Longleftrightarrow t_\Sigma u + C_\Sigma[g] = -A_\tau^{-1}[g] \\ &\Longleftrightarrow \frac{1}{2}(\lim_{\mathrm{nt}} \varphi_+ + \lim_{\mathrm{nt}} \varphi_-) = -iA_\tau^{-1}(\alpha \cdot N))(\lim_{\mathrm{nt}} \varphi_+ - \lim_{\mathrm{nt}} \varphi_-) \\ &\Longleftrightarrow \left(\frac{1}{2} + iA_\tau^{-1}(\alpha \cdot N)\right) \lim_{\mathrm{nt}} \varphi_+ = -\left(\frac{1}{2} - iA_\tau^{-1}(\alpha \cdot N)\right) \lim_{\mathrm{nt}} \varphi_-. \end{aligned} \tag{3.1.19}$$

From this, we get the following properties:

(P3) $(1/2 \pm iA_\tau^{-1}(\alpha \cdot N))$ are projectors in $L^2(\Sigma)^4$.

(P4) $\mathrm{sgn}(\tau) = -4$ and $\widetilde{A}_\tau(\alpha \cdot N) = (\alpha \cdot N)A_\tau$.

Then, the following proposition illustrates the phenomenon of confinement for non-critical parameters.

Proposition 3.1.3. *Let H_τ be as in (3.1.4) with a non-critical parameter $\tau \in \mathbb{R}^n$. If (P3) or (P4) holds, then H_τ generates confinement and we have*

$$H_\tau \varphi = H_\tau^{\Omega_+} \varphi_+ \oplus H_\tau^{\Omega_-} \varphi_- = (-i\alpha \cdot \nabla + m\beta)\, \varphi_+ \oplus (-i\alpha \cdot \nabla + m\beta)\, \varphi_-,$$

where $H_\tau^{\Omega_\pm}$ are the self-adjoint Dirac operators defined on

$$\begin{aligned} \mathrm{dom}(H_\tau^{\Omega_\pm}) = \Big\{ u_{\Omega_\pm} + \Phi_{\Omega_\pm}[g] : u_{\Omega_\pm} \in H^1(\Omega_\pm)^4, g \in L^2(\Sigma)^4 \textit{ and} \\ \left(\frac{1}{2} \pm iA_\tau^{-1}(\alpha \cdot N)\right)(t_\Sigma u_{\Omega_\pm} + C_\pm[g]) = 0 \Big\}. \end{aligned}$$

Proof. If (P3) holds true, then the proof follows directly from (3.1.19). Assume that (P4) holds true, then a simple computation yields that

$$\begin{aligned} &\left(\frac{1}{2} \pm iA_\tau^{-1}(\alpha \cdot N)\right) A_\tau \left(\frac{1}{2} \pm iA_\tau^{-1}(\alpha \cdot N)\right) = -4 \left(\frac{1}{2} \pm iA_\tau^{-1}(\alpha \cdot N)\right) \\ &\left(\frac{1}{2} \pm iA_\tau^{-1}(\alpha \cdot N)\right) A_\tau \left(\frac{1}{2} \mp iA_\tau^{-1}(\alpha \cdot N)\right) = 0, \end{aligned}$$

Again, using (3.1.19) we get the desired result. □

Now, in the case of a critical parameter, one need to replace (P3) and (P4) by the following properties:

(P′3) $(1/2 \pm iA_\tau^{-1}(\alpha \cdot N))$ are projectors in $H^{-1/2}(\Sigma)^4$.

(P′4) $\mathrm{sgn}(\tau) = -4$ and $\widetilde{A}_\tau(\alpha \cdot N) = (\alpha \cdot N)A_\tau$.

Here A_τ (respectively $\widetilde{A}_\tau$) is the extension given by the property (P1). Then, using Proposition 3.1.2 and following essentially the same arguments as Proposition 3.1.3, we get the following result for the confinement in this case.

Proposition 3.1.4. *Let $\overline{H_\tau}$ be as in (3.1.4) with a critical parameter $\tau \in \mathbb{R}^n$. If (P′3) or (P′4) holds true, then $\overline{H_\tau}$ generates confinement and we have*

$$\overline{H_\tau}\varphi = H_\tau^{\Omega_+}\varphi_+ \oplus H_\tau^{\Omega_-}\varphi_- = (-i\alpha \cdot \nabla + m\beta)\,\varphi_+ \oplus (-i\alpha \cdot \nabla + m\beta)\,\varphi_-,$$

where $H_\tau^{\Omega_\pm}$ are the self-adjoint Dirac operators defined on

$$\mathrm{dom}(H_\tau^{\Omega_\pm}) = \left\{\varphi_\pm \in L^2(\Omega_\pm)^4 : (\alpha \cdot \nabla)\varphi_\pm \in L^2(\Omega_\pm)^4 \text{ and } \left(\frac{1}{2} \pm iA_\tau^{-1}(\alpha \cdot N)\right) t_\Sigma\varphi_\pm = 0\right\}.$$

where the boundary conditions holds in $H^{-1/2}(\Sigma)^4$.

3.1.4 The β and the γ transformations of the electrostatic and the magnetic δ-potentials

In this part, we introduce the β and the γ transformations of the electrostatic and the magnetic δ-potentials. We emphasise that we are not formulating a theory here, but rather describing facts based on our observations.

Let $\epsilon, \eta \in \mathbb{R}$, recall that the electrostatic and the magnetic δ-shell interactions of strength ϵ and η, respectively, supported on Σ are defined by

$$V_\epsilon := \epsilon I_4 \delta_\Sigma \;\text{ and }\; V_\eta = \eta(\alpha \cdot N)\delta_\Sigma. \tag{3.1.20}$$

Then the β transformation, which we denote by Γ_β is the multiplication operator by β that preserves the symmetry of the above δ-potentials, that is

$$\Gamma_\beta(V_\epsilon) := \epsilon\beta\delta_\Sigma \;\text{ and }\; \Gamma_\beta(V_\eta) = i\eta\beta(\alpha \cdot N)\delta_\Sigma. \tag{3.1.21}$$

Thus, the β transformation of the electrostatic δ-potential gives the Lorentz scalar δ-potential, and the β transformation of the magnetic δ-potential gives what we called in Section 2.4 (and independently in [41] in the 2D case) the *anomalous magnetic* δ-potential.

Similarly, the γ transformation denoted by Γ_γ, is the multiplication operator by γ_5

$$\gamma_5 := -i\alpha_1\alpha_2\alpha_3 = \begin{pmatrix} 0 & I_2 \\ I_2 & 0 \end{pmatrix}, \tag{3.1.22}$$

that preserves the symmetry, thus we get the potentials

$$\Gamma_\gamma(V_\epsilon) := \epsilon\gamma_5\delta_\Sigma \;\text{ and }\; \Gamma_\gamma(V_\eta) = \eta\gamma_5(\alpha \cdot N)\delta_\Sigma. \tag{3.1.23}$$

Again, the γ transformation of the electrostatic δ-potential was already considered in Chapter 2, and we have seen in Remark 2.4.2 that $\pm 2\gamma_5\delta_\Sigma$ coincided with the electrostatic δ-potential of constant strength ∓ 2, so we called it here the *modified electrostatic* δ-potential. Also we call $\eta\gamma_5(\alpha \cdot N)\delta_\Sigma$ the *modified magentic* δ-potential.

Finally, we have the composition of the β transformation and the γ transformation which gives us the following potentials

$$\Gamma_\beta\Gamma_\gamma(V_\epsilon) := i\epsilon\gamma_5\beta\delta_\Sigma \;\text{ and }\; \Gamma_\beta\Gamma_\gamma(V_\eta) = i\eta\gamma_5\beta(\alpha \cdot N)\delta_\Sigma, \tag{3.1.24}$$

and we call them respectively the *modified Lorentz scalar* δ-potential and the *modified anomalous magnetic* δ-potential.

To put things in order we use the following notations:

$$V_{\tilde{\epsilon}} = \tilde{\epsilon}\gamma_5\delta_\Sigma, \quad V_\mu = \mu\beta\delta_\Sigma, \quad V_{\tilde{\mu}} = i\tilde{\mu}\gamma_5\beta\delta_\Sigma, \quad \tilde{\epsilon}, \mu, \tilde{\mu} \in \mathbb{R}. \tag{3.1.25}$$

$$V_{\tilde{\eta}} = \tilde{\eta}\gamma_5(\alpha \cdot N)\delta_\Sigma, \quad V_\upsilon = i\upsilon\beta(\alpha \cdot N)\delta_\Sigma, \quad V_{\tilde{\upsilon}} = i\tilde{\upsilon}\gamma_5\beta(\alpha \cdot N)\delta_\Sigma, \quad \tilde{\eta}, \upsilon, \tilde{\upsilon} \in \mathbb{R}. \tag{3.1.26}$$

The reader may wonder why we introduced such transformations, and what is the interest behind that. In fact, the answer is:

- The γ transformation preserves the characteristics of the potentials given by (3.1.25) and (3.1.26). That is, the characteristics of the potentials are stable under the γ transformation in the sense that, for any potential $V_\bullet$ from (3.1.25) or (3.1.26), if the parameter is critical then it remains critical after applying the γ transformation, and the same holds true to the case of the confinement.

- The characteristics of the potentials given by (3.1.25) and (3.1.26) are not stable under the β transformation, in the sense that, if $V_\bullet$ has a critical parameter, then $\Gamma_\beta(V_\bullet)$ does not have a critical parameter and vice versa. Similarly, if $V_\bullet$ does not generate confinement for any values of the parameter, then $\Gamma_\beta(V_\bullet)$ can generate confinement for certain values of the parameter and vice versa.

As a simple example, one can consider the electrostatic δ-potential. As is well-known [90, 19], V_ϵ has a critical parameter which is $\epsilon = \pm 2$, and it does not generate confinement for all $\epsilon \in \mathbb{R}$. Also we know that V_μ generates confinement for $\mu = \pm 2$; cf. [11]. Moreover, from Section 2.4 we know that $V_{\tilde{\epsilon}}$ has a critical parameter which is $\tilde{\epsilon} = \pm 2$. More generally, one can prove the above facts using directly Definition 3.1.1, (P3), (P4), (P$'$3) and (P$'$4). Thus we conclude that

- V_μ and $V_{\tilde{\mu}}$ generate confinement (for $\mu = \tilde{\mu} = \pm 2$) without critical parameters.

- V_υ and $V_{\tilde{\upsilon}}$ generate confinement for the critical parameters $\upsilon = \tilde{\upsilon} = \pm 2$.

We are going to show this in detail in the next section.

3.2 Delta interactions of electrostatic and magnetic type

As the title of this section indicates, here we focus on the spectral study of the Dirac operator H_τ when V_τ is a combination of the δ-potentials given by (3.1.25) and (3.1.26). We first consider the following Dirac operator

$$H_\kappa = H + V_\kappa = H + (\epsilon I_4 + \mu\beta + \eta(\alpha \cdot N))\delta_\Sigma, \quad \kappa := (\epsilon, \mu, \eta) \in \mathbb{R}^3,$$

which has already been studied in Chapter 2 for critical and non-critical parameters, when Ω_+ is a C^2-smooth domain. Thus, we only focus on the spectral properties of H_κ for non-critical parameter in the case of UR domains.

For the convenience of the reader, we begin our study with the subclass of bounded Lipschitz domains with VMO normals, where we can discuss the spectral properties of H_κ for all $\mathrm{sgn}(\kappa) \neq 0, 4$. Subsequently, we discuss the Sobolev regularity of $\mathrm{dom}(H_\kappa)$ in the case of bounded $C^{1,\omega}$-smooth domains. Finally, we separately study the couplings $(H + V_\epsilon + V_\mu)$

and $(H + V_\eta)$ for general UR domains. Then in Subsection 3.2.4, we consider the following Dirac operators

$$\begin{aligned} H_{\tilde\mu} &= H + V_{\tilde\mu} = H + i\tilde\mu\gamma_5\beta\delta_\Sigma, \quad \tilde\mu \in \mathbb{R}, \\ H_{\tilde\upsilon} &= H + V_{\tilde\upsilon} = H + i\tilde\upsilon\gamma_5\beta(\alpha\cdot N)\delta_\Sigma, \quad \tilde\upsilon \in \mathbb{R}, \end{aligned} \tag{3.2.1}$$

which deserve to be analysed in detail. Since $V_{\tilde\epsilon}$ (resp. $V_{\tilde\eta}$) can be treated in a similar way as V_ϵ (resp. V_η), and the potential V_υ has been studied in Section 2.4, to avoid repetition we will only make some remarks on the latter potentials.

3.2.1 δ-interactions supported on the boundary of a Lipschitz domain with a normal in VMO

In what follows, unless otherwise specified, we always suppose that Σ satisfies the following property:

(H3) $\Sigma = \partial\Omega_+$ with Ω_+ a bounded Lipschitz domain with a normal $N \in \mathrm{VMO}(\partial\Omega, \mathrm{d}\sigma)^3$.

Roughly speaking, the above assumption implies smallness of the Lipschitz constant of Ω_+. Another way to reformulate the assumption (H3) is to say that Ω_+ belongs to the intersection of the class of bounded Lipschitz domains and the class of regular SKT domains, see the proof of Proposition 3.2.1.

Recall that $\mathrm{sgn}(\kappa) = \epsilon^2 - \mu^2 - \eta^2$, and the operators $\Lambda^z_{\kappa,\pm}$ are given by

$$\Lambda^z_{\kappa,\pm} = \frac{1}{\mathrm{sgn}(\kappa)}(\epsilon I_4 \mp (\mu\beta + \eta(\alpha\cdot N))) \pm \mathscr{C}^z_\Sigma, \quad \forall z \in \mathbb{C}\setminus((-\infty,-m]\cup[m,\infty)). \tag{3.2.2}$$

Now we can state the main result about the spectral properties of the Dirac operator H_κ.

Theorem 3.2.1. *Let $\kappa \in \mathbb{R}^3$ be such that $\mathrm{sgn}(\kappa) \neq 0, 4$, and assume that Σ satisfies* (H3), *and let H_κ be as in* (3.1.4). *Then H_κ is self-adjoint. Moreover, the following hold true:*

(i) For all $z \in \mathbb{C}\setminus\mathbb{R}$, it holds that

$$(H_\kappa - z)^{-1} = (H - z)^{-1} - \Phi^z(\Lambda^z_{\kappa,+})^{-1} t_\Sigma (H - z)^{-1}. \tag{3.2.3}$$

(ii) $\mathrm{Sp}_{\mathrm{ess}}(H_\kappa) = (-\infty,-m]\cup[m,+\infty)$.

(iii) $\mathrm{Sp}_{\mathrm{disc}}(H_\kappa)\cap(-m,m)$ *is finite.*

(iv) $a \in \mathrm{Sp}_{\mathrm{disc}}(H_\kappa)$ if and only if $a \in \mathrm{Sp}_{\mathrm{disc}}(H_{\widetilde\kappa})$, where $\widetilde\kappa$ is given by

$$\widetilde\kappa = \left(-\frac{4\epsilon}{\mathrm{sgn}(\kappa)}, -\frac{4\mu}{\mathrm{sgn}(\kappa)}, \frac{4\eta}{\mathrm{sgn}(k)}\right).$$

Before proving this result, we first give a characterization of the assumption (H3) via the compactness of the anticommutator $\{\alpha\cdot N, \mathscr{C}^z_\Sigma\}$.

Let $g \in L^2(\Sigma)$, then the harmonic double layer K and the Riesz transforms $(R_k)_{1\leqslant k\leqslant 3}$ on Σ are defined by

$$\begin{aligned} K[g](x) &= \lim_{\rho\searrow 0}\int_{|x-y|>\rho}\frac{N(y)\cdot(x-y)}{4\pi|x-y|^3}g(y)\mathrm{d}\sigma(y), \\ R_k[g](x) &= \lim_{\rho\searrow 0}\int_{|x-y|>\rho}\frac{x_k-y_k}{4\pi|x-y|^3}g(y)\mathrm{d}\sigma(y). \end{aligned} \tag{3.2.4}$$

The following proposition is implicitly contained in [63], but we state and prove it here for the sake of completeness.

Proposition 3.2.1. *Assume that Σ satisfies* (H3)*. Then, the harmonic double layer K and the commutators $[N_j, R_k]$, $1 \leqslant j, k \leqslant 3$, are compact operators on $L^2(\Sigma)$.*

Before giving the proof, we need to introduce the notion of bounded regular Semmes-Kenig-Toro domains (regular SKT domains for short) developed by S. Hofmann, M. Mitrea and M. Taylor in [63].

Definition 3.2.1 (regular SKT Domains)**.** *We say that a bounded open set $\Omega \subset \mathbb{R}^3$ is a regular Semmes-Kenig-Toro domain, or briefly regular SKT domain, provided Ω is two-sided NTA domain, $\partial\Omega$ is ADR and whose geometric measure theoretic outward unit normal $\nu \in \mathrm{VMO}(\partial\Omega, \mathrm{d}\sigma)^3$.*

Remark 3.2.1. *We mention that Definition 3.2.1 is a characterization of regular SKT domains, for the precise definition we refer to [63, Definition 4.8].*

Proof of Proposition 3.2.1. The result follows from the fact that Ω_+ is a regular SKT domain. To see this, note that bi-Lipschitz mappings preserve the class of two-sided NTA domains with Ahlfors-David regular boundaries, and the class of regular SKT domains is invariant under continuously differentiable diffeomorphisms, see [62]. Now, by definition Ω_+ is locally the region above the graph of a Lipschitz function $\phi : \mathbb{R}^2 \longrightarrow \mathbb{R}$. Therefore, one may (and do) assume (via a partition of unity and a local flattening of the boundary) that

$$\Omega_+ = \{x = (\overline{x}, x_3) \in \mathbb{R}^2 \times \mathbb{R} : x_3 > \phi(\overline{x})\}.$$

Let $F : \mathbb{R}^3 \longrightarrow \mathbb{R}^3$ be defined for all $(\overline{x}, x_3) \in \mathbb{R}^2 \times \mathbb{R}$ as $F(\overline{x}, x_3) := (\overline{x}, x_3 + \phi(\overline{x}))$. Then, it easily follows that F is a bijective function with inverse $F^{-1} : \mathbb{R}^3 \longrightarrow \mathbb{R}^3$ given by $F^{-1}(\overline{y}, y_3) := (\overline{y}, y_3 - \phi(\overline{y}))$ for all $(\overline{y}, y_3) \in \mathbb{R}^2 \times \mathbb{R}$. Moreover, F and F^{-1} are both Lipschitz functions with constants $L_F, L_{F^{-1}} \leqslant (1 + ||\nabla\phi||_{L^\infty})$. It is clear that Ω_+ (resp. Ω_-) is the image of $\mathbb{R}^3_+$ (resp. $\mathbb{R}^3_-$) under the bi-Lipschitz homeomorphism F, which also maps $\mathbb{R}^2 \times \{0\}$ onto Σ. From this, it follows that Ω_+ is a two-sided NTA domain and Σ is ADR (because $\mathbb{R}^3_+$ is a two sided NTA domain and $\mathbb{R}^2 \times \{0\}$ is ADR). Since $N \in \mathrm{VMO}(\Sigma)^3$ by assumption, thanks to [63, Theorem 4.21], we know that Ω_+ is a regular SKT domain. Therefore the claimed result follows by [63, Theorem 4.47]. □

Lemma 3.2.1. *Assume that Σ satisfies* (H3)*. Then $\{\alpha \cdot N, \mathscr{C}^z_\Sigma\}$ is a compact operator on $L^2(\Sigma)^4$, for all $z \in \mathbb{C} \setminus ((-\infty, -m] \cup [m, \infty))$.*

Proof. Given $g \in L^2(\Sigma)^4$, then a straightforward computation shows that

$$\{\alpha \cdot N, \mathscr{C}^z_\Sigma\}[g](x) = T_{K_1}[g](x) + T_{K_2}[g](x), \tag{3.2.5}$$

where the kernels K_j, $j = 1, 2$, are given by

$$\begin{aligned} K_1(x,y) =& \frac{e^{i\sqrt{z^2-m^2}|x-y|}}{4\pi|x-y|}(\alpha \cdot N(x))\left(z + m\beta + \sqrt{z^2-m^2}\left(\alpha \cdot \frac{x-y}{|x-y|}\right)\right) \\ &+ \frac{e^{i\sqrt{z^2-m^2}|x-y|}}{4\pi|x-y|}\left(z + m\beta + \sqrt{z^2-m^2}\left(\alpha \cdot \frac{x-y}{|x-y|}\right)\right)(\alpha \cdot N(y)) \\ &+ \frac{e^{i\sqrt{z^2-m^2}|x-y|} - 1}{4\pi|x-y|^3}\left[(\alpha \cdot N(x))(i\alpha \cdot (x-y)) + (i\alpha \cdot (x-y))(\alpha \cdot N(y))\right]. \end{aligned}$$

$$K_2(x,y) = \frac{i}{4\pi|x-y|^3}\left((N(x))(\alpha \cdot (x-y)) + \alpha \cdot (x-y))(N(y))\right).$$

Using the estimate

$$\left|e^{i\sqrt{z^2-m^2}|x|}-1\right| \leqslant \left|\sqrt{z^2-m^2}\right| |x|, \tag{3.2.6}$$

it easily follows that

$$\sup_{1\leqslant k,j\leqslant 4} |K_1(x-y)| = \mathcal{O}(|x-y|^{-1}) \quad \text{when } |x-y| \longrightarrow 0. \tag{3.2.7}$$

Once (3.2.7) has been established, working component by component and using [53, Lemma 3.11], one can show that T_{K_1} is a compact operator in $L^2(\Sigma)^4$. Now it is straightforward to check that

$$T_{K_2}[g](x) = \widetilde{K}[g](x) + \widetilde{K}^*[g](x) + \sum_{j=1}^{3}\sum_{\substack{k=1\\k\neq j}}^{3} \alpha_j\alpha_k \left[N_j, \mathcal{R}_k\right][g](x). \tag{3.2.8}$$

where $\widetilde{K}$ denotes the matrix valued harmonic double layer, $\widetilde{K}^*$ is the associated adjoint operator, and $\mathcal{R}_k$ are the matrix versions of the Riesz transforms. That is, for $x\in\Sigma$ and $g\in L^2(\Sigma)^4$, we have

$$\begin{aligned}
\widetilde{K}[g](x) &= \lim_{\rho\searrow 0}\int_{|x-y|>\rho} \frac{N(y)\cdot(x-y)}{4\pi|x-y|^3} I_4 g(y)\mathrm{d}\sigma(y),\\
\widetilde{K}^*[g](x) &= \lim_{\rho\searrow 0}\int_{|x-y|>\rho} \frac{N(x)\cdot(x-y)}{4\pi|x-y|^3} I_4 g(y)\mathrm{d}\sigma(y),\\
\mathcal{R}_k[g](x) &= \lim_{\rho\searrow 0}\int_{|x-y|>\rho} \frac{x_k-y_k}{4\pi|x-y|^3} I_4 g(y)\mathrm{d}\sigma(y).
\end{aligned} \tag{3.2.9}$$

Since the adjoint of a compact operator is a compact operator and α_j's are constants matrices, using Proposition 3.2.1 and working component by component, we get that T_{K_2} is a compact operator in $L^2(\Sigma)^4$. Therefore $\{\alpha\cdot N, \mathscr{C}_\Sigma^z\}$ is a compact operator in $L^2(\Sigma)^4$ and this finishes the proof of the lemma. □

Note that Lemma 3.2.1 is not valid for general Lipschitz surfaces. In fact, it turns out that assuming (H3) means that we are excluding the special class of corner domains. Indeed, from the proof of Proposition 3.2.1 we know that any bounded Lipschitz domain Ω_+ is an NTA domain and Σ is ADR. However, the presence of any angle $\theta\neq 0$, implies that

$$\operatorname{dist}(N, \mathrm{VMO}(\Sigma,\mathrm{d}\sigma)^3) > 0,$$

where the distance is taken in $\mathrm{BMO}(\Sigma,\mathrm{d}\sigma)^3$, cf. [63, Proposition 4.38] and the discussion that precedes it. Hence, Ω_+ is not a regular SKT domain and then by [63, Theorem 4.47] , the principale value of the harmonic double layer K and the commutators $[N_j, R_k]$, $1\leqslant j,k\leqslant 3$, are not compact on $L^2(\Sigma)$. So, $\{\alpha\cdot N, \mathscr{C}_\Sigma\}$ is not a compact operator on $L^2(\Sigma)^4$, and thus the assumption (H3) is sharp. To make this clearer, we have the following result.

Theorem 3.2.2. *Given $z\in\mathbb{C}\setminus((-\infty,-m]\cup[m,\infty))$ and let Ω_+ be a bounded Lipschitz domain, such that the decomposition $\mathbb{R}^3=\Omega_+\cup\Sigma\cup\Omega_-$ holds, where $\partial\Omega_+=\Sigma$. Then, Σ satisfies* (H3) *if and only if $\{\alpha\cdot N, \mathscr{C}_\Sigma^z\}$ is compact in $L^2(\Sigma)^4$.*

Proof. The first implication follows from Lemma 3.2.1. Let us prove the reverse implication, so assume that $\{\alpha\cdot N, \mathscr{C}_\Sigma^z\}$ is compact in $L^2(\Sigma)^4$. Recall the definition of the operator W from (1.3.6). Then, from (3.2.5) it holds that

$$\{\alpha\cdot N, \mathscr{C}_\Sigma^z\} = T_{K_1} + \begin{pmatrix} \{\sigma\cdot N, W\} & 0\\ 0 & \{\sigma\cdot N, W\}\end{pmatrix}, \tag{3.2.10}$$

where T_{K_1} is a compact operator in $L^2(\Sigma)^4$. Using this, it follows that

$$\{\alpha \cdot N, \mathscr{C}_\Sigma\} \text{ is compact in } L^2(\Sigma)^4 \Longleftrightarrow \{\sigma \cdot N, W\} \text{ is compact in } L^2(\Sigma)^2. \tag{3.2.11}$$

Hence, it remains to show that

$$\{\sigma \cdot N, W\} \text{ is compact in } L^2(\Sigma)^2 \Longrightarrow \Sigma \text{ satisfies (H3)}. \tag{3.2.12}$$

For this, note that from the proof of Proposition 3.2.1 we know that Ω_+ is a two-sided NTA domain and Σ is ADR. So Ω_+ satisfies the two-sided corkscrew condition with an ADR boundary. Hence, Ω_+ is a UR domain by [63, Corollary 3.9] . Next, we claim that there exists $C > 0$ depending only on the uniform rectifiability and the ADR constants of Σ, such that

$$\operatorname{dist}\left(N, \mathrm{VMO}(\partial\Omega, \mathrm{d}\sigma)^3\right) \leqslant C \operatorname{dist}\left(\{\sigma \cdot N, W\}, \mathscr{K}(L^2(\Sigma)^2)\right), \tag{3.2.13}$$

where the distance in the right-hand side is measured in $\mathscr{B}(L^2(\Sigma)^2)$. Let us now suppose that (3.2.13) is true. Since $\{\sigma \cdot N, W\}$ is compact in $L^2(\Sigma)^2$, by (3.2.13), it holds that $N \in \mathrm{VMO}(\partial\Omega, \mathrm{d}\sigma)^3$. Therefore, Σ satisfies (H3), which proves the theorem. Let us now return to the proof of (3.2.13). Given $x, y \in \mathbb{R}^3$, we define the following multiplication operator

$$x \odot y := (i\sigma \cdot x)(i\sigma \cdot y) = (\sigma \cdot x)(-\sigma \cdot y). \tag{3.2.14}$$

Using the anticommutation properties of the Pauli matrices, it is easy to check that:

$$x \odot x := -|x|^2, \quad x \odot y + y \odot x = -2(x \cdot y) I_2, \quad \forall x, y \in \mathbb{R}^3.$$

Now, we make the observation that the multiplication operator defined by (3.2.14) has the same properties as the multiplication operator in the Clifford algebra $\mathcal{C}l_3$ (see [63, Section 4.6] for the precise definition). Moreover, $W(\sigma \cdot N)$ plays the same role as the Cauchy-Clifford operator defined on $L^2(\Sigma) \otimes \mathcal{C}l_3$ (i.e. it acts on $\mathcal{C}l_3$-valued functions), cf. [63, Section 4.6]. Thus, one can adapt the same arguments of [63, Theorem 4.46] and show that the claim (3.2.13) holds true, we leave the details for the reader. This completes the proof of the theorem. □

As it was done in [63, Theorem 4.47], one can also characterize the class of bounded regular SKT domains via the compactness of the anticommutators $\{\sigma \cdot N, W\}$ in $L^2(\Sigma)^2$, or equivalently via the compactness of the anticommutator $\{\alpha \cdot N, \mathscr{C}_\Sigma\}$ in $L^2(\Sigma)^4$. This is the purpose of the following proposition.

Proposition 3.2.2. *Let $\Omega \subset \mathbb{R}^3$ be a bounded two-sided NTA domain with a compact, ADR boundary. Then the following statements are equivalent:*

(i) Ω is a regular SKT domain.

(ii) The harmonic double layer K and the commutators $[N_j, R_k]$, $1 \leqslant j, k \leqslant 3$, are compact operators on $L^2(\partial\Omega)$.

(iii) $\{\alpha \cdot N, \mathscr{C}^z_{\partial\Omega}\}$ is a compact operator on $L^2(\partial\Omega)^4$, for all $z \in \mathbb{C} \setminus ((-\infty, -m] \cup [m, \infty))$.

(iv) $\{\sigma \cdot N, W\}$ is a compact operator on $L^2(\partial\Omega)^2$.

Proof. (i) ⇒ (ii) is a consequence of [63, Theorem 4.21] and [63, Theorem 4.47]. (ii) ⇒ (iii) readily follows from (3.2.5) and (3.2.8). (iii) ⇒ (iv) is an immediate consequence of (3.2.11). Finally, (iv) ⇒ (i) follows from (3.2.13) and [63, Theorem 4.21]. □

Corollary 3.2.1. *Let $z \in \mathbb{C} \setminus ((-\infty, -m] \cup [m, \infty))$, then $\Lambda^z_{\kappa,\pm}$ is a Fredholm operator on $L^2(\Sigma)^4$.*

Proof. Fix $z \in \mathbb{C} \setminus ((-\infty, -m] \cup [m, \infty))$. Observe that

$$\{\beta, \mathscr{C}^z_\Sigma\}[g](x) = 2(mI_4 + z\beta)S^z[g](x). \tag{3.2.15}$$

Using this, it follows that

$$\Lambda^z_{\kappa,\mp}\Lambda^z_{\kappa,\pm} = \frac{1}{\operatorname{sgn}(\kappa)} - \frac{1}{4} - \mathscr{C}^z_\Sigma(\alpha\cdot N)\{\alpha\cdot N, \mathscr{C}^z_\Sigma\} + \frac{2\mu}{\operatorname{sgn}(\kappa)}(mI_4 + z\beta)S^z + \frac{\eta}{\operatorname{sgn}(\kappa)}\{\alpha\cdot N, \mathscr{C}^z_\Sigma\}, \tag{3.2.16}$$

As S^z is bounded from $L^2(\Sigma)^4$ to $H^{1/2}(\Sigma)^4$ (see [81, Theorem 6.11] for example), and the injection $H^{1/2}(\Sigma)^4$ into $L^2(\Sigma)^4$ is compact, it follows that S^z is a compact operator in $L^2(\Sigma)^4$. Now, using that $\mathscr{C}^z_\Sigma(\alpha\cdot N)$ is bounded in $L^2(\Sigma)^4$ and that $\{\alpha\cdot N, \mathscr{C}^z_\Sigma\}$ is a compact operator on $L^2(\Sigma)^4$ by Lemma 3.2.1, we thus obtain that $\mathscr{C}^z_\Sigma(\alpha\cdot N)\{\alpha\cdot N, \mathscr{C}^z_\Sigma\}$ is a compact operator on $L^2(\Sigma)^4$. Hence $\Lambda^z_{\kappa,\mp}\Lambda^z_{\kappa,\pm}$ is Fredholm operator and therefore $\Lambda^z_{\kappa,\pm}$ is Fredholm operator by [2, Theorem 1.46 (iii)]. This finishes the proof of the corollary. □

Now we are in position to give the proof of Theorem 3.2.1.

Proof of Theorem 3.2.1 Since $\Lambda^z_{\kappa,+}$ is Fredholm for all $z \in \mathbb{C} \setminus ((-\infty, -m] \cup [m, \infty))$, a direct application of Theorem 3.1.1 yields that H_κ is self-adjoint which proves the first statement of the theorem. Assertions (i), (ii) and (iii) are consequences of Proposition 3.1.1. Finally, it remains to show (iv). For this, if we let

$$\widetilde{\kappa} = \left(-\frac{4\epsilon}{\operatorname{sgn}(\kappa)}, -\frac{4\mu}{\operatorname{sgn}(\kappa)}, \frac{4\eta}{\operatorname{sgn}(k)}\right),$$

then we have

$$\Lambda^a_{\widetilde{\kappa},+} = \frac{1}{4}(-\epsilon I_4 + \mu\beta - \eta(\alpha\cdot N)) + \mathscr{C}^a_\Sigma. \tag{3.2.17}$$

Using Proposition 3.1.1-(i) and Lemma 1.3.2 it follows that

$$\begin{aligned}
0 \in \mathrm{Sp}_{\mathrm{disc}}(\Lambda^a_{\kappa,+}) &\Longleftrightarrow \text{ there is } 0 \neq g \in L^2(\Sigma)^4 : -\frac{1}{\operatorname{sgn}(\kappa)}(\epsilon I_4 - \mu\beta - \eta(\alpha\cdot N))g = \mathscr{C}^a_\Sigma[g] \\
&\Longleftrightarrow \frac{4}{\operatorname{sgn}(\kappa)}(\epsilon I_4 - \mu\beta - \eta(\alpha\cdot N))((\alpha\cdot N)\mathscr{C}^a_\Sigma)^2[g] = \mathscr{C}^a_\Sigma[g] \\
&\Longleftrightarrow \mathscr{C}^a_\Sigma((\alpha\cdot N)\mathscr{C}^a_\Sigma)[g] = \frac{1}{4}(\epsilon I_4 - \mu\beta + \eta(\alpha\cdot N))(\alpha\cdot N)\mathscr{C}^a_\Sigma[g] \\
&\Longleftrightarrow \text{ there is } 0 \neq f = ((\alpha\cdot N)\mathscr{C}^a_\Sigma)[g] \in L^2(\Sigma)^4 : \Lambda^a_{\widetilde{\kappa},+}[f] = 0 \\
&\Longleftrightarrow a \in \mathrm{Sp}_{\mathrm{disc}}(H_{\widetilde{\kappa}}) \cap (-m, m).
\end{aligned}$$

Therefore, $a \in \mathrm{Sp}_{\mathrm{disc}}(H_\kappa)$ if and only if $a \in \mathrm{Sp}_{\mathrm{disc}}(H_{\widetilde{\kappa}})$, which proves (iv). This completes the proof of the theorem. □

The reader interested on the confinement may wonder if the Dirac operator H_κ generates this phenomenon under the assumption that $\mathrm{sgn}(\kappa) = -4$. To clarify and provide an answer to this question, pick $\varphi = u + \Phi[g] \in \mathrm{dom}(H_\kappa)$ and recall the decomposition 3.1.18. Then

$$\begin{aligned}\lim_{\mathrm{nt}} \varphi_\pm &= t_\Sigma u + \lim_{\mathrm{nt}} \Phi_{\Omega_\pm}[g] = t_\Sigma u + (\mathscr{C}_\Sigma \mp \frac{i}{2}(\alpha \cdot N))[g] \\ &= \left(\frac{1}{4}(\epsilon - \mu\beta - \eta(\alpha \cdot N)) \mp \frac{i}{2}(\alpha \cdot N)\right) g,\end{aligned} \tag{3.2.18}$$

where in the last equality we used that $t_\Sigma u = -\Lambda_{\kappa,+}[g]$. Now, multiplying the identity (3.2.18) by

$$\left(\frac{1}{2}(\epsilon + \mu\beta + \eta(\alpha \cdot N)) \pm i(\alpha \cdot N)\right),$$

we get

$$\left(\frac{1}{2}(\epsilon + \mu\beta + \eta(\alpha \cdot N)) \pm i(\alpha \cdot N)\right) \lim_{\mathrm{nt}} \varphi_\pm = \mp i\eta g. \tag{3.2.19}$$

As consequence, if $\mathrm{sgn}(\kappa) = -4$ and $\eta \neq 0$, then H_κ cannot generate confinement. Hence Σ is penetrable. Clearly, if we set $\eta = 0$ in (3.2.19), then H_κ generates confinement, but we postpone this case to subsection 3.2.3, where we establish that for Lipschitz surfaces.

We finish this part by pointing the following result. Thanks to Proposition 3.2.2, if Ω_+ is bounded SKT domain then the same arguments used in the proof of Theorem 3.2.1 yields that $\Lambda^z_{\kappa,+}$ is Fredholm for all $z \in \mathbb{C} \setminus ((-\infty, -m] \cup [m, \infty))$. In addition, the compactness in $L^2(\Sigma)^4$ of the anticommutator $\{\alpha \cdot N, \mathscr{C}^z_\Sigma\}$ implies that $\mathrm{Sp}_{\mathrm{disc}}(H_\kappa) \cap (-m, m)$ is finite when $\mu = \eta = 0$. Indeed, we have:

Proposition 3.2.3. *Suppose that Ω_+ is a bounded SKT domain and let H_κ be as in (3.1.4). Then for all $\kappa \in \mathbb{R}^3$ such that $\mathrm{sgn}(\kappa) \neq 0, 4$, H_κ is self-adjoint. If in addition $\mu = \eta = 0$, then $\mathrm{Sp}_{\mathrm{disc}}(H_\kappa) \cap (-m, m)$ is finite.*

Proof. The proof of the first statement follows directly by Theorem 3.1.1 and the Fredholmness of $\Lambda^z_{\kappa,+}$ all $z \in \mathbb{C} \setminus ((-\infty, -m] \cup [m, \infty))$. The second assertion is consequence of $\{\alpha \cdot N, \mathscr{C}^z_\Sigma\}$ from Lemma 3.2.1. Indeed, assume that $\mu = \eta = 0$, and hence $\Lambda^z_{\kappa,\pm} = (1/2 \pm \mathscr{C}^a_\Sigma$ for $a \in (-m, m)$. Now, notice that

$$C_0 := \sup_{a \in [-m,m]} \|\mathscr{C}^z_\Sigma\| < \infty. \tag{3.2.20}$$

This follows in the same way as in [11, Lemma 3.2]. Next, recall that for all $a \in (-m, m)$ we have

$$\Lambda^z_{\kappa,\mp}\Lambda^z_{\kappa,\pm} = \frac{1}{4} - (\mathscr{C}^a_\Sigma)^2. \tag{3.2.21}$$

Thus, there exists a finite or countable family of continuous and non-decreasing functions $\lambda_j : [-m, m] \to [1/4C_0, C_0]$ such that

$$\mathrm{Sp}(\mathscr{C}^a_\Sigma) = \left\{\pm\frac{1}{2}\right\} \cup \{\lambda_j(a) : j \in \mathbb{N}\} \cup \left\{-\frac{1}{4\lambda_j(a)} : j \in \mathbb{N}\right\}. \tag{3.2.22}$$

Now, if we assume that $\mathrm{Sp}_{\mathrm{disc}}(H_\kappa) \cap (-m, m)$ is not finite, then the same arguments as in the proof of [16, Theorem 4.4 (iii)] yields that $\epsilon = 2$ or $\epsilon = -2$, which contradicts the fact that $\epsilon \neq \pm 2$. This achieves the proof. ☐

3.2.2 Sobolev regularity of $\mathrm{dom}(H_\kappa)$ for δ-interactions supported on the boundary of a $C^{1,\omega}$-domain

In this part, we discuss how the smoothness of the surface supporting the singular perturbation affects the Sobolev regularity of $\mathrm{dom}(H_\kappa)$ in the non-critical case. As shown in Section 2.2 we know that if Σ is a C^2-smooth compact surface, then $\mathrm{dom}(H_\kappa) \subset H^1(\mathbb{R}^3 \setminus \Sigma)^4$. However, such a result may fail if Σ is less regular. In fact, there are two obstacles that prevent us from obtaining such a result. The first is that $(\alpha \cdot N)\Lambda_{\kappa,+}[g]$ should belong to $H^{1/2}(\Sigma)^4$, which clearly fails if Σ is only C^1-smooth, for example. The second reason is that we also need to extend the anticommutator $\{\alpha \cdot N, \mathscr{C}_\Sigma\}$ to a bounded operator from $L^2(\Sigma)^4$ to $H^{1/2}(\Sigma)^4$. Although again, we know that behind this operator there are components of the Riesz transforms as well as the principal value of the harmonic double layer operator and its adjoint, which do not have this property, even if Σ is $C^{1,\omega}$-smooth with $\omega < 1/2$.

In the following, we assume that Ω_+ is a bounded $C^{1,\omega}$-smooth domain with $\gamma \in (0,1)$. The main result of this subsection reads as follows:

Theorem 3.2.3. *Let $\kappa \in \mathbb{R}^3$ be such that $\mathrm{sgn}(\kappa) \neq 0, 4$ and let H_κ be as in Theorem 3.2.1. Then H_κ is self adjoint and the following hold:*

(i) If $\omega \leqslant 1/2$, then for all $s < \omega$, we have

$$\mathrm{dom}(H_\kappa) \subset \Big\{u + \Phi[g] : u \in H^1(\mathbb{R}^3)^4, g \in H^s(\Sigma)^4, t_\Sigma u = -\Lambda_{\kappa,+}[g]\Big\} \subset H^{1/2+s}(\mathbb{R}^3 \setminus \Sigma)^4.$$

(ii) If $\omega > 1/2$, then

$$\mathrm{dom}(H_\kappa) = \Big\{u + \Phi[g] : u \in H^1(\mathbb{R}^3)^4, g \in H^{1/2}(\Sigma)^4, t_\Sigma u = -\Lambda_{\kappa,+}[g]\Big\} \subset H^1(\mathbb{R}^3 \setminus \Sigma)^4.$$

Lemma 3.2.2. *There is a constant $C > 0$ such that for all $x, y \in \Sigma$, it holds that*

$$|N(x) \cdot (x - y)| \leqslant C|x - y|^{1+\omega}. \tag{3.2.23}$$

Proof. Note first that if $|x - y| > 1$, then the Cauchy-Schwarz inequality yields that

$$\frac{1}{|x - y|^{1+\omega}} |N(x) \cdot (x - y)| \leqslant 1. \tag{3.2.24}$$

which gives the result for $|x - y| > 1$, so it remains to prove the statement for $|x - y| < 1$. Without loss of generality (after translation and rotation if necessary), we may assume that $x = 0$ and $N(x) = (0, 0, 1)$. There is a $C^{1,\omega}$-smooth function $\phi : B(0,1) \subset \mathbb{R}^2 \longrightarrow \mathbb{R}$ such that $\phi(0) = 0$, $|\nabla\phi(0)| = 0$ and

$$B(0,1) \cap \Sigma = \{x = (x_1, x_2, x_3) : x_3 = \phi(x_1, x_2)\}.$$

Then we get

$$|N(x) \cdot (x - y)| = |y_3| = |\phi(y_1, y_2)| \leqslant C|y|^{1+\omega}. \tag{3.2.25}$$

Therefore the statement is proven since Σ is compact. $\square$

In the following proposition, we prove that $\{\alpha \cdot N, \mathscr{C}_\Sigma\}$ is bounded from $L^2(\Sigma)^4$ to $H^s(\Sigma)^4$, for all $s \in (0, \omega)$. This result should be compared to [21, Proposition 3.10], where the authors showed that for Σ a C^2-smooth compact surface, the commutator of the Cauchy operator $\mathscr{C}_\Sigma$ with a Hölder continuous function of order $a \in (0, 1)$ is bounded from $L^2(\Sigma)^4$ to $H^s(\Sigma)^4$, for all $s \in (0, a)$. In fact, both results are identical modulo a slight change of the assumptions.

Lemma 3.2.3. *Suppose that Σ is $C^{1,\omega}$. Then, for all $s \in (0,\omega)$, the anticommutator $\{\alpha \cdot N, \mathscr{C}_\Sigma\}$ is a bounded operator from $L^2(\Sigma)^4$ to $H^s(\Sigma)^4$.*

Proof. Let $g \in L^2(\Sigma)^4$, in the same manner as in the proof of Lemma 3.2.1, one can check that

$$\{\alpha \cdot N, \mathscr{C}_\Sigma\}[g](x) = \int_{y\in\Sigma} K'(x,y)g(y)\mathrm{dS}(y) + \widetilde{K}^*[g](x) := T_{K'}[g](x) + \widetilde{K}^*[g](x), \quad (3.2.26)$$

where $\widetilde{K}^*$ is defined by (3.2.9) and the kernel K' is given by

$$\begin{aligned} K'(x,y) =& \phi(x-y)(\alpha\cdot(N(y)-N(x)) - m\frac{e^{-m|x-y|}}{2i\pi|x-y|^2}(N(x)\cdot(x-y))I_4 \\ &- \frac{e^{-m|x-y|}-1}{2i\pi|x-y|^3}(N(x)\cdot(x-y))I_4. \end{aligned}$$

As Σ is $C^{1,\omega}$-smooth, there is a constant $C>0$ such that $|N(x)-N(y)| \leqslant C|x-y|$. Using this, the estimate (3.2.6) and Lemma 4.4.5, we obtain that $|K'(x,y)| \leqslant C|x-y|^{-1}$. This implies that the integral operator $T_{K'}$ is not singular. Since N is in the Hölder class $C^{0,\omega}(\Sigma)^4$, for $x,y,z\in\Sigma$ such that $|x-y| \leqslant |x-z|/4$, following the same arguments as in [21, Proposition 3.10] one can show that

$$|K'(x,z) - K'(y,z)| \leqslant C\frac{|x-y|}{|x-z|^2}.$$

Thus, [21, Lemma A.3] yields that $T_{K'}$ is bounded from $L^2(\Sigma)^4$ to $H^1(\Sigma)^4$, and hence $T_{K'}$ is bounded from $L^2(\Sigma)^4$ to $H^s(\Sigma)^4$, for all $s\in(0,\omega)$. Finally, the fact that $\widetilde{K}^*$ is bounded from $L^2(\Sigma)^4$ onto $H^s(\Sigma)^4$, for all $s\in(0,\omega)$, follows by [101, p. 165] . This completes the proof of the lemma. □

We are now in a position to give the proof of Theorem 3.2.3:

Proof of Theorem 3.2.3. The first statement is a direct consequence of Theorem 3.2.1. The second statement follows by the same method as in Theorem 2.2.1. Indeed, fix $\omega\in(0,1)$ and assume that Σ is $C^{1,\omega}$, and let $g\in L^2(\Sigma)^4$ be such that $\Lambda_{\kappa,+}[g]\in H^{1/2}(\Sigma)^4$. Note that the multiplication by N is bounded in $H^s(\Sigma)^4$ for all $s\in[0,\omega)$ (see, e.g., [21, Lemma A.2]) and $\mathscr{C}_\Sigma$ is bounded from $H^{1/2}(\Sigma)^4$ into itself. Therefore, we obtain that $\Lambda_{\kappa,-}\Lambda_{\kappa,+}[g]\in H^s(\Sigma)^4$, for all $s\in[0,\omega)$. Now, observe that

$$\Lambda_{\kappa,-}\Lambda_{\kappa,+} = \frac{1}{\mathrm{sgn}(\kappa)} - \frac{1}{4} - \{\alpha\cdot N,\mathscr{C}_\Sigma\}(\alpha\cdot N)\mathscr{C}_\Sigma + \frac{2m\mu}{\mathrm{sgn}(\kappa)}S + \frac{\eta}{\mathrm{sgn}(\kappa)}\{\alpha\cdot N,\mathscr{C}_\Sigma\},$$

here we used the fact that

$$\mathscr{C}_\Sigma(\alpha\cdot N)\{\alpha\cdot N,\mathscr{C}_\Sigma\} = \{\alpha\cdot N,\mathscr{C}_\Sigma\}(\alpha\cdot N)\mathscr{C}_\Sigma.$$

Thus we get

$$g = \frac{4(\mathrm{sgn}(\kappa))}{4-\mathrm{sgn}(\kappa)}\left(\Lambda_{\kappa,-}\Lambda_{\kappa,+} + \{\alpha\cdot N,\mathscr{C}_\Sigma\}(\alpha\cdot N)\mathscr{C}_\Sigma - \frac{\eta}{\mathrm{sgn}(\kappa)}\{\alpha\cdot N,\mathscr{C}_\Sigma\} - \frac{2m\mu}{\mathrm{sgn}(\kappa)}S\right)[g], \quad (3.2.27)$$

As $\mathscr{C}_\Sigma(\alpha\cdot N)$ is bounded from $L^2(\Sigma)^4$ into itself and S is bounded from $L^2(\Sigma)^4$ to $H^{1/2}(\Sigma)^4$, by combining Lemma 3.2.3 and (3.2.27) it follows that $g\in H^s(\Sigma)^4$, for all $s\in[0,\omega)$. Notice that for all $\omega\in[0,1/2]$ and all $s\in(0,\omega)$, the operator Φ gives rise to a bounded operator

$\Phi : H^s(\Sigma)^4 \longrightarrow H^{1/2+s}(\mathbb{R}^3 \setminus \Sigma)^4$. Indeed, recall that for any $g \in H^s(\Sigma)^4$ we have $\Phi[g] = (-i\alpha \cdot \nabla + m\beta)\mathcal{S}[g]$, where $\mathcal{S}$ is the single layer potential associated to $(-\Delta + m^2)$, that is

$$\mathcal{S}[g](x) = \int_\Sigma \frac{e^{-m|x-y|}}{4\pi|x-y|} I_4 g(y)\mathrm{d}\sigma(y), \quad \forall x \in \mathbb{R}^3 \setminus \Sigma.$$

By [81, Theorem 6.13] we know that $\mathcal{S}$ is bounded from $H^s(\Sigma)^4$ to $H^{3/2+s}(\mathbb{R}^3 \setminus \Sigma)^4$ for any $s \in (0, \omega)$, which means that Φ is bounded from $H^s(\Sigma)^4$ to $H^{1/2+s}(\mathbb{R}^3 \setminus \Sigma)^4$. Hence, from the above considerations we get the inclusions in (i). Finally, if $\omega > 1/2$, we then obtain that $g \in H^{1/2}(\Sigma)^4$ and therefore $\Phi[g] \in H^1(\mathbb{R}^3 \setminus \Sigma)^4$ holds by Proposition 1.3.3, which gives the equality in (ii) and completes the proof of the theorem. □

Remark 3.2.2. *Note that if* $\mathrm{sgn}(\kappa) \notin \{0, 4\}$, *and* Σ *is* $C^{1,\omega}$*-smooth with* $\gamma \in (1/2, 1)$, *then using the same technique as in Section 2.2 one can show that* H_κ *is self-adjoint. In fact, as* $\{\alpha \cdot N, \mathscr{C}_\Sigma\}$ *is self-adjoint, and bounded from* $L^2(\Sigma)^4$ *to* $H^{1/2}(\Sigma)^4$, *by duality, we can extend it to a bounded operator from* $H^{-1/2}(\Sigma)^4$ *to* $L^2(\Sigma)^4$. *Hence, by iterating twice the same argument of the proof of Theorem 2.2.1, we then get that*

$$\mathrm{dom}(H_\kappa^*) = \left\{ u + \Phi[g] : u \in H^1(\mathbb{R}^3)^4, g \in H^{1/2}(\Sigma)^4, t_\Sigma u = -\Lambda_{\kappa,+}[g] \right\},$$

which proves the self-adjointness of H_κ *in this case.*

3.2.3 δ-interactions supported on the boundary of a bounded uniformly rectifiable domain

Here we discuss special cases where we can show the self-adjointness of H_κ, when Ω_+ is bounded uniformly rectifiable and $\eta = 0$. The idea is to identify some situations where the operator $\Lambda_{\kappa,+}$ gives rise to a Fredholm operator, and thereby use Theorem 3.1.1 to get the self-adjointness of H_κ. So in this subsection the domain Ω_+ is UR unless stated otherwise, and we suppose that $\eta = 0$. Thus, H_κ coincides with $H_{\epsilon,\mu}$, the Dirac operator with electrostatic and Lorentz scalar δ-shell interactions supported on Σ. The first main result on the spectral properties of the Dirac operator $H_{\epsilon,\mu}$ reads as follows:

Theorem 3.2.4. *Let* $(\epsilon, \mu) \in \mathbb{R}^2$ *be such that* $0 < |\epsilon^2 - \mu^2| < 1/\|\mathscr{C}_\Sigma\|^2_{L^2(\Sigma)^4 \to L^2(\Sigma)^4}$, *then* $H_{\epsilon,\mu}$ *is self-adjoint. In particular, if* Ω_+ *is Lipschitz and there is* $z_0 \in \mathbb{C} \setminus \mathbb{R}$, *such that* $|\epsilon^2 - \mu^2| < 1/\| C_\Sigma^{z_0} \|^2_{L^2(\Sigma)^4 \to L^2(\Sigma)^4}$, *then it holds that*

$$\mathrm{Sp}_{\mathrm{ess}}(H_{\epsilon,\mu}) = (-\infty, -m] \cup [m, +\infty). \tag{3.2.28}$$

Proof. Fix $\epsilon, \mu \in \mathbb{R}$ such that

$$0 < |\epsilon^2 - \mu^2| < 1/\|\mathscr{C}_\Sigma^z\|^2_{L^2(\Sigma)^4 \to L^2(\Sigma)^4},$$

holds for some $z \in \mathbb{C} \setminus ((-\infty, -m] \cup [m, \infty))$. Then, from the proof of Corollary 3.2.1 we have

$$\Lambda^z_{(\epsilon,\mu),\mp}\Lambda^z_{(\epsilon,\mu),\pm} = \frac{1}{\epsilon^2 - \mu^2} - (\mathscr{C}_\Sigma^z)^2 + \frac{2\mu}{\epsilon^2 - \mu^2}(mI_4 + z\beta)S^z, \tag{3.2.29}$$

Recall that $\mathscr{C}_\Sigma^z$ is bounded in $L^2(\Sigma)^4$. Using Neumann's lemma, it follows that

$$M_z := \left(I - (\epsilon^2 - \mu^2)(\mathscr{C}_\Sigma^z)^2 \right),$$

is a bounded invertible operator in $L^2(\Sigma)^4$. Now, since $(mI_4 + z\beta)$ is bounded and S is compact on $L^2(\Sigma)^4$, we therefore get that $K_z := \frac{2\mu}{\epsilon^2-\mu^2}(mI_4 + z\beta)S^z$ is compact on $L^2(\Sigma)^4$. Combining this with (3.2.29), we obtain that

$$\begin{aligned} I - (\epsilon^2 - \mu^2)M_z^{-1}\Lambda^z_{(\epsilon,\mu),-}\Lambda^z_{(\epsilon,\mu),+} &= -(\epsilon^2 - \mu^2)M_z^{-1}K_z, \\ I - (\epsilon^2 - \mu^2)\Lambda^z_{(\epsilon,\mu),+}\Lambda^z_{(\epsilon,\mu),-}M_z^{-1} &= -(\epsilon^2 - \mu^2)K_z M_z^{-1}. \end{aligned} \tag{3.2.30}$$

As $M_z^{-1}\Lambda^z_{(\epsilon,\mu),-}$ and $\Lambda^z_{(\epsilon,\mu),-}M_z^{-1}$ are bounded operators on $L^2(\Sigma)^4$, $M_z^{-1}K_z$ and $K_z M_z^{-1}$ are compact on $L^2(\Sigma)^4$, then [2, Theorem 1.50 and Theorem 1.51] yields that $\Lambda^z_{(\epsilon,\mu),+}$ is Fredholm. Hence, the first statement is a direct consequence of Theorem 3.1.1 and the fact that $\Lambda_{(\epsilon,\mu),+}$ is a self-adjoint, Fredholm operator on $L^2(\Sigma)^4$. Since $\Lambda^{z_0}_{(\epsilon,\mu),+}$ is Fredholm by assumption, by Proposition 3.1.1 we easily get the last statement. □

Remark 3.2.3. *From Lemma 1.3.2(iv) we know that $\|\mathscr{C}^z_\Sigma\| \geqslant 1/2$, which implies that $|\epsilon^2 - \mu^2| < 4$. Hence, the combination of coupling constants ϵ and μ is not critical. Of course, we already know that the above result is false in the case $\epsilon^2 - \mu^2 = 4$. Also, note that Theorem 3.2.4 remains valid if one control the norm of the Cauchy operator instead of controlling $|\epsilon^2 - \mu^2|$. However, this may affect the geometric characterization of Σ, leading to an increase in regularity.*

As mentioned in the introduction, the existence of a unique self-adjoint realization of the two dimensional Dirac operator with pure Lorentz scalar δ-interactions was shown in [92] for $m = 0$ and $\mu \in (-2, 2)$, where Σ is a closed curve with finitely many corners. It seems that their assumption (i.e., the restriction that μ must lie in $(-2, 2)$) is related to the assumption we made in the Theorem 3.2.4.

Although Theorem 3.2.4 gives an upper bound for $|\epsilon^2 - \mu^2|$ so that $H_{\epsilon,\mu}$ is self-adjoint, this is not satisfactory in the sense that this bound involves $\|\mathscr{C}_\Sigma\|^2_{L^2(\Sigma)^4\to L^2(\Sigma)^4}$, which is not easy to quantify. In what follow, we are going to remove this restriction by imposing a better quantitative assumption than the one of Theorem 3.2.4.

Theorem 3.2.5. *Let $(\epsilon, \mu) \in \mathbb{R}^2$ be such that $|\epsilon| \neq |\mu|$, and let $(H_{\epsilon,\mu}, \mathrm{dom}(H_{\epsilon,\mu}))$ be as above. Assume that ϵ and μ satisfy one of the the following assumptions:*

(a) $\epsilon^2 - \mu^2 < 1/\|W\|^2_{L^2(\Sigma)^2\to L^2(\Sigma)^2}$.

(b) $\epsilon^2 - \mu^2 > 16\|W\|^2_{L^2(\Sigma)^2\to L^2(\Sigma)^2}$.

Then $H_{\epsilon,\mu}$ is self-adjoint. In particular, if Ω_+ is Lipschitz, then the following statements hold true:

(i) *Given $a \in (-m, m)$, then* $\mathrm{Kr}(H_{\epsilon,\mu} - a) \neq \{0\} \iff \mathrm{Kr}(\Lambda^a_{(\epsilon,\mu),+}) \neq \{0\}$.

(ii) $\mathrm{Sp}_{\mathrm{disc}}(H_{\epsilon,\mu}) \cap (-m, m)$ *is finite.*

(iii) *For all $z \in \mathbb{C} \setminus \mathbb{R}$, it holds that*

$$(H_{\epsilon,\mu} - z)^{-1} = (H - z)^{-1} - \Phi^z(\Lambda^z_{(\epsilon,\mu),+})^{-1} t_\Sigma (H - z)^{-1}.$$

(iv) $\mathrm{Sp}_{\mathrm{ess}}(H_{\epsilon,\mu}) = (-\infty, -m] \cup [m, +\infty)$.

(v) *$a \in \mathrm{Sp_p}(H_{\epsilon,\mu})$ if and only if $a \in \mathrm{Sp_p}(H_{\frac{-4\epsilon}{\epsilon^2-\mu^2}, \frac{-4\mu}{\epsilon^2-\mu^2}})$, for all $a \in (-m, m)$.*

(vi) *$C_0 := \sup_{a\in[-m,m]} \|\mathscr{C}^a_\Sigma\| < \infty$. Moreover, $\mathrm{Sp}_{\mathrm{disc}}(H_{\epsilon,\mu}) \cap (-m, m) = \emptyset$ either if $|\epsilon - \mu| < 1/C_0$ and $|\epsilon + \mu| < 1/C_0$, or if $|\epsilon - \mu| > 4C_0$ and $|\epsilon + \mu| > 4C_0$.*

(vii) If $\epsilon = 0$ and $\mu > 0$, then $\mathrm{Sp}_{\mathrm{disc}}(H_{\epsilon,\mu}) \cap (-m, m) = \emptyset$.

Proof. To prove the theorem, in both situations, we show that $\Lambda^z_{(\epsilon,\mu),+}$ is Fredholm for all $z \in \mathbb{C} \setminus ((-\infty, -m] \cup [m, \infty))$. Once this is shown, we use the fact that $\Lambda_{(\epsilon,\mu),+}$ is a bounded self-adjoint operator, and we conclude by using Theorem 3.1.1 to obtain the first statement of the theorem. So, fix $\epsilon, \mu \in \mathbb{R}$ such that $|\epsilon| \neq |\mu|$, and let $z \in \mathbb{C} \setminus ((-\infty, -m] \cup [m, \infty))$. Then, from the definition of $\mathscr{C}^z_\Sigma$ it follows that

$$\mathscr{C}^z_\Sigma = T^z_K + \begin{pmatrix} 0 & W \\ W & 0 \end{pmatrix} := T^z_K + \widetilde{W}, \tag{3.2.31}$$

where the kernel K satisfies

$$\sup_{1 \leqslant k,j \leqslant 4} |K(x-y)| = \mathcal{O}\left(|x-y|^{-1}\right) \qquad \text{when } |x-y| \longrightarrow 0. \tag{3.2.32}$$

Hence, T^z_K is compact in $L^2(\Sigma)^4$. Therefore, in the same way as in (3.2.29) we get that

$$\begin{aligned} \Lambda^z_{(\epsilon,\mu),\mp}\Lambda^z_{(\epsilon,\mu),\pm} &= \frac{1}{\epsilon^2-\mu^2} - \widetilde{W}^2 + (T^z_K)^2 + \{T^z_K, \widetilde{W}\} + \frac{2\mu}{\epsilon^2-\mu^2}(mI_4 + z\beta)S^z \\ &:= \frac{1}{\epsilon^2-\mu^2} - \widetilde{W}^2 + T_K, \end{aligned} \tag{3.2.33}$$

where T_K is compact in $L^2(\Sigma)^4$. Now, observe that

$$\widetilde{W}^2 = \begin{pmatrix} W^2 & 0 \\ & W^2 \end{pmatrix}.$$

As W is a bounded self-adjoint operator in $L^2(\Sigma)^2$, it follows that $\widetilde{W}^2$ is a nonnegative, self-adjoint operator on $L^2(\Sigma)^4$. Hence, we get

$$\mathrm{Sp}(\widetilde{W}^2) \subset \left(0, \|W\|^2_{L^2(\Sigma)^2 \to L^2(\Sigma)^2}\right].$$

From this, it follows that $1/(\epsilon^2 - \mu^2)$ belongs to the resolvent set of $\widetilde{W}^2$ when $\epsilon^2 < \mu^2$. Similarly, if $0 < \epsilon^2 - \mu^2 < 1/\|W\|^2_{L^2(\Sigma)^2 \to L^2(\Sigma)^2}$ holds, then $1/(\epsilon^2 - \mu^2) > \|W\|^2_{L^2(\Sigma)^2 \to L^2(\Sigma)^2}$, and thus $1/(\epsilon^2 - \mu^2)$ is not in the spectrum of $\widetilde{W}^2$. Hence, if assumption (a) holds true, then $I_4 - (\epsilon^2 - \mu^2)\widetilde{W}^2$ in invertible on $L^2(\Sigma)^4$. In that case, similar arguments to those of the proof of Theorem 3.2.4 yield that $\Lambda^z_{(\epsilon,\mu),+}$ is Fredholm.

Now assume that assumption (b) holds true. Then, from Lemma 1.3.2 we know that W is invertible on $L^2(\Sigma)^2$ and $W^{-1} = -4(\sigma \cdot N)W(\sigma \cdot N)$. Thus, from (3.2.33) it follows that

$$\begin{aligned} (\epsilon^2-\mu^2)(\widetilde{W}^{-1})^2\Lambda^z_{(\epsilon,\mu),-}\Lambda^z_{(\epsilon,\mu),+} &= (\widetilde{W}^{-1})^2 - (\epsilon^2-\mu^2)I_4 + (\epsilon^2-\mu^2)(\widetilde{W}^{-1})^2 T_K, \\ (\epsilon^2-\mu^2)\Lambda^z_{(\epsilon,\mu),+}\Lambda^z_{(\epsilon,\mu),-}(\widetilde{W}^{-1})^2 &= (\widetilde{W}^{-1})^2 - (\epsilon^2-\mu^2)I_4 + (\epsilon^2-\mu^2)T_K(\widetilde{W}^{-1})^2. \end{aligned} \tag{3.2.34}$$

As $\|\widetilde{W}\|_{L^2(\Sigma)^4 \to L^2(\Sigma)^4} = \|W\|_{L^2(\Sigma)^2 \to L^2(\Sigma)^2}$, using again Lemma 1.3.2 we get that

$$\|\widetilde{W}^{-1}\|_{L^2(\Sigma)^4 \to L^2(\Sigma)^4} \leqslant 4\|\widetilde{W}\|_{L^2(\Sigma)^4 \to L^2(\Sigma)^4} = 4\|W\|_{L^2(\Sigma)^2 \to L^2(\Sigma)^2} \tag{3.2.35}$$

Hence, if $\epsilon^2 - \mu^2 > 16\|W\|^2_{L^2(\Sigma)^2 \to L^2(\Sigma)^2}$, then $\epsilon^2 - \mu^2 > \|\widetilde{W}^{-1}\|^2_{L^2(\Sigma)^4 \to L^2(\Sigma)^4}$. Thus $\epsilon^2 - \mu^2$ is not in the spectrum of $(\widetilde{W}^{-1})^2$. Thereby $\widetilde{W}^{-1} - (\epsilon^2 - \mu^2)I_4$ is invertible on $L^2(\Sigma)^4$. Now, from (3.2.34) it follows that

$$\begin{aligned} I_4 - (\epsilon^2-\mu^2)\left((\widetilde{W}^{-1})^2 - (\epsilon^2-\mu^2)I_4\right)^{-1}(\widetilde{W}^{-1})^2\Lambda^z_{(\epsilon,\mu),-}\Lambda^z_{(\epsilon,\mu),+} &= T_{K_1}, \\ I_4 - (\epsilon^2-\mu^2)\Lambda^z_{(\epsilon,\mu),+}\Lambda^z_{(\epsilon,\mu),-}(\widetilde{W}^{-1})^2\left((\widetilde{W}^{-1})^2 - (\epsilon^2-\mu^2)I_4\right)^{-1} &= T_{K_2}. \end{aligned} \tag{3.2.36}$$

where $T_{K_1}, T_{K_2} \in \mathcal{K}(L^2(\Sigma)^4)$. Thereby, [2, Theorem 1.50 and Theorem 1.51] yields that $\Lambda^z_{(\epsilon,\mu),+}$ is Fredholm, and this finishes the proof of the first statement.

Item (i) is a consequence of Proposition 3.1.1. The proof of the assertions (ii), (iii), (iv) and (v) runs as in the proof of Theorem 3.2.1. Now we turn to the proof of item (vi). The first claim of statement is contained in [11, Lemma 3.2] (see also [16, Proposition 3.5]), for C^2-compact surfaces, and the same arguments apply to the Lipschitz case. To prove the last claim of (v), note that for all $a \in (-m, m)$ we have

$$0 \in \mathrm{Sp}_{\mathrm{disc}}(\Lambda^a_{(\epsilon,\mu),+}) \Longleftrightarrow -1 \in \mathrm{Sp}_{\mathrm{disc}}((\epsilon I_4 + \mu\beta)\mathscr{C}^a_\Sigma). \tag{3.2.37}$$

Using the first claim of (vi), it follows that if $|\epsilon - \mu| < 1/C_0$ and $|\epsilon + \mu| < 1/C_0$, then

$$\|(\epsilon I_4 + \mu\beta)\mathscr{C}^a_\Sigma\|_{L^2(\Sigma)^4 \to L^2(\Sigma)^4} < 1.$$

Therefore, $-1 \notin \mathrm{Sp}_{\mathrm{disc}}((\epsilon I_4 + \mu\beta)\mathscr{C}^a_\Sigma)$. Hence, (3.2.37) together with assertion (i) yield that

$$\mathrm{Sp}_{\mathrm{disc}}(H_{\epsilon,\mu}) \cap (-m, m) = \emptyset.$$

Using the equivalence given by (v), and iterating the previous arguments we easily recover the case $|\epsilon - \mu| > 4C_0$ and $|\epsilon + \mu| > 4C_0$, which gives (vi).

Finally, the assertion (vii) is a consequence of (i). Indeed, suppose that $\epsilon = 0$ and fix $a \in (-m, m)$. Then we have

$$(\Lambda^a_{(0,\mu),+})^2 = \frac{1}{\mu^2} + (\mathscr{C}^a_\Sigma)^2 + \frac{2}{\mu}(mI_4 + a\beta)S^a.$$

As S^a is a positive operator in $L^2(\Sigma)^4$ for all $a \in (-m, m)$; cf. [11, Lemma 4.2], it follows that

$$(\mathscr{C}^a_\Sigma)^2 + \frac{2}{\mu}(mI_4 + a\beta)S^a,$$

is also a positive operator for $\mu > 0$. Therefore, $0 \notin \mathrm{Sp}(\Lambda^a_{(0,\mu),+})$ for all $a \in (-m, m)$, which proves (vi). This completes the proof of theorem. □

Remark 3.2.4. *Assume that Ω_+ is Lipschitz. Then, using essentially the same arguments as in the proof of Theorem 3.2.5, one can show that, if for all $a \in (-m, m)$ one of the following assumptions holds*

$$\text{(a) } 16\|\mathscr{C}^a_\Sigma\|^2_{L^2(\Sigma)^4 \to L^2(\Sigma)^4} < \epsilon^2 - \mu^2, \qquad \text{(b) } \epsilon^2 - \mu^2 < 1/\|\mathscr{C}^a_\Sigma\|^2_{L^2(\Sigma)^4 \to L^2(\Sigma)^4},$$

then $H_{\epsilon,\mu}$ is self-adjoint. Moreover, if $\mu = 0$, then from Theorem 3.2.5-(v) it follows that

$$\mathrm{Sp}_{\mathrm{disc}}(H_{\epsilon,0}) \cap (-m, m) = \emptyset,$$

see also [11, Theorem 3.3] and [16, Theorem 4.4] for a similar result.

Remark 3.2.5. *Assume that Ω_+ is UR. Then, using exactly the same technique as in the proof of Theorem 3.2.5, one can show that the coupling $(H + \tilde{\epsilon}\gamma_5\delta_\Sigma)$ is self-adjoint under the assumption* (a) *or* (b), *with $\mu = 0$.*

Remark 3.2.6. *Note that in Theorem 3.2.5, the combination of the coupling constants ϵ and μ is not critical. Moreover, there is an interval $J \subset \mathbb{R}_+$, such that we have no information on the self-adjointness character of $H_{\epsilon,\mu}$, if $\epsilon^2 - \mu^2 \in J$. We would also note that if Ω_+ is a ball, the interval reduces to the point $J = \{4\}$, since $\|W\| = 1/2$; cf. [12, Lemma 4.2]*

Next, we discuss the particular case $\epsilon^2 - \mu^2 = -4$. Assume that Ω_+ is Lipschitz, then it is clear that (P4) holds true. Thus, if we let

$$P_\pm = \left(1 \mp \frac{i}{2}(\epsilon + \mu\beta)(\alpha \cdot N)\right).$$

As a consequence of proposition 3.1.3 we have the following result.

Proposition 3.2.4. *Assume that Ω_+ is Lipschitz. Let $(\epsilon, \mu) \in \mathbb{R}^2$ be such that $\epsilon^2 - \mu^2 = -4$, and let $H_{\epsilon,\mu}$ be as in Theorem 3.2.5. Then Σ is impenetrable and it holds that*

$$H_{\epsilon,\mu}\varphi = H^{\Omega_+}_{\epsilon,\mu}(\varphi_+) \oplus H^{\Omega_-}_{\epsilon,\mu}(\varphi_-) = (-i\alpha \cdot \nabla + m\beta)\,\varphi_+ \oplus (-i\alpha \cdot \nabla + m\beta)\,\varphi_- \tag{3.2.38}$$

where $H^{\Omega_\pm}_{\epsilon,\mu}$ are the self-adjoint Dirac operators defined on

$$\mathrm{dom}(H^{\Omega_\pm}_{\epsilon,\mu}) = \left\{\varphi_\pm := u_{\Omega_\pm} + \Phi_{\Omega_\pm}[g], u_{\Omega_\pm} \in H^1(\Omega_\pm)^4, g \in L^2(\Sigma)^4 : P_\pm \lim_{\mathrm{nt}} \varphi_\pm = 0\right\}.$$

Remark 3.2.7. *By Taking $\epsilon = 0$ in Theorem 3.2.5* (a)*, we conclude that if Ω_+ is UR, then $H_{0,\mu}$ is always self-adjoint. Moreover, $H_{0,\mu}$ generates confinement when $\mu = \pm 2$, for any compact Lipschitz surface Σ.*

The reason we assumed that $\eta = 0$ is purely technical. The following proposition is about the self-adjointness of the coupling $H + \eta(\alpha \cdot N)\delta_\Sigma$.

Proposition 3.2.5. *Assume that Ω_+ is UR. Let $\eta \in \mathbb{R} \setminus \{0\}$, set $\kappa = (0, 0, \eta)$ and let H_κ be as above. Then H_κ is self-adjoint and we have*

$$\mathrm{dom}(H_\kappa) = \left\{u + \Phi[-4\eta^2(\eta^2+4)^{-1}(\alpha \cdot N)\Lambda_{\kappa,-}(\alpha \cdot N)[t_\Sigma u]] : u \in H^1(\mathbb{R}^3)^4\right\}.$$

Moreover, If Ω_+ is Lipschitz, then the spectrum of H_κ is given by

$$\mathrm{Sp}(H_\kappa) = \mathrm{Sp}_{\mathrm{ess}}(H_\kappa) = (-\infty, -m] \cup [m, +\infty). \tag{3.2.39}$$

Remark 3.2.8. *It is worth noting that in 2D the analog of the coupling $H + \eta(\alpha \cdot N)\delta_\Sigma$ is unitarily equivalent to the two-dimensional Dirac operator, see [41, Theorem 2.1] for more details.*

Proof. Assume that $\eta \in \mathbb{R} \setminus \{0\}$ and fix $z \in \mathbb{C} \setminus ((-\infty, -m] \cup [m, \infty))$. Recall that $\Lambda^z_{\kappa,\pm}$ are given by

$$\Lambda^z_{\kappa,\pm} = \frac{1}{\eta}(\alpha \cdot N) \pm \mathscr{C}^z_\Sigma.$$

Now, using Lemma 1.3.2, a simple computation yields

$$(\eta(\alpha \cdot N))\Lambda^z_{\kappa,-}(\eta(\alpha \cdot N))\Lambda^z_{\kappa,+} = \Lambda^z_{\kappa,+}(\eta(\alpha \cdot N))\Lambda^z_{\kappa,-}(\eta(\alpha \cdot N)) = 1 + \frac{\eta^2}{4}.$$

Therefore, $\Lambda^z_{\kappa,+}$ is invertible with $(\Lambda^z_{\kappa,+})^{-1} = 4\eta^2(\eta^2+4)^{-1}(\alpha \cdot N)\Lambda^z_{\kappa,-}(\alpha \cdot N)$. In particular, $\Lambda^z_{\kappa,+}$ is Fredholm for all $z \in \mathbb{C} \setminus ((-\infty, -m] \cup [m, \infty))$. As $\Lambda_{\kappa,+}$ is invertible and self-adjoint in $L^2(\Sigma)^4$, using Theorem 3.1.1 we then get the first statement. That $\mathrm{Sp}(H_\kappa)$ is characterized by (3.2.39) is a consequence of Proposition 3.1.1. This completes the proof of the proposition. ☐

To finish this part, we briefly discuss the particular case $\mu = \pm\epsilon$. Assume that Ω_+ is Lipschitz and given $\epsilon \in \mathbb{R} \setminus \{0\}$, recall that $H_{\epsilon,\mu}$ is defined on the domain

$$\mathrm{dom}(H_{\epsilon,\pm\epsilon}) = \Big\{ u + \Phi[g] : u \in H^1(\mathbb{R}^3)^4, g \in P_\pm L^2(\Sigma)^4 \text{ and } P_\pm t_\Sigma u = -\Lambda_{\epsilon,+}[g] \Big\}, \quad (3.2.40)$$

where $\Lambda_{\epsilon,\pm}$ are given by

$$\Lambda_{\epsilon,+} = P_+ \left(1/2\epsilon + \mathscr{C}_\Sigma\right) P_+ \text{ and } \Lambda_{\epsilon,-} = P_+ \left(1/2\epsilon - \mathscr{C}_\Sigma\right) P_+, \quad \text{if } \mu = \epsilon,$$
$$\Lambda_{\epsilon,+} = P_- \left(1/2\epsilon + \mathscr{C}_\Sigma\right) P_- \text{ and } \Lambda_{\epsilon,-} = P_- \left(1/2\epsilon - \mathscr{C}_\Sigma\right) P_-, \quad \text{if } \mu = -\epsilon,$$

where $P_\pm = (I_4 \pm \beta)/2$, see Proposition 2.2.4.

The following proposition is about the self-adjointness of $H_{\epsilon,\pm\epsilon}$. Its proof follows exactly the same lines as the proof of Theorem 3.1.1, so we will only reproduce the main ideas here. In the proof, we use the notations $\langle\, ,\, \rangle_{\mathbb{R}^3}$ and $\langle\, ,\, \rangle_\Sigma$ for the scalar product in $L^2(\mathbb{R}^3)^4$ and $L^2(\Sigma)^4$, respectively.

Proposition 3.2.6. *Let $\epsilon \in \mathbb{R} \setminus \{0\}$ and assume that Ω_+ is a bounded Lipschitz domain. Then $H_{\epsilon,\pm\epsilon}$ is self-adjoint and it holds that*

$$\mathrm{dom}(H_{\epsilon,\pm\epsilon}) = \Big\{ u + \Phi[g] : u \in H^1(\mathbb{R}^3)^4, g \in P_\pm H^{1/2}(\Sigma)^4, P_\pm t_\Sigma u = -\Lambda_{\epsilon,+}[g] \Big\}. \quad (3.2.41)$$

Proof. The cases $\epsilon = \mu$ and $\epsilon = \mu$ are almost identical, so we only sketch a proof for $\epsilon = \mu$. It is clear that $H_{\epsilon,\epsilon}$ is symmetric and densely defined on $\mathrm{dom}(H_{\epsilon,\epsilon})$. Hence, it remains to prove the inclusions $H^*_{\epsilon,\epsilon} \subset H_{\epsilon,\epsilon}$ and that $\mathrm{dom}(H_{\epsilon,\epsilon})$ is given by (3.2.41). First, observe that

$$\Lambda_{\epsilon,-}\Lambda_{\epsilon,+} = \Lambda_{\epsilon,+}\Lambda_{\epsilon,-} = \frac{1}{4\epsilon^2} P_+ - P_+\mathscr{C}_\Sigma P_+ \mathscr{C}_\Sigma P_+ = \frac{1}{4\epsilon^2} P_+ - m^2(S)^2 P_+. \quad (3.2.42)$$

where in the last equality the anticommutation relations of the Dirac matrices were used. As $\Lambda_{\epsilon,\pm}$ is bounded and self-adjoint in $P_+L^2(\Sigma)^4$, and S is bounded from $H^{-1/2}(\Sigma)^4$ to $H^{1/2}(\Sigma)^4$, we get by [2, Theorem 1.46 (iii)] that $\Lambda_{\epsilon,\pm}$ is a Fredholm operator in $P_+L^2(\Sigma)^4$. Therefore $\{\Phi[g] : g \in \mathrm{Kr}(\Lambda_{\epsilon,+})\}$ is closed and the following decomposition holds

$$P_+L^2(\Sigma)^4 = \mathrm{Kr}(\Lambda_{\epsilon,+}) \oplus \mathrm{Rn}(\Lambda_{\epsilon,+}). \quad (3.2.43)$$

Now we are going to show that $H^*_{\epsilon,\epsilon} \subset H_{\epsilon,\epsilon}$. To this end, it is sufficient to prove that $\mathcal{G}(H^*_{\epsilon,\epsilon}) \subset \mathcal{G}(H_{\epsilon,\epsilon})$, where $\mathcal{G}(H^*_{\epsilon,\epsilon})$ (resp. $\mathcal{G}(H_{\epsilon,\epsilon})$) denotes the graph of $H^*_{\epsilon,\epsilon}$ (resp. $H_{\epsilon,\epsilon}$). Once we know this, it follows immediately from the regularization property of S and (3.2.42) that, if $u + \Phi[g] \in \mathrm{dom}(H_{\epsilon,\epsilon})$ then $g \in P_+H^{1/2}(\Sigma)^4$, which implies that $\mathrm{dom}(H_{\epsilon,\epsilon})$ is given by (3.2.41).

In what follows we will adapt the proof of Theorem 3.1.1 to the current case. Let $(\psi, G) \in \mathcal{G}(H^*_{\epsilon,\epsilon})$, then it holds that

$$\langle H_{\epsilon,\epsilon}\varphi, \psi\rangle_{\mathbb{R}^3} = \langle \varphi, G\rangle_{\mathbb{R}^3}, \quad \forall \varphi = u + \Phi[g] \in \mathrm{dom}(H_{\epsilon,\epsilon}).$$

As $H^{-1}G \in H^1(\mathbb{R}^3)^4$, from (3.2.43) it follows that $P_+t_\Sigma H^{-1}G = h + \Lambda_{\epsilon,+}[f]$, with $h \in \mathrm{Kr}(\Lambda_{\epsilon,+})$. Since $\Phi[h] \in \mathrm{dom}(H_{\epsilon,\epsilon})$ and $H_{\epsilon,\epsilon}\Phi[h] = 0$, we thus get

$$0 = \langle H_{\epsilon,\epsilon}\Phi[h], \psi\rangle_{\mathbb{R}^3} = \langle \Phi[h], G\rangle_{\mathbb{R}^3} = \langle h, t_\Sigma H^{-1}G\rangle_\Sigma = \langle h, P_+t_\Sigma H^{-1}G\rangle_\Sigma,$$

where in the last equalities [10, Lemma 2.10] was used. As $P_+t_\Sigma H^{-1}G = h + \Lambda_{\epsilon,+}[f]$ and $\Lambda_{\epsilon,+}[h] = 0$, using the self-adjointness of $\Lambda_{\epsilon,+}$ we obtain that $0 = \langle h, P_+t_\Sigma H^{-1}G\rangle_\Sigma = \langle h, h\rangle_\Sigma$.

From this, we conclude that $P_+ t_\Sigma H^{-1} G = \Lambda_{\epsilon,+}[f]$. Hence, the previous conclusion together with [10, Lemma 2.10] yield that

$$\begin{aligned}\langle Hu, \psi\rangle_{\mathbb{R}^3} &= \langle u + \Phi[g], G\rangle_{\mathbb{R}^3} = \langle Hu, H^{-1}G\rangle_{\mathbb{R}^3} + \langle g, t_\Sigma H^{-1} G\rangle_{L^2(\Sigma)^4} \\ &= \langle Hu, H^{-1}G\rangle_{\mathbb{R}^3} + \langle g, \Lambda_{\epsilon,+}[f]\rangle_\Sigma = \langle Hu, H^{-1}G\rangle_{\mathbb{R}^3} - \langle t_\Sigma u, f\rangle_\Sigma,\end{aligned}$$

for any $\varphi = u + \Phi[g] \in \mathrm{dom}(H_{\epsilon,\epsilon})$. Notice that

$$P_+ t_\Sigma u = P_+ t_\Sigma H H^{-1} u = t_\Sigma H H^{-1} P_+ u = t_\Sigma P_+ u. \tag{3.2.44}$$

Using this, from the above computations it follows that $\langle Hu, \psi\rangle_{\mathbb{R}^3} = \langle Hu, H^{-1}G - \Phi[f]\rangle_{\mathbb{R}^3}$. Hence, we get

$$\langle Hu, \psi - (H^{-1}G - \Phi[f])\rangle_{\mathbb{R}^3} = 0 \quad \text{for all } u \in H^1(\mathbb{R}^3)^4 \text{ such that } P_+ t_\Sigma u \in \mathrm{Rn}(\Lambda_{\epsilon,+}).$$

As $\Lambda_{\epsilon,+}$ is Fredholm and self-adjoint, we get by [10, Lemma 2.10] and (3.2.44) that: $P_+ t_\Sigma u \in \mathrm{Rn}(\Lambda_{\epsilon,+})$ if and only if $0 = \langle t_\Sigma u, h\rangle_\Sigma = \langle Hu, \Phi[h]\rangle_{\mathbb{R}^3}$ for all $h \in \mathrm{Kr}(\Lambda_{\epsilon,+})$. Which implies that $\psi - H^{-1}G + \Phi[f] \in \{\Phi[g] : g \in \mathrm{Kr}(\Lambda_{\epsilon,+})\}$. Thus, for all $(\psi, G) \in \mathcal{G}(H^*_{\epsilon,\epsilon})$, there exist $(h_j)_{j\in\mathbb{N}} \subset \mathrm{Kr}(\Lambda_{\epsilon,+})$ and $f \in \mathrm{Rn}(\Lambda_{\epsilon,+})$ such that the following hold:

$$\begin{aligned}\lim_{j\to\infty} \Phi[h_j] &= \Phi[h] \in \mathrm{dom}(H_{\epsilon,\epsilon}) \text{ with } h \in \mathrm{Kr}(\Lambda_{\epsilon,+}),\\ \psi = \lim_{j\to\infty}(H^{-1}G - \Phi[f] + \Phi[h_j]) &= H^{-1}G - \Phi[f] + \Phi[h] \text{ in } L^2(\mathbb{R}^3)^4.\end{aligned}$$

Since $H_{\epsilon,\epsilon}(H^{-1}G - \Phi[f] + \Phi[h_j]) = G$ for all $j \in \mathbb{N}$, we then get $\mathcal{G}(H^*_{\epsilon,\epsilon}) \subset \mathcal{G}(H_{\epsilon,\epsilon})$, which completes the proof. □

3.2.4 Spectral properties of $H_{\tilde\mu}$ and $H_{\tilde\upsilon}$

In this part, we briefly discuss the spectral properties of the Dirac operators $H_{\tilde\mu}$ and $H_{\tilde\upsilon}$ defined by (3.2.1). Recall that for $\tilde\mu, \tilde\upsilon \in \mathbb{R}\setminus\{0\}$, the operators $\Lambda^z_{\tilde\mu,\pm}$ and $\Lambda^z_{\tilde\upsilon,\pm}$ are given by

$$\Lambda^z_{\tilde\mu,\pm} = \frac{i}{\tilde\mu}\gamma_5\beta \pm \mathscr{C}^z_\Sigma \text{ and } \Lambda^z_{\tilde\upsilon,\pm} = \frac{1}{\tilde\upsilon}\gamma_5\beta(\alpha\cdot N) \pm \mathscr{C}^z_\Sigma. \tag{3.2.45}$$

The following two propositions summarise the main spectral properties of $H_{\tilde\mu}$. We remark that $H_{\tilde\mu}$ has almost the same properties as the coupling $(H + \mu\beta\delta_\Sigma)$, and this is the reason why we called the potential $V_{\tilde\mu}$ the *modified Lorentz scalar* δ-potential.

Proposition 3.2.7. *Let $\tilde\mu \in \mathbb{R}\setminus\{0\}$ and assume that Ω_+ is UR, then $(H_{\tilde\mu}, \mathrm{dom}(H_{\tilde\mu}))$ is self-adjoint. In particular, if Ω_+ is Lipschitz, then the following hold:*

(i) $\mathrm{Sp}_{\mathrm{ess}}(H_{\tilde\mu}) = (-\infty, -m] \cup [m, +\infty)$.

(ii) If $\tilde\mu^2 = 4$, then $H_{\tilde\mu}$ generates confinement and we have

$$H_{\tilde\mu}\varphi = H^{\Omega_+}_{\tilde\mu}\varphi_+ \oplus H^{\Omega_-}_{\tilde\mu}\varphi_- = (-i\alpha\cdot\nabla + m\beta)\,\varphi_+ \oplus (-i\alpha\cdot\nabla + m\beta)\,\varphi_-,$$

where $H^{\Omega_\pm}_{\tilde\mu}$ are the self-adjoint Dirac operators defined on

$$\mathrm{dom}(H^{\Omega_\pm}_{\tilde\mu}) = \Big\{ u_{\Omega_\pm} + \Phi_{\Omega_\pm}[g] : u_{\Omega_\pm} \in H^1(\Omega_\pm)^4, g \in L^2(\Sigma)^4 \text{ and } \left(\frac{1}{2} \mp \frac{1}{\tilde\mu}\gamma_5\beta(\alpha\cdot N)\right)(t_\Sigma u_{\Omega_\pm} + C_\pm[g]) = 0 \Big\}.$$

Proof. Fix $z \in \mathbb{C} \setminus ((-\infty, -m] \cup [m, \infty))$, and observe that

$$\{\gamma_5\beta, \mathscr{C}_\Sigma^z\} = 2z\gamma_5\beta S^z. \tag{3.2.46}$$

Now, using (3.2.31), similar arguments as in the proof of Theorem 3.2.5 yield that

$$(\Lambda^z_{\tilde\mu,+})^2 = \frac{1}{\tilde\mu^2} + \widetilde{W}^2 + \frac{i}{\tilde\mu}\{\gamma_5\beta, \mathscr{C}_\Sigma^z\} + T_z, \tag{3.2.47}$$

where $T_z \in \mathscr{K}(L^2(\Sigma)^4)$. Thus $(\Lambda^z_{\tilde\mu,+})$ is Fredholm, for all $z \in \mathbb{C} \setminus ((-\infty, -m] \cup [m, \infty))$. Therefore, $H_{\tilde\mu}$ is self-adjoint by Theorem 3.1.1. Assertion (i) follows by Proposition 3.1.1. Now it is easy to check that $(1/2 \mp \frac{1}{\tilde\mu}\gamma_5\beta(\alpha\cdot N))$ are projectors, thus the property (P3) holds true. Therefore, (ii) is a direct consequence of Proposition 3.1.3. This completes the proof of the proposition. □

The following proposition gives us more information about the spectrum of $H_{\tilde\mu}$ in the case of $C^{1,\omega}$ domains. The arguments of the proof are rather standard, so we are not going to give a complete proof.

Proposition 3.2.8. *Assume that Ω_+ is $C^{1,\omega}$-smooth with $\gamma > 1/2$, and let $H_{\tilde\mu}$ be as in Proposition 3.2.7. Then, the following is true:*

(i) The spectrum of $H_{\tilde\mu}$ is symmetric with respect to 0.

(ii) $\mathrm{Sp}_{\mathrm{disc}}(H_{\tilde\mu}) \cap (-m, m)$ is finite, and every eigenvalue of $H_{\tilde\mu}$ has even multiplicity.

(iii) $H_{\tilde\mu}$ is unitarily equivalent to $H_{-\tilde\mu}$.

(iv) $a \in \mathrm{Sp}_{\mathrm{p}}(H_{\tilde\mu})$ if and only if $a \in \mathrm{Sp}_{\mathrm{p}}(H_{\frac{-4}{\tilde\mu}})$, for all $a \in (-m, m)$.

(v) There is $C_0 > 0$ such that $\mathrm{Sp}_{\mathrm{disc}}(H_{\tilde\mu}) \cap (-m, m) = \emptyset$ either if $|\tilde\mu| < 1/C_0$ or if $|\tilde\mu| > 4C_0$.

Proof. First, observe that for all $\tilde\mu \in \mathbb{R} \setminus \{0\}$, $\mathrm{dom}(H_{\tilde\mu}) \subset H^1(\mathbb{R}^3 \setminus \Sigma)^4$ (this follows in the same way as in Theorem 3.2.3). Moreover, $H_{\tilde\mu}$ acts in the sense of distributions as

$$H_{\tilde\mu}\varphi = (-i\nabla\cdot\alpha + m\beta)\,\varphi_+ \oplus (-i\nabla\cdot\alpha + m\beta)\,\varphi_-, \tag{3.2.48}$$

on the domain

$$\mathrm{dom}(H_{\tilde\mu}) = \Big\{\varphi = (\varphi_+, \varphi_-) \in H^1(\Omega_+)^4 \oplus H^1(\Omega_-)^4 : \\ \left(\frac{1}{2} - \frac{1}{\tilde\mu}\gamma_5\beta(\alpha\cdot N)\right) t_\Sigma\varphi_+ = -\left(\frac{1}{2} + \frac{1}{\tilde\mu}\gamma_5\beta(\alpha\cdot N)\right) t_\Sigma\varphi_-\Big\}.$$

Now assertions (i) and the fact that every eigenvalue of $H_{\tilde\mu}$ has even multiplicity can be proved as much as [66, Theorem 2.3]. Also, that $\mathrm{Sp}_{\mathrm{disc}}(H_{\tilde\mu}) \cap (-m, m)$ is finite can be deduced by applying the same arguments as Theorem 2.3.2.

In order to prove (iii) we define the operator

$$T(\psi) = \gamma_5\beta\psi, \quad \forall\psi \in L^2(\mathbb{R}^3)^4. \tag{3.2.49}$$

Then, a simple computation yields that $T^2(\psi) = -\psi$ and $T(H(\psi)) = -H(T(\psi))$. Moreover, it is easy to verify that

$$\left(\frac{1}{2} \pm \frac{1}{\tilde\mu}\gamma_5\beta(\alpha\cdot N)\right)(\gamma_5\beta t_\Sigma\varphi_\pm) = \gamma_5\beta\left(\frac{1}{2} \mp \frac{1}{\tilde\mu}\gamma_5\beta(\alpha\cdot N)\right) t_\Sigma\varphi_\pm.$$

Hence, we conclude that $\varphi \in \mathrm{dom}(H_{\tilde{\mu}})$ if and only if $T(\varphi) \in \mathrm{dom}(H_{-\tilde{\mu}})$, which proves (iii). Finally, the assertions (iv) and (v) can be proved in the same way as Theorem 3.2.5(v)-(vi). □

We now move on to the spectral study of the operator $H_{\tilde{\upsilon}}$. Again, we note that $H_{\tilde{\upsilon}}$ has almost the same spectral properties as $(H + i\upsilon\beta(\alpha \cdot N)\delta_\Sigma)$. In the following proposition, we are only interested in the self-adjointness character of $H_{\tilde{\upsilon}}$, we omit the other specific spectral properties since they can be derived from Theorem 2.4.1 and Theorem 2.4.2

Proposition 3.2.9. *Let $\tilde{\upsilon} \in \mathbb{R} \setminus \{0\}$ and let $(H_{\tilde{\upsilon}}, \mathrm{dom}(H_{\tilde{\upsilon}}))$ be as in (3.1.4). Then, the following hold true:*

(i) If Ω_+ is a regular SKT domain and $\tilde{\upsilon}^2 \neq 4$, then $(H_{\tilde{\upsilon}}, \mathrm{dom}(H_{\tilde{\upsilon}}))$ is self-adjoint.

(ii) If Ω_+ is a C^2-smooth domain and $\tilde{\upsilon}^2 = 4$, then $(H_{\tilde{\upsilon}}, \mathrm{dom}(H_{\tilde{\upsilon}}))$ is essentially self-adjoint and generates confinement, and we have

$$\overline{H_{\tilde{\upsilon}}}\varphi = H_{\tilde{\upsilon}}^{\Omega_+}\varphi_+ \oplus H_{\tilde{\upsilon}}^{\Omega_-}\varphi_- = (-i\alpha \cdot \nabla + m\beta)\,\varphi_+ \oplus (-i\alpha \cdot \nabla + m\beta)\,\varphi_-,$$

where $H_{\tilde{\upsilon}}^{\Omega_\pm}$ are the self-adjoint Dirac operators defined on

$$\mathrm{dom}(H_{\tilde{\upsilon}}^{\Omega_\pm}) = \Big\{\varphi_\pm \in L^2(\Omega_\pm)^4 : (\alpha \cdot \nabla)\varphi_\pm \in L^2(\Omega_\pm)^4 \text{ and } \Big(\frac{1}{2} \pm \frac{i}{\tilde{\upsilon}}\gamma_5\beta\Big)\, t_\Sigma\varphi_\pm = 0\Big\}.$$

Proof. Let $z \in \mathbb{C} \setminus ((-\infty, -m] \cup [m, \infty))$, then

$$\Lambda_{\tilde{\upsilon},\mp}^z \Lambda_{\tilde{\upsilon},\pm}^z = \frac{1}{\tilde{\upsilon}^2} - (\mathscr{C}_\Sigma^z)^2 \pm \frac{1}{\tilde{\upsilon}}[\gamma_5\beta(\alpha \cdot N), \mathscr{C}_\Sigma^z]. \tag{3.2.50}$$

Now, observe that

$$\frac{1}{\tilde{\upsilon}}[\gamma_5\beta(\alpha \cdot N), \mathscr{C}_\Sigma^z] = m[\gamma_5(\alpha \cdot N), S^z] + \gamma_5\beta(T_z + \{\alpha \cdot N, \widetilde{W}\}), \tag{3.2.51}$$

where $\widetilde{W}$ is given by (3.2.31), and T_z is an integral operator with kernel K_z given by:

$$\begin{aligned} K_z(x,y) =& \sqrt{z^2 - m^2}\frac{e^{i\sqrt{z^2-m^2}|x-y|}}{4\pi|x-y|^2}\left((\alpha \cdot N(x))\alpha \cdot (x-y) + \alpha \cdot (x-y)(\alpha \cdot N(y))\right) \\ &+ \frac{e^{i\sqrt{z^2-m^2}|x-y|} - 1}{4\pi|x-y|^3}\left[(\alpha \cdot N(x))(i\alpha \cdot (x-y)) + (i\alpha \cdot (x-y))\,(\alpha \cdot N(y))\right]. \end{aligned}$$

Clearly, $T_z, [\gamma_5(\alpha \cdot N), S^z] \in \mathscr{K}(L^2(\Sigma)^4)$. Thus, using Proposition 3.2.2 we get that

$$\Lambda_{\tilde{\upsilon},-}^z \Lambda_{\tilde{\upsilon},+}^z = \frac{4 - \tilde{\upsilon}^2}{4\tilde{\upsilon}^2} - \widetilde{T}_z, \tag{3.2.52}$$

with $\widetilde{T}_z \in \mathscr{K}(L^2(\Sigma)^4)$. Thus, if Ω_+ is a regular SKT domain and $\tilde{\upsilon}^2 \neq 4$, then similar arguments to those of the proof of Theorem 3.2.5 yield that $\Lambda_{\tilde{\upsilon},+}^z$ is Fredholm, for all $z \in \mathbb{C} \setminus ((-\infty, -m] \cup [m, \infty))$. Therefore, (i) follows by Theorem 3.1.1.

Now we are going to prove (ii), we only consider the case $\tilde{\upsilon} = 2$, since the case $\tilde{\upsilon} = -2$ can be treated analogously. So assume that Ω_+ is a C^2-smooth, then it is clear that $\tilde{\upsilon} = 2$ is a critical parameter, and (P1) holds true. Thus, $\Lambda_{2,\pm}$ extends to a bounded operator from $H^{-1/2}(\Sigma)^4$ onto itself by Proposition 1.3.3.

Since $\widetilde{\Lambda}_{2,+} + \widetilde{\Lambda}_{2,-} = \gamma_5\beta(\alpha \cdot N)$, we then deduce that

$$\widetilde{\Lambda}_{2,+}(\gamma_5\beta(\alpha \cdot N))\widetilde{\Lambda}_{2,-} = \Lambda_{2,+}\widetilde{\Lambda}_{2,+}\widetilde{\Lambda}_{2,-} + \widetilde{\Lambda}_{2,+}\widetilde{\Lambda}_{2,-}\widetilde{\Lambda}_{2,-}, \tag{3.2.53}$$

Thus, using the same arguments as in the proof of Lemma 1.3.5 one can show that $\widetilde{\Lambda}_{2,+}\widetilde{\Lambda}_{2,-}$ and $\widetilde{\Lambda}_{2,+}\widetilde{\Lambda}_{2,-}$ are bounded from $H^{-1/2}(\Sigma)^4$ to $H^{1/2}(\Sigma)^4$. Hence, (P2) also holds true and thus H_2 is essentially self-adjoint and generates confinement by Theorem 3.1.2 and Proposition 3.1.4, because (P′3) also holds true. This proves (ii) and complets the proof of the proposition. □

3.3 On the confinement induced by delta interactions involving the Cauchy operator

In this section, we are interested in the families of Dirac operators given by

$$\begin{aligned} &(-m,m) \ni a \longmapsto H_{a,\lambda} = H + \lambda \mathscr{C}^a_\Sigma \delta_\Sigma, \quad \lambda \in \mathbb{R}\setminus\{0\},\\ &(-m,m) \ni a \longmapsto H_{a,\lambda'} = H + \lambda'(\alpha \cdot N)\mathscr{C}^a_\Sigma(\alpha \cdot N)\delta_\Sigma, \quad \lambda' \in \mathbb{R}\setminus\{0\}. \end{aligned} \tag{3.3.1}$$

As we have already mentioned in the beginning of this chapter, the above families of Dirac operators involve the Calderón projectors and their adjoint operator:

$$\left(\frac{1}{2} \mp i\mathscr{C}^a_\Sigma(\alpha \cdot N)\right) \text{ and } \left(\frac{1}{2} \mp i(\alpha \cdot N)\mathscr{C}^a_\Sigma\right), \tag{3.3.2}$$

for $\lambda, \lambda' \in \{-4, 4\}$, and hence they induce confinement. So throughout this section we focus only on those two cases.

First, we study the Dirac operators $H_{a,\lambda}$. As usual we let

$$\Lambda^z_{\lambda,\pm} = -\frac{4}{\lambda}(\alpha \cdot N)\mathscr{C}^a_\Sigma(\alpha \cdot N) \pm \mathscr{C}^z_\Sigma. \tag{3.3.3}$$

and

$$\mathrm{dom}(H_{a,\lambda}) = \left\{u + \Phi[g] : u \in H^1(\mathbb{R}^3)^4, g \in L^2(\Sigma)^4 \text{ and } t_\Sigma u = -\Lambda_{\lambda,+}[g]\right\}. \tag{3.3.4}$$

The following proposition is about the basic spectral properties of $H_{a,\lambda}$.

Proposition 3.3.1. *Let $H_{a,\lambda}$ be as in (4.5.2). The following hold true:*

(i) If Ω_+ is a UR domain and $\lambda = 4$, then $(H_{a,\lambda}, \mathrm{dom}(H_{a,\lambda}))$ is self-adjoint for all $a \in (-m,m)$. Moreover, if Ω_+ is Lipschitz, then $a \notin \mathrm{Sp}(H_{a,\lambda})$, Σ is impenetrable and the following hold:

(a) $H_{a,\lambda}\varphi = H^{\Omega_+}_{a,\lambda}\varphi_+ \oplus H^{\Omega_-}_{a,\lambda}\varphi_- = (-i\alpha \cdot \nabla + m\beta)\varphi_+ \oplus (-i\alpha \cdot \nabla + m\beta)\varphi_-$, where $H^{\Omega_\pm}_{a,\lambda}$ are the self-adjoint Dirac operators defined on

$$\mathrm{dom}(H^{\Omega_\pm}_{a,\lambda}) = \Big\{u_{\Omega_\pm} + \Phi_{\Omega_\pm}[g] : u_{\Omega_\pm} \in H^1(\Omega_\pm)^4, g \in L^2(\Sigma)^4 \text{ and } \left(\frac{1}{2} \mp i(\alpha \cdot N)\mathscr{C}^a_\Sigma\right)(t_\Sigma u_{\Omega_\pm} + C_\pm[g]) = 0\Big\}.$$

(b) $\mathrm{Sp}_{\mathrm{ess}}(H_{a,\lambda}) = (-\infty, -m] \cup [m, +\infty)$.

(ii) If Ω_+ is a C^2-smooth domain and $\lambda = -4$, then $(H_{a,\lambda}, \mathrm{dom}(H_{a,\lambda}))$ is essentially self-adjoint. Moreover, we have

$$\overline{H_{a,\lambda}}\varphi = H^{\Omega_+}_{a,\lambda}\varphi_+ \oplus H^{\Omega_-}_{a,\lambda}\varphi_- = (-i\alpha\cdot\nabla + m\beta)\,\varphi_+ \oplus (-i\alpha\cdot\nabla + m\beta)\,\varphi_-,$$

where $H^{\Omega_\pm}_{a,\lambda}$ are the self-adjoint Dirac operators defined on

$$\mathrm{dom}(H^{\Omega_\pm}_{a,\lambda}) = \left\{\varphi_\pm \in L^2(\Omega_\pm)^4 : (\alpha\cdot\nabla)\varphi_\pm \in L^2(\Omega_\pm)^4 \text{ and } \left(\frac{1}{2} \pm i(\alpha\cdot N)\widetilde{\mathscr{C}^a_\Sigma}\right) t_\Sigma\varphi_\pm = 0\right\}.$$

Proof. First we prove (i), so assume that Ω_+ is a UR domain and $\lambda = 4$. Fix $a \in (-m, m)$, then using the decomposition (3.2.31) we obtain that

$$\Lambda^z_{\lambda,+} = -(\alpha\cdot N)\widetilde{W}(\alpha\cdot N) + \widetilde{W} + T^z_K = -4(\alpha\cdot N)\widetilde{W}(\alpha\cdot N)(\frac{1}{4} + \widetilde{W}^2) + T^z_K \tag{3.3.5}$$

where $T^z_K \in \mathscr{K}(L^2(\Sigma)^4)$. Since $(\alpha\cdot N)\widetilde{W}(\alpha\cdot N)$ and $(1/4 + \widetilde{W}^2)$ are invertible in $L^2(\Sigma)^4$, by [2, Theorem 1.50 and Theorem 1.51] it follows that $\Lambda_{\lambda,+}$ is a Fredholm operator. As $\Lambda_{\lambda,+}$ is self-adjoint in $L^2(\Sigma)^4$, by Theorem 3.1.1 we conclude that $(H_{a,\lambda}, \mathrm{dom}(H_{a,\lambda}))$ is self-adjoint for all $a \in (-m, m)$, which proves the first statement of (i). Now assume that Ω_+ is Lipschitz, and observe that

$$\Lambda^a_{\lambda,+} = -(\alpha\cdot N)\mathscr{C}^a_\Sigma(\alpha\cdot N) + \mathscr{C}^a_\Sigma = -4(\alpha\cdot N)\mathscr{C}^a_\Sigma(\alpha\cdot N)(\frac{1}{4} + (\mathscr{C}^a_\Sigma)^2). \tag{3.3.6}$$

Then, the same reasoning as before yields that $\Lambda^a_{\lambda,+}$ is invertible for all $a \in (-m, m)$. Therefore, by Proposition 3.1.1-(i) it follows that $a \notin \mathrm{Sp}(H_{a,\lambda})$. Item (a) and (b) are consequences of Proposition 1.3.2 and Proposition 3.1.3, respectively. This finishes the proof of (i).

Now, we prove (ii), so assume that Ω_+ is C^2-smooth and $\lambda = -4$. It is clear that $\Lambda^a_{\lambda,+} \in \mathscr{K}(L^2(\Sigma)^4)$, therefore $\lambda = -4$ is a critical parameter. Also, observe that the properties (P1) and (P′3) hold true by Proposition 1.3.3. Thus, the only thing left to check is the property (P2). To this end, recall again the decomposition (3.2.31), then we make the observation that in order to prove that $\{\alpha\cdot N, \mathscr{C}^a_\Sigma\}$ extends to a bounded operator from $H^{-1/2}(\Sigma)^4$ to $H^{1/2}(\Sigma)^4$ (see the proof of Lemma 1.3.5 and Remark 1.3.5, see also [90, Proposition 2.8]), the most delicate part is to show that $\{\alpha\cdot N, \widetilde{W}\}$ extends to a bounded operator from $H^{-1/2}(\Sigma)^4$ to $H^{1/2}(\Sigma)^4$, because the kernel of T^a_K behaves locally as $|x-y|^{-1}$ and thus T^a_K extends to a bounded operator from $H^{-1/2}(\Sigma)^4$ to $H^{1/2}(\Sigma)^4$, even if Σ is Lipschitz. Now, a straightforward computation shows that

$$\begin{aligned}\widetilde{\Lambda}_{\lambda,+}\widetilde{\mathscr{C}^a_\Sigma}\widetilde{\Lambda}_{\lambda,-} &= \Big((\alpha\cdot N)T^a_K(\alpha\cdot N) + T^0_K + \Big((\alpha\cdot N)\widetilde{W}(\alpha\cdot N) + \widetilde{W}\Big)\Big)\widetilde{\mathscr{C}^a_\Sigma}\widetilde{\Lambda}_{\lambda,-}\\ &= \Big((\alpha\cdot N)T^a_K(\alpha\cdot N) + T^0_K + (\alpha\cdot N)\{\alpha\cdot N, \widetilde{W}\}\Big)\widetilde{\mathscr{C}^a_\Sigma}\widetilde{\Lambda}_{\lambda,-}.\end{aligned} \tag{3.3.7}$$

Combining this with the above observation, and taking into account the fact that N is C^1-smooth we then get the property (P2). Therefore, item (ii) follows by Theorem 3.1.2 and Proposition 3.1.4. This achieves the proof of the proposition. □

Now we turn to the analysis of the Dirac operator $H_{a,\lambda'}$. We recall that

$$\Lambda^z_{\lambda',+} = -\frac{4}{\lambda'}\mathscr{C}^a_\Sigma + \mathscr{C}^z_\Sigma, \qquad \text{for all } (a,\lambda') \neq (0,4). \tag{3.3.8}$$

The case $(a, \lambda') = (0, 4)$ is special, we will discuss it separately in the end of this section. The main result about the self-adjointness of $H_{a,\lambda'}$ reads as follows.

Proposition 3.3.2. *Let $(H_{a,\lambda'}, \mathrm{dom}(H_{a,\lambda'}))$ be as above. The following hold:*

(i) If Ω_+ is a UR domain and $\lambda' = -4$, then $(H_{a,\lambda'}, \mathrm{dom}(H_{a,\lambda'}))$ is self-adjoint. Moreover, if Ω_+ is Lipschitz, then $a \notin \mathrm{Sp}(H_{a,\lambda'})$, Σ is impenetrable and we have

$$H_{a,\lambda'}(\varphi) = H^{\Omega_+}_{a,\lambda'}(\varphi_+) \oplus H^{\Omega_-}_{a,\lambda'}(\varphi_-) = (-i\alpha\cdot\nabla + m\beta)\,\varphi_+ \oplus (-i\alpha\cdot\nabla + m\beta)\,\varphi_- \quad (3.3.9)$$

where $H^{\Omega_\pm}_{a,\lambda'}$ are the self-adjoint Dirac operators defined on

$$\mathrm{dom}(H^{\Omega_\pm}_{a,\lambda'}) = \Big\{ u_{\Omega_\pm} + \Phi_{\Omega_\pm}[g] : u_{\Omega_\pm} \in H^1(\Omega_\pm)^4, g \in L^2(\Sigma)^4 \textit{ and } \left(\frac{1}{2} \pm i\mathscr{C}^a_\Sigma(\alpha\cdot N)\right)(t_\Sigma u_{\Omega_\pm} + C_\pm[g]) = 0 \Big\}.$$

(ii) If Ω_+ is a C^2-smooth domain, $\lambda' = 4$ and $a \neq 0$, then $(H_{a,\lambda'}, \mathrm{dom}(H_{a,\lambda'}))$ is essentially self-adjoint. furthermore we have

$$\overline{H_{a,\lambda'}}(\varphi) = H^{\Omega_+}_{a,\lambda'}(\varphi_+) \oplus H^{\Omega_-}_{a,\lambda'}(\varphi_-) = (-i\alpha\cdot\nabla + m\beta)\,\varphi_+ \oplus (-i\alpha\cdot\nabla + m\beta)\,\varphi_-,$$

where $H^{\Omega_\pm}_{a,\lambda'}$ are the self-adjoint Dirac operators defined on

$$\mathrm{dom}(H^{\Omega_\pm}_{a,\lambda'}) = \Big\{ \varphi_\pm \in L^2(\Omega_\pm)^4 : (\alpha\cdot\nabla)\varphi_\pm \in L^2(\Omega_\pm)^4 \textit{ and } \left(\frac{1}{2} \mp i\widetilde{\mathscr{C}^a_\Sigma}(\alpha\cdot N)\right) t_\Sigma\varphi_\pm = 0 \Big\}.$$

We omit the proof of this proposition, since it is easier than, and can easily be extracted from the proof of Proposition 3.3.1.

In the following, we describe the property of the confinement induced by $H_{a,\lambda'}$ when $(a, \lambda') = (0, 4)$. From (3.3.8), we notice that $\Lambda_{\lambda',+}$ vanishes in this case. Indeed, let $\varphi = u + \Phi[g]$ with $u \in H^1(\mathbb{R}^3)^4$ and $g \in L^2(\Sigma)^4$, then

$$H_{a,\lambda'}(\varphi) = H(u) + (\alpha\cdot N)\mathscr{C}_\Sigma(\alpha\cdot N)t_\Sigma u, \quad (3.3.10)$$

holds in the sense of distributions. Thus, we need to assume that $u \in H^1_0(\mathbb{R}^3\setminus\Sigma)^4$ in order to ensure that $H_{a,\lambda'}(\varphi) \in L^2(\mathbb{R}^3)^4$. Hence, we cannot define $H_{a,\lambda'}$ as we did before. To work around this problem, note that for $\varphi = (\varphi_+, \varphi_-) \in H^1(\Omega_+)^4 \oplus H^1(\Omega_-)^4$, a simple computation in the sense of distributions yields

$$\begin{aligned} H_{0,\lambda'}(\varphi) =& H(\varphi) + 2(\alpha\cdot N)\mathscr{C}_\Sigma(\alpha\cdot N)(t_\Sigma\varphi_+ + t_\Sigma\varphi_-)\delta_\Sigma \\ =& H(\varphi_+) \oplus H(\varphi_-) + i\alpha\cdot N(t_\Sigma\varphi_+ - t_\Sigma\varphi_-)\delta_\Sigma + 2(\alpha\cdot N)\mathscr{C}_\Sigma(\alpha\cdot N)(t_\Sigma\varphi_+ + t_\Sigma\varphi_-)\delta_\Sigma. \end{aligned}$$

Thus, if we let

$$\left(\frac{1}{2} - i\mathscr{C}_\Sigma(\alpha\cdot N)\right) t_\Sigma\varphi_+ = \left(\frac{1}{2} + i\mathscr{C}_\Sigma(\alpha\cdot N)\right) t_\Sigma,\varphi_-, \quad (3.3.11)$$

then $H_{0,\lambda'}(\varphi) \in L^2(\mathbb{R}^3)^4$. In particular, this leads us to define $H_{0,\lambda'}$ as follows:

$$\mathrm{dom}(H_{0,\lambda'}) = \Big\{ \varphi = (\varphi_+, \varphi_-) \in H^1(\Omega_+)^4 \oplus H^1(\Omega_-)^4 : (3.3.11) \text{ holds in } H^{1/2}(\Sigma)^4 \Big\}. \quad (3.3.12)$$

Clearly, $H_{0,\lambda'}$ is symmetric. Moreover, if we let $P_{\mp} = 1/2 \mp i\mathscr{C}_\Sigma(\alpha\cdot N)$, then it is straightforward to check that

$$H_{0,\lambda'}(\varphi) = H_{\Omega_+}(\varphi_+) \oplus H_{\Omega_-}(\varphi_-) = (-i\alpha\cdot\nabla + m\beta)\,\varphi_+ \oplus (-i\alpha\cdot\nabla + m\beta)\,\varphi_-, \qquad (3.3.13)$$

where $H_{\Omega_\pm}$ are the symmetric Dirac operators defined on

$$\mathrm{dom}(H_{\Omega_\pm}) = \left\{\varphi_\pm \in H^1(\Omega_\pm)^4 : \left(\frac{1}{2} \mp i\mathscr{C}_\Sigma(\alpha\cdot N)\right) t_\Sigma\varphi_\pm = 0\right\}.$$

Then, we have the following theorem about the self-adjointness of $H_{a,\lambda'}$ when $(a,\lambda') = (0,4)$. In the proof, we use the notation $\langle\, ,\rangle_{H^{-1/2},H^{1/2}}$ for the duality pairing between $H^{-1/2}(\Sigma)^4$ and $H^{1/2}(\Sigma)^4$.

Theorem 3.3.1. *Assume that $(a,\lambda') = (0,4)$ and let $H_{a,\lambda'}$ be as in (3.3.12). Then $H_{a,\lambda'}$ is self-adjoint, the restriction $\overline{H_{a,\lambda'}} \upharpoonright H^1(\mathbb{R}^3\setminus\Sigma)^4$ is essentially self-adjoint. Moreover, Σ is impenetrable and we have $\overline{H_{a,\lambda'}} = \overline{H_{\Omega_+}} \oplus \overline{H_{\Omega_-}}$, with*

$$\mathrm{dom}(\overline{H_{\Omega_\pm}}) = \left\{\psi \in L^2(\Omega_+)^4 : (\alpha\cdot\nabla)\psi \in L^2(\Omega_+)^4 \text{ and } P_{\mp}t_\Sigma\psi = 0\right\}, \qquad (3.3.14)$$

where the boundary condition has to be understood as an equality in $H^{-1/2}(\Sigma)^4$.

Proof. The proof is standard and follows essentially the same idea as [90, Theorem 3.2 and Theorem 4.2]. Indeed, due to the decomposition (3.3.13), it is sufficient to prove that both H_{Ω_+} and H_{Ω_-} are self-adjoint. In what follows we deal with the self-adjointness of H_{Ω_+} only, since H_{Ω_-} can be treated analogously. For the convenience of the reader, the proof is divided into two streps as follows:

(a) The domain of $H^*_{\Omega_+}$ is given by

$$\mathrm{dom}(H^*_{\Omega_+}) = \left\{\psi \in L^2(\Omega_+)^4 : (\alpha\cdot\nabla)\psi \in L^2(\Omega_+)^4 \text{ and } P_- t_\Sigma\psi = 0\right\}, \qquad (3.3.15)$$

where the boundary condition has to be understood as an equality in $H^{-1/2}(\Sigma)^4$.

(b) The inclusion $\overline{H_{\Omega_+}} \subset H^*_{\Omega_+}$ holds.

Once (a) and (b) are proved, we use the fact that H_{Ω_+} is symmetric and then we conclude that $\overline{H_{\Omega_+}} = H^*_{\Omega_+}$.

Proof of (a)**.** Denote by D be the set on the right-hand of (3.3.15). First, we show the inclusion $D \subset \mathrm{dom}(H^*_{\Omega_+})$, for this let $\varphi \in \mathrm{dom}(H_{\Omega_+})$ and $\psi \in D$. Then, using the Green's formula from Ref. 1.2.4 it follows that

$$\langle H(\psi),\varphi\rangle_{L^2(\Omega_+)^4} = \langle\psi, H(\varphi)\rangle_{L^2(\Omega_+)^4} + \langle -i(\alpha\cdot N)t_\Sigma\psi, t_\Sigma\varphi\rangle_{H^{-1/2},H^{1/2}}. \qquad (3.3.16)$$

Now, using (1.3.23) and the fact that $-i(\alpha\cdot N)t_\Sigma\psi = 2(\alpha\cdot N)\mathscr{C}_\Sigma(\alpha\cdot N)t_\Sigma\psi$, it follows that

$$\begin{aligned}\langle -i(\alpha\cdot N)t_\Sigma\psi, t_\Sigma\varphi\rangle_{H^{-1/2},H^{1/2}} &= \langle 2(\alpha\cdot N)\mathscr{C}_\Sigma(\alpha\cdot N)t_\Sigma\psi, t_\Sigma\varphi\rangle_{H^{-1/2},H^{1/2}}\\ &= \langle -i(\alpha\cdot N)t_\Sigma\psi, -2i\mathscr{C}_\Sigma(\alpha\cdot N)t_\Sigma\varphi\rangle_{H^{-1/2},H^{1/2}}.\end{aligned} \qquad (3.3.17)$$

Similarly, using that $t_\Sigma\varphi = 2i\mathscr{C}_\Sigma(\alpha\cdot N)t_\Sigma\varphi$, we get that

$$\langle -i(\alpha\cdot N)t_\Sigma\psi, t_\Sigma\varphi\rangle_{H^{-1/2},H^{1/2}} = -\langle -i(\alpha\cdot N)t_\Sigma\psi, -2i\mathscr{C}_\Sigma(\alpha\cdot N)t_\Sigma\varphi\rangle_{H^{-1/2},H^{1/2}}. \qquad (3.3.18)$$

From this, we conclude that

$$\langle -i(\alpha\cdot N)t_\Sigma\psi, t_\Sigma\varphi\rangle_{H^{-1/2},H^{1/2}} = 0. \tag{3.3.19}$$

Therefore, we obtain

$$\langle H(\psi),\varphi\rangle_{L^2(\Omega_+)^4} = \langle \psi, H(\varphi)\rangle_{L^2(\Omega_+)^4},$$

which yields the inclusion $D\subset \mathrm{dom}(H^*_{\Omega_+})$. We now prove the converse inclusion. Given $\varphi\in\mathscr{D}(\Omega_+)^4$ and let $\psi\in\mathrm{dom}(H^*_{\Omega_+})$. Then by definition there exists $\chi\in L^2(\Omega_+)^4$ such that

$$\langle H(\psi),\varphi\rangle_{\mathscr{D}'(\Omega_+)^4,\mathscr{D}(\Omega_+)^4} = \langle \psi, H(\varphi)\rangle_{\mathscr{D}'(\Omega_+)^4,\mathscr{D}(\Omega_+)^4} = \langle \psi, H(\varphi)\rangle_{L^2(\Omega_+)^4} = \langle \psi,\chi\rangle_{\mathscr{D}'(\Omega_+)^4,\mathscr{D}(\Omega_+)^4}.$$

Thus, we get that $H(\psi)=\chi$ in $\mathscr{D}'(\Omega_+)^4$ and then in $L^2(\Omega_+)^4$. Hence, $\psi,(\alpha\cdot\nabla)\psi\in L^2(\Omega_+)^4$, so it remains to show that $P_-t_\Sigma\psi=0$ in $H^{-1/2}(\Sigma)^4$. To this end, recall the definition of the extension operator E_{Ω_+} from Subsection 1.2.1. Observe that $\mathscr{E}_{\Omega_+}(P_+g)\in\mathrm{dom}(H_{\Omega_+})$, for all $g\in H^{1/2}(\Sigma)^4$. Hence, from (3.3.16) and (3.3.19) it follows that

$$\langle -i(\alpha\cdot N)t_\Sigma\psi, P_+g\rangle_{H^{-1/2},H^{1/2}} = 0. \tag{3.3.20}$$

Thus, we get

$$\langle -i(\alpha\cdot N)t_\Sigma\psi, g\rangle_{H^{-1/2},H^{1/2}} = \langle -i(\alpha\cdot N)t_\Sigma\psi, P_-g\rangle_{H^{-1/2},H^{1/2}}. \tag{3.3.21}$$

Now, using (1.3.23) and the identity $-4(\mathscr{C}_\Sigma(\alpha\cdot N))^2 = I_4$, a simple computation yields

$$\begin{aligned}\langle -i(\alpha\cdot N)t_\Sigma\psi, g\rangle_{H^{-1/2},H^{1/2}} &= \langle -i(\alpha\cdot N)t_\Sigma\psi, -4P_-(\mathscr{C}_\Sigma(\alpha\cdot N))^2 g\rangle_{H^{-1/2},H^{1/2}}\\ &= \langle 2i\mathscr{C}_\Sigma(\alpha\cdot N)t_\Sigma\psi, i(\alpha\cdot N)P_-g\rangle_{H^{-1/2},H^{1/2}}.\end{aligned} \tag{3.3.22}$$

Therefore, we get

$$\langle\Big(\frac{1}{2} - i\mathscr{C}_\Sigma(\alpha\cdot N)\Big)t_\Sigma\psi, g\rangle_{H^{-1/2},H^{1/2}} = 0. \tag{3.3.23}$$

Since this is true for all $g\in H^{1/2}(\Sigma)^4$, it follows that $\psi\in D$. Hence $\mathrm{dom}(H^*_{\Omega_+})\subset D$, which proves (a).

Proof of (b)**.** Fix $\psi\in\mathrm{dom}(H^*_{\Omega_+})$ and let $(g_j)_{j\in\mathbb{N}} = (P_+h_j)_{j\in\mathbb{N}}\subset H^{1/2}(\Sigma)^4$ be a sequence of functions that converges to $t_\Sigma\psi$ in $H^{-1/2}(\Sigma)^4$. Set

$$\psi_j = \psi + \Phi_{\Omega_+}[i(\alpha\cdot N)(g_j - t_\Sigma\psi]) + \mathscr{E}_{\Omega_+}(\{\alpha\cdot N,\mathscr{C}_\Sigma\}(\alpha\cdot N)(g_j - t_\Sigma\psi)) := \psi + F_1 + F_2. \tag{3.3.24}$$

Clearly, $\psi_j,(\alpha\cdot\nabla)\psi_j\in L^2(\Omega_+)^4$, for all $j\in\mathbb{N}$. Now observe that

$$t_\Sigma F_1 = P_+(g_j - t_\Sigma\psi) \ \text{ and } \ t_\Sigma F_2 = \{\alpha\cdot N,\mathscr{C}_\Sigma\}(\alpha\cdot N)(g_j - t_\Sigma\psi). \tag{3.3.25}$$

Hence we get

$$t_\Sigma\psi_j = g_j + \{\alpha\cdot N,\mathscr{C}_\Sigma\}(\alpha\cdot N)(g_j - t_\Sigma\psi). \tag{3.3.26}$$

Since $\{\alpha\cdot N,\mathscr{C}_\Sigma\}$ is bounded from $H^{-1/2}(\Sigma)^4$ into $H^{1/2}(\Sigma)^4$, it follows that $t_\Sigma\psi_j\in H^{1/2}(\Sigma)^4$. Therefore, $\psi_j\in H^1(\Omega_+)^4$ holds by Proposition 1.2.4-(ii). As $P_-g_j = 0 = P_-t_\Sigma\psi$, we get that

$$2i\mathscr{C}_\Sigma(\alpha\cdot N)\{\alpha\cdot N,\mathscr{C}_\Sigma\}(\alpha\cdot N)(g_j - t_\Sigma\psi) = \{\alpha\cdot N,\mathscr{C}_\Sigma\}(\alpha\cdot N)(g_j - t_\Sigma\psi).$$

Using this and the fact that $g_j = P_+ g_j$, from (3.3.26) it follows that $P_- t_\Sigma \psi_j = 0$. Thus, $\psi_j \in \mathrm{dom}(H_{\Omega_+})$, for all $j \in \mathbb{N}$. Now, by Proposition 1.3.3 (i)-(ii), we obtain that

$$\psi_j \xrightarrow[j\to\infty]{} \psi \text{ in } L^2(\Omega_+)^4. \tag{3.3.27}$$

Next, by Proposition 1.3.3-(i) and the trace theorem, there is $C > 0$ such that

$$\|H(\psi_j - \psi)\|^2_{L^2(\Omega_+)^4} \leqslant \|t_\Sigma \psi_j - t_\Sigma \psi\|^2_{H^{-1/2}(\Sigma)^4}. \tag{3.3.28}$$

Thus

$$H(\psi_j) \xrightarrow[j\to\infty]{} H(\psi) \text{ in } L^2(\Omega_+)^4. \tag{3.3.29}$$

Summing up, we have proved that $(\psi_j, H_{\Omega_+}(\psi_j))$ convergences to $(\psi, H^*_{\Omega_+}(\psi))$ when j tends to infinity. Therefore, $\overline{H_{\Omega_+}} \subset H^*_{\Omega_+}$ and this completes the proof of (b).

Finally, it remains to prove that $\overline{H_{\Omega_+}} \not\subset H_{\Omega_+}$. Pick $g \in H^{-1/2}(\Sigma)^4 \setminus L^2(\Sigma)^4$ and set $\psi = \mathcal{E}_{\Omega_+}(P_+ g)$. Then $\psi \in \mathrm{dom}(\overline{H_{\Omega_+}})$ and $\psi \notin \mathrm{dom}(H_{\Omega_+})$, as otherwise $g \in H^{1/2}(\Sigma)^4$ by Proposition 1.3.3-iv). This achieves the proof of the theorem. □

Remark 3.3.1. *It should be noted that the reason $H_{a,\lambda} \upharpoonright H^1(\mathbb{R}^3\setminus\Sigma)^4$ and $H_{a,\lambda'} \upharpoonright H^1(\mathbb{R}^3\setminus\Sigma)^4$ are not self-adjoint for critical parameters is that we are projecting in the wrong direction. In other words, we have forced the terms (more precisely, the projectors associated with each problem) that allow us to regularize the functions in* $\mathrm{dom}(\overline{H_{a,\lambda}})$ *(respectively in* $\mathrm{dom}(\overline{H_{a,\lambda'}})$*) to be zero; see Proposition 1.3.3-*(iv)*.*

□

Chapter 4

Poincaré-Steklov operators for the MIT bag Model

In this chapter, we will describe the results obtained in the article [31] in collaboration with Vincent Bruneau and Mahdi Zreik.

4.1 Introduction

Throughout this chapter, for $m > 0$ we use the symbol D_m to denote the Dirac operator $(-i\alpha \cdot \nabla + m\beta)$. For a Lipschitz domain $\Omega \subset \mathbb{R}^3$ with a compact boundary Σ, we let $r_\Omega : L^2(\mathbb{R}^3)^4 \to L^2(\Omega)^4$ be the restriction operator on Ω and $e_\Omega : L^2(\Omega)^4 \to L^2(\mathbb{R}^3)^4$ is the extension by 0 outside of Ω. We set

$$\Omega_i = \Omega \text{ and } \Omega_e = \mathbb{R}^3 \setminus \overline{\Omega}, \quad \Sigma = \partial\Omega,$$

and we denote by n and σ the outward pointing normal to Ω_i and the surface measure on Σ, respectively. We denote by $P_\pm$ the orthogonal projections along the boundary Σ defined by

$$P_\pm := \frac{1}{2}\left(I_4 \mp i\beta(\alpha \cdot n(x))\right), \quad x \in \Sigma. \tag{4.1.1}$$

In the previous chapter, we have seen that the coupling $(D_m + \mu\beta\delta_\Sigma)$ generates confinement when $\mu = \pm 2$ (see Theorem 3.2.4), and gives rise to the so-called Dirac operator with the MIT bag boundary condition on Ω_i, $(H_{\text{MIT}}(m), \text{dom}(H_{\text{MIT}}(m)))$, or simply the MIT bag operator, which is defined on the domain

$$\text{dom}(H_{\text{MIT}}(m)) := \left\{\psi \in H^{1/2}(\Omega_i)^4 : (\alpha \cdot \nabla)u \in L^2(\Omega_i)^4 \text{ and } P_- t_\Sigma \psi = 0 \text{ on } \Sigma\right\}, \tag{4.1.2}$$

by $H_{\text{MIT}}(m)\psi = D_m\psi$, for all $\psi \in \text{dom}(H_{\text{MIT}}(m))$, and where the boundary condition holds in $L^2(\Sigma)^4$. We recall that if Ω is in the class of Hölder's domains $C^{1,\omega}$, with $\omega \in (1/2, 1)$, then Theorem 3.2.3 yields that $H_{\text{MIT}}(m)$ is self-adjoint and

$$\text{dom}(H_{\text{MIT}}(m)) := \left\{\psi \in H^1(\Omega)^4 : P_- t_\Sigma \psi = 0 \text{ on } \Sigma\right\}.$$

Among all Dirac operators acting on domains arising in the context of confining δ-shell interactions, the MIT bag operator stands out among the latter by the fact that it can also be obtained as a limit of Dirac operators

$$H_M \varphi = (D_m + M\beta 1_{\Omega_e})\varphi, \quad \forall \varphi \in \text{dom}(H_M) := H^1(\mathbb{R}^3)^4,$$

as $M \longrightarrow \infty$, where 1_{Ω_e} is characteristic function of Ω_e. This idea was originally introduced by Bogolioubov in the late 60's [33], and has been revised by the MIT physicists almost 52 years ago. Recently, under the assumption that Ω_i is bounded smooth domain (C^3-smooth to be precise), in [99] it is shown that in the massless case (i.e., $m = 0$) the spectral projections of bidimensional analogue of H_M converge to those of the bidimensional analogue of $H_{\text{MIT}}(m)$. In the same setting, based on a resolvent identity, in [14] it was shown that the convergence in the norm resolvent sense holds with a convergence rate of $\mathcal{O}(M^{-1/2})$. In three dimensional case, it was shown that in the limite $M \to \infty$, any eigenvalue of $H_{\text{MIT}}(m)$ is a limit of eigenvalues of H_M, cf. [6, 87].

The main goal of this chapter is to relate the resolvents of H_M and $H_{\text{MIT}}(m)$ via a Krein-type resolvent formula and answer the following question:

Let $M_0 > 0$ be large enough and fix $M \geqslant M_0$. Given $f \in L^2(\mathbb{R}^3)^4$ and $U \in H^1(\mathbb{R}^3)^4$, what is the boundary value problem on Ω_i whose solutions closely approximate those of $(D_m + M\beta - z)U = f$?

Throughout this chapter, for $z \in \rho(D_m)$ we denote by $\Phi^{\Omega}_{z,m}$ the restriction on Ω of the mapping Φ^z defined by (1.3.4), and by $\mathscr{C}_{z,m}$ the Cauchy operator associated with $(D_m - z)$, i.e.,

$$\mathscr{C}_{z,m}[f](x) = \lim_{\rho \searrow 0} \int_{|x-y|>\rho} \phi^z_m(x-y) f(y) \mathrm{d}\sigma(y), \quad \text{for } \sigma\text{-a.e. } x \in \partial\Omega,\ f \in L^2(\Sigma)^4, \tag{4.1.3}$$

and we set

$$\Lambda^z_m = \frac{1}{2}\beta + \mathscr{C}_{z,m}, \quad \text{for all } z \in \rho(D_m), \tag{4.1.4}$$

The following lemma is a consequence of Theorem 3.2.5 and Proposition 2.3.1.

Lemma 4.1.1. *For any $z \in \rho(D_m)$, the operator Λ^z_m is bounded invertible in $L^2(\Sigma)^4$. If in addition Ω is C^2-smooth, then $\Lambda^z_m : H^{1/2}(\Sigma)^4 \longrightarrow H^{1/2}(\Sigma)^4$ is bounded invertible.*

Proof. From assertions (i) and (vi) of Theorem 3.2.5 and its proof, we know that $\mathrm{Kr}(\Lambda^z_m) = \{0\}$ and that Λ^z_m is Fredholm operator with index 0, which implies the first statement of the lemma. The second statement follows from this and Proposition 2.3.1. □

As we will see in Section 4.5, to obtain an explicit formula for the resolvent of H_M we will need to treat certain boundary integral operators as pseudodifferential operators and use symbol calculus in order to ensure their invertibility in $H^{1/2}(\Sigma)^4$. In the following part, we recall the basic facts concerning the classes of pseudodifferential operators that will serve in the rest of this chapter.

4.1.1 Symbol classes and Pseudodifferential operators

We recall here the basic facts concerning the classes of pseudodifferential operators that will serve in the rest of the paper.

Let $\mathscr{M}_4(\mathbb{C})$ be the set of 4×4 matrices over $\mathbb{C}$. For $d \in \mathbb{N}^*$ we let $\mathcal{S}^m(\mathbb{R}^d \times \mathbb{R}^d)$ be the standard symbol class of order $m \in \mathbb{R}$ whose elements are matrix-valued functions a in the space $C^\infty(\mathbb{R}^d \times \mathbb{R}^d; \mathscr{M}_4(\mathbb{C}))$ such that

$$|\partial^\alpha_x \partial^\beta_\xi a(x,\xi)| \leqslant C_{\alpha\beta}(1 + |\xi|^2)^{m-|\beta|}, \quad \forall (x,\xi) \in \mathbb{R}^d \times \mathbb{R}^d,\ \forall \alpha \in \mathbb{N}^k,\ \forall \beta \in \mathbb{N}^k. \tag{4.1.5}$$

Let $\mathscr{S}(\mathbb{R}^d)$ be the Schwartz class of functions. Then, for each $a \in \mathcal{S}^m(\mathbb{R}^d \times \mathbb{R}^d)$, for $h \in (0,1]$ we associate a semiclassical pseudodifferential operator $Op^h(a) : \mathscr{S}(\mathbb{R}^d)^4 \to \mathscr{S}(\mathbb{R}^d)^4$ via the standard formula

$$Op^h(a)u(x) = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} e^{i\xi\cdot x} a(x, h\xi)\mathcal{F}[u](\xi)\mathrm{d}\xi, \quad \forall u \in \mathscr{S}(\mathbb{R}^d)^4.$$

If $a \in \mathcal{S}^0(\mathbb{R}^d \times \mathbb{R}^d)$, then Calderón-Vaillancourt theorem's [36] yields that $Op^h(a)$ extends to a bounded operator from $L^2(\mathbb{R}^d)^4$ into itself, and there exists $C, N_C > 0$ such that

$$\left|\left|Op^h(a)\right|\right|_{L^2\to L^2} \leqslant C \max_{|\alpha+\beta|\leqslant N_C} \left|\left|\partial_x^\alpha \partial_\xi^\beta a\right|\right|_{L^\infty}. \tag{4.1.6}$$

Given a C^∞-smooth domain $\Omega \subset \mathbb{R}^3$ with a compact boundary $\Sigma = \partial\Omega$. Then Σ is a 2-dimensional parameterized surface, which in the sense of differential geometry, can also be viewed as a smooth 2-dimensional manifold immersed into $\mathbb{R}^3$. Then, Σ can be covered by an atlas $\mathbb{A} = \{(U_j, V_j, \varphi_j) | j \in \{1, \cdots, N\}\}$ (i.e., a collection of smooth charts) where $N \in \mathbb{N}^*$. That is

$$\Sigma = \bigcup_{j=1}^{N} U_j,$$

and for each $j \in \{1, \cdots, N\}$, U_j is an open set of Σ, $V_j \subset \mathbb{R}^2$ is an open set of the parametric space $\mathbb{R}^2$, and $\varphi_j : U_j \to V_j$ is a C^∞- diffeormorphism. Moreover, by definition of a smooth manifold, if $U_j \cap U_k \neq \emptyset$ then

$$\varphi_k \circ (\varphi_j)^{-1} \in C^\infty\Big(\varphi_j(U_j \cap U_k);\, \varphi_k(U_j \cap U_k)\Big).$$

As usual, we define the pull-back $(\varphi_j^{-1})^*$ and the pushforward φ_j^* by

$$(\varphi_j^{-1})^* u = u \circ \varphi_j^{-1} \quad \text{and} \quad \varphi_j^* v = v \circ \varphi_j,$$

for u and v functions on U_j and V_j, respectively. We also recall that a function u on Σ is said to be in the class $C^k(\Sigma)$ if for every chart the pushforward has the property $(\varphi_j^{-1})^* u \in C^k(V_j)$.

Following Zworski [106, Part 4]), we define pseudodifferential operators on the boundary Σ as follows:

Definition 4.1.1. *Let $\mathscr{A} : C^\infty(\Sigma)^4 \to C^\infty(\Sigma)^4$ be a continuous linear operator. Then $\mathscr{A}$ is said to be a h-pseudodifferential operator of order $m \in \mathbb{R}$ on Σ, and we write $\mathscr{A} \in Op^h\mathcal{S}^m(\Sigma)$, if*

(1) for every chart (U_j, V_j, φ_j) there exists a symbol $a \in \mathcal{S}^m$ such that

$$\psi_1 \mathscr{A}(\psi_2 u) = \psi_1 \varphi_j^* Op^h(a)(\varphi_j^{-1})^*(\psi_2 u),$$

for any $\psi_1, \psi_2 \in C_0^\infty(U_j)$ and $u \in C^\infty(\Sigma)^4$.

(2) for all $\psi_1, \psi_2 \in C^\infty(\Sigma)$ such that $\mathrm{supp}(\psi_1) \cap \mathrm{supp}(\psi_2) = \emptyset$ and for all $N \in \mathbb{N}$ we have

$$\|\psi_1 \mathscr{A} \psi_2\|_{H^{-N}(\Sigma)^4 \to H^N(\Sigma)^4} = \mathcal{O}(h^\infty).$$

For h fixed (for example $h = 1$), $\mathscr{A}$ is called a pseudodifferential operator.

Since the study of a given pseudodifferential operator on Σ reduce to the local study on local charts, in what follows, we shall recall the specific local coordinates and the notations of surface geometry we will use in the rest of the paper.

We always fix an open set $U \subset \Sigma$, and we let $\chi : V \to \mathbb{R}$ to be a C^∞-function (where $V \subset \mathbb{R}^2$ is open) such that its graph coincides with U. Set $\varphi(\tilde{x}) = (\tilde{x}, \chi(\tilde{x}))$, then for $x \in U$ we write $x = \varphi(\tilde{x})$ with $\tilde{x} \in V$. Here and also in what follows, $\partial_1\chi$ and $\partial_2\chi$ stand for the partial derivatives $\partial_{\tilde{x}_1}\chi$ and $\partial_{\tilde{x}_2}\chi$, respectively. Recall that the first fundamental form, I, and the metric tensor $G(\tilde{x}) = (g_{jk}(\tilde{x}))$, have the form

$$\mathrm{I} = g_{11} d\tilde{x}_1^2 + 2g_{12} d\tilde{x}_1 d\tilde{x}_2 + g_{22} d\tilde{x}_2^2,$$

$$G(\tilde{x}) = (g_{jk}(\tilde{x})) = \begin{pmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{pmatrix}(\tilde{x}) := \begin{pmatrix} 1 + |\partial_1\chi|^2 & \partial_1\chi\partial_2\chi \\ \partial_1\chi\partial_2\chi & 1 + |\partial_2\chi|^2 \end{pmatrix}(\tilde{x}).$$

As $G(\tilde{x})$ is symmetric, it follows that it is diagonalizable by an orthogonal matrix. Indeed, let

$$Q(\tilde{x}) := \begin{pmatrix} \frac{|\partial_2\chi|}{|\nabla\chi|} & \frac{\partial_1\chi\partial_2\chi}{|\partial_2\chi||\nabla\chi|} \\ -\frac{\partial_1\chi\partial_2\chi}{|\partial_2\chi||\nabla\chi|} & \frac{|\partial_2\chi|}{|\nabla\chi|}, \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & g^{-1/2} \end{pmatrix}(\tilde{x}). \tag{4.1.7}$$

where g stands for the determinant of G. Then, it is straightforward to check that

$$Q^{\mathrm{t}} G Q(\tilde{x}) = I_2, \quad QQ^{\mathrm{t}}(\tilde{x}) = G^{-1}(\tilde{x}) =: \left(g^{jk}(\tilde{x})\right), \quad \det(Q) = \det(Q^{\mathrm{t}}) = g^{-1/2}. \tag{4.1.8}$$

4.2 Basic properties of the MIT bag operator

In this section, we give a brief review of the basic spectral properties of the Dirac operator with the MIT bag boundary condition on Lipschitz domains. Then, we establish some results concerning the regularization properties of the resolvent and the Sobolev regularity of the eigenfunctions in the case of smooth domains.

In order to stress the notations, we often write Ω instead of Ω_i. The following theorem gathers the basic properties of the MIT bag operator. We mention that some of theses properties are well-known in the case of smooth domains, see, e.g., [6, 7, 9, 21, 90].

Theorem 4.2.1. *Let $(H_{MIT}(m), \mathrm{dom}(H_{MIT}(m)))$ be as in (4.1.2), then*

$$(H_{MIT}(m) - z)^{-1} = r_\Omega (D_m - z)^{-1} e_\Omega - \Phi^{\Omega}_{z,m} (\Lambda^z_m)^{-1} t_\Sigma (D_m - z)^{-1} e_\Omega, \quad \forall z \in \rho(D_m). \tag{4.2.1}$$

Moreover, the following statements hold true:

(i) If Ω is bounded, then $\mathrm{Sp}(H_{MIT}(m)) = \mathrm{Sp}_{\mathrm{disc}}(H_{MIT}(m)) \subset \mathbb{R} \setminus [-m, m]$.

(ii) If Ω is unbounded, then $\mathrm{Sp}(H_{MIT}(m)) = \mathrm{Sp}_{\mathrm{ess}}(H_{MIT}(m)) = (-\infty, -m] \cup [m, +\infty)$. Moreover, if Ω is connected then $\mathrm{Sp}(H_{MIT}(m))$ is purely continuous.

(iii) Let $z \in \rho(H_{MIT}(m))$ be such that $2|z| < m$, then for all $f \in L^2(\Omega)^4$ it holds that

$$\left\| (H_{MIT}(m) - z)^{-1} f \right\|_{L^2(\Omega)^4} \lesssim \frac{1}{m} \|f\|_{L^2(\Omega)^4}.$$

Proof. Recall that for any $\varphi, \psi \in \mathrm{dom}(H_{\mathrm{MIT}}(m))$, density arguments yield the Green's formula

$$\langle(-i\alpha\cdot\nabla)\varphi,\psi\rangle_{L^2(\Omega)^4} - \langle\varphi,(-i\alpha\cdot\nabla)\psi\rangle_{L^2(\Omega)^4} = \langle(-i\alpha\cdot n)t_\Sigma\varphi, t_\Sigma\psi\rangle_{L^2(\Sigma)^4}. \tag{4.2.2}$$

We first check the resolvent formula (4.2.1). So let $f \in L^2(\Omega)^4$, $z \in \rho(D_m)$ and set

$$\psi = r_\Omega(D_m - z)^{-1}e_\Omega f - \Phi^\Omega_{z,m}(\Lambda^z_m)^{-1}t_\Sigma(D_m - z)^{-1}e_\Omega f. \tag{4.2.3}$$

Since $(D_m - z)^{-1}e_\Omega$ is bounded from $L^2(\Omega)^4$ into $H^1(\mathbb{R}^3)^4$ and $(\Lambda^z_m)^{-1}$ is well-defined by Lemma 4.1.1, it follows that

$$u = r_\Omega(D_m - z)^{-1}e_\Omega f \in H^1(\Omega)^4 \quad \text{and} \quad g = -(\Lambda^z_m)^{-1}t_\Sigma(D_m - z)^{-1}e_\Omega f \in L^2(\Sigma)^4.$$

The properties of $\Phi^\Omega_{z,m}$ from Proposition 1.3.1 imply that $\psi \in H^{1/2}(\Omega)^4$. Next, using Lemmas 4.1.1 (i) and 1.3.2 we easily get

$$t_\Sigma\psi = P_+\beta(\Lambda^z_m)^{-1}t_\Sigma(D_m - z)^{-1}e_\Omega f,$$

thus $P_- t_\Sigma\psi = 0$ on Σ, which means that $\psi \in \mathrm{dom}(H_{\mathrm{MIT}}(m))$. Using that $(D_m - z)\Phi^\Omega_{z,m}[g] = 0$, it follows that $(H_{\mathrm{MIT}}(m) - z)\psi = f$ and the formula (4.2.1) is proved.

Now, we are going to prove assertions (i) and (ii). First, note that for $\psi \in \mathrm{dom}(H_{\mathrm{MIT}}(m))$ a straightforward application of the Green formula (4.2.2) yields that

$$\|H_{\mathrm{MIT}}(m)\psi\|^2_{L^2(\Omega)^4} = \|(-i\alpha\cdot\nabla)\psi\|^2_{L^2(\Omega)^4} + m^2\|\psi\|^2_{L^2(\Omega)^4} + m\|P_+t_\Sigma\psi\|^2_{L^2(\Sigma)^4}. \tag{4.2.4}$$

Thus $\|H_{\mathrm{MIT}}(m)\psi\|^2_{L^2(\Omega)^4} \geqslant m^2\|\psi\|^2_{L^2(\Omega)^4}$ which entails that $\mathrm{Sp}(H_{\mathrm{MIT}}(m)) \subset (-\infty,-m] \cup [m,+\infty)$. Note that this fact can be seen immediately from the formula (4.2.1). Next, we show that $\{-m, m\} \notin \mathrm{Sp}_{\mathrm{disc}}(H_{\mathrm{MIT}}(m))$. Assume that there is $0 \neq \psi \in \mathrm{dom}(H_{\mathrm{MIT}}(m))$ such that $(H_{\mathrm{MIT}}(m) - m)\psi = 0$ in Ω. Then, from (4.2.4) we have that

$$\|(-i\alpha\cdot\nabla)\psi\|^2_{L^2(\Omega)^4} + m\|P_+t_\Sigma\psi\|^2_{L^2(\Sigma)^4} = 0.$$

Since $m > 0$ it follows that $P_+t_\Sigma\psi = 0$, and thus $t_\Sigma\psi = 0$. Using this and the above equation, an integration by parts (using density arguments) gives

$$\|(-i\alpha\cdot\nabla)\psi\|_{L^2(\Omega)^4} = \|\nabla\psi\|_{L^2(\Sigma)^4} = 0.$$

From this we conclude that ψ vanishes identically, which contradicts the fact that $\psi \neq 0$, and thus $m \notin \mathrm{Sp}_{\mathrm{disc}}(H_{\mathrm{MIT}}(m))$. Following the same lines as above we also get that $-m \notin \mathrm{Sp}_{\mathrm{disc}}(H_{\mathrm{MIT}}(m))$. Thus, if Ω is bounded, then the above considerations and the fact that $\mathrm{dom}(H_{\mathrm{MIT}}(m)) \subset H^{1/2}(\Omega)^4$ is compactly embedded in $L^2(\Omega)^4$ yield that $\mathrm{Sp}(H_{\mathrm{MIT}}(m)) = \mathrm{Sp}_{\mathrm{disc}}(H_{\mathrm{MIT}}(m)) \subset \mathbb{R}\setminus[-m,m]$, which shows the assertion (i).
Lest us now complete the proof of (ii), so suppose that Ω is unbounded. We first show that $(-\infty,-m] \cup [m,+\infty) \subset \mathrm{Sp}_{\mathrm{ess}}(H_{\mathrm{MIT}}(m))$ by constructing Weyl sequences as in the case of half-space, see Theorem 2.3.3. As Ω is unbounded it follows that there is $R_1 > 0$ such that the half-space $\{x = (x_1,x_2,x_3) \in \mathbb{R}^3 : x_3 > R_1\}$ is strictly contained in Ω and $\mathbb{R}^3\setminus\overline{\Omega} \subset B(0,R_1)$. Fix $\lambda \in (-\infty,-m) \cup (m,+\infty)$ and let $\xi = (\xi_1,\xi_2)$ be such that $|\xi|^2 = \lambda^2 - m^2$. We define the function $\varphi : \mathbb{R}^3 \longrightarrow \mathbb{C}^4$ by

$$\varphi(\overline{x},x_3) = \left(\frac{\xi_1 - i\xi_2}{\lambda - m}, 0, 0, 1\right)^t e^{i\xi\cdot\overline{x}}, \quad \text{with } \overline{x} = (x_1,x_2).$$

Clearly we have $(D_m - \lambda)\varphi = 0$. Now, fix $R_2 > R_1$ and let $\eta \in C_0^\infty(\mathbb{R}^2, \mathbb{R})$ and $\chi \in C_0^\infty(\mathbb{R}, \mathbb{R})$ be such that $\mathrm{supp}(\chi) \subset [R_1, R_2]$. For $n \in \mathbb{N}^\star$, we define the sequences of functions

$$\varphi_n(\overline{x}, x_3) = n^{-\frac{3}{2}} \varphi(\overline{x}, x_3)\eta(\overline{x}/n)\chi(x_3/n), \quad \text{for } (\overline{x}, x_3) \in \Omega.$$

Then, as in the proof of Theorem 2.3.3, it is easy to check that $\varphi_n \in H_0^1(\Omega) \subset \mathrm{dom}(H_{\mathrm{MIT}}(m))$, $(\varphi_n)_{n\in\mathbb{N}^\star}$ converges weakly to zero, and that

$$\|\varphi_n\|^2_{L^2(\Omega)^4} = \frac{2\lambda}{\lambda - m}\|\chi\|^2_{L^2(\mathbb{R}^2)}\|\theta\|^2_{L^2(\mathbb{R})} > 0, \quad \frac{\|\,(D_m - \lambda)\,\varphi_n\|_{L^2(\Omega)^4}}{\|\varphi_n\|_{L^2(\Omega)^4}} \xrightarrow[n\to\infty]{} 0.$$

Therefore, Weyl's criterion yields that $(-\infty, -m) \cup (m, +\infty) \subset \mathrm{Sp}_{\mathrm{ess}}(H_{\mathrm{MIT}}(m))$. Since the spectrum of a self-adjoint operator is closed, we then get the first statement of (ii). Now, if we assume in addition that Ω is connected, then using the same arguments as in the proof of [11, Theorem 3.7] (i.e., using Rellich's lemma and the unique continuation property) one can verifies that $H_{\mathrm{MIT}}(m)$ has no eigenvalues in $\mathbb{R} \setminus [-m, m]$. As $\{-m, m\} \notin \mathrm{Sp}_{\mathrm{disc}}(H_{\mathrm{MIT}}(m))$ it follows that $H_{\mathrm{MIT}}(m)$ has a purely continuous spectrum.

Now we prove (iii). Let $\psi \in \mathrm{dom}(H_{\mathrm{MIT}}(m))$, then (4.2.4) yields that

$$m^2 \|\psi\|^2_{L^2(\Omega)^4} \leqslant \|H_{\mathrm{MIT}}(m)\psi\|^2_{L^2(\Omega)^4},$$

and thus

$$m \|\psi\|_{L^2(\Omega)^4} \leqslant \|H_{\mathrm{MIT}}(m)\psi\|_{L^2(\Omega)^4} \leqslant \|(H_{\mathrm{MIT}}(m) - z)\psi\|_{L^2(\Omega)^4} + |z| \|\psi\|_{L^2(\Omega)^4}$$

Therefore, for $2|z| < m$ with $z \in \rho(H_{\mathrm{MIT}}(m))$, we get that

$$\|\psi\|_{L^2(\Omega)^4} \leqslant 2m^{-1} \|(H_{\mathrm{MIT}}(m) - z)\psi\|_{L^2(\Omega)^4}.$$

Thus, (iii) follows by taking $\psi = (H_{\mathrm{MIT}}(m) - z)^{-1} f$. □

Now we establish regularity results which concerns the regularization property of the resolvent and the Sobolev regularity of the eigenfunctions of $H_{\mathrm{MIT}}(m)$. The first statement of the theorem will be crucial in Section 4.4 when studying the semiclassical pseudodifferential properties of the Poincaré-Steklov operator.

Theorem 4.2.2. *Let $k \geqslant 1$ be an integer and assume that Ω is C^{2+k}-smooth. Then the following statements hold true:*

(i) The mapping $(H_{MIT}(m) - z)^{-1} : H^k(\Omega)^4 \longrightarrow H^{k+1}(\Omega)^4 \cap \mathrm{dom}(H_{MIT}(m))$ is well-defined and bounded for all $m > 0$ and all $z \in \rho(H_{MIT}(m))$. In particular, for $m_0 > 0$ and all $z \in \rho(H_{\mathrm{MIT}}(m_0)) \cap \rho(H_{MIT}(m))$ we have

$$\|(H_{MIT}(m) - z)^{-1}\|_{H^k(\Omega)^4 \longrightarrow H^{k+1}(\Omega)^4} \lesssim 1,$$

uniformly on $m \geqslant m_0$.

(ii) If ϕ is an eigenfunction associated with an eigenvalue $z \in \mathrm{Sp}(H_{MIT}(m))$, i.e., $(H_{MIT}(m) - z)\phi = 0$, then $\phi \in H^{1+k}(\Omega)^4$. In particular, if Ω is C^∞-smooth, then $\phi \in C^\infty(\Omega)^4$.

To prove this theorem we need the following classical regularity result.

Proposition 4.2.1. *Let k be a nonnegative integer. Assume that Ω is C^{3+k}-smooth and $u \in H^1(\Omega)$. If u solves the Neumann problem*

$$-\Delta u = f \in H^k(\Omega) \quad \text{and} \quad \partial_n u = g \in H^{1/2+k}(\Sigma), \tag{4.2.5}$$

then $u \in H^{2+k}(\Omega)$.

Proof. First, assume that $k = 0$. As Ω is C^3-smooth we know that the Neumann trace $\partial_n : H^2(\Omega) \to H^{1/2}(\Sigma)$ is surjective. Thus, there is $G \in H^2(\Omega)$ such that $\partial_n G = g$ in Σ. Note that the function $\widetilde{u} = u - G$ satisfies the homogeneous Neumann problem

$$-\Delta \widetilde{u} = f + \Delta G \ \text{ in } \Omega \quad \text{and} \quad \partial_n \widetilde{u} = 0 \ \text{ on } \Sigma.$$

Therefore, $\widetilde{u} \in H^2(\Omega)$ by [84, Theorem 5, p. 217], which implies that $u \in H^2(\Omega)$ and this proves the result for $k = 0$. If $k \geqslant 1$, then the result follows by [58, Theorem 2.5.1.1]. □

Proof of theorem 4.2.2. The theorem will be proved by induction on k. First, we show (i), so fix $z \in \rho(H_{\mathrm{MIT}}(m))$ and assume that $k = 1$. Let $\phi = (\phi_1, \phi_2)^\top \in \mathrm{dom}(H_{\mathrm{MIT}}(m))$ be such that $(D_m - z)\phi = f$ in Ω, with $f = (f_1, f_2)^\top \in H^1(\Omega)^4$. By assumption we have $(\Delta + m^2 - z^2)\phi = (D_m - z)f$ in $\mathscr{D}'(\Omega)^4$, and then in $L^2(\Omega)^4$. We next prove that $\partial_n \phi \in H^{1/2}(\Sigma)^4$. To this end, consider $\Omega_\epsilon := \{x \in \mathbb{R}^3 : \mathrm{dist}(x, \Sigma) < \epsilon\}$ for $\epsilon > 0$. Then, for $\delta > 0$ small enough and $0 < \epsilon \leqslant \delta$ the mapping $\Psi : \Sigma \times (-\epsilon, \epsilon) \to \Omega_\epsilon$, defined by

$$\Psi(x_\Sigma, t) = x_\Sigma + t n(x_\Sigma), \quad x_\Sigma \in \Sigma,\, t \in (-\epsilon, \epsilon) \tag{4.2.6}$$

is a C^2-diffeomorphism and $\Omega_\epsilon := \{x + tn(x) : x \in \Sigma,\, t \in (-\epsilon, \epsilon)\}$.

Let $\widetilde{P_-} : L^2(\Omega_\epsilon \cap \Omega)^4 \to L^2(\Omega_\epsilon \cap \Omega)^4$ be the bounded operator defined by

$$\widetilde{P_-}\varphi(\Psi(x,t)) = \frac{1}{2}(I_4 + i\beta(\alpha \cdot n(x)))\varphi(\Psi(x,t)), \quad \Psi(x,t) \in \Omega_\epsilon \cap \Omega.$$

Let x_Σ^0 be an arbitrary point on the boundary Σ, fix $0 < r < \epsilon/2$, and let $\zeta : \mathbb{R}^3 \to [0,1]$ be a C^∞-smooth and compactly supported function such that $\zeta = 1$ on $B(x_\Sigma^0, r)$ and $\zeta = 0$ on $\mathbb{R}^3 \setminus B(x_\Sigma^0, 2r)$. We claim that $\widetilde{P_-}\zeta\phi$ satisfies the elliptic problem

$$\begin{cases} -\Delta(\widetilde{P_-}\zeta\phi) = g & \text{in } \Omega, \\ t_\Sigma(\widetilde{P_-}\zeta\phi) = 0 & \text{on } \Sigma, \end{cases} \tag{4.2.7}$$

with $g \in L^2(\Omega)^4$. Indeed, set $\mathscr{B}(x) = i\beta(\alpha \cdot n(x))$ for $x \in \Sigma$, and observe that

$$(D_m - z)(\widetilde{P_-}\zeta\phi) = \left(\widetilde{P_-}\zeta f + \frac{1}{2}[D_m, \zeta]\phi\right) + \frac{1}{2}[D_m, \zeta\mathscr{B}]\phi =: I(\phi, f) + \frac{1}{2}[D_m, \zeta\mathscr{B}]\phi.$$

Since n is C^2-smooth, ζ is infinitely differentiable and $\psi, f \in H^1(\Omega)^4$, it is clear that $I(\phi, f) \in H^1(\Omega)^4$ and $[D_m, \zeta\mathscr{B}]\phi \in L^2(\Omega)^4$. Now, applying $(D_m + z)$ to the above equation yields that $-\Delta(\widetilde{P_-}\zeta\phi) = g$ with

$$g := (z^2 - m^2)\widetilde{P_-}\zeta\phi + (D_m + z)I(\phi, f) + \frac{z}{2}[D_m, \zeta\mathscr{B}]\phi + \frac{1}{2}D_m[D_m, \zeta\mathscr{B}]\phi.$$

As before, it is clear that the first three terms are square integrable. Next, observe that

$$\begin{aligned} D_0[D_0, \zeta\mathscr{B}]\phi &= \{D_0, [D_0, \zeta\mathscr{B}]\}\phi - [D_0, \zeta\mathscr{B}](f - (m\beta - z)\phi) \\ &= [-\Delta, \zeta\mathscr{B}]\phi - [D_0, \zeta\mathscr{B}](f - (m\beta - z)\phi). \end{aligned}$$

Using this together with the smoothness assumption on n and the fact $(D_m - z)\phi = f \in H^1(\Omega)^4$, we easily see that $D_0[D_0, \zeta\mathscr{B}]\phi \in L^2(\Omega)^4$. Hence, $D_m[D_m, \zeta\mathscr{B}]\phi$ is square integrable, which means that $g \in L^2(\Omega)^4$. As $P_- t_\Sigma \phi = 0$ and $t_\Sigma(\widetilde{P_- \zeta\phi}) = t_\Sigma \zeta P_- t_\Sigma \phi = 0$ on Σ, by [56, Theorem 8.12] it follows that $\widetilde{P_- \zeta\phi} \in H^2(\Omega_\epsilon \cap \Omega)^4$, which implies that

$$\zeta(\phi_1 + i(\sigma\cdot n)\phi_2) \in H^2(B(x_\Sigma^0, 2r)\cap\Omega)^2 \quad \text{and} \quad \zeta(-i(\sigma\cdot n)\phi_1 + \phi_2) \in H^2(B(x_\Sigma^0, 2r)\cap\Omega)^2.$$

Consequently, we get

$$\phi_1 + i(\sigma\cdot n)\phi_2 \in H^2(B(x_\Sigma^0, r)\cap\Omega)^2 \quad \text{and} \quad -i(\sigma\cdot n)\phi_1 + \phi_2 \in H^2(B(x_\Sigma^0, r)\cap\Omega)^2. \tag{4.2.8}$$

Since $-i(\sigma\cdot\nabla)\phi_2 = (z-m)\phi_1 + f_1$ and $-i(\sigma\cdot\nabla)\phi_1 = (z+m)\phi_2 + f_2$ hold in $H^1(\Omega)^2$, it follows from (4.2.8) that

$$(\sigma\cdot\nabla)\phi_j \in H^1(B(x_\Sigma^0, r))^2 \quad \text{and} \quad (\sigma\cdot\nabla)(\sigma\cdot n)\phi_j \in H^1(B(x_\Sigma^0, r))^2, \quad j = 1, 2. \tag{4.2.9}$$

Using this and the fact that n is C^2-smooth, we easily get that

$$(\sigma\cdot n)(\sigma\cdot\nabla)\phi_j + (\sigma\cdot\nabla)(\sigma\cdot n)\phi_j = \langle n, \nabla\rangle I_2\phi_j + F_j \in H^1(B(x_\Sigma^0, r))^2, \tag{4.2.10}$$

with $F_j \in H^1(B(x_\Sigma^0, r)\cap\Omega)^2$. As a consequence, we get that $\langle n, \nabla\rangle I_2\phi_j \in H^1(B(x_\Sigma^0, r)\cap\Omega)^2$. Since this holds true for all $x_\Sigma^0 \in \Sigma$, using the compactness of Σ it follows that $\partial_n\phi \in H^{1/2}(\Sigma)^4$. Therefore, Propositions 4.2.1 yields that $\phi \in H^2(\Omega)^4$.

Next, assume $k \geqslant 2$, Ω is C^{2+k}-smooth and $\phi, f \in H^k(\Omega)^4$. Since n is C^{1+k}-smooth and Ψ defined by (4.2.6) is a C^{1+k}-diffeomorphism, following the same arguments as above we then conclude that $\partial_n\phi \in H^{k+1/2}(\Sigma)^4$. Note also that $-\Delta\phi = (z^2 - m^2)\phi + (D_m - z)f \in H^{k-1}(\Omega)^4$. Therefore, thanks to Propositions 4.2.1, we conclude that $\phi \in H^{k+1}(\Omega)^4$, which proves the first statement of (i).

Now, the second statement of (i) is a direct consequence of the first one, and this completes the proof of (i).

Finally, the proof of the first statement of (ii) follows the same lines as the one of (i). In particular, if Ω is C^∞-smooth, we then get $\phi \in H^{k+1}(\Omega)^4$ for any $k \geqslant 0$, which implies that ϕ is infinitely differentiable in Ω, and the theorem is proved. □

4.3 Principal symbol of the Poincaré-Steklov operator

The main purpose of this section is to define the Poincaré-Steklov operator $\mathscr{A}_m$ associated with the Dirac operator and to prove that it fits into the framework of pseudodifferential operators.

Throughout this section, let Ω be a smooth domain with a compact boundary Σ, let $P_\pm$ be as in (4.1.1) and set

$$S\cdot X = -\gamma_5(\alpha\cdot X) \ \text{ for all } \forall X \in \mathbb{R}^3, \quad \gamma_5 := -i\alpha_1\alpha_2\alpha_3 = \begin{pmatrix} 0 & I_2 \\ I_2 & 0 \end{pmatrix}. \tag{4.3.1}$$

Using the anticommutation relations of the Dirac's matrices we easily get the following identities

$$\begin{aligned} &i(\alpha\cdot X)(\alpha\cdot Y) = iX\cdot Y + S\cdot(X\wedge Y), \\ &\{S\cdot X, \alpha\cdot Y\} = -(X\cdot Y)\gamma_5, \quad [S\cdot X, \beta] = 0, \quad \forall X, Y \in \mathbb{R}^3. \end{aligned} \tag{4.3.2}$$

We next give the rigorous definition of the Poincaré-Steklov operator $\mathscr{A}_m$.

Definition 4.3.1. *(PS operator) Let $z \in \rho(H_{MIT}(m))$ and $g \in P_-H^{1/2}(\Sigma)^4$. We denote by $E_m^\Omega(z) : P_+H^{1/2}(\Sigma)^4 \to H^1(\Omega)^4$ the lifting operator associated with the elliptic problem*

$$\begin{cases} (D_m - z)v = 0 & \text{in } \Omega, \\ P_-t_\Sigma v = g & \text{on } \Sigma. \end{cases} \tag{4.3.3}$$

That is, $E_m^\Omega(z)g$ is the unique function in $H^1(\Omega)^4$ satisfying $(D_m - z)E_m^\Omega(z)g = 0$ in Ω and $P_-t_\Sigma E_m^\Omega(z)g = g$ on Σ. Then the Poincaré-Steklov (PS) operator $\mathscr{A}_m : P_-H^{1/2}(\Sigma)^4 \longrightarrow P_+H^{1/2}(\Sigma)^4$ associated with the system (4.3.3) is defined by

$$\mathscr{A}_m g = P_+t_\Sigma E_m^\Omega(z)g.$$

Recall the definitions of $\Phi_{z,m}^\Omega$ and Λ_m^z from Subsection 4.1. Then, the following proposition justifies the existence and the unicity of the solution to the elliptic problem (4.3.3), and gives in particular the explicit formula of the PS operator in terms the operator $(\Lambda_m^z)^{-1}$ when $z \in \rho(D_m)$. The second assertion of the proposition will be particularly important in Section 4.4 when studying the PS operator from the semiclassical point of view.

Proposition 4.3.1. *For any $z \in \rho(H_{MIT}(m))$ and $g \in P_-H^{1/2}(\Sigma)^4$, the elliptic problem (4.3.3) has a unique solution $E_m^\Omega(z)[g] \in H^1(\Omega)^4$. Moreover, the following hold true*

(i) $\left(E_m^\Omega(z)\right)^* = -\beta P_+t_\Sigma(H_{MIT}(m) - \overline{z})^{-1}$.

(ii) For any compact set $K \subset \mathbb{C}$, there is $m_0 > 0$ such that for all $m \geqslant m_0$ it holds that $K \subset \rho(H_{MIT}(m))$, and for all $z \in K$ we have

$$\left|\left|E_m^\Omega(z)g\right|\right|_{L^2(\Omega)^4} \lesssim \frac{1}{\sqrt{m}} \left|\left|g\right|\right|_{L^2(\Sigma)^4}, \quad \forall g \in P_-H^{1/2}(\Sigma)^4.$$

(iii) If $z \in \rho(D_m)$, then $E_m^\Omega(z)$ and $\mathscr{A}_m$ are explicitly given by

$$E_m^\Omega(z) = \Phi_z^\Omega(\Lambda_m^z)^{-1} \quad \text{and} \quad \mathscr{A}_m = -P_+\beta(\Lambda_m^z)^{-1}P_-. \tag{4.3.4}$$

Proof. We first show that the boundary value problem (4.3.3) has a unique solution. For this, assume that u_1 and u_2 are both solutions of (4.3.3), then $(D_m - z)(u_1 - u_2) = 0$ in Ω, and $P_-t_\Sigma(u_1 - u_2) = 0$ on Σ. Thus, $(u_1 - u_2) \in \mathrm{dom}(H_{\mathrm{MIT}}(m))$, and since $H_{\mathrm{MIT}}(m)$ is self-adjoint by Theorem 4.2.1 it follows that $u_1 = u_2$, which proves the uniqueness. Next, observe that the function

$$v_g = \mathscr{E}_\Omega(P_-g) - (H_{\mathrm{MIT}}(m) - z)^{-1}(D_m - z)\mathscr{E}_\Omega(P_-g)$$

is a solution to (4.3.3). Indeed, we have $\mathscr{E}_\Omega(P_-g) \in H^1(\Omega)^4$ and thus $v_g \in H^1(\Omega)^4$, moreover, we clearly have that $P_-t_\Sigma v_g = g$ and $(D_m - z)v_g = 0$. Since we already know that the solution to (4.3.3) is unique, it follows that v_g is independent of the extension operator $\mathscr{E}_\Omega$, and hence there is a unique solution in $H^1(\Omega)^4$ to the elliptic problem (4.3.3).

Let us show the assertion (i). Let $\psi \in P_-H^{1/2}(\Sigma)^4$ and $f \in L^2(\Omega)^4$, then using the Green's formula and the fact that $P_+(-i\alpha \cdot n) = (-i\alpha \cdot n)P_-$ we get that

$$\begin{aligned} \langle E_m^\Omega(z)\psi, f\rangle_{L^2(\Omega)^4} &= \langle E_m^\Omega(z)\psi, (H_{\mathrm{MIT}}(m) - \overline{z})(H_{\mathrm{MIT}}(m) - \overline{z})^{-1}f\rangle_{L^2(\Omega)^4} \\ &= \langle E_m^\Omega(z)\psi, (D_m - \overline{z})(H_{\mathrm{MIT}}(m) - \overline{z})^{-1}f\rangle_{L^2(\Omega)^4} \\ &= \langle (D_m - z)E_m^\Omega(z)\psi, (H_{\mathrm{MIT}}(m) - \overline{z})^{-1}f\rangle_{L^2(\Omega)^4} \\ &+ \langle (-i\alpha \cdot n)t_\Sigma E_m^\Omega(z)\psi, t_\Sigma(H_{\mathrm{MIT}}(m) - \overline{z})^{-1}f\rangle_{L^2(\Sigma)^4} \\ &= \langle (-i\alpha \cdot n)P_-t_\Sigma E_m^\Omega(z)\psi, P_+t_\Sigma(H_{\mathrm{MIT}}(m) - \overline{z})^{-1}f\rangle_{L^2(\Sigma)^4} \\ &= \langle \psi, -\beta P_+t_\Sigma(H_{\mathrm{MIT}}(m) - \overline{z})^{-1}f\rangle_{L^2(\Sigma)^4} \end{aligned}$$

which entails that $-\beta P_+ t_\Sigma (H_{\mathrm{MIT}}(m) - \overline{z})^{-1}$ is the adjoint of $E_m^\Omega(z)$ and proves (i).

Now we are going to show the assertion (ii). So, let K be a compact set of $\mathbb{C}$, and note that for all $m > \sup\{|\mathrm{Re}(z)| : z \in K\}$ it holds that $K \subset \rho(D_m) \subset \rho(H_{\mathrm{MIT}}(m))$. Hence, $v := E_m^\Omega(z) g$ is well defined for any $z \in K$ and $g \in P_- H^{1/2}(\Sigma)^4$. Then a straightforward application of the Green's formula yields that

$$\begin{aligned} 0 = ||(D_m - z)v||^2_{L^2(\Omega)^4} &= ||(i\alpha \cdot \nabla - z)v||^2_{L^2(\Omega)^4} + m^2\, ||v||^2_{L^2(\Omega)^4} \\ &+ m\left(\langle -i(\alpha \cdot n) t_\Sigma v, \beta t_\Sigma v\rangle_{L^2(\Sigma)^4} - 2\mathrm{Re}(z)\langle v, \beta v\rangle_{L^2(\Omega)^4} \right). \end{aligned} \tag{4.3.5}$$

Observe that

$$\langle -i(\alpha \cdot n) t_\Sigma v, \beta t_\Sigma v\rangle_{L^2(\Sigma)^4} = \langle (P_+ - P_-) t_\Sigma v, t_\Sigma v\rangle_{L^2(\Sigma)^4} = ||P_+ t_\Sigma v||^2_{L^{!2}(\Sigma)^4} - ||P_- t_\Sigma v||^2_{H^{1/2}(\Sigma)^4}.$$

Since $P_- t_\Sigma v = g$ and $P_+ t_\Sigma v = \mathscr{A}_m(g)$ hold by definition, and that

$$-\mathrm{Re}(z)\langle v, \beta v\rangle_{L^2(\Omega_e)^4} \geqslant -|\mathrm{Re}(z)|\, ||v||^2_{L^2(\Omega_e)^4}$$

holds by Cauchy-Schwarz inequality, it follows from (4.3.5) that

$$||g||^2_{L^2(\Sigma)^4} \geqslant m\, ||v||^2_{L^2(\Omega)^4} - 2|\mathrm{Re}(z)|\, ||v||^2_{L^2(\Omega)^4} + ||\mathscr{A}_m(g)||^2_{L^{!2}(\Sigma)^4}.$$

Thus, if we take $m_0 \geqslant 4\sup\{|\mathrm{Re}(z)| : z \in K\}$, then

$$||\mathscr{A}_m(g)||^2_{L^2(\Sigma)^4} + \frac{m}{2}\, ||v||^2_{L^2(\Omega)^4} \leqslant ||g||^2_{L^2(\Sigma)^4} \tag{4.3.6}$$

holds for any $m \geqslant m_0$, which prove the desired estimate for $E_m^\Omega(z)$.

Let us now show the assertion (iii), so let $z \in \rho(D_m)$ and recall that $\Phi^\Omega_{z,m}(\Lambda^z_m)^{-1} : H^{1/2}(\Sigma)^4 \to H^1(\Omega)^4$ is well defined and bounded by Lemma 4.1.1. Since ϕ^z_m is a fundamental solution of $(D_m - z)$, it holds that

$$(D_m - z)\Phi^\Omega_{z,m}(\Lambda^z_m)^{-1}[g] = 0 \ \text{ in } L^2(\Omega)^4, \quad \forall g \in H^{1/2}(\Sigma)^4.$$

Next, observe that if $g \in P_- H^{1/2}(\Sigma)^4$, then a direct application of the jump formula from Lemma 1.3.2 yields that

$$t_\Sigma \Phi^\Omega_{z,m}(\Lambda^z_m)^{-1}[g] = \left(-\frac{i}{2}(\alpha \cdot n) + \mathscr{C}_{z,m} \right)(\Lambda^z_m)^{-1}[g] = g - P_+\beta(\Lambda^z_m)^{-1}[g].$$

Consequently, we get

$$P_- t_\Sigma \Phi^\Omega_{z,m}(\Lambda^z_m)^{-1}[g] = g \ \text{ and } \ P_+ t_\Sigma \Phi^\Omega_{z,m}(\Lambda^z_m)^{-1}[g] = -P_+\beta(\Lambda^z_m)^{-1}[g],$$

which means that $E_m^\Omega(z)[g] = \Phi^\Omega_{z,m}(\Lambda^z_m)^{-1}[g]$ is the unique solution to the boundary value problem (4.3.3), and proves the identity $\mathscr{A}_m = -P_+\beta(\Lambda^z_m)^{-1}P_-$. This completes the proof of the proposition. □

Remark 4.3.1. *The proof above gives more, namely that for all $m_0 > 0$, $K \subset \rho(D_{m_0})$ a compact set and $z \in K$, there is $m_1 \gg 1$ such that*

$$\sup_{m \geqslant m_1} ||\mathscr{A}_m||^2_{P_- H^{1/2}(\Sigma)^4 \longrightarrow P_+ L^2(\Sigma)^4} \lesssim 1.$$

Remark 4.3.2. *It is worthwhile to note that if $z \in \rho(D_m)$, then the assertion* (i) *of Proposition 4.3.1 is a direct consequence of the resolvent formula* (4.2.1)*. Indeed, let $\psi \in P_- H^{1/2}(\Sigma)^4$ and $f \in L^2(\Omega)^4$, then thanks to Lemma 1.3.3 and Proposition 4.3.1-* (iii) *we have*

$$\begin{aligned}\langle f, E_m^{\Omega}(z)\psi\rangle_{L^2(\Omega)^4} &= \langle e_\Omega f, -\Phi_{z,m}(\Lambda_m^z)^{-1}\psi\rangle_{L^2(\mathbb{R}^3)^4} \\ &= \langle -P_-(\Lambda_m^{\overline{z}})^{-1} t_\Sigma (D_m - \overline{z})^{-1} e_\Omega f, \psi\rangle_{L^2(\Sigma)^4},\end{aligned} \tag{4.3.7}$$

where $\Phi_{z,m}$ is the mapping given by (1.3.4)*, which is defined from $H^{1/2}(\Sigma)^4$ to $H^1(\mathbb{R}^3 \setminus \Sigma)^4$. Now, from the explicit formula of $(H_{MIT}(m) - \overline{z})^{-1}$ (see* (4.2.1)*) it is easy to check that*

$$P_+ t_\Sigma (H_{MIT}(m) - \overline{z})^{-1} e_\Omega f = -\beta P_-(\Lambda_m^{\overline{z}})^{-1} t_\Sigma (D_m - \overline{z})^{-1} e_\Omega f.$$

From this and (4.3.7) *we obtain that $-\beta P_+ t_\Sigma (H_{MIT}(m) - \overline{z})^{-1}$ is the adjoint of $E_m^{\Omega}(z)$.*

Remark 4.3.3. *Note that if Ω is a Lipschitz domain, then $E_m^{\Omega}(z)$ is the unique solution in $H^{1/2}(\Omega)^4$ to the system* (4.3.3) *for datum in $L^2(\Sigma)^4$. Moreover, the PS operator $\mathscr{A}_m = -P_+\beta(\Lambda_m^z)^{-1}P_-$ is well-defined and bounded as an operator from $P_- L^2(\Sigma)^4$ to $P_+ L^2(\Sigma)^4$.*

In the rest of this section, we will only address the case $z \in \rho(D_m)$ and we show that the Poincaré-Steklov operator $\mathscr{A}_m$ from Definition 4.3.1 is a homogeneous pseudodifferential operators of order 0 and capture its principal symbol in local coordinates. To this end, we first study the pseudodifferential properties of the Cauchy operator $\mathscr{C}_{z,m}$. Once this is done, we use the explicit formula of $\mathscr{A}_m$ given by (4.3.4) and the symbol calculus to obtain the principal symbol of $\mathscr{A}_m$.

Recall the definition of ϕ_m^z from (1.3.1), and observe that

$$\phi_m^z(x-y) = k^z(x-y) + w(x-y),$$

where

$$\begin{aligned} k^z(x-y) &= \frac{e^{i\sqrt{z^2-m^2}|x-y|}}{4\pi|x-y|}\left(z + m\beta + \sqrt{z^2-m^2}\,\alpha\cdot\frac{x-y}{|x-y|}\right) + i\frac{e^{i\sqrt{z^2-m^2}|x-y|}-1}{4\pi|x-y|^3}\alpha\cdot(x-y), \\ w(x-y) &= \frac{i}{4\pi|x-y|^3}\alpha\cdot(x-y). \end{aligned}$$

Using this, it follows that

$$\begin{aligned}\mathscr{C}_{z,m}[f](x) = &\lim_{\rho\searrow 0}\int_{|x-y|>\rho} w(x-y)f(y)\mathrm{d}\sigma(y) + \int_\Sigma k^z(x-y)f(y)\mathrm{d}\sigma(y) \\ =&W[f](x) + K[f](x).\end{aligned} \tag{4.3.8}$$

As $|k^z(x-y)| = \mathcal{O}(|x-y|^{-1})$ when $|x-y| \to 0$, using the standard layer potential techniques (see, e.g. [101, Chap. 3, Sec. 4] or [100, Chap. 7, Sec. 11]) it is not hard to prove that the integral operator K gives rise to a pseudodifferential operator of order -1, i.e. $K \in Op\mathcal{S}^{-1}(\Sigma)$. Thus, we can (formally) write

$$\mathscr{C}_{z,m} = W \mod Op\mathcal{S}^{-1}(\Sigma), \tag{4.3.9}$$

which means that the strongly singular operator W encodes the main contribution in the pseudodifferential character of $\mathscr{C}_{z,m}$. So we only need to focus on the study of the pseudodifferential properties of W. The following theorem makes this heuristic more rigorous. Its proof follows similar arguments as in [4, 85, 86].

Theorem 4.3.1. *Let $\mathscr{C}_{z,m}$ be as (4.1.3), W as in (4.3.8) and $\mathscr{A}_m$ as in Definition 4.3.1. Then $\mathscr{C}_{z,m}$, W and $\mathscr{A}_m$ are homogeneous pseudodifferential operators of order 0, and we have*

$$\begin{aligned}\mathscr{C}_{z,m} &= \frac{1}{2}\alpha\cdot\frac{\nabla_\Sigma}{\sqrt{-\Delta_\Sigma}} \quad \mathrm{mod}\ Op\mathcal{S}^{-1}(\Sigma),\\ \mathscr{A}_m &= \frac{1}{\sqrt{-\Delta_\Sigma}}S\cdot(\nabla_\Sigma\wedge n)P_- \quad \mathrm{mod}\ Op\mathcal{S}^{-1}(\Sigma),\end{aligned} \tag{4.3.10}$$

where, in local coordinates, the symbol of $\nabla_\Sigma(-\Delta_\Sigma)^{-1/2}$ is given by

$$\langle G^{-1}\xi,\xi\rangle^{-1/2}\begin{pmatrix} G^{-1}\xi \\ \langle\nabla\chi(\tilde{x}),G^{-1}\xi\rangle\end{pmatrix}.$$

In particular, in local coordinates, $\mathscr{A}_m$ has principal symbol

$$p_{\mathscr{A}_m}(\tilde{x},\xi) = S\cdot\left(\frac{\xi\wedge n(x)}{\sqrt{\xi\wedge n(x)}}\right)P_-. \tag{4.3.11}$$

Proof. We first deal with the operator W. So, let $\psi_k:\Sigma\to,\mathbb{R}$, $k=1,2$, be a C^∞-smooth function. Clearly, if $\mathrm{supp}(\psi_2)\cap\mathrm{supp}(\psi_1)=\emptyset$, then $\psi_2 W\psi_1$ gives rise to a bounded operator from $H^{-j}(\Sigma)^4$ into $H^j(\Sigma)^4$, for all $j\geqslant 0$.
Now, fix a local chart (U,V,φ) as in Subsection 4.1.1 and recall the definition of first fundamental form I and the metric tensor $G(\tilde{x})$. That is, for all $x\in U$ we have $x=\varphi(\tilde{x})=(\tilde{x},\chi(\tilde{x}))$ with $\tilde{x}\in V$, and where the graph of $\chi:V\to\mathbb{R}$ coincides with U. Notice that if we assume that ψ_k is compactly supported with $\mathrm{supp}(\psi_k)\subset U$, then, in this setting, the operator $\psi_2 W\psi_1$ has the form

$$\begin{aligned}\psi_2 W[\psi_1 f](x) =& \psi_2(x)\mathrm{p.v}\int_V i\alpha\cdot\frac{\varphi(\tilde{x})-\varphi(\tilde{y})}{4\pi|\varphi(\tilde{x})-\varphi(\tilde{y})|^3}\psi_1(\varphi(\tilde{y}))f(\varphi(\tilde{y}))\sqrt{g(\tilde{y})}\mathrm{d}\tilde{y}\\ =&\psi_2(x)\sqrt{g(\tilde{x})}\mathrm{p.v}\int_V i\alpha\cdot\frac{\varphi(\tilde{x})-\varphi(\tilde{y})}{4\pi|\varphi(\tilde{x})-\varphi(\tilde{y})|^3}\psi_1(\varphi(\tilde{y})f(\varphi(\tilde{y}))\mathrm{d}\tilde{y}\\ &+\psi_2(x)\int_V i\alpha\cdot\frac{\varphi(\tilde{x})-\varphi(\tilde{y})}{4\pi|\varphi(\tilde{x})-\varphi(\tilde{y})|^3}f(\varphi(\tilde{y}))\left(\sqrt{g(\tilde{y})}-\sqrt{g(\tilde{x})}\right)\mathrm{d}\tilde{y}.\end{aligned} \tag{4.3.12}$$

where g is the determinant of the metric tensor G. Since $g(\cdot)$ is smooth, it follows that

$$|\sqrt{g(\tilde{y})}-\sqrt{g(\tilde{x})}|\lesssim|\tilde{x}-\tilde{y}|.$$

Therefore, the last integral operator on the right-hand side of (4.3.12) has a non singular kernel and does not require to write it as an integral operator in the principal value sense. Next, let $x,y\in U$ such that $x=\varphi(\tilde{x})$ and $y=\varphi(\tilde{y})$, with $\tilde{x},\tilde{y}\in V$. Then, a simple computation using Taylor's formula shows that

$$|x-y|^2=|\varphi(\tilde{x})-\varphi(\tilde{y})|^2=\langle\tilde{x}-\tilde{y},G(\tilde{x})(\tilde{x}-\tilde{y})\rangle(1+\mathcal{O}|\tilde{x}-\tilde{y}|),$$

where the definition of I was used in the last equality. It follows from the above computations that

$$|x-y|^{-3}=\frac{1}{\langle\tilde{x}-\tilde{y},G(\tilde{x})(\tilde{x}-\tilde{y})\rangle^{3/2}}+k_1(\tilde{x},\tilde{y}),$$

where the kernel k_1 satisfies $|k_1(\tilde{x},\tilde{y})| = \mathcal{O}(|\tilde{x}-\tilde{y}|^{-2})$, when $|\tilde{x}-\tilde{y}| \to 0$. Consequently, we get that

$$\frac{x_j - y_j}{|x-y|^3} = \begin{cases} \dfrac{\tilde{x}_j - \tilde{y}_j}{\langle \tilde{x}-\tilde{y}, G(\tilde{x})(\tilde{x}-\tilde{y})\rangle^{3/2}} + (\tilde{x}_j - \tilde{y}_j)k_1(\tilde{x},\tilde{y}), & \text{for } j = 1,2, \\ \dfrac{\langle \nabla\chi, \tilde{x}-\tilde{y}\rangle}{\langle \tilde{x}-\tilde{y}, G(\tilde{x})(\tilde{x}-\tilde{y})\rangle^{3/2}} + k_2(\tilde{x},\tilde{y}), & \text{for } j = 3, \end{cases}$$

with $|k_2(\tilde{x},\tilde{y})| = \mathcal{O}(|\tilde{x}-\tilde{y}|^{-1})$, when $|\tilde{x}-\tilde{y}| \to 0$. Note that this implies

$$\alpha \cdot \left(\frac{x-y}{|x-y|^3}\right) = \alpha \cdot \frac{(\tilde{x}-\tilde{y}, \langle \nabla\chi, \tilde{x}-\tilde{y}\rangle)}{\langle \tilde{x}-\tilde{y}, G(\tilde{x})(\tilde{x}-\tilde{y})\rangle^{3/2}} + \mathcal{O}(|\tilde{x}-\tilde{y}|^{-1})I_4.$$

Combining the above computations and (4.3.12),we deduce that

$$\psi_2 W[\psi_1 f](x) = \psi_2(x)\sqrt{g(\tilde{x})}\text{p.v}\int_V i\alpha \frac{(\tilde{x}-\tilde{y}, \langle \nabla\chi, \tilde{x}-\tilde{y}\rangle)}{\langle \tilde{x}-\tilde{y}, G(\tilde{x})(\tilde{x}-\tilde{y})\rangle^{3/2}} f(\varphi(\tilde{y}))\mathrm{d}\tilde{y} + \psi_2(x)L[\psi_1 f](x), \tag{4.3.13}$$

where L is an integral operator with a kernel $l(x,y)$ satisfying

$$|l(x,y)| = \mathcal{O}(|x-y|^{-1}) \ \text{ when } \ |x-y| \to 0.$$

Thus, similar arguments as the ones in [100, Chap. 7, Sec. 11] yield that L is a pseudodifferential operator of order -1. Now, for $h \in L^2(\mathbb{R}^2)$ and $k = 1,2$, observe that if we set

$$R_k[h](\tilde{x}) = \frac{i\sqrt{g(\tilde{x})}}{4\pi}\int_{\mathbb{R}^2} r_k(\tilde{x}, \tilde{x}-\tilde{y})h(\tilde{y})\mathrm{d}(\tilde{y}),$$

where

$$r_k(\tilde{x}, \tilde{x}-\tilde{y}) = \frac{\tilde{x}_k - \tilde{y}_k}{\langle \tilde{x}-\tilde{y}, G(\tilde{x})(\tilde{x}-\tilde{y})\rangle^{3/2}}, \quad \tilde{x} \neq \tilde{y}.$$

Then the standard formula connecting a pseudodifferential operator and its symbol yields

$$R_k[h](\tilde{x}) = \frac{i\sqrt{g(\tilde{x})}}{(2\pi)^2}\int_{\mathbb{R}^2}\int_{\mathbb{R}^2} e^{i\langle \tilde{x}-\tilde{y}, \xi\rangle} q_k(\tilde{x},\xi)h(\tilde{y})\mathrm{d}\xi\mathrm{d}\tilde{y},$$

where

$$q_k(\tilde{x},\xi) = \frac{i\sqrt{g(\tilde{x})}}{2}\int_{\mathbb{R}^2} e^{-i\langle\omega,\xi\rangle} r_k(\tilde{x},\omega)\mathrm{d}\xi.$$

Recall the definition of Q from (4.1.7) and set $\omega = Q(\tilde{x})\tau$. Also recall that

$$\int_{\mathbb{R}^2} e^{-i\langle\omega,\xi\rangle}\frac{\omega_k}{|\omega|^3}\mathrm{d}\omega = -i\frac{\xi_k}{|\xi|}, \quad k = 1,2. \tag{4.3.14}$$

Thus, the above change of variables together with the properties (4.1.8) and (4.3.14) yield that

$$q_k(\tilde{x},\xi) = \frac{i}{2}\int_{\mathbb{R}^2} e^{-i\langle\tau, Q^{\mathrm{t}}(\tilde{x})\xi\rangle}\frac{(Q^{\mathrm{t}}(\tilde{x})\tau)_k}{|\tau|^3}\mathrm{d}\tau = \frac{(G^{-1}(\tilde{x})\xi)_k}{2\langle G^{-1}(\tilde{x})\xi,\xi\rangle^{1/2}} = \frac{g_{k1}\xi_1 + g_{k2}\xi_2}{2\langle G^{-1}(\tilde{x})\xi,\xi\rangle^{1/2}}, \tag{4.3.15}$$

which means that $q_k(\tilde{x},\xi)$ is homogeneous of degree 0 in ξ. Therefore R_k is a homogeneous pseudodifferential operators of degree 0. It is worth mentioning that $(G^{-1}(\tilde{x})\xi, \langle \nabla\chi(\tilde{x}), G^{-1}\xi\rangle)^{\mathrm{t}}$ and $\langle G^{-1}(\tilde{x})\xi, \xi\rangle$ are the symbols of the surface gradient ∇_Σ and the Laplace-Beltrami operator Δ_Σ, respectively. From the above observation and (4.3.13) if follows that

$$\psi_2 W \psi_1 = \psi_2 \alpha \cdot (R_1, R_2, \partial_1\chi(\tilde{x})R_1 + \partial_2\chi(\tilde{x})R_2)\,\psi_1 + \psi_2 L \psi_1. \tag{4.3.16}$$

Since L is a pseudodifferential operator of order -1 we deduce that W is a homogeneous pseudodifferential operators of order 0, and we obtain that

$$W = \frac{1}{2}\alpha \cdot \frac{\nabla_\Sigma}{\sqrt{-\Delta_\Sigma}} \quad \mathrm{mod}\ Op\mathcal{S}^{-1}(\Sigma). \tag{4.3.17}$$

Thanks to (4.3.9) and (4.3.17), we deduce that the Cauchy operator $\mathscr{C}_{z,m}$ has the same principal symbol as the operator W.

Now we are going to deal with the operator $\mathscr{A}_m$. Note that we have

$$\frac{1}{2}\left(\beta + \alpha \cdot \frac{\nabla_\Sigma}{\sqrt{-\Delta_\Sigma}}\right)^2 = I_4, \tag{4.3.18}$$

and as $\mathscr{A}_m$ is given by the formula

$$\mathscr{A}_m = -P_+\beta\left(\frac{1}{2}\beta + \mathscr{C}_{z,m}\right)^{-1} P_-,$$

using (4.3.18) and the standard mollification arguments, it follows from the product formula for calculus of pseudodifferential operators that, in local coordinates, the symbol of $\mathscr{A}_m$ denoted by $q_{\mathscr{A}_m}$ has the form

$$q_{\mathscr{A}_m}(\tilde{x},\xi) = -P_+\beta\left(\beta + \alpha \cdot \left(\frac{(\sum_k g^{1k}\xi_k, \sum_k g^{2k}\xi_k, \langle \nabla\chi(\tilde{x}), G^{-1}\xi\rangle)^\top}{\langle G^{-1}\xi, \xi\rangle^{1/2}}\right)\right) P_- + p(\tilde{x},\xi),$$

where $p \in \mathcal{S}^{-1}(\Sigma)$. Therefore, we get

$$q_{\mathscr{A}_m}(\tilde{x},\xi) = -P_+\beta\alpha \cdot \left(\frac{(\sum_k g^{1k}\xi_k, \sum_k g^{2k}\xi_k, \langle \nabla\chi(\tilde{x}), G^{-1}\xi\rangle)^\top}{\langle G^{-1}\xi, \xi\rangle^{1/2}}\right) P_- + p(\tilde{x},\xi).$$

Hence, using the fact that $P_\pm$ are projectors, a computation shows

$$q_{\mathscr{A}_m}(\tilde{x},\xi) = -\frac{1}{2}\left[i\alpha \cdot n(x), \alpha \cdot \frac{(\sum_k g^{1k}\xi_k, \sum_k g^{2k}\xi_k, \langle \nabla\chi(\tilde{x}), G^{-1}\xi\rangle)^\top}{\langle G^{-1}\xi, \xi\rangle^{1/2}}\right] P_- + p(\tilde{x},\xi), \tag{4.3.19}$$

where $[\,,]$ is the commutator bracket. Hence, the formula (4.3.2) together with the fact that

$$\begin{pmatrix} G^{-1}\xi \\ \langle \nabla\chi(\tilde{x}), G^{-1}\xi\rangle \end{pmatrix} \wedge n(x) = \xi \wedge n(x), \quad \langle G^{-1}\xi, \xi\rangle^{1/2} = |\xi \wedge n(x)|,$$

give that

$$p_{\mathscr{A}_m}(\tilde{x},\xi) = S \cdot \left(\frac{\xi \wedge n(x)}{\sqrt{\xi \wedge n(x)}}\right) P_- + p(\tilde{x},\xi),$$

$$\mathscr{A}_m = \frac{1}{\sqrt{-\Delta_\Sigma}} S \cdot (\nabla_\Sigma \wedge n(x)) P_- \quad \mathrm{mod}\ Op\mathcal{S}^{-1}(\Sigma),$$

which proves the formula (4.3.11) and the fact that $\mathscr{A}_m$ is a homogeneous pseudodifferential operators of order 0. This completes the proof of the theorem. □

Remark 4.3.4. *It is worth pointing out that the above result might be generalized for less regular surface. Indeed, we first notice that the arguments used in the proof remain valid if one assumes for example that Ω is $C^{2+\alpha}$-smooth, $\alpha > 0$. In this setting, Theorem 4.3.1 can be generalized without any difficulties by changing slightly the definition of pseudodifferential operators, see, e.g., [4, 85, 86]. More generally, if we assume that Ω is a Lipschitz domain with an outward unit normal having vanishing mean oscillations on Σ, then Theorem 4.3.1 can be recovered using the symbol calculus introduced in [64], see also [100].*

4.4 Approximation of the Poincaré-Steklov operators for large mass

Although the technique used in the last section allows us to treat the layer potential operator $\mathscr{A}_m$ as pseudodifferential operator and to derive its principal symbol. However, it does not allow us to capture the dependence on m. The main goal of this section is to study the Poincaré-Steklov operator, $\mathscr{A}_m$, as a m-dependent pseudodifferential operator when m is large enough. For this purpose, we consider $h = 1/m$ as a semiclassical parameter (for $m \gg 1$) and use the system (4.3.3) instead of the layer potential formula of $\mathscr{A}_m$. Roughly speaking, we will look for a local approximate formula for the solution of (4.3.3). Once this is done, we use the regularization property of the resolvent of the MIT bag operator to catch the semiclassical principal symbol of $\mathscr{A}_m$.

Throughout this section, we assume that $m > 1$, $z \in \rho(H_{\mathrm{MIT}}(m))$ and that Ω is smooth with a compact boundary $\Sigma := \partial\Omega$. We next introduce the semiclassical parameter $h = m^{-1} \in (0, 1]$, and we set $\mathscr{A}^h := \mathscr{A}_m$. Recall the definition of the spin angular momentum S from (4.3.1).

The following theorem is the main result of this section, it ensures that $\mathscr{A}^h$ is a h-pseudodifferential operator of order 0 and gives its semiclassical principal symbol.

Theorem 4.4.1. *Let $h \in (0, 1]$ and $z \in \rho(H_{MIT}(m))$, and let $\mathscr{A}^h$ be as above. Then for any $N \in \mathbb{N}$, there exists a h-pseudodifferential operator of order 0, $\mathscr{A}^h_N \in Op^h\mathcal{S}^0(\Sigma)$ such that for h sufficiently small, and any $0 \le l \le N + \frac{1}{2}$*

$$\|\mathscr{A}^h - \mathscr{A}^h_N\|_{H^{\frac{1}{2}}(\Sigma)\to H^{N+\frac{3}{2}-l}(\Sigma)} = O(h^{N+\frac{1}{2}+l}), \tag{4.4.1}$$

and

$$\mathscr{A}^h_N = S \cdot \left(\frac{h\nabla_\Sigma \wedge n}{\sqrt{-h^2\Delta_\Sigma + I} + I} \right) P_- \quad \mathrm{mod}\ hOp^h\mathcal{S}^{-1}(\Sigma).$$

Let us consider $\mathbb{A} = \{(U_{\varphi_j}, V_{\varphi_j}, \varphi_j) | j \in \{1, \cdots, N\}\}$ an atlas of Σ and $(U_\varphi, V_\varphi, \varphi) \in \mathbb{A}$. As in Section 4.3 we consider the case where U_φ is the graph of a smooth function χ, and we assume that Ω corresponds locally to the side $x_3 > \chi(x_1, x_2)$. Then, for

$$U_\varphi = \{(x_1, x_2, \chi(x_1, x_2)); \, (x_1, x_2) \in V_\varphi\}; \quad \varphi((x_1, x_2, \chi(x_1, x_2)) = (x_1, x_2) \tag{4.4.2}$$

$$\mathcal{V}_{\varphi,\varepsilon} := \{(y_1, y_2, y_3 + \chi(y_1, y_2)); \, (y_1, y_2, y_3) \in V_\varphi \times (0, \varepsilon)\} \subset \Omega, \tag{4.4.3}$$

with ε sufficiently small, we have the following homeomorphism:

$$\begin{aligned} \phi : \mathcal{V}_{\varphi,\varepsilon} &\longrightarrow V_\varphi \times (0, \varepsilon) \\ (x_1, x_2, x_3) &\mapsto (x_1, x_2, x_3 - \chi(x_1, x_2)). \end{aligned}$$

Then the pull-back

$$\begin{aligned} \phi^* : C^\infty(V_\varphi \times (0,\varepsilon)) &\longrightarrow C^\infty(\mathcal{V}_{\varphi,\varepsilon}) \\ v &\mapsto \phi^* v := v \circ \phi \end{aligned}$$

transforms the differential operator D_m restricted on $\mathcal{V}_{\varphi,\varepsilon}$ into the following operator on $V_\varphi \times (0,\varepsilon)$:

$$\begin{aligned} \widetilde{D}_m^\varphi := (\phi^{-1})^* D_m (\phi)^* &= -i\left(\alpha_1\partial_{y_1} + \alpha_2\partial_{y_2} - (\alpha_1\partial_{x_1}\chi + \alpha_2\partial_{x_2}\chi - \alpha_3)\partial_{y_3}\right) + m\beta \\ &= -i(\alpha_1\partial_{y_1} + \alpha_2\partial_{y_2}) + \sqrt{1+|\nabla\chi|^2}(i\alpha\cdot n^\varphi)(\tilde{y})\partial_{y_3} + m\beta, \end{aligned} \tag{4.4.4}$$

where $\tilde{y} = (y_1, y_2)$, and $n^\varphi = (\varphi^{-1})^* n$ is the pull-back of the outward pointing normal to Ω restricted on V_φ:

$$n^\varphi(\tilde{y}) = \frac{1}{\sqrt{1+|\nabla\chi|^2}} \begin{pmatrix} \partial_{x_1}\chi \\ \partial_{x_2}\chi \\ -1 \end{pmatrix} (y_1, y_2). \tag{4.4.5}$$

For the projectors $P_\pm$, we have:

$$P_\pm^\varphi := (\varphi^{-1})^* P_\pm (\varphi)^* = \frac{1}{2}\Big(I_4 \mp i\beta\,\alpha\cdot n^\varphi(\tilde{y})\Big).$$

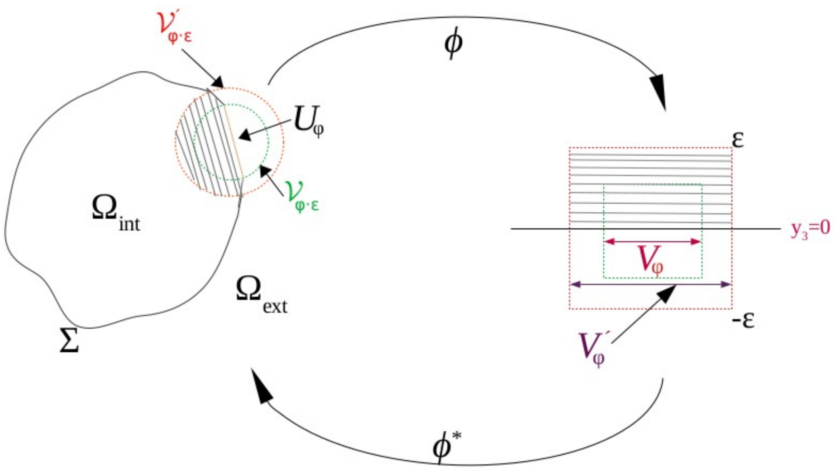

Figure 4.1: Flattening the boundary Σ

Hence, in the variable $y \in V_\varphi \times (0,\varepsilon)$, the equation (4.3.3) becomes:

$$\begin{cases} (\widetilde{D}_m^\varphi - z)u = 0, & \text{in } V_\varphi \times (0,\varepsilon), \\ \Gamma_-^\varphi u = g^\varphi = g\circ\varphi^{-1}, & \text{on } V_\varphi \times \{0\}, \end{cases} \tag{4.4.6}$$

where $\Gamma_\pm^\varphi = P_\pm^\varphi t_{\{y_3=0\}}$.
By isolating the derivative with respect to y_3, and using that $(i\alpha\cdot n^\varphi)^{-1} = -i\alpha\cdot n^\varphi$, the system (4.4.6) becomes:

$$\begin{cases} \partial_{y_3} u = \dfrac{i\alpha\cdot n^\varphi(\tilde{y})}{\sqrt{1+|\nabla\chi(\tilde{y})|^2}}\Big(-i\alpha_1\partial_{y_1} - i\alpha_2\partial_{y_2} + m\beta - z\Big)u, & \text{in } V_\varphi \times (0,\varepsilon), \\ \Gamma_-^\varphi u = g^\varphi, & \text{on } V_\varphi \times \{0\}. \end{cases} \tag{4.4.7}$$

Let us now introduce the matrices-valued symbols

$$L_0(\tilde{y},\xi) := \frac{i\alpha\cdot n^\varphi(\tilde{y})}{\sqrt{1+|\nabla\chi(\tilde{y})|^2}}\Big(\alpha\cdot\xi+\beta\Big); \qquad L_1(\tilde{y}) := \frac{-iz\alpha\cdot n^\varphi(\tilde{y})}{\sqrt{1+|\nabla\chi(\tilde{y})|^2}}, \tag{4.4.8}$$

with $\xi=(\xi_1,\xi_2)$ identified with $(\xi_1,\xi_2,0)$. Then (4.4.7) is equivalent to

$$\begin{cases} h\partial_{y_3}u = L_0(\tilde{y},hD_{\tilde{y}})u + hL_1(\tilde{y})u, & \text{in } V_\varphi\times(0,\varepsilon),\\ \Gamma^\varphi_- u = g^\varphi, & \text{on } V_\varphi\times\{0\}. \end{cases} \tag{4.4.9}$$

Before constructing an approximate solution of the system (4.4.9), let us give some properties of L_0.

4.4.1 Algebric properties of L_0

The following lemma will be used in the sequel, it gathers some useful properties which allow us to simplify the expression of $L_0(\tilde{y},\xi)$. We omit the proof since it is an easy consequence of the anticommutation relations of the Dirac's matrices and the formulas (4.3.2).

Lemma 4.4.1. *Let n^φ and ξ be as above, and let S be as in (4.3.1). Then, for any $z\in\mathbb{C}$ and any $\tau\in\mathbb{R}^3$ such that $\tau\perp n^\varphi$, the following identities hold:*

$$(S\cdot\tau - im\beta(\alpha\cdot n^\varphi(\tilde{y})))^2 = \Big(|\tau|^2+m^2\Big)I_4. \tag{4.4.10}$$

$$P^\varphi_\pm(S\cdot\tau) = (S\cdot\tau)P^\varphi_\mp \quad \textit{and} \quad P^\varphi_\pm(i\alpha\cdot n^\varphi) = (i\alpha\cdot n^\varphi)P^\varphi_\mp. \tag{4.4.11}$$

The next proposition gathers the main properties of the operator L_0.

Proposition 4.4.1. *Let $L_0(\tilde{y},\xi)$ be as in (4.4.8), then we have*

$$\begin{aligned} L_0(\tilde{y},\xi) &= \frac{1}{\sqrt{1+|\nabla\chi(\tilde{y})|^2}}\Big(i\xi\cdot n^\varphi(\tilde{y}) + S\cdot(n^\varphi(\tilde{y})\wedge\xi) - i\beta(\alpha\cdot n^\varphi(\tilde{y}))\Big),\\ &= \xi\cdot\tilde{n}^\varphi(\tilde{y}) + \frac{\lambda(\tilde{y},\xi)}{\sqrt{1+|\nabla\chi(\tilde{y})|^2}}\Pi_+(\tilde{y},\xi) - \frac{\lambda(\tilde{y},\xi)}{\sqrt{1+|\nabla\chi(\tilde{y})|^2}}\Pi_-(\tilde{y},\xi) \end{aligned}$$

where

$$\begin{aligned} \lambda(\tilde{y},\xi) :=& \sqrt{|n^\varphi\wedge\xi|^2+1},\\ \tilde{n}^\varphi(\tilde{y}) :=& \frac{1}{\sqrt{1+|\nabla\chi|^2}}n^\varphi(\tilde{y}),\\ \Pi_\pm(\tilde{y},\xi) :=& \frac{1}{2}\left(I_4 \pm \frac{S\cdot(n^\varphi(\tilde{y})\cdot\xi) - i\beta(\alpha\cdot n^\varphi(\tilde{y}))}{\lambda(\tilde{y},\xi)}\right). \end{aligned} \tag{4.4.12}$$

In particular, the symbol $L_0(\tilde{y},\xi)$ is elliptic in $\mathcal{S}^1$ and it admits two eigenvalues $\rho_\pm(\cdot,\cdot)\in\mathcal{S}^1$ of multiplicity 2 which are given by

$$\rho_\pm(\tilde{y},\xi) = \frac{in^\varphi(\tilde{y})\cdot\xi \pm \lambda(\tilde{y},\xi)}{\sqrt{1+|\nabla\chi|^2}}, \tag{4.4.13}$$

and for which there exists $c>0$ such that

$$\pm\Re\rho_\pm(\tilde{y},\xi) > c\langle\xi\rangle, \tag{4.4.14}$$

uniformly with respect to $\tilde{y}$. *Moreover,* $\Pi_\pm(\tilde{y},\xi)$ *are the projections onto* $\mathrm{Kr}(L_0(\tilde{y},\xi) - \rho_\pm(\tilde{y},\xi)I_4)$*, belong to the symbol class* $\mathcal{S}^0$ *and satisfy:*

$$P_\pm^\varphi \, \Pi_\pm(\tilde{y},\xi) \, P_\pm^\varphi = k_+^\varphi(\tilde{y},\xi) P_\pm^\varphi \quad \textit{and} \;\; P_\pm^\varphi \, \Pi_\mp(\tilde{y},\xi) \, P_\mp^\varphi = \mp\Theta^\varphi(\tilde{y},\xi) P_\mp^\varphi, \tag{4.4.15}$$

with

$$k_\pm^\varphi(\tilde{y},\xi) = \frac{1}{2}\left(1 \pm \frac{1}{\lambda(\tilde{y},\xi)}\right), \quad \Theta^\varphi(\tilde{y},\xi) = \frac{1}{2\lambda(\tilde{y},\xi)}\left(S \cdot (n^\varphi(\tilde{y}) \wedge \xi)\right). \tag{4.4.16}$$

That is, k_+^φ *is a positive function of* $\mathcal{S}^0$*,* $(k_+^\varphi)^{-1} \in \mathcal{S}^0$ *and* $\Theta^\varphi \in \mathcal{S}^0$*.*

Remark 4.4.1. *Thanks to the property* (4.4.15) *a* 4×4*-matrix* A *is uniquely determined by* $P_-^\varphi A$ *and* $\Pi_+ A$ *and we have:*

$$A = P_-^\varphi A + P_+^\varphi A = P_-^\varphi A + \frac{1}{k_+^\varphi} P_+^\varphi \Pi_+ P_+^\varphi A = \Big(I - \frac{P_+^\varphi \Pi_+}{k_+^\varphi}\Big) P_-^\varphi A + \frac{P_+^\varphi}{k_+^\varphi} \Pi_+ A.$$

Proof of Proposition 4.4.1. By definition it is clear that $L_0(\tilde{y},\xi)$ belongs to the symbol class $\mathcal{S}^1$, $\Pi_\pm(\tilde{y},\xi), \Theta^\varphi \in \mathcal{S}^0$, k_+^φ a positive function of $\mathcal{S}^0$ and $(k_+^\varphi)^{-1} \in \mathcal{S}^0$. Now, by (4.3.2) we obtain that

$$L_0(\tilde{y},\xi) = \frac{1}{\sqrt{1+|\nabla\chi(\tilde{y})|^2}}\Big(i\xi \cdot n^\varphi(\tilde{y}) + S \cdot (n^\varphi(\tilde{y}) \wedge \xi) - i\beta(\alpha \cdot n^\varphi(\tilde{y}))\Big),$$

and since $(n^\varphi \wedge \xi) \perp n^\varphi$, Lemma 4.4.1 yields that

$$\left(S \cdot (n^\varphi(\tilde{y}) \wedge \xi) - i\beta(\alpha \cdot n^\varphi(\tilde{y}))\right)^2 = |n^\varphi \wedge \xi|^2 + 1 = (\lambda(\tilde{y},\xi))^2,$$

with λ as in (4.4.12). From this we deduce that $L_0(\tilde{y},\xi)$ has two eigenvalues $\rho_\pm$ which are given by (4.4.13) and $\Pi_\pm(\tilde{y},\xi)$ are the corresponding projectors onto $\mathrm{Kr}(L_0(\tilde{y},\xi) - \rho_\pm(\tilde{y},\xi)I_4)$. Next, using that

$$|n^\varphi \wedge \xi|^2 = (1+|\nabla\chi|^2)^{-1}(|\xi|^2 + (\xi_1\partial\chi_2 - \xi_2\partial\chi_1)^2),$$

and the fact that $|\nabla\chi(\tilde{y})| \lesssim 1$ holds uniformly with respect to $\tilde{y}$, we get for some $c > 0$ independent of $\tilde{y}$ that

$$\pm\Re\rho_\pm(\tilde{y},\xi) = \frac{\sqrt{|n^\varphi \wedge \xi|^2 + 1}}{\sqrt{1+|\nabla\chi|^2}} \geqslant c(1+|\xi|),$$

which gives (4.4.14) and shows that $\rho_\pm$ are elliptic in $\mathcal{S}^1$. Consequently, we also get that $L_0(\tilde{y},\xi)$ is elliptic in $\mathcal{S}^1$. Now, using Lemma 4.4.1 and the properties (4.3.1), a simple computation shows that

$$\begin{aligned} P_+^\varphi \Pi_\pm &= k_\pm^\varphi P_+^\varphi \pm \frac{1}{2\lambda}\left(S \cdot (n^\varphi(\tilde{y}) \wedge \xi)\right) P_-^\varphi, \\ P_-^\varphi \Pi_\pm &= k_\mp^\varphi P_-^\varphi \pm \frac{1}{2\lambda}\left(S \cdot (n^\varphi(\tilde{y}) \wedge \xi)\right) P_+^\varphi, \end{aligned} \tag{4.4.17}$$

with $k_\pm^\varphi$ as in (4.4.16). Hence, (4.4.15) directly follows from the above formulas. $\square$

4.4.2 Semiclassical parametrix for the boundary problem

In this subsection, we construct the approximate solution of the system (4.3.3) mentioned in the introduction of this section. For simplicity of notations, in the sequel we will use y and $P_\pm$ instead of $\tilde{y}$ and $P_\pm^\varphi$, respectively.

We are going to construct a local approximate solution of the following first order system:

$$\begin{cases} h\partial_\tau u^h = L_0(y, hD_y)u^h + hL_1(y)u^h, & \text{in } \mathbb{R}^2 \times (0, +\infty), \\ P_- u^h = f, & \text{on } \mathbb{R}^2 \times \{0\}, \end{cases} \tag{4.4.18}$$

where $L_0(y,\xi) = l_{0,0}(y) + l_{0,1}(y)\cdot\xi$ with $l_{0,0}$, $l_{0,1}$ and L_1 matrices-valued symbols of $\mathcal{S}^0$, such that the properties of Proposition 4.4.1 hold for L_0 and $P_\pm$.

To be precise, we will look for a solution u^h in the following form:

$$u^h(y,\tau) = Op^h(A^h(\cdot,\cdot,\tau))f = \int_{\mathbb{R}^2} A^h(y, h\xi, \tau)e^{iy\cdot\xi}\hat{f}(\xi)\mathrm{d}\xi, \tag{4.4.19}$$

with $A^h(\cdot,\cdot,\tau) \in \mathcal{S}^0$ for any $\tau > 0$ constructed inductively in the form:

$$A^h(y,\xi,\tau) \sim \sum_{j\geq 0} h^j A_j(y,\xi,\tau).$$

The action of $h\partial_\tau - L_0(y, hD_y) - hL_1(y)$ on $A^h(y, hD_y, \tau)f$ is given by $T^h(y, hD_y, \tau)f$, with

$$T^h(y,\xi,\tau) = h(\partial_\tau A)(y,\xi,\tau) - L_0(y,\xi)A(y,\xi,\tau) + h\Big(L_1(y)A(y,\xi,\tau) - \partial_\xi L_0(y,\xi)\cdot\partial_y A(y,\xi,\tau)\Big).$$

Then we look for A_0 satisfying:

$$\begin{cases} h\partial_\tau A_0(y,\xi,\tau) = L_0(y,\xi)A_0(y,\xi,\tau), \\ P_-(y)A_0(y,\xi,\tau) = P_-(y), \end{cases} \tag{4.4.20}$$

and for $j \geq 1$,

$$\begin{cases} h\partial_\tau A_j(y,\xi,\tau) = L_0(y,\xi)A_j(y,\xi,\tau) + L_1(y)A_{j-1}(y,\xi,\tau) - \partial_\xi L_0(y,\xi)\cdot\partial_y A_{j-1}(y,\xi,\tau), \\ P_-(y)A_j(y,\xi,\tau) = 0, \end{cases} \tag{4.4.21}$$

Proposition 4.4.2. *Let A_0 be the solution of (4.4.20), then*

$$A_0(y,\xi,\tau) = \frac{\Pi_-(y,\xi)P_-(y)}{k_+^\varphi(y,\xi)}\, e^{h^{-1}\tau\rho_-(y,\xi)}.$$

In particular, $A_0(\cdot,\cdot,\tau) \in \mathcal{S}^0$, and for all $(k,l) \in \mathbb{N}^2$ it holds that

$$\tau^k\partial_\tau^l A_0(\cdot,\cdot,\tau) \in h^{k-l}\mathcal{S}^{-k+l}.$$

Proof. The solutions of the differential system $h\partial_\tau A_0 = L_0 A_0$ are

$$A_0(y,\xi,\tau) = e^{h^{-1}\tau L_0(y,\xi)}A_0(y,\xi,0).$$

By definition of $\rho_\pm$ and $\Pi_\pm$, we have:

$$e^{h^{-1}\tau L_0(y,\xi)} = e^{h^{-1}\tau\rho_-(y,\xi)}\Pi_-(y,\xi) + e^{h^{-1}\tau\rho_+(y,\xi)}\Pi_+(y,\xi). \tag{4.4.22}$$

It follows from (4.4.14) that A_0 belongs to $\mathcal{S}^0$ for any $\tau > 0$ if and only if $\Pi_+(y,\xi)A_0(y,\xi,0) = 0$. Moreover, the boundary condition $P_- A_0 = P_-$ implies $P_-(y)A_0(y,\xi,0) = P_-(y)$. Thus, thanks to Remark 4.4.1, we deduce that

$$A_0(y,\xi,0) = P_-(y) - \frac{P_+\Pi_+P_-}{k_+^\varphi}(y,\xi) = P_-(y) + \frac{P_+\Pi_-P_-}{k_+^\varphi}(y,\xi) = \frac{\Pi_-P_-}{k_+^\varphi}(y,\xi).$$

Hence, for τ fixed the properties of ρ_-, Π_-, P_- and k_+ given in Proposition 4.4.1, imply that

$$\frac{\Pi_-P_-}{k_+^\varphi} \in \mathcal{S}^0 \quad \text{and} \quad \tau^k\partial_\tau^l(e^{h^{-1}\tau\rho_-(y,\xi)}) \in h^{k-l}\mathcal{S}^{-k+l},$$

for all $(k,l) \in \mathbb{N}^2$. This concludes the proof of Proposition 4.4.2. □

Next we treat the term A_1, after that we see more clearly in which symbol class we should construct the terms A_j, $j \geq 2$. Set $a_0(y) := i\alpha \cdot \tilde{n}(y)$, and define $A_1(y,\xi,\tau)$, then we have:

Proposition 4.4.3. *Let A_1 be the solution to the system*

$$\begin{cases} h\partial_{y_3}A_1(y,\xi,\tau) = L_0(y,\xi)A_1(y,\xi,\tau) + a_0(y)(-i\alpha\cdot\partial_y - z)A_0(y,\xi,\tau), \\ \Gamma_-^\varphi A_1(y,\xi,0) = 0, \end{cases} \tag{4.4.23}$$

Then

$$A_1(y,\xi,\tau) = e^{h^{-1}\tau\rho_-}\left[B_{1,0}(y,\xi) + h^{-1}\tau B_{1,1}(y,\xi) + h^{-2}\tau^2B_{1,2}(y,\xi)\right],$$

with $B_{1k} \in h^1\mathcal{S}^{-1}$ for $k \in \{0,1,2\}$.

Proof. We have

$$\begin{aligned} A_1(y,\xi,\tau) =& e^{h^{-1}L_0\,\tau}A_{1|\tau=0} + e^{h^{-1}L_0\,\tau}\int_0^\tau e^{-h^{-1}sL_0}a_0(y)(-i\alpha\cdot\partial_y - z)A_0(y,\xi,s)\mathrm{d}s, \\ &:= I_1(\tau) + I_2(\tau) \end{aligned}$$

with

$$I_1(\tau) = \left(e^{h^{-1}\tau\rho_-}\Pi_- + e^{h^{-1}\tau\rho_+}\Pi_+\right)A_{1|\tau=0},$$

and

$$\begin{aligned} I_2(\tau) &= e^{h^{-1}\tau L_0}\int_0^\tau e^{-h^{-1}sL_0}a_0(y)(i\alpha\cdot\partial_y - z)A_{0|y_3=0}\,\mathrm{d}s \\ &= \left(e^{h^{-1}y_3\rho_-}\Pi_- + e^{h^{-1}y_3\rho_+}\Pi_+\right)\int_0^{y_3} e^{-h^{-1}L_0\,s}a_0(y)(-i\alpha\cdot\partial_y - z)A_{0|\tau=0}\,\mathrm{d}s, \end{aligned}$$

Using the decomposition of $e^{-h^{-1}sL_0}$ as (4.4.22), we get that

$$\int_0^{y_3} e^{-h^{-1}L_0s}a_0(y)(-i\alpha\cdot\partial_y + z)A_{0|y_3=0}\,ds = J_1(y_3) + J_2(y_3),$$

where

$$J_1(\tau) = \int_0^\tau e^{-h^{-1}s\rho_-}\Pi_-a_0(y)(-i\alpha\cdot\partial_y)\left(e^{h^{-1}s\rho_-}\Pi_-A_{0|s=0}\right)\mathrm{d}s,$$

$$J_2(y_3) = \int_0^{y_3} e^{-h^{-1}s\rho_+}\Pi_+ a_0(y)(-i\alpha\cdot\partial_y - z)\left(e^{s\rho_-}\Pi_- A_{0|s=0}\right)\mathrm{d}s,$$

A simple computation shows that

$$J_1(\tau) = \Pi_- a_0\left(-h^{-1}\frac{\tau^2}{2}i\alpha\cdot\partial_y\rho_- - i\tau\alpha\cdot\partial_y\right)\Pi_- A_{0|\tau=0},$$

and that

$$\begin{aligned}
J_2(\tau) :=& \int_0^{\tau} e^{h^{-1}s(\rho_- - \rho_+)}\Pi_+ a_0\left(-ih^{-1}s\alpha\cdot\partial_y\rho_- - i\alpha\cdot\partial_y - z\right)\Pi_- A_{0|s=0}\,\mathrm{d}s\\
&= \Pi_+ a_0\left[\frac{-i\tau\alpha\cdot\partial_y\rho_-}{\rho_- - \rho_+} + \frac{i\alpha\cdot\partial_y\rho_-}{h^{-1}(\rho_- - \rho_+))^2}\right]e^{h^{-1}\tau(\rho_- - \rho_+)}\Pi_- A_{0|\tau=0}\\
&+ \Pi_+ a_0\left[\frac{(-i\alpha\cdot\partial_y - z)}{h^{-1}(\rho_- - \rho_+)}\right]e^{h^{-1}\tau(\rho_- - \rho_+)}\Pi_- A_{0|\tau=0}\\
&- \Pi_+ a_0\left[\frac{i\alpha\cdot\partial_y\rho_-}{h^{-1}(\rho_- - \rho_+)^2}) + \frac{(-i\alpha\cdot\partial_y + z)}{h^{-1}(\rho_- - \rho_+)}\right]\Pi_- A_{0|\tau=0}.
\end{aligned}$$

Thus, we get

$$\begin{aligned}
A_1(y,\xi,\tau) =& \left(e^{h^{-1}\tau\rho_-}\Pi_- + e^{h^{-1}\tau\rho_+}\Pi_+\right)A_{1|\tau=0}\\
&+ e^{h^{-1}\tau\rho_-}\Pi_- a_0\left(-h^{-1}\frac{\tau^2}{2}i\alpha\cdot\partial_y\rho_- - i\tau\alpha\cdot\partial_y\right)\Pi_- A_{0|\tau=0}\\
&+ e^{h^{-1}\tau\rho_-}\Pi_+ a_0\left[\left(\frac{\tau(-i\alpha\cdot\partial_y\rho_-)}{(\rho_- - \rho_+)} + \frac{i\alpha\cdot\partial_y\rho_-}{h^{-1}(\rho_- - \rho_+))^2}\right)\right]\Pi_- A_{0|y_3=0}\\
&+ e^{h^{-1}\tau\rho_-}\Pi_+ a_0\left[\frac{(-i\alpha\cdot\partial_y - z)}{h^{-1}(\rho_- - \rho_+)}\right]\Pi_- A_{0|\tau=0}\\
&- e^{h^{-1}\tau\rho_+}\Pi_+ a_0\left[\frac{i\alpha\cdot\partial_y\rho_-}{h^{-1}(\rho_- - \rho_+)^2}) + \frac{(-i\alpha\cdot\partial_y - z)}{h^{-1}(\rho_- - \rho_+)}\right]\Pi_- A_{0|\tau=0}.
\end{aligned}$$

As the terms involving $e^{h^{-1}\tau\rho_+}$ are not square integrable, it follows that

$$\Pi_+ A_{1|y_3=0} = \Pi_+ a_0\left[\frac{i\alpha\cdot\partial_y\rho_-}{h^{-1}(\rho_- - \rho_+)^2} + \frac{(-i\alpha\cdot\partial_y + z)}{h^{-1}(\rho_- - \rho_+)}\right]\Pi_- A_{0|y_3=0}, \tag{4.4.24}$$

Thanks to Remark 4.4.1, we deduce that

$$A_1(y,\xi,y_3) = e^{h^{-1}y_3\rho_-}\left[B_{1,0}(y,\xi) + h^{-1}y_3 B_{1,1}(y,\xi) + h^{-2}y_3^2 B_{1,2}(y,\xi)\right],$$

with

$$B_{1,0}(y,\xi) = -h\Pi_+ a_0\left(\frac{(z + i\alpha\cdot\partial_y)}{2\lambda} - \frac{i\alpha\cdot\partial_y\rho_-}{4\lambda^2}\right)\Pi_- A_0(y,\xi,0),$$

$$B_{1,1}(y,\xi) = h\Pi_+ a_0\left(\frac{-i\alpha\cdot\partial_y\rho_-}{\lambda} - (i\alpha\cdot\partial_y)\right]\Pi_- A_{0|y_3=0},$$

$$B_{1,2}(y,\xi) = h\,\Pi_- a_0\left[-\frac{1}{2}i\alpha\cdot\partial_y\rho_-\right]\Pi_- A_{0|y_3=0}.$$

From this we see that $B_{1k} \in h^1 \mathcal{S}^{-1}$ for $k \in \{0, 1, 2\}$, and this completes the proof. □

The construction of the terms A_0 and A_1 leads us to introduce the following class of parametrized symbols

$$\mathcal{P}_h^m := \{b(\cdot,\cdot,\tau) \in \mathcal{S}^m;\ \forall (k,l) \in \mathbb{N}^2,\ \tau^k \partial_\tau^l b(\cdot,\cdot,\tau) \in h^{k-l}\mathcal{S}^{m-k+l}\}; \quad m \in \mathbb{Z}, \tag{4.4.25}$$

in which we shall construct the other terms A_j, $j \geq 2$. Indeed, we have

Proposition 4.4.4. *Let A_0 be defined by Proposition 4.4.2. Then for any $j \geq 1$, there exists $A_j \in h^j \mathcal{P}_h^{-j}$ solution of (4.4.21) which has the form:*

$$A_j(y,\xi,\tau) = e^{h^{-1}\tau\rho_-(y,\xi)} \sum_{k=0}^{2j} (h^{-1}\tau\langle\xi\rangle)^k B_{j,k}(y,\xi), \tag{4.4.26}$$

with $B_{j,k} \in h^j \mathcal{S}^{-j}$.

Proof. Since A_1 has already the claimed form by Proposition 4.4.3, thus for A_j with $j \geq 2$, it is sufficient to prove the induction step. Let us assume there exists $A_j \in h^j \mathcal{P}_h^{-j}$ solution of (4.4.21) satisfying the above property and let us prove that the same holds for A_{j+1}. In order to be a solution of the differential system $h\partial_\tau A_{j+1} = L_0 A_{j+1} + L_1 A_j - \partial_\xi L_0 \cdot \partial_y A_j$, A_{j+1} :

$$A_{j+1} = e^{h^{-1}\tau L_0} A_{j+1|\tau=0} + e^{h^{-1}\tau L_0} \int_0^\tau e^{-h^{-1}sL_0}(L_1 A_j - \partial_\xi L_0 \cdot \partial_y A_j)\mathrm{d}s, \tag{4.4.27}$$

where $L_1 A_j$ has still the form (4.4.26), and we have

$$\partial_y A_j = e^{h^{-1}\tau\rho_-} \left(h^{-1}\tau\partial_y\rho_- + \partial_y\right) \sum_{k=0}^{2j} (h^{-1}\tau\langle\xi\rangle)^k B_{j,k}.$$

Thus, thanks to the properties ρ_- and $B_{j,k}$, the quantity $(L_1 A_j - \partial_\xi L_0 \cdot \partial_y A_j)(y,\xi,s)$ has the form:

$$e^{h^{-1}s\rho_-(y,\xi)} \sum_{k=0}^{2j+1} (h^{-1}\tau\langle\xi\rangle)^k \widetilde{B}_{j,k}(y,\xi) \tag{4.4.28}$$

with $\widetilde{B}_{j,k} \in h^j \mathcal{S}^{-j}$. So, by using the decomposition (4.4.22), for the second term of the r.h.s. of (4.4.27) we have:

$$e^{h^{-1}\tau L_0} \int_0^\tau e^{-h^{-1}sL_0}(L_1 A_j - \partial_\xi L_0 \cdot \partial_y A_j)\mathrm{d}s = e^{h^{-1}\tau\rho_-}\Pi_- I_-^j(\tau) + e^{h^{-1}\tau\rho_+}\Pi_+ I_+^j(\tau) \tag{4.4.29}$$

with

$$I_\pm^j(\tau) = \int_0^\tau e^{h^{-1}s(\rho_- - \rho_\pm)} \sum_{k=0}^{2j+1} (h^{-1}s\langle\xi\rangle)^k \widetilde{B}_{j,k}\mathrm{d}s,$$

For I_-^j, the exponential term is equal to 1 and by integration of s^k, we obtain:

$$I_-^j(\tau) = \sum_{k=0}^{2j+1} (h^{-1}\tau\langle\xi\rangle)^{k+1} \frac{h\langle\xi\rangle^{-1}}{k+1} \widetilde{B}_{j,k}. \tag{4.4.30}$$

For I_+^j, let us introduce P_k the polynomial of degree k such that

$$\int_0^\tau e^{\lambda s} s^k \mathrm{d}s = \frac{1}{\lambda^{k+1}}(e^{\tau\lambda}P_k(\tau\lambda) - P_k(0)),$$

for any $\lambda \in \mathbb{C}^*$. With this notation in hand, we easily see that the term $e^{\tau^h \rho_+} \Pi_+ I_+^j(\tau)$ has the following form:

$$e^{\tau^h \rho_+} \Pi_+ I_+^j(\tau) = \Pi_+ \sum_{k=0}^{2j+1} \frac{h\langle\xi\rangle^k}{(\rho_- - \rho_+)^{k+1}} \widetilde{B}_{j,k} \Big(e^{\tau^h \rho_-} P_k(\tau^h(\rho_- - \rho_+)) - e^{\tau^h \rho_+} P_k(0) \Big), \quad (4.4.31)$$

where $\tau^h := h^{-1}\tau$. Thus, by combining (4.4.30) and (4.4.31) with (4.4.27), (4.4.29) and (4.4.22), we obtain:

$$A_{j+1} = e^{h^{-1}\tau\rho_+} \Big(\Pi_+ A_{j+1|\tau=0} - \widetilde{B^+_{j+1}} \Big) + e^{h^{-1}\tau\rho_-} \Big(\Pi_- A_{j+1|\tau=0} + \sum_{k=0}^{2(j+1)} (h^{-1}\tau\langle\xi\rangle)^k \widetilde{B^-_{j+1,k}} \Big), \quad (4.4.32)$$

where

$$\widetilde{B^+_{j+1}} = \Pi_+ \sum_{k=0}^{2j+1} \frac{h\langle\xi\rangle^k}{(\rho_- - \rho_+)^{k+1}} P_k(0) \widetilde{B}_{j,k} \in h^{j+1} \mathcal{S}^{-j-1},$$

and $\widetilde{B^-_{j+1,k}} \in h^{j+1}\mathcal{S}^{-j-1}$ as a linear combination of products of $\Pi_- \in \mathcal{S}^0$, $h\langle\xi\rangle^{-1}$ (or $h\langle\xi\rangle^k(\rho_- - \rho_+)^{-k-1}$) belonging to $h\mathcal{S}^{-1}$ and of $\widetilde{B}_{j,k} \in h^j \mathcal{S}^{-j}$.

Now, in order to have $A_{j+1} \in \mathcal{S}^0$, we let the contribution of the exponentially growing term vanish by choosing

$$\Pi_+ A_{j+1}(y,\xi,0) = \widetilde{B^+_{j+1}}(y,\xi). \quad (4.4.33)$$

Then, thanks to Remark 4.4.1, the boundary condition $P_-(y)A_{j+1}(y,\xi,0) = 0$ gives

$$A_{j+1}(y,\xi,0) = \frac{P_+\Pi_+}{k_+^\varphi} \widetilde{B^+_{j+1}}(y,\xi). \quad (4.4.34)$$

Finally, we have

$$A_{j+1}(y,\xi,\tau) = e^{h^{-1}\tau\rho_-(y,\xi)} \Big(\frac{\Pi_- P_+ \Pi_+}{k_+^\varphi} \widetilde{B^+_{j+1}}(y,\xi) + \sum_{k=0}^{2(j+1)} (h^{-1}\tau\langle\xi\rangle)^k \widetilde{B^-_{j+1,k}}(y,\xi) \Big),$$

and Proposition 4.4.4 is proven with

$$B_{j+1,0} = \frac{\Pi_- P_+ \Pi_+}{k_+^\varphi} \widetilde{B^+_{j+1}} + \widetilde{B^-_{j+1,0}},$$

and for $k \geq 1$, $B_{j+1,k} = \widetilde{B^-_{j+1,k}}$. □

Thanks to the relation (4.4.19), to any $A^h \in \mathcal{P}_h^0$ we associate a bounded operator from $L^2(\mathbb{R}^2)$ into $L^2(\mathbb{R}^2 \times (0,+\infty))$. The boundedness in the variable $y \in \mathbb{R}^2$ is a consequence of the Calderon-Vaillancourt theorem (see 4.1.6), and in the variable $\tau \in (0,+\infty)$ it is essentially the multiplication by an L^∞-function. Moreover, for A_j of the form (4.4.26), we have the following mapping property which captures the Sobolev space regularity.

Proposition 4.4.5. *Let A_j, $j \geq 0$, be of the form (4.4.26). Then, for any $s \geq -j - \frac{1}{2}$, the operator $\mathcal{A}_j$ defined by*

$$\mathcal{A}_j : f \longmapsto (\mathcal{A}_j f)(y, y_3) = \int_{\mathbb{R}^2} A_j(y, h\xi, y_3) e^{iy\cdot\xi} \hat{f}(\xi) \mathrm{d}\xi$$

gives rise to a bounded operator from $H^s(\mathbb{R}^2)$ into $H^{s+j+\frac{1}{2}}(\mathbb{R}^2 \times (0,+\infty))$. Moreover, for any $l \in [0, j+\frac{1}{2}]$ we have:

$$\|\mathcal{A}_j\|_{H^s \to H^{s+j+\frac{1}{2}-l}} = O(h^{l-s}). \quad (4.4.35)$$

Proof. First, let us prove the result for $s = k - j - \frac{1}{2}$, $k \in \mathbb{N}$, between the semiclassical Sobolev spaces

$$\begin{aligned} H^s_{\text{scl}}(\mathbb{R}^2) &:= \langle hD_y\rangle^{-s} L^2(\mathbb{R}^2) \\ H^k_{\text{scl}}(\mathbb{R}^2 \times (0,+\infty)) &:= \{u \in L^2;\ \langle hD_y\rangle^{k_1}(h\partial_{y_3})^{k_2} u \in L^2 \text{ for } (k_1,k_2) \in \mathbb{N}^2, k_1 + k_2 = k\}, \end{aligned}$$

where $\langle hD_y\rangle = \sqrt{-h^2\Delta_{\mathbb{R}^2} + I}$. Then, for $f \in H^s(\mathbb{R}^2)^4$, we have:

$$\begin{aligned} \|\mathcal{A}_j f\|^2_{H^k_{\text{scl}}(\mathbb{R}^2\times(0,+\infty))} &= \sum_{k_1+k_2=k} \|\langle hD_y\rangle^{k_1}(h\partial_{y_3})^{k_2}\mathcal{A}_j f\|^2_{L^2(\mathbb{R}^2\times(0,+\infty))} \\ &= \sum_{k_1+k_2=k} \int_0^{+\infty} \|\langle hD_y\rangle^{k_1}(h\partial_{y_3})^{k_2}(\mathcal{A}_j f)(\cdot,y_3)\|^2_{L^2(\mathbb{R}^2)} \mathrm{d}y_3. \end{aligned} \tag{4.4.36}$$

Thanks to the ellipticity property (4.4.14), for A_j given by Proposition 4.4.4 we have:

$$(h\partial_{y_3})^{k_2} A_j(y,\xi,y_3) = h^j b_j(y,\xi;y_3) e^{-h^{-1}y_3\frac{c}{2}\langle\xi\rangle}\langle\xi\rangle^{k_2-j},$$

with b_j satisfying, for any $(\alpha,\beta) \in \mathbb{N}^2 \times \mathbb{N}^2$ there exists $C_{\alpha,\beta} > 0$ such that:

$$|\partial_y^\alpha \partial_\xi^\beta b_j(y,\xi;y_3)| \leq C_{\alpha,\beta}, \quad \forall (y,\xi;y_3) \in \mathbb{R}^2 \times \mathbb{R}^2 \times (0,+\infty).$$

Consequently, from the Calderón-Vaillancourt theorem's (see (4.1.6)), we can write:

$$\langle hD_y\rangle^{k_1}(h\partial_{y_3})^{k_2}\mathcal{A}_j = h^j \mathcal{B}_j(y_3)\langle hD_y\rangle^{k_1+k_2-j} e^{-h^{-1}y_3\frac{c}{2}\langle hD_y\rangle},$$

with $(\mathcal{B}_j(y_3))_{y_3>0}$ a family of bounded operators on $L^2(\mathbb{R}^2)$, and uniformly bounded with respect to $y_3 > 0$. Then, for $f \in H^s(\mathbb{R}^2)^4$, we have:

$$\|\langle hD_y\rangle^{k_1}(h\partial_{y_3})^{k_2}(\mathcal{A}_j f)(\cdot,y_3)\|^2_{L^2(\mathbb{R}^2)} \lesssim h^j \|\langle hD_y\rangle^{k_1+k_2-j} e^{-h^{-1}y_3\frac{c}{2}\langle hD_y\rangle} f\|^2_{L^2(\mathbb{R}^2)},$$

and from (4.4.36) we deduce that

$$\|\mathcal{A}_j f\|^2_{H^k_{\text{scl}}(\mathbb{R}^2\times(0,+\infty))} \lesssim h^{2j+1}\|\langle hD_y\rangle^{k-j-\frac{1}{2}} f\|^2_{L^2(\mathbb{R}^2)} = h^{2j+1}\|f\|^2_{H^{k-j-\frac{1}{2}}_{\text{scl}}(\mathbb{R}^2)},$$

where we used that for any $l \in \mathbb{N}$, $f \in H^{l-\frac{1}{2}}_{\text{scl}}(\mathbb{R}^2)$,

$$\begin{aligned} \|\langle hD_y\rangle^l e^{-h^{-1}y_3\frac{c}{2}\langle hD_y\rangle} f\|^2_{L^2(\mathbb{R}^2)} &= \langle e^{-h^{-1}y_3 c\langle hD_y\rangle}\langle hD_y\rangle^l f\,,\, \langle hD_y\rangle^l f\rangle_{L^2} \\ &= -\frac{h}{c}\frac{\partial}{\partial_{y_3}}\langle e^{-h^{-1}y_3 c\langle hD_y\rangle}\langle hD_y\rangle^{l-1} f\,,\, \langle hD_y\rangle^l f\rangle_{L^2}. \end{aligned}$$

By interpolation arguments we thus deduce that for any $j \in \mathbb{N}$, $s \geq -j - \frac{1}{2}$, it holds that

$$\|\mathcal{A}_j\|_{H^s_{\text{scl}} \to H^{s+j+\frac{1}{2}}_{\text{scl}}} = O(h^{j+\frac{1}{2}}). \tag{4.4.37}$$

proving the estimate (4.4.35) and completing the proof of the proposition. □

Proposition 4.4.6. *Let $f \in H^s(\mathbb{R}^2)$ and A_j, $j \geq 0$, be defined as in Propositions 4.4.2 and 4.4.4. Then for any $N \geq -s - \frac{1}{2}$, the function $u^h_N = \sum_{j=0}^N h^j \mathcal{A}_j f$ satisfies:*

$$\begin{cases} h\partial_\tau u^h_N - L_0(y,hD_y)u^h_N - hL_1(y)u^h_N = h^{N+1}\mathcal{R}^h_N f, & \textit{in } \mathbb{R}^2 \times (0,+\infty), \\ P_- u^h_N = f, & \textit{on } \mathbb{R}^2 \times \{0\}, \end{cases} \tag{4.4.38}$$

with

$$\mathcal{R}_N^h : f \longmapsto \int_{\mathbb{R}^2} \Big(L_1 A_N - \partial_\xi L_0 \cdot \partial_y A_N\Big)(y, h\xi, \tau) e^{iy\cdot\xi} \hat{f}(\xi) \mathrm{d}\xi,$$

a bounded operator from $H^s(\mathbb{R}^2)$ *into* $H^{s+N+\frac{1}{2}}(\mathbb{R}^2 \times (0,+\infty))$ *satisfying for any* $l \in [0, N+\frac{1}{2}]$*:*

$$\|\mathcal{R}_N^h\|_{H^s \to H^{s+N+\frac{1}{2}-l}} = O(h^{l-s}). \tag{4.4.39}$$

Proof. By construction of the sequence $(A_j)_{j\in\{0,\cdots,N-1\}}$ we have the system (4.4.38) with $\mathcal{R}_N^h = Op^h(r_N^h(\cdot,\cdot,\tau))$,

$$r_N^h(y,\xi,\tau) = \Big(L_1 A_N - \partial_\xi L_0 \cdot \partial_y A_N\Big)(y,\xi,\tau),$$

(see the beginning of Section 4.4.2). As in the proof of Proposition 4.4.4, r_N^h has the form (4.4.28) (with $j = N$). Then, in similar way as in the proof of Proposition 4.4.5 we obtain the estimate (4.4.39). □

4.4.3 Proof of Theorem 4.4.1

In this section, we apply the above construction in order to prove Theorem 4.4.1. Let $g \in P_- H^{1/2}(\partial\Omega)^4$, $(U_\varphi, V_\varphi, \varphi)$ a chart of the atlas $\mathbb{A}$ and $\psi_1, \psi_2 \in C_0^\infty(U_\varphi)$. Then $f := (\varphi^{-1})^*(\psi_2 g)$ is a function of $H^{1/2}(V_\varphi)^4$ which can be extended by 0 to a function of $H^{1/2}(\mathbb{R}^2)^4$. Then for $h = 1/m$ and any $N \in \mathbb{N}$, the previous construction provides a function $u_N^h \in H^1(\mathbb{R}^2 \times (0,+\infty))^4$ satisfying

$$\begin{cases} (\widetilde{D}_m^\varphi - z) u_N^h = h^{N+1} \mathcal{R}_N^h f, & \text{in } \mathbb{R}^2 \times (0,\varepsilon), \\ \Gamma_- u_N^h = f, & \text{on } \mathbb{R}^2 \times \{0\}, \end{cases} \tag{4.4.40}$$

with $u_N^h = \sum_{j=0}^N h^j \mathcal{A}_j f$ (see Proposition 4.4.5) and $\mathcal{R}_N^h f \in H^{N+1}(\mathbb{R}^2 \times (0,\varepsilon))$ with norm in H^{N+1-l}, $l \in [0, N+\frac{1}{2}]$, bounded by $O(h^{l-\frac{1}{2}})$. Consequently, $v_N^h := \phi^* u_N^h$, defined on $\mathcal{V}_{\varphi,\varepsilon}$, satisfies:

$$\begin{cases} (D_m - z) v_N^h = h^{N+1} \phi^*(\mathcal{R}_N^h f), & \text{in } \mathcal{V}_{\varphi,\varepsilon}, \\ \Gamma_- v_N^h = \psi_2 g, & \text{on } U_\varphi. \end{cases} \tag{4.4.41}$$

Now, let $E_m^\Omega(z)[\psi_2 g] \in H^1(\Omega)^4$ be as in Definition 4.3.1. Since $\Gamma_- v_N^h = \Gamma_- E_m^\Omega(z)[\psi_2 g] = \psi_2 g$, then the following equality holds in $\mathcal{V}_{\varphi,\varepsilon}$:

$$v_N^h - E_m^\Omega(z)[\psi_2 g] = h^{N+1} (H_{\mathrm{MIT}}(m) - z)^{-1} \phi^* \Big(\mathcal{R}_N^h (\varphi^{-1})^*(\psi_2 g)\Big).$$

From this, we deduce that

$$\psi_1 \mathscr{A}_m \psi_2(g) := \psi_1 \Gamma_+ E_m^\Omega(z)[\psi_2 g] = \psi_1 \Gamma_+ v_N^h - h^{N+1} \psi_1 \Gamma_+ (H_{\mathrm{MIT}}(m) - z)^{-1} \phi^* \Big(\mathcal{R}_N^h (\varphi^{-1})^*(\psi_2 g)\Big).$$

Since $\phi\restriction_{U_\varphi} = \varphi$, for any $u \in H^1(V_\varphi \times (0,\varepsilon))^4$, we have that

$$\Gamma_+ \phi^*(u) = \varphi^*(P_+ u\restriction_{V_\varphi \times \{0\}}), \quad \psi_1 \Gamma_+ v_N^h = \psi_1 \varphi^* Op^h(a_N^h)(\varphi^{-1})^* \psi_2 g,$$

with

$$a_N^h(\tilde{y},\xi) = \sum_{j=0}^N h^j P_+ A_j(y,\xi,0) = \sum_{j=0}^N h^j P_+ B_{j,0}(y,\xi), \tag{4.4.42}$$

where $B_{j,0} \in h^j \mathcal{S}^{-j}$ are introduced in Proposition 4.4.4. Thus, in local coordinates, the principal semiclassical symbol of $\mathscr{A}_m$ is given by

$$P_+ B_{0,0}(y,\xi) = P_+ A_0(y,\xi,0) = \frac{P_+ \Pi_- P_-}{k_+^\varphi}(y,\xi).$$

Thanks to the property (4.4.15) it is equal to

$$-\Theta^\varphi P_-(y,\xi) = \frac{S \cdot (\xi \wedge n^\varphi(y))}{\sqrt{|n^\varphi \wedge \xi|^2 + 1} + 1} P_-(y,\xi).$$

We conclude the proof of Theorem 4.4.1 by proving the following Lemma which is a consequence of the above considerations, the regularity estimates from Theorem 4.2.1-(iii), Theorem 4.2.2-(i) and Proposition 4.3.1.

Lemma 4.4.2. *Let $\psi_1, \psi_2 \in C^\infty(\Sigma)$ such that* $\mathrm{supp}(\psi_1) \cap \mathrm{supp}(\psi_2) = \emptyset$. *Then, for $m_0 > 0$ sufficiently large, $m \geqslant m_0$, and for any $(k, N) \in \mathbb{N}^* \times \mathbb{N}^*$ it holds that*

$$\|\psi_1 \mathscr{A}_m \psi_2\|_{P_- H^{1/2}(\Sigma)^4 \to P_+ H^k(\Sigma)^4} = \mathcal{O}(m^{-N}).$$

Proof. Let $\psi_1, \psi_2 \in C^\infty(\Sigma)$ with disjoint supports. Thanks to Theorem 4.2.1-(iii) and Theorem 4.2.2-(i), to prove the lemma it suffices to show that for any $(N_1, N_2) \in \mathbb{N}^2$, there exists C_{N_1,N_2} such that

$$\begin{aligned} \|(\psi_1 \mathscr{A}_m \psi_2) g\|_{P_+ H^{N_2+\frac{1}{2}}(\Sigma)^4} \leq & \frac{C_{N_1,N_2}}{\sqrt{m}} \left(\Pi_{k=0}^{N_2-1} \|(H_{\mathrm{MIT}}(m) - z)^{-1}\|_{H^k(\Omega)^4 \to H^{k+1}(\Omega)^4} \right) \\ & \times \|(H_{\mathrm{MIT}}(m) - z)^{-1}\|_{L^2(\Omega)^4 \to L^2(\Omega)^4}^{N_1} \|g\|_{P_- H^{1/2}(\Sigma)^4}. \end{aligned} \tag{4.4.43}$$

For this, let us introduce $\Phi_1 \in C_0^\infty(\overline{\Omega})$ such that $\Phi_1 = 1$ near $\mathrm{supp}(\psi_1)$ and $\Phi_1 = 0$ near $\mathrm{supp}(\psi_2)$. Thus, for $g \in P_- H^{1/2}(\partial\Omega)^4$ and $E_m^\Omega(z)[\psi_2 g] \in H^1(\Omega)$ as in Definition 4.3.1, the function $u_{1,2} := \Phi_1 E_m^\Omega(z)[\psi_2 g]$ satisfies:

$$\begin{cases} (D_m - z) u_{1,2} = [D_0\,,\, \Phi_1] E_m^\Omega(z)[\psi_2 g], & \text{in } \Omega, \\ \Gamma_- u_{1,2} = \Phi_1 \restriction_\Sigma \psi_2 g = 0, & \text{on } \Sigma. \end{cases} \tag{4.4.44}$$

Then, $u_{1,2} = (H_{\mathrm{MIT}}(m) - z)^{-1}[D_0\,,\, \Phi_1] E_m^\Omega(z)[\psi_2 g]$, and for any $\widetilde{\Phi_1} \in C_0^\infty(\overline{\Omega})$ equals to 1 near $\mathrm{supp}(\psi_1)$ we have:

$$\psi_1 \mathscr{A}_m \psi_2(g) = \psi_1 \Gamma_+ \widetilde{\Phi_1} (H_{\mathrm{MIT}}(m) - z)^{-1} [D_0\,,\, \Phi_1] E_m^\Omega(z)[\psi_2 g].$$

Moreover, by choosing $\widetilde{\Phi_1}$ such that $\widetilde{\Phi_1} \prec \Phi_1$, that is $\Phi_1 = 1$ on $\mathrm{supp}(\widetilde{\Phi_1})$, both functions $\widetilde{\Phi_1}$ and $[D_0\,,\, \Phi_1]$ have disjoint supports, and we can apply the following telescopic formula:

$$\begin{aligned} \widetilde{\Phi_1}(H_{\mathrm{MIT}}(m) - z)^{-1}(1 - \chi_1) = & \widetilde{\Phi_1}(H_{\mathrm{MIT}}(m) - z)^{-1}[D_0, \chi_N] \cdots (H_{\mathrm{MIT}}(m) - z)^{-1}[D_0, \chi_2] \\ & (H_{\mathrm{MIT}}(m) - z)^{-1}(1 - \chi_1), \end{aligned}$$

for $(\chi_i)_{1 \leq i \leq N}$ a family of compactly supported smooth functions such that $\widetilde{\Phi_1} \prec \chi_N \prec \chi_{N-1} \prec \cdots \prec \chi_1 \prec \Phi_1$. Since $[D_0\,,\, \Phi_1] = (1 - \chi_1)[D_0\,,\, \Phi_1]$, the above telescopic formula allows us to write $\psi_1 \mathscr{A}_m \psi_2(g)$ as a product of N cutoff resolvents of $H_{\mathrm{MIT}}(m)$. Now, by Proposition 4.3.1 we have

$$\left|\left| E_m^\Omega(z)[\psi_2 g] \right|\right|_{L^2(\Omega)^4} \lesssim \frac{1}{\sqrt{m}} \|g\|_{L^2(\Sigma)^4}.$$

Thus, using the continuity of Γ_+ from $H^{N_2+1}(\Omega)$ to $H^{N_2+\frac{1}{2}}(\Sigma)$, we then get the estimation (4.4.43) for $N = N_1 + N_2$, finishing the proof of the lemma. ☐

Remark 4.4.2. *Note that for any $m > 0$ and $z \in \rho(H_{MIT}(m))$, the parametrix we have constructed for $\mathscr{A}_m$ is valid from the classical pseudodifferentiel point of view. Actually, Lemma 4.4.2 is the only result where the assumption that m is big enough has been assumed, and it is exclusively required to ensures that away from the diagonal the operator $\mathscr{A}_m$ is negligible in $1/m$. In the same vein, if m is fixed then the proof of Lemma 4.4.2 still ensures that away from the diagonal $\mathscr{A}_m$ is regularizing. Consequently, we deduce that for any $m > 0$ and $z \in \rho(H_{MIT}(m))$, the operator $\mathscr{A}_m$ is a homogeneous pseudodifferential operator of order 0, and that*

$$\mathscr{A}_m = \frac{1}{\sqrt{-\Delta_\Sigma}} S \cdot (\nabla_\Sigma \wedge n) P_- \quad \mathrm{mod}\ Op\mathcal{S}^{-1}(\Sigma),$$

which is in accordance with Theorem 4.3.1.

Remark 4.4.3. *If Ω is the upper half-plane $\{(x_1, x_2, x_3) \in \mathbb{R}^3;\ x_3 > 0\}$, we easily obtain that $\mathscr{A}_m$ is a Fourier multiplier with symbol*

$$a_m(\xi) = -\frac{i\alpha_3(\alpha_1\xi_1 + \alpha_2\xi_2 - z)}{\sqrt{|\xi|^2 + m} + m} P_-.$$

Note that this result is straight forward and can be easily derived from the Fourier side, since by Theorem 2.3.3 $\mathrm{Sp}(H_{MIT}(m)) = \mathrm{Sp}(D_m)$, *and thus $\mathscr{A}_m$ has the explicit formula given in Proposition 4.3.1-*(iii).

4.5 Krein-type resolvent formula and resolvent convergence to the MIT bag operator

In the whole section, we let $\Omega \subset \mathbb{R}^3$ be a bounded smooth domain. As in the introduction of this chapter, we set

$$\Omega_i = \Omega \ \text{and} \ \Omega_e = \mathbb{R}^3 \setminus \overline{\Omega}, \quad \partial\Omega = \Sigma.$$

Fix $m > 0$ and let $M > 0$. Recall that the Dirac operator H_M is defined by

$$H_M\varphi = (D_m + M\beta 1_{\Omega_e})\varphi, \quad \forall\varphi \in \mathrm{dom}(H_M) := H^1(\mathbb{R}^3)^4,$$

where 1_{Ω_e} is characteristic function of Ω_e. By Kato-Rellich theorem and Weyl's theorem, it is easy to see that $(H_M, \mathrm{dom}(H_M))$ is self-adjoint and that

$$\mathrm{Sp}_{\mathrm{ess}}(H_M) = (-\infty, -(m+M)] \cup [m+M, +\infty),$$
$$\mathrm{Sp}(H_M) \cap (-(m+M), m+M) \text{ is purely discrete.}$$

We also recall that the MIT bag operator acting on $L^2(\Omega_i)^4$, is defined by

$$H_{\mathrm{MIT}}(m)v = D_m v \quad \forall v \in \mathrm{dom}(H_{\mathrm{MIT}}(m)) := \left\{ v \in H^1(\Omega_i)^4 : P_- t_\Sigma v = 0 \text{ on } \Sigma \right\}, \tag{4.5.1}$$

where t_Σ is the trace operator and $P_\pm$ are the orthogonal projections defined by (4.1.1).

The aim of this section is to use the properties of the Poincaré-Steklov operators carried out in the previous sections to study the resolvent of H_M when M is large enough. Namely, we give a Krein-type resolvent formula in terms of the resolvent of $H_{\mathrm{MIT}}(m)$, and we show that the convergence of H_M toward $H_{\mathrm{MIT}}(m)$, in the norm resolvent sense, holds with a convergence rate of $\mathcal{O}(M^{-1})$.

Before stating the main results of this section, we need to introduce some notations and definitions. First, we introduce the following Dirac auxiliary operator

$$\widetilde{H}_M u = D_{m+M} u, \quad \forall u \in \mathrm{dom}(\widetilde{H}_M) := \Big\{ u \in H^1(\Omega_e)^4 : P_+ t_\Sigma u = 0 \text{ on } \Sigma \Big\}. \tag{4.5.2}$$

Notice that $\widetilde{H}_M$ is the MIT bag operator on Ω_e. Since Ω_e is unbounded, Theorem 4.2.1 implies that $(\widetilde{H}_M, \mathrm{dom}(\widetilde{H}_M))$ is self-adjoint, and that

$$\mathrm{Sp}(\widetilde{H}_M) = \mathrm{Sp}_{\mathrm{ess}}(\widetilde{H}_M) = (-\infty, -(m+M)] \cup [m+M, +\infty).$$

Let $z \in \rho(H_{\mathrm{MIT}}(m)) \cap \rho(H_M)$ and $g, h \in H^{1/2}(\Sigma)^4$. We denote by $E_m^{\Omega_i}(z) : P_- H^{1/2}(\Sigma)^4 \to H^1(\Omega_i)^4$ the unique solution of the following boundary value problem:

$$\begin{cases} (D_m - z)v = 0, & \text{in } \Omega_i, \\ P_- t_\Sigma v = g, & \text{in } \Sigma. \end{cases} \tag{4.5.3}$$

Similarly, we denote by $E_{m+M}^{\Omega_e}(z) : P_+ H^{1/2}(\Sigma)^4 \to H^1(\Omega_e)^4$ the unique solution of the following boundary value problem:

$$\begin{cases} (D_{m+M} - z)u = 0, & \text{in } \Omega_e, \\ P_+ t_\Sigma u = h, & \text{in } \Sigma. \end{cases} \tag{4.5.4}$$

Define the Poincaré-Steklov operators associated to the above problems by

$$\mathscr{A}_m^i = P_+ t_\Sigma E_m^{\Omega_i}(z) P_- \quad \text{and} \quad \mathscr{A}_{m+M}^e = P_- t_\Sigma E_{m+M}^{\Omega_e}(z) P_+.$$

Then, from Proposition 4.3.1 we have the explicit formulas

$$\begin{aligned} E_m^{\Omega_i}(z) &= \Phi_z^{\Omega_i} (\Lambda_m^z)^{-1} P_-, \quad \mathscr{A}_m^i = -P_+ \beta (\Lambda_m^z)^{-1} P_-, \quad \forall z \in \rho(D_m), \\ E_{m+M}^{\Omega_e}(z) &= \Phi_{z,m+M}^{\Omega_e} (\Lambda_{m+M}^z)^{-1} P_+, \quad \mathscr{A}_{m+M}^e = -P_- \beta (\Lambda_{m+M}^z)^{-1} P_+, \quad \forall z \in \rho(D_{m+M}). \end{aligned} \tag{4.5.5}$$

Notation 4.5.1. *In the sequel we shall denote by $R_M(z)$, $\widetilde{R}_M(z)$ and $R_{MIT}(z)$ the resolvent of H_M, $\widetilde{H}_M$ and $H_{MIT}(m)$, respectively. We also use the notations:*

- $\Gamma_\pm = P_\pm t_\Sigma$ *and* $\Gamma = \Gamma_+ r_{\Omega_i} + \Gamma_- r_{\Omega_e}$.
- $E_M(z) = e_{\Omega_i} E_m^{\Omega}(z) P_- + e_{\Omega_e} E_{m+M}^{\Omega_e}(z) P_+$.
- $\widetilde{R}_{MIT}(z) = e_{\Omega_i} R_{MIT}(z) r_{\Omega_i} + e_{\Omega_e} \widetilde{R}_M(z) r_{\Omega_e}$.

With these notations in hand, we can state the main results of this section.

Theorem 4.5.1. *There is $M_0 > 0$ such that for all $M > M_0$ and all $z \in \rho(H_{MIT}(m)) \cap \rho(H_M)$, the operator $\Psi_M(z) := \Big(I - \mathscr{A}_m^i - \mathscr{A}_{m+M}^e\Big)$ is bounded invertible in $H^{1/2}(\Sigma)^4$, and it holds that*

$$R_M(z) = \widetilde{R}_{\mathrm{MIT}}(z) + E_M(z) \Psi^{-1}(z) \Gamma \widetilde{R}_{\mathrm{MIT}}(z). \tag{4.5.6}$$

Moreover, for any $a \in (-(m+M), m+M) \setminus \rho(H_{MIT}(m))$ we have $a \in \mathrm{Sp_p}(H_M) \Leftrightarrow 0 \in \mathrm{Sp_p}(\Psi_M(a))$, and it holds that

$$\mathrm{Kr}(H_M - a) = \{ E_M(a) g : g \in \mathrm{Kr}(\Psi_M(a)) \}.$$

Remark 4.5.1. *By Proposition 4.3.1* (ii) *we have that*

$$\left(E_m^{\Omega_i}(z)\right)^* = -\beta\Gamma_+ R_{\mathrm{MIT}}(\overline{z}) \quad \text{and} \quad \left(E_{m+M}^{\Omega_e}(z)\right)^* = -\beta\Gamma_- \widetilde{R}_M(\overline{z}),$$

for any $z \in \rho(H_{MIT}(m)) \cap \rho(H_M)$. Thus, the resolvent formula (4.5.6) can be written in the form:

$$R_M(z) = \widetilde{R}_{\mathrm{MIT}}(z) - (\beta\Gamma\widetilde{R}_{\mathrm{MIT}}(\overline{z}))^*\Psi^{-1}(z)\Gamma\widetilde{R}_{\mathrm{MIT}}(z).$$

Before going through the proof of Theorem 4.5.1 we first establish a regularity result that will play a crucial role in the rest of this section. It concerns the dependence on the parameter M of the norm of an auxiliary operator which involves the composition of the operators $\mathscr{A}_m^i$ and $\mathscr{A}_{m+M}^e$. In the proof we use the symbols $\hat{u}$ and $\mathcal{F}[u]$ to denote the Fourier transform of u.

Theorem 4.5.2. *Let $\mathscr{A}_m^i$ and $\mathscr{A}_{m+M}^e$ be as above. Then, there is $M_0 > 0$ such that for every $\infty > M > M_0$ and all $z \in \rho(H_{MIT}(m)) \cap \rho(H_M)$ the following hold true:*

(i) For any $s \in \mathbb{R}$ the operator $\Xi_M(z) : H^s(\Sigma)^4 \longrightarrow H^s(\Sigma)^4$ defined by

$$\Xi_M(z) = \left(I_4 - \mathscr{A}_m^i\mathscr{A}_{m+M}^e - \mathscr{A}_{m+M}^e\mathscr{A}_m^i\right)^{-1}, \tag{4.5.7}$$

is everywhere defined and uniformly bounded with respect to M.

(ii) The Poincaré-Steklov operator, $\mathscr{A}_{m+M}^e$, satisfies the estimate

$$||\mathscr{A}_{m+M}^e||_{P_+H^{s+1}(\Sigma)^4 \to P_-H^s(\Sigma)^4} \lesssim \frac{1}{M}, \quad \forall s \in \mathbb{R}. \tag{4.5.8}$$

Proof. (i) Set $\tau := (m+M)$, then the result essentially follows from the fact that $\Xi_M(z)$ is a $1/\tau$-pseudodifferential operator of order 0. Fix $z \in \rho(H_{\mathrm{MIT}}(m)) \cap \rho(H_M)$ and set $h = \tau^{-1}$. From Theorem 4.3.1 and Remark 4.4.2 we know that $\mathscr{A}_m^i$ is a homogeneous pseudodifferential operator of order 0. Thus $\mathscr{A}_m^i$ can also be viewed as a h-pseudodifferential operators of order 0. That is, $\mathscr{A}_m^i \in Op^h\mathcal{S}^0(\Sigma)$, and in local coordinates, its semiclassical principal symbol is given by

$$p_{h,\mathscr{A}_m^i}(x,\xi) = \frac{S\cdot(\xi \wedge n(x))P_-}{|\xi \wedge n(x)|}.$$

Similarly, thanks to Theorem 4.4.1, we also know that for h_0 sufficiently small (and hence M_0 big enough) and all $h < h_0$, $\mathscr{A}_{m+M}^e$ is a h-pseudodifferential operator and that

$$\mathscr{A}_{m+M}^e \in Op^h\mathcal{S}^0(\Sigma), \quad p_{h,\mathscr{A}_{m+M}^e}(x,\xi) = -\frac{S\cdot(\xi \wedge n(x))P_+}{\sqrt{|\xi \wedge n(x)|^2 + 1} + 1}.$$

Therefore, the symbol calculus yields for all $h < h_0$ that $\left(I_4 - \mathscr{A}_m^i\mathscr{A}_{m+M}^e - \mathscr{A}_{m+M}^{ex}\mathscr{A}_m^i\right)$ is a h-pseudodifferential operator of order 0. Now, a simple computation using Lemma 4.4.1 yields that

$$\frac{S\cdot(\xi \wedge n(x))P_\pm S\cdot(\xi \wedge n(x))P_\mp}{|\xi \wedge n(x)|(\sqrt{|\xi \wedge n(x)|^2+1}+1)} = \frac{|\xi \wedge n(x)|P_\mp}{\sqrt{|\xi \wedge n(x)|^2+1}+1}.$$

Thus

$$I_4 - p_{h,\mathscr{A}^i_m}(x,\xi)p_{h,\mathscr{A}^e_{m+M}}(x,\xi) - p_{h,\mathscr{A}^e_{m+M}}(x,\xi)p_{h,\mathscr{A}^i_m}(x,\xi) = I_4 + \frac{|\xi \wedge n(x)|}{\sqrt{|\xi \wedge n(x)|^2+1}+1}$$
$$= \frac{\sqrt{|\xi \wedge n(x)|^2+1}+1+|\xi \wedge n(x)|}{\sqrt{|\xi \wedge n(x)|^2+1}+1} \gtrsim 1.$$

From this, we deduce that $\left(I_4 - \mathscr{A}^i_m\mathscr{A}^e_{m+M} - \mathscr{A}^{ex}_{m+M}\mathscr{A}^i_m\right)$ is elliptic in $Op^h\mathcal{S}^0(\Sigma)$. Thus, $\Xi_M(z) \in Op^h\mathcal{S}^0(\Sigma)$, and in local coordinates, its semiclassical principal symbol is given by

$$p_{h,\Xi_M(z)}(x,\xi) = \frac{\sqrt{|\xi \wedge n(x)|^2+1}+1}{\sqrt{|\xi \wedge n(x)|^2+1}+1+|\xi \wedge n(x)|}.$$

As $\Xi_M(z)$ is a h-pseudodifferential operators of order 0, it follows that for any $s \in \mathbb{R}$, $\Xi_M(z) : H^s(\Sigma)^4 \to H^s(\Sigma)^4$ is well-defined and bounded uniformly with respect to M, proving the statement (i) of the theorem.

The proof of the statement (ii) follows the standard arguments of the proof of the boundedness of classical pseudodifferential operators. Indeed, since Σ is compact, it suffices to show for $\varphi \in C^2_0(\mathbb{R}^2)$ that $Op(\varphi p_{\mathscr{A}^e_\tau}) = \varphi Op(p_{\mathscr{A}^e_\tau})$ satisfies the estimate

$$||\varphi Op(p_{\mathscr{A}^e_\tau})f||_{H^s(\mathbb{R}^2)^4} \lesssim \frac{1}{\tau}\,||f||_{H^{s+1}(\mathbb{R}^2)^4}, \quad \forall f \in \mathcal{S}(\mathbb{R}^2)^4, \tag{4.5.9}$$

where $p_{\mathscr{A}^e_\tau}$ is the principal symbol of $\mathscr{A}^e_\tau$, i.e.,

$$p_{\mathscr{A}^e_\tau}(x,\xi) = -\frac{S\cdot(\xi \wedge n(x))P_+}{\sqrt{|\xi \wedge n(x)|^2+\tau^2}+\tau}, \qquad \tau = m+M.$$

Set $a_\tau(x,\xi) = \varphi(x)p_{\mathscr{A}^e_\tau}(x,\xi)$. Thus, a_τ is compactly supported with respect to x and satisfies the estimate

$$|a_\tau(x,\xi)| \leqslant C\left(\frac{1+|\xi|}{\tau+|\xi|}\right), \quad \forall (x,\xi) \in \mathbb{R}^2 \times \mathbb{R}^2.$$

We set $\langle D\rangle^k = Op(\langle\xi\rangle^k) \in Op\mathcal{S}^k$, $B_s := \langle D\rangle^s\varphi Op(a_\tau)\langle D\rangle^{-(s+1)}$, and we let $g = \langle D\rangle^{s+1}f$. Then (4.5.9) is equivalent to

$$||B_s g||_{L^2(\mathbb{R}^2)^4} \lesssim \frac{1}{\tau}\,||g||_{L^2(\mathbb{R}^2)^4}.$$

Observe that

$$y^\alpha \hat{a}_\tau(y,\xi) = \int_{\mathbb{R}^2} e^{-ix\cdot y}y^\alpha a_\tau(x,\xi)\mathrm{d}x = \int_{\mathbb{R}^2} e^{-ix\cdot y}D^\alpha_x a_\tau(x,\xi)\mathrm{d}x, \quad \forall \alpha,\, y,$$

where in the last equality the support condition on a_τ was used. From this it follows for any $N > 0$, there is $C_N > 0$ (independent of ξ) such that

$$|\hat{a}_\tau(y,\xi)| \leqslant C_N\langle y\rangle^{-N}\left(\frac{1+|\xi|}{\tau+|\xi|}\right), \quad \forall (y,\xi) \in \mathbb{R}^2 \times \mathbb{R}^2. \tag{4.5.10}$$

Notice that for $g \in \mathcal{S}(\mathbb{R}^2)^4$, we have that $\hat{B}_s g(y) = \langle y\rangle^s\mathcal{F}[Op(a_\tau)\langle D\rangle^{-(s+1)}]$, and that

$$\mathcal{F}[Op(a_\tau)\langle D\rangle^{-(s+1)}]g(y) = \int_{\mathbb{R}^2} e^{-ix\cdot y}\left(\int_{\mathbb{R}^2} e^{ix\cdot\xi}a_\tau(x,\xi)\langle\xi\rangle^{-(s+1)}\hat{g}(\xi)\mathrm{d}\xi\right)\mathrm{d}x$$
$$= \int_{\mathbb{R}^2}\left(\int_{\mathbb{R}^2} e^{-ix\cdot(y-\xi)}a_\tau(x,\xi)\langle\xi\rangle^{-(s+1)}\hat{g}(\xi)\mathrm{d}x\right)\mathrm{d}\xi$$
$$= \int_{\mathbb{R}^2}\hat{a}_\tau(y-\xi,\xi)\langle\xi\rangle^{-(s+1)}\hat{g}(\xi)\mathrm{d}\xi.$$

Thus

$$\hat{B}_s g(y) = \langle y \rangle^s \int_{\mathbb{R}^2} \hat{a}_\tau(y-\xi,\xi)\langle \xi \rangle^{-(s+1)} \hat{g}(\xi)\mathrm{d}\xi = \int_{\mathbb{R}^2} K(y,\xi)\hat{g}(\xi)\mathrm{d}\xi.$$

Hence, Peetre's inequality: $\langle y \rangle^s \langle \xi \rangle^{-s} \leqslant 2^{|s|-1}\langle y-\xi \rangle^{|s|}$, together with (4.5.10) yield that

$$\begin{aligned}|K(y,\xi)| &\lesssim \langle y \rangle^s \langle y-\xi \rangle^{-N} \langle \xi \rangle^{-(s+1)} \left(\frac{1+|\xi|}{\tau+|\xi|}\right) \lesssim \frac{\langle y \rangle^s \langle \xi \rangle^{-s} \langle y-\xi \rangle^{-N}}{(\tau+|\xi|)} \\ &\lesssim \frac{\langle y-\xi \rangle^{-N+|s|}}{(\tau+|\xi|)}.\end{aligned}$$

Since (4.5.10) holds true for any $N>0$, choosing N sufficiently large we get that

$$\int_{\mathbb{R}^2} |K(y,\xi)|\mathrm{d}\xi \lesssim \frac{1}{\tau} \quad \text{and} \quad \int_{\mathbb{R}^2} |K(y,\xi)|\mathrm{d}y \lesssim \frac{1}{\tau}.$$

Therefore, Schur's test from Theorem 1.3.1 implies that

$$||B_s g||_{L^2(\mathbb{R}^2)^4} = \left|\left|\widehat{B_s g}\right|\right|_{L^2(\mathbb{R}^2)^4} \lesssim \frac{1}{\tau} ||g||_{L^2(\mathbb{R}^2)^4},$$

which gives the desired estimate and finishes the proof of (ii). □

We can now give the proof of Theorem 4.5.1.

Proof of Theorem 4.5.1. Let M_0 be as in Theorem 4.5.2 and $M > M_0$, fix $z \in \rho(H_{\mathrm{MIT}}(m)) \cap \rho(H_M)$ and let $f \in L^2(\mathbb{R}^3)^4$. We set

$$v = r_{\Omega_i} R_M(z) f \quad \text{and} \quad u = r_{\Omega_e} R_M(z) f.$$

Then u and v satisfy the following system

$$\begin{cases} (D_m - z)v = f & \text{in } \Omega_i, \\ (D_{m+M} - z)u = f & \text{in } \Omega_e, \\ \Gamma_- v = \Gamma_- u & \text{on } \Sigma, \\ \Gamma_+ v = \Gamma_+ u & \text{on } \Sigma. \end{cases} \tag{4.5.11}$$

Not that if we let

$$\varphi = \Gamma_- u \quad \text{and} \quad \psi = \Gamma_+ v, \tag{4.5.12}$$

then it holds that

$$\begin{cases} (D_m - z)E_m^{\Omega_i}(z)\varphi = 0 & \text{in } \Omega_i, \\ (D_{m+M} - z)E_{m+M}^{\Omega_e}(z)\psi = 0 & \text{in } \Omega_e, \\ \Gamma_- E_m^{\Omega_i}(z)\varphi = \varphi & \text{on } \Sigma, \\ \Gamma_+ E_{m+M}^{\Omega_e}(z)\psi = \psi & \text{on } \Sigma. \end{cases}$$

Since by definition we have that

$$\begin{cases} (D_m - z)R_{\mathrm{MIT}}(z) r_{\Omega_i} f = f & \text{in } \Omega_i, \\ (D_{m+M} - z)\widetilde{R}_M(z) r_{\Omega_e} f = f & \text{in } \Omega_e, \\ \Gamma_- R_{\mathrm{MIT}}(z) r_{\Omega_i} f = 0 & \text{on } \Sigma, \\ \Gamma_+ \widetilde{R}_M(z) r_{\Omega_e} f = 0 & \text{on } \Sigma, \end{cases}$$

from this we deduce that
$$\begin{cases} v = R_{\mathrm{MIT}}(z) r_{\Omega_i} f + E_m^{\Omega_i}(z)\varphi, \\ u = \widetilde{R}_M(z) r_{\Omega_e} f + E_{m+M}^{\Omega_e}(z)\psi. \end{cases} \tag{4.5.13}$$
Thus, to get an explicit formula for $R_M(z)$ it remains to find the unknowns φ and ψ. For this, note that from (4.5.13) we have
$$\begin{cases} \psi = \Gamma_+ r_{\Omega_i} R_M(z) f = \Gamma_+ R_{\mathrm{MIT}}(z) r_{\Omega_i} f + \Gamma_+ E_m^{\Omega_i}(z)[\varphi], \\ \varphi = \Gamma_- r_{\Omega_e} R_M(z) f = \Gamma_- \widetilde{R}_M(z) r_{\Omega_e} f + \Gamma_- E_{m+M}^{\Omega_e}(z)[\psi]. \end{cases} \tag{4.5.14}$$
Substituting the values of ψ and φ (from (4.5.14)) into the system (4.5.13), we obtain
$$\begin{aligned} R_M(z) =& e_{\Omega_i} R_{\mathrm{MIT}}(z) r_{\Omega_i} + e_{\Omega_e} \widetilde{R}_M(z) r_{\Omega_e} \\ &+ \left(e_{\Omega_i} E_m^{\Omega_i}(z)\Gamma_- r_{\Omega_e} + e_{\Omega_e} E_{m+M}^{\Omega_e}(z)\Gamma_+ r_{\Omega_i} \right) R_M(z) \\ =& \widetilde{R}_{\mathrm{MIT}}(z) + E_M(z)\Gamma R_M(z). \end{aligned} \tag{4.5.15}$$
Note that, by definition of the Poincaré-Steklov operators, (4.5.14) is equivalent to
$$\begin{cases} \psi = \Gamma_+ R_{\mathrm{MIT}}(z) r_{\Omega_i} f + \mathscr{A}_m^i(\varphi), \\ \varphi = \Gamma_- \widetilde{R}_M(z) r_{\Omega_e} f + \mathscr{A}_{m+M}^e(\psi). \end{cases} \tag{4.5.16}$$
Thus, applying Γ to the identity (4.5.15) yields that
$$\Gamma \widetilde{R}_{\mathrm{MIT}}(z) = \left(I - \mathscr{A}_m^i - \mathscr{A}_{m+M}^e \right) \Gamma R_M(z) = \Psi_M(z)\Gamma R_M(z). \tag{4.5.17}$$
Now, we apply $(I + \mathscr{A}_m^i + \mathscr{A}_{m+M}^e)$ to the last identity and we get
$$\left(I + \mathscr{A}_m^i + \mathscr{A}_{m+M}^e \right) \Gamma \widetilde{R}_{\mathrm{MIT}}(z) = \left(I - \mathscr{A}_m^i \mathscr{A}_{m+M}^e - \mathscr{A}_{m+M}^e \mathscr{A}_m^i \right) \Gamma R_M(z) = (\Xi_M(z))^{-1}\Gamma R_M(z).$$
Thanks to Theorem 4.5.2, we know that for $M > M_0$ the operator $(\Xi_M(z))^{-1}$ is bounded invertible from $H^{1/2}(\Sigma)^4$ into itself, which actually means that Ψ_M is bounded invertible from $H^{1/2}(\Sigma)^4$ into itself and that
$$\Psi_M^{-1}(z) = \Xi_M(z) \left(I + \mathscr{A}_m^i + \mathscr{A}_{m+M}^e \right) \quad \text{and} \quad \Gamma R_M(z) = \Psi_M^{-1}(z)\Gamma \widetilde{R}_{\mathrm{MIT}}(z).$$
Thereby, the identity (4.5.6) follows from the above computations and (4.5.15).

Now we turn to the proof the second statement. Let us first prove the implication ($\Longrightarrow$). Let $a \in (-(m+M), m+M) \setminus \rho(H_{\mathrm{MIT}}(m))$ be such that $(H_M - a)\varphi = 0$ for some $0 \neq \varphi \in H^1(\mathbb{R}^3)^4$. Set $\varphi_+ = \varphi_{|\Omega_i}$ and $\varphi_- = \varphi_{|\Omega_e}$. Then, it is clear that φ_+ solves the system (4.5.3) with $g = \Gamma_- \varphi$, and φ_- solves the system (4.5.4) with $h = \Gamma_+ \varphi$. Thus, $\varphi_+ = E_m^{\Omega_i}(a)\Gamma_- \varphi$ and $\varphi_- = E_{m+M}^{\Omega_e}(a)\Gamma_+ \varphi$. Hence, $\varphi = E_M(a) t_\Sigma \varphi$ and $\Gamma_\pm \varphi \neq 0$, as otherwise φ would be zero. Using this and the definition of the Poincaré-Steklov operators, we obtain that
$$(I_4 + \mathscr{A}_m^i)\Gamma_- \varphi := t_\Sigma \varphi_+ = t_\Sigma \varphi = t_\Sigma \varphi_- := (I_4 + \mathscr{A}_{m+M}^e)\Gamma_- \varphi,$$
and since $t_\Sigma \varphi \neq 0$ it follows that
$$\Psi_M(a) t_\Sigma \varphi = (I_4 + \mathscr{A}_m^i + \mathscr{A}_{m+M}^e) t_\Sigma \varphi = 0,$$
which means that $0 \in \mathrm{Sp_p}(\Psi_M(a))$ and proves the inclusion $\mathrm{Kr}(H_M - a) \subset \{E_M(a)g : g \in \mathrm{Kr}(\Psi_M(a))\}$.

We now prove the implication ($\Longleftarrow$). Let $a \in (-(m+M), m+M) \setminus \rho(H_{\rm MIT}(m))$ and assume that 0 is an eigenvalue of $\Psi_M(a)$. Then, there is $g \in H^{1/2}(\Sigma)^4 \setminus \{0\}$ such that $\Psi_M(a)g = 0$ on Σ. Note that this is equivalent to

$$(P_- + \mathscr{A}_m^i)g = (P_+ + \mathscr{A}_{m+M}^e)g. \tag{4.5.18}$$

Since $a \in (-(m+M), m+M) \setminus \rho(H_{\rm MIT}(m))$, the operators $E_m^{\Omega_i}(a) : P_- H^{1/2}(\Sigma)^4 \to H^1(\Omega_i)^4$ and $E_{m+M}^{\Omega_e}(a) : P_+ H^{1/2}(\Sigma)^4 \to H^1(\Omega_e)^4$ are well-defined and bounded. Thus, if we let $\varphi = E_M(a)g = (E_m^{\Omega_i}(a)P_- g, E_{m+M}^{\Omega_e}(a)P_+ g)$, then $\varphi \neq 0$ and we have that $(D_m - a)\varphi = 0$ in Ω_i, and that $(D_{m+M} - a)\varphi = 0$ in Ω_e. Now, using the definition of the Poincaré-Steklov operators and the equation (4.5.18) we get that

$$t_\Sigma E_m^{\Omega_i}(a) P_- g = (P_- + \mathscr{A}_m^i)g = (P_+ + \mathscr{A}_{m+M}^e)g = t_\Sigma E_{m+M}^{\Omega_e}(a) P_+ g.$$

Thanks to the boundedness properties of $E_m^{\Omega_i}(a)$ and $E_{m+M}^{\Omega_e}(a)$, it follows from the above computations that $\varphi = E_M(a)g \in H^1(\mathbb{R}^3)^4 \setminus \{0\}$ and satisfies the equation $(H_M - a)\varphi = 0$. Therefore, $a \in {\rm Sp_p}(H_M)$ and the inclusion $\{E_M(a)g : g \in {\rm Kr}(\Psi_M(a))\} \subset {\rm Kr}(H_M - a)$ holds true, and this achieves the proof of the theorem. □

As an immediate consequence of Theorem 4.5.2 and Theorem 4.5.1 we have:

Corollary 4.5.1. *There is $M_0 > 0$ such that for every $M > M_0$ and all $z \in \rho(H_{MIT}(m)) \cap \rho(H_M)$, the operators $\Xi_M^\pm(z) : P_\pm H^s(\Sigma)^4 \to P_\pm H^s(\Sigma)^4$ defined by*

$$\Xi_M^+(z) = \left(I - \mathscr{A}_m^i \mathscr{A}_{m+M}^e\right)^{-1} \quad \text{and} \quad \Xi_M^-(z) = \left(I - \mathscr{A}_{m+M}^e \mathscr{A}_m^i\right)^{-1},$$

are everywhere defined and uniformly bounded with respect to M, for any $s \in \mathbb{R}$. Moreover, if $v \in H^1(\mathbb{R}^3)^4$ solves $(D_m + M\beta 1_{\Omega_e} - z)v = e_{\Omega_i} f$, for some $f \in L^2(\Omega_i)^4$. Then, $r_{\Omega_i} v$ satisfies the following boundary value problem

$$\begin{cases} (D_m - z) r_{\Omega_i} v = f & \text{in } \Omega_i, \\ \qquad \Gamma_- v = \Xi_M^-(z) \mathscr{A}_{m+M}^e \Gamma_+ R_{\rm MIT}(z) f & \text{on } \Sigma, \\ \qquad \Gamma_+ v = \Gamma_+ R_{\rm MIT}(z) f + \mathscr{A}_m^i \Gamma_- v & \text{on } \Sigma. \end{cases} \tag{4.5.19}$$

Proof. We first note that $\Xi_M^\pm(z) = P_\pm \Xi_M(z) P_\pm$. Thus, the first statement follows immediately from Theorem 4.5.2 . Now, let $f \in L^2(\Omega_i)^4$, and suppose tha $v \in H^1(\mathbb{R}^3)^4$ solves $(D_m + M\beta 1_{\Omega_e} - z)v = e_{\Omega_i} f$. Thus $(D_m - z) r_{\Omega_i} v = f$ in Ω_i, and if we set

$$\varphi = P_- t_\Sigma v \quad \text{and} \quad \psi = P_+ t_\Sigma v, \tag{4.5.20}$$

Then, from (4.5.16) we easily get

$$\varphi = \Xi_M^-(z) \mathscr{A}_{m+M}^e \Gamma_+ R_{\rm MIT}(z) f \quad \text{and} \quad \psi = \Gamma_+ R_{\rm MIT}(z) f + \mathscr{A}_m^i \varphi,$$

which means that $r_{\Omega_i} v$ satisfies (4.5.19), and this completes the proof of the corollary. □

Remark 4.5.2. *Notice that from (4.5.16) we have that*

$$\begin{pmatrix} \Gamma_+ r_{\Omega_i} R_M(z) f \\ \Gamma_- r_{\Omega_e} R_M(z) f \end{pmatrix} = \begin{pmatrix} \Xi_M^+(z) \\ \Xi_M^-(z) \end{pmatrix} \begin{pmatrix} I_4 & \mathscr{A}_m^i \\ \mathscr{A}_{m+M}^e & I_4 \end{pmatrix} \begin{pmatrix} \Gamma_+ R_{MIT}(z) r_{\Omega_i} f \\ \Gamma_- \widetilde{R}_M(z) r_{\Omega_e} f \end{pmatrix}.$$

With this observation, we remark that the resolvent formula (4.5.6) can also be written in the following matrix form

$$\begin{pmatrix} r_{\Omega_i} R_M(z) \\ r_{\Omega_e} R_M(z) \end{pmatrix} = \begin{pmatrix} R_{MIT}(z) r_{\Omega_i} \\ \widetilde{R}_M(z) r_{\Omega_e} \end{pmatrix} + \begin{pmatrix} E_m^{\Omega_i}(z) \Xi_M^-(z) \\ E_{m+M}^{\Omega_e}(z) \Xi_M^+(z) \end{pmatrix} \begin{pmatrix} \mathscr{A}_{m+M}^e & I_4 \\ I_4 & \mathscr{A}_m^i \end{pmatrix} \begin{pmatrix} \Gamma_+ R_{MIT}(z) r_{\Omega_i} \\ \Gamma_- \widetilde{R}_M(z) r_{\Omega_e} \end{pmatrix}.$$

We finish this section by providing an asymptotic expansion of $R_M(z)$ and proving its norm convergence toward $R_{\text{MIT}}(z)$ and estimate the rate of convergence.

Proposition 4.5.1. *For any compact set $K \subset \rho(H_{MIT}(m))$, there is $M_0 > 0$ such that for all $M > M_0$, $K \subset \rho(H_M)$, and for all $z \in K$ the resolvent R_M admits an asymptotic expansion in $\mathcal{L}(L^2(\mathbb{R}^3)^4)$ of the form:*

$$R_M(z) = e_{\Omega_i} R_{MIT}(z) r_{\Omega_i} + \frac{1}{M}\left(K_M(z) + L_M(z)\right), \tag{4.5.21}$$

where $K_M(z)$ and $L_M(z)$ are bounded from $L^2(\mathbb{R}^3)^4$ into itself independently of M, and we have

$$r_{\Omega_i} K_M(z) e_{\Omega_i} = 0 = r_{\Omega_e} K_M(z) e_{\Omega_e}.$$

In particular, it holds that

$$||R_M(z) - e_{\Omega_i} R_{MIT}(z) r_{\Omega_i}||_{L^2(\mathbb{R}^3)^4 \to L^2(\mathbb{R}^3)^4} = \mathcal{O}\left(\frac{1}{M}\right).$$

Before giving the proof, we need the following estimates:

Lemma 4.5.1. *Let $K \subset \mathbb{C}$ be a compact set. Then, there is $M_0 > 0$ such that for all $M > M_0$: $K \subset \rho(\widetilde{H}_M)$ and for every $z \in K$ the following estimates hold:*

$$\begin{aligned}
\left|\left|\widetilde{R}_M(z) f\right|\right|_{L^2(\Omega_e)^4} &\lesssim \frac{1}{M} ||f||_{L^2(\Omega_e)^4}, \quad \forall f \in L^2(\Omega_e)^4,\\
\left|\left|\Gamma_- \widetilde{R}_M(z) f\right|\right|_{L^2(\Sigma)^4} &\lesssim \frac{1}{\sqrt{M}} ||f||_{L^2(\Omega_e)^4}, \quad \forall f \in L^2(\Omega_e)^4,\\
\left|\left|\Gamma_- \widetilde{R}_M(z) f\right|\right|_{H^{-1/2}(\Sigma)^4} &\lesssim \frac{1}{M} ||f||_{L^2(\Omega_e)^4}, \quad \forall f \in L^2(\Omega_e)^4,\\
\left|\left|E^{\Omega_e}_{m+M}(z)\psi\right|\right|_{L^2(\Omega_e)^4} &\lesssim \frac{1}{\sqrt{M}} ||\psi||_{L^2(\Sigma)^4}, \quad \forall \psi \in P_+ L^2(\Sigma)^4,\\
\left|\left|E^{\Omega_e}_{m+M}(z)\psi\right|\right|_{L^2(\Omega_e)^4} &\lesssim \frac{1}{M} ||\psi||_{H^{1/2}(\Sigma)^4}, \quad \forall \psi \in P_+ H^{1/2}(\Sigma)^4.
\end{aligned}$$

Proof. Fix a compact set $K \subset \mathbb{C}$, and note that for $M_1 > \sup_{z\in K}\{|\text{Re}(z)| - m\}$ it holds that $K \subset \rho(\widetilde{H}_{M_1})$, and hence $K \subset \rho(\widetilde{H}_M)$ for all $M > M_1$. We next show the claimed estimates for $\widetilde{R}_M(z)$ and $\Gamma_- \widetilde{R}_M(z)$. For this, given $z \in K$ and assume that $M > M_1$. Let $\varphi \in \text{dom}(\widetilde{H}_M)$, then a straightforward application of the Green's formula yields that

$$\|\widetilde{H}_M \varphi\|^2_{L^2(\Omega_e)^4} = \|(\alpha\cdot\nabla)\varphi\|^2_{L^2(\Omega_e)^4} + (m+M)^2 ||\varphi||^2_{L^2(\Omega_e)^4} + (m+M) ||P_- t_\Sigma \varphi||^2_{L^2(\Sigma)^4}.$$

Using this and the Cauchy-Schwarz inequality we obtain that

$$\begin{aligned}
\|(\widetilde{H}_M - z)\varphi\|^2_{L^2(\Omega_e)^4} &= \|\widetilde{H}_M\varphi\|^2_{L^2(\Omega_e)^4} + |z|^2 \|\varphi\|^2_{L^2(\Omega_e)^4} - 2\text{Re}(z)\langle \widetilde{H}_M\varphi, \varphi\rangle_{L^2(\Omega_e)^4}\\
&\geqslant \|\widetilde{H}_M\varphi\|^2_{L^2(\Omega_e)^4} + |z|^2\|\varphi\|^2_{L^2(\Omega_e)^4} - \frac{1}{2}\|\widetilde{H}_M\varphi\|^2_{L^2(\Omega_e)^4} - 2|\text{Re}(z)|^2\|\varphi\|^2_{L^2(\Omega_e)^4}\\
&\geqslant \left(\frac{(m+M)^2}{2} + |\text{Im}(z)|^2 - |\text{Re}(z)|^2\right) ||\varphi||^2_{L^2(\Omega_e)^4} + \frac{M}{2} ||P_- t_\Sigma\varphi||^2_{L^2(\Sigma)^4}.
\end{aligned}$$

Therefore, taking $\widetilde{R}_M(z) f = \varphi$ and $M \geqslant M_2 \geqslant \sup_{z\in K}\{\sqrt{|\text{Re}(z)|^2 - |\text{Im}(z)|^2} - m\}$ we obtain the inequality

$$\left|\left|\widetilde{R}_M(z) f\right|\right|_{L^2(\Omega_e)^4} \lesssim \frac{1}{M} ||f||_{L^2(\Omega_e)^4} \quad \text{and} \quad \left|\left|\Gamma_- \widetilde{R}_M(z) f\right|\right|_{L^2(\Sigma)^4} \lesssim \frac{1}{\sqrt{M}} ||f||_{L^2(\Omega_e)^4}.$$

Since Γ_- is bounded from $L^2(\Omega_e)^4$ into $H^{-1/2}(\Sigma)^4$, using the above inequality we get that

$$\left|\left|\Gamma_-\widetilde{R}_M(z)f\right|\right|_{H^{-1/2}(\Sigma)^4} \lesssim ||\Gamma_-||_{L^2(\Omega_e)^4\to H^{-1/2}(\Sigma)^4} \left|\left|\widetilde{R}_M(z)f\right|\right|_{H^{-1/2}(\Sigma)^4} \lesssim \frac{1}{M} ||f||_{L^2(\Omega_e)^4},$$

for any $f \in L^2(\Omega_e)^4$, which gives the second inequality.

Let us now turn to the proof of the claimed estimates for $E^{\Omega_e}_{m+M}(z)$. Let $\psi \in P_+L^2(\Sigma)^4$, then from the proof of Proposition 4.3.1 (ii) we have

$$||\psi||^2_{L^2(\Sigma)^4} \geqslant (m+M)\left|\left|E^{\Omega_e}_{m+M}(z)\psi\right|\right|^2_{L^2(\Omega_e)^4} - 2|\mathrm{Re}(z)|\left|\left|E^{\Omega_e}_{m+M}(z)\psi\right|\right|^2_{L^2(\Omega_e)^4}.$$

Thus, for any $M \geqslant M_3 \geqslant \sup_{z\in K}\{4|\mathrm{Re}(z)| - m\}$, we get that

$$M\left|\left|E^{\Omega_e}_{m+M}(z)\psi\right|\right|^2_{L^2(\Omega_e)^4} \leqslant 2\,||\psi||^2_{L^2(\Sigma)^4},$$

and this proves the first estimate for $E^{\Omega_e}_{m+M}(z)$. Finally, the last inequality is a consequence of the first one and Proposition 4.3.1. Indeed, from Proposition 4.3.1 (ii) we know that $\beta\Gamma_-\widetilde{R}_M(\overline{z})$ is the adjoint of the operator $E^{\Omega_e}_{m+M}(z) : P_+H^{1/2}(\Sigma)^4 \longrightarrow H^1(\Omega_e)^4$. Using this and the estimate fulfilled by $\Gamma_-\widetilde{R}_M(\overline{z})$ we obtain that

$$\begin{aligned}\left|\langle f, E^{\Omega_e}_{m+M}(z)\psi\rangle_{L^2(\Omega_e)^4}\right| &= \left|\langle \Gamma_-\widetilde{R}_M(\overline{z})f, \beta\psi\rangle_{H^{-1/2}(\Sigma)^4, H^{1/2}(\Sigma)^4}\right| \\ &\leqslant \left|\left|\Gamma_-\widetilde{R}_M(z)f\right|\right|_{H^{-1/2}(\Sigma)^4} ||\psi||_{H^{1/2}(\Sigma)^4} \\ &\lesssim \frac{1}{M}||f||_{L^2(\Omega_e)^4}\,||\psi||_{H^{1/2}(\Sigma)^4}.\end{aligned}$$

Since this is true for all $f \in L^2(\Omega_e)^4$, by duality it follows that

$$\left|\left|E^{\Omega_e}_{m+M}(z)\psi\right|\right|_{L^2(\Omega_e)^4} \lesssim \frac{1}{M}||\psi||_{H^{1/2}(\Sigma)^4}, \quad \forall\psi \in P_+H^{1/2}(\Sigma)^4,$$

which proves the last inequality. Hence, the lemma follows by taking $M_0 = \max\{M_1, M_2, M_3\}$. □

Proof of Proposition 4.5.1. We first show the result for some $M_0' > 0$ and any $z \in \mathbb{C}\backslash\mathbb{R}$. So, let's fix such a z and let $f \in L^2(\mathbb{R}^3)^4$. Then, it is clear that $z \in \rho(H_{\mathrm{MIT}}(m)) \cap \rho(H_M)$, and from Theorem 4.5.1 and Remark 4.5.2 we know that there is $M_0' > 0$ such that for all $M > M_0'$ it holds that

$$\begin{aligned}||(R_M(z) - e_{\Omega_i}R_{\mathrm{MIT}}(z)r_{\Omega_i})f||_{L^2(\mathbb{R}^3)^4} \leqslant{} & \left|\left|E^{\Omega_i}_m(z)\Xi^-_M(z)\Gamma_-\widetilde{R}_M(z)r_{\Omega_e}f\right|\right|_{L^2(\Omega_i)^4} \\ &+ \left|\left|E^{\Omega_e}_{m+M}(z)\Xi^+_M(z)\Gamma_+R_{\mathrm{MIT}}(z)r_{\Omega_i}f\right|\right|_{L^2(\Omega_e)^4} \\ &+ \left|\left|E^{\Omega_i}_m(z)\Xi^-_M(z)\mathscr{A}^e_{m+M}\Gamma_+R_{\mathrm{MIT}}(z)r_{\Omega_i}f\right|\right|_{L^2(\Omega_i)^4} \\ &+ \left|\left|E^{\Omega_e}_{m+M}(z)\Xi^+_M(z)\mathscr{A}^i_m\Gamma_-\widetilde{R}_M(z)r_{\Omega_e}f\right|\right|_{L^2(\Omega_e)^4} \\ &+ \left|\left|\widetilde{R}_M(z)r_{\Omega_e}f\right|\right|_{L^2(\Omega_e)^4} =: J_1 + J_2 + J_3 + J_4 + J_5.\end{aligned}$$

From Lemma 4.5.1 we immediately get that $J_5 \lesssim M^{-1}||f||$. Next, observe that $\Gamma_+R_{\mathrm{MIT}}(z) : L^2(\Omega_i)^4 \to H^{1/2}(\Sigma)^4$, $\mathscr{A}^i_m : H^{1/2}(\Sigma)^4 \to H^{1/2}(\Sigma)^4$ and $E^{\Omega_i}_m(z) : H^{-1/2}(\Sigma)^4 \to H(\alpha,\Omega_i) \subset L^2(\Omega_i)^4$ (where $H(\alpha,\Omega_i)$ is defined by (1.2.4)) are bounded operators and do not depend on

M. Moreover, thanks to Corollary 4.5.1 we know that for all $s \in \mathbb{R}$ there is $C > 0$ independent of M such that

$$\left|\left|\Xi^{\pm}_{M}(z)\right|\right|_{P_{\pm}H^{s}(\Sigma)^4 \to P_{\pm}H^{s}(\Sigma)^4} \leqslant C.$$

Using this and the above observation, for $j \in \{1,2,3,4\}$, we can estimate J_k as follows

$$\begin{aligned}
J_1 &\lesssim \left|\left|E^{\Omega_i}_{m}(z)\Xi^{-}_{M}(z)\right|\right|_{H^{-1/2}(\Sigma)^4 \to L^2(\Omega_i)^4} \left|\left|\Gamma_{-}\widetilde{R}_M(z)r_{\Omega_e}f\right|\right|_{H^{-1/2}(\Sigma)^4},\\
J_2 &\lesssim \left|\left|E^{\Omega_e}_{m+M}(z)\right|\right|_{H^{1/2}(\Sigma)^4 \to L^2(\Omega_e)^4} \left|\left|\Xi^{+}_{M}(z)\Gamma_{+}R_{\mathrm{MIT}}(z)r_{\Omega_i}f\right|\right|_{H^{1/2}(\Sigma)^4},\\
J_3 &\lesssim \left|\left|E^{\Omega_i}_{m}(z)\Xi^{-}_{M}(z)\right|\right|_{P_{-}H^{-1/2}(\Sigma)^4 \to L^2(\Omega_i)^4} ||\mathscr{A}^{e}_{m+M}||_{H^{1/2}(\Sigma)^4 \to H^{-1/2}(\Sigma)^4} ||\Gamma_{+}R_{\mathrm{MIT}}(z)r_{\Omega_i}f||_{H^{1/2}(\Sigma)^4},\\
J_4 &\lesssim \left|\left|E^{\Omega_e}_{m+M}(z)\right|\right|_{L^2(\Sigma)^4 \to L^2(\Omega_e)^4} \left|\left|\Xi^{+}_{M}(z)\mathscr{A}^{i}_{m}\right|\right|_{L^2(\Sigma)^4 \to L^2(\Sigma)^4} \left|\left|\Gamma_{-}\widetilde{R}_M(z)r_{\Omega_e}f\right|\right|_{L^2(\Sigma)^4}.
\end{aligned}$$

Therefore, Theorem 4.5.2-(ii) together with Lemma 4.5.1 yield that

$$J_k \lesssim \frac{1}{M}\,||f||_{L^2(\mathbb{R}^3)^4}, \quad \text{for any } j \in \{1,2,3,4\}.$$

Thus, we obtain the estimate

$$||(R_M(z) - e_{\Omega_i}R_{\mathrm{MIT}}(z)r_{\Omega_i})f||_{L^2(\mathbb{R}^3)^4} \leqslant \frac{C}{M}\,||f||_{L^2(\mathbb{R}^3)^4}. \tag{4.5.22}$$

Moreover, the asymptotic expansion (4.5.21) holds with

$$\begin{aligned}
L_M(z) =& M(e_{\Omega_e}\widetilde{R}_M(z)r_{\Omega_e} + e_{\Omega_i}E^{\Omega_i}_{m}(z)\Xi^{-}_{M}(z)\mathscr{A}^{e}_{m+M}\Gamma_{+}R_{\mathrm{MIT}}(z)r_{\Omega_i}\\
&+ e_{\Omega_e}E^{\Omega_e}_{m+M}(z)\Xi^{+}_{M}(z)\mathscr{A}^{i}_{m}\Gamma_{-}\widetilde{R}_M(z)r_{\Omega_e}),
\end{aligned}$$

and

$$K_M(z) = M\left(e_{\Omega_i}E^{\Omega_i}_{m}(z)\Xi^{-}_{M}(z)\Gamma_{-}\widetilde{R}_M(z)r_{\Omega_e} + e_{\Omega_e}E^{\Omega_e}_{m+M}(z)\Xi^{+}_{M}(z)\Gamma_{+}R_{\mathrm{MIT}}(z)r_{\Omega_i}\right),$$

and we clearly see that $r_{\Omega_i}K_M(z)e_{\Omega_i} = 0 = r_{\Omega_e}K_M(z)e_{\Omega_e}$.

Finally, since (4.5.22) holds true for any $z \in \mathbb{C}\setminus\mathbb{R}$, for any fixed compact subset $K \subset \rho(H_{\mathrm{MIT}}(m))$, one can show by arguments similar to those in the proof of [14, Lemma A.1] that there is $M_0 > M_0'$ such that $K \subset \rho(H_M)$. Therefore, the proposition follows with the same arguments as before. □

We conclude this part by pointing out the following remarks.

Remark 4.5.3. *Notice that the rate of convergence given in Proposition 4.5.1 is sharp. Indeed, since the resolvent $\widetilde{R}_M(z)$ can be viewed as a semiclassical pseudodifferantial operator of order -1, the L^2-norm estimate of $\widetilde{R}_M(z)$ given in Lemma 4.5.1 can not be ameliorated.*

Remark 4.5.4. *We mention that by mean of the min-max characterization and optimizations techniques, a first-order asymptotic expansion of the eigenvalues of H_M in terms of the eigenvalues of $H_{MIT}(m)$ has been established in [6] when $M \to \infty$. Note that it is also possible to obtain such a result using the Krein formula from Theorem 4.5.1 and finite-dimensional perturbation theory (cf. Kato [74] for example), see, e.g., [28, 34] for similar arguments. Note also that the asymptotic expansion of the eigenvalues of H_M depends only on the term*

$E_m^{\Omega_i}(z)\Xi_M^-(z)\mathscr{A}_{m+M}^e\Gamma_+R_{MIT}(z)r_{\Omega_i}$. Indeed, let λ_{MIT} be an eigenvalue of $H_{MIT}(m)$ with multiplicity l, and let $(f_1,\cdots,f_l)$ be an $L^2(\Omega_i)^4$-orthonormal basis of $\mathrm{Kr}(H_{MIT}(m)-\lambda_{MIT}I_4)$. Then, using the Krein resolvent formula from Theorem 4.5.1 we see that

$$\begin{aligned}\langle R_M(z)e_{\Omega_i}f_k, e_{\Omega_i}f_j\rangle_{L^2(\mathbb{R}^3)^4} &= \langle E_m^{\Omega_i}(z)\Xi_M^-(z)\mathscr{A}_{m+M}^e\Gamma_+R_{MIT}(z)f_k, f_j\rangle_{L^2(\Omega_i)^4}\\ &= \langle \Xi_M^-(z)\mathscr{A}_{m+M}^e\Gamma_+R_{MIT}(z)f_k, -\beta\Gamma_+R_{MIT}(\overline{z})f_j\rangle_{L^2(\Sigma)^4}\\ &= \frac{1}{(z-\lambda_{MIT})^2}\langle \Xi_M^-(z)\mathscr{A}_{m+M}^e\Gamma_+f_k, -\beta\Gamma_+f_j\rangle_{L^2(\Sigma)^4},\end{aligned}$$

which means that $E_m^{\Omega_i}(z)\Xi_M^-(z)\mathscr{A}_{m+M}^e\Gamma_+R_{MIT}(z)r_{\Omega_i}$ is the only term that intervenes in the asymptotic expansion of the eigenvalues of H_M. Since the principle symbol of $\Xi_M^-(z)\mathscr{A}_{m+M}^e$ is given by

$$q_M(x,\xi)=\frac{|\xi\wedge n(x)|}{\sqrt{|\xi\wedge n(x)|^2+(m+M)^2}+|\xi\wedge n(x)|+(m+M)}.$$

Using this, we formally deduce that for sufficiently large M, H_M has exactly l eigenvalues $(\lambda_k^M)_{1\leqslant k\leqslant l}$ counted according to their multiplicities (in $B(\lambda_{MIT},\eta)$ with $B(\lambda_{MIT},\eta)\cap \mathrm{Sp}(H_{MIT}(m))=\{\lambda_{MIT}\}$) and these eigenvalues admit an asymptotic expansion of the form

$$\lambda_k^M=\lambda_{MIT}+\frac{1}{M}\mu_k+\sum_{j=2}^{N}\frac{1}{M^j}\mu_k^j+O\left(M^{-N-\frac{1}{2}}\right). \tag{4.5.23}$$

where $(\mu_k)_{1\leqslant k\leqslant l}$ are the eigenvalues of the matrix $\mathcal{M}$ with coefficients:

$$m_{kj}=-\langle\beta Op(q(x,\frac{\xi}{M})\Gamma_+f_k,\Gamma_+f_j\rangle_{L^2(\Sigma)^4}=-\langle\beta Op^{1/M}(q(x,\xi)\Gamma_+f_k,\Gamma_+f_j\rangle_{L^2(\Sigma)^4}.$$

4.6 Appendix A. Resolvent convergence: the case of C^2-smooth domains

We establish in this part the convergence of H_M to $H_{\mathrm{MIT}}(m)$ in the norm resolvent sense in the case of C^2-smooth domains. More precisely, with the same notations of the preceding section and assuming that Ω_i is a bounded C^2-smooth domain, we have the following result:

Proposition 4.6.1. *Let $K\subset\rho(H_{MIT}(m))$ be a compact set, then there is $M_0>0$ such that for all $M>M_0$: $K\subset\rho(H_{MIT}(m))\cap\rho(H_M)$ and for any $z\in K$ it holds that*

$$||(R_M(z)-e_{\Omega_i}R_{MIT}(z)r_{\Omega_i})f||_{L^2(\mathbb{R}^3)^4}\lesssim\frac{1}{\sqrt{M}}$$

To prove this result without using the properties of the Poincaré-Steklov operators we need the next statement which follows from [6, Propistion 2.1. (i)].

Lemma 4.6.1. *There exist $C, M_0>0$ such that, for all $M\geqslant M_0$ and all $\varphi\in H^1(\Omega_e)^4$ it holds that*

$$||\varphi||^2_{L^2(\Omega_e)^4}+M^2\,||\nabla\varphi||^2_{L^2(\Omega_e)^4}\geqslant(M-C)\,||t_\Sigma\varphi||^2_{L^2(\Sigma)^4}.$$

Proof of Proposition 4.6.1. As in the proof of Proposition 4.5.1 it suffices to prove the result for $z\in\mathbb{C}\setminus\mathbb{R}$. So, Let $f\in L^2(\mathbb{R}^3)^4$ and fix $z\in\mathbb{C}\setminus\mathbb{R}$. Set

$$v=r_{\Omega_i}R_M(z)f\quad\text{ and }\quad u=r_{\Omega_e}R_M(z)f.$$

Then from the proof of Theorem 4.5.1(ii) and Remark 4.3.3 we know that

$$\begin{cases} v = R_{\mathrm{MIT}}(z) r_{\Omega_i} f + E_m^{\Omega_i}(z) \Gamma_- r_{\Omega_e} R_M(z) f, \\ u = \widetilde{R}_M(z) r_{\Omega_e} f + E_{m+M}^{\Omega_e}(z) \Gamma_+ r_{\Omega_i} R_M(z) f, \end{cases} \tag{4.6.1}$$

and that

$$\begin{cases} \Gamma_+ r_{\Omega_i} R_M(z) f = \Gamma_+ R_{\mathrm{MIT}}(z) r_{\Omega_i} f + \Gamma_+ E_m^{\Omega_i}(z) \Gamma_- r_{\Omega_e} R_M(z) f \\ \Gamma_- r_{\Omega_e} R_M(z) f = \Gamma_- \widetilde{R}_M(z) r_{\Omega_e} f + \Gamma_- E_{m+M}^{\Omega_e}(z) \Gamma_+ r_{\Omega_i} R_M(z) f. \end{cases}$$

which is by definition equivalent to

$$\begin{cases} \Gamma_+ r_{\Omega_i} R_M(z) f = \Gamma_+ R_{\mathrm{MIT}}(z) r_{\Omega_i} f + \mathscr{A}_m^i(\Gamma_- r_{\Omega_e} R_M(z) f), \\ \Gamma_- r_{\Omega_e} R_M(z) f = \Gamma_- \widetilde{R}_M(z) r_{\Omega_e} f + \mathscr{A}_{m+M}^e(\Gamma_+ r_{\Omega_i} R_M(z) f). \end{cases} \tag{4.6.2}$$

Now, we make the observation that from the proof of Lemma 4.5.1 we see that the estimates

$$\left|\left| E_{m+M}^{\Omega_e}(z)\psi \right|\right|_{L^2(\Omega_e)^4} \lesssim \frac{1}{\sqrt{M}} ||\psi||_{L^2(\Sigma)^4}, \quad \forall \psi \in P_+ L^2(\Sigma)^4,$$
$$\left|\left| \widetilde{R}_M(z) f \right|\right|_{L^2(\Omega_e)^4} \lesssim \frac{1}{M} ||f||_{L^2(\Omega_e)^4}, \quad \forall f \in L^2(\Omega_e)^4,$$
$$\left|\left| \Gamma_- \widetilde{R}_M(z) f \right|\right|_{L^2(\Sigma)^4} \lesssim \frac{1}{\sqrt{M}} ||f||_{L^2(\Omega_e)^4}, \quad \forall f \in L^2(\Omega_e)^4,$$

are still hold true for Ω_i a bounded Lipschitz domain, and that, there exists $M_1 > 0$ such that

$$\sup_{M \geqslant M_1} ||\mathscr{A}_{m+M}^e||^2_{P_+ L^2(\Sigma)^4 \longrightarrow P_- L^2(\Sigma)^4} \lesssim 1. \tag{4.6.3}$$

(note that this last fact follows also from Remark 4.3.1). Using this observation and (4.6.1) it follows that there is $M_2 > M_1$ such that for all $M > M_2$ we have

$$\begin{aligned} ||(R_M(z) - e_{\Omega_i} R_{\mathrm{MIT}}(z) r_{\Omega_i}) f||_{L^2(\mathbb{R}^3)^4} &\leqslant \left|\left| E_m^{\Omega_i}(z) \Gamma_- r_{\Omega_e} R_M(z) f \right|\right|_{L^2(\Omega_i)^4} + \left|\left| \widetilde{R}_M(z) r_{\Omega_e} f \right|\right|_{L^2(\Omega_e)^4} \\ &\quad + \left|\left| E_{m+M}^{\Omega_e}(z) \Gamma_+ r_{\Omega_i} R_M(z) f \right|\right|_{L^2(\Omega_e)^4} \\ &\lesssim ||\Gamma_- r_{\Omega_e} R_M(z) f||_{L^2(\Sigma)^4} + \frac{1}{M} ||f||_{L^2(\mathbb{R}^3)^4} \\ &\quad + \frac{1}{\sqrt{M}} ||\Gamma_+ r_{\Omega_i} R_M(z) f||_{L^2(\Sigma)^4}. \end{aligned}$$

To achieve the proof, it remains to show that

$$||\Gamma_- r_{\Omega_e} R_M(z) f||_{L^2(\Sigma)^4} \lesssim \frac{1}{\sqrt{M}} ||f||_{L^2(\mathbb{R}^3)^4}, \quad ||\Gamma_+ r_{\Omega_i} R_M(z) f||_{L^2(\Sigma)^4} \lesssim ||f||_{L^2(\mathbb{R}^3)^4}. \tag{4.6.4}$$

For this, observe that from (4.6.2) we have

$$\begin{aligned} ||\Gamma_+ r_{\Omega_i} R_M(z) f||_{L^2(\Sigma)^4} &\leqslant ||\Gamma_+ R_{\mathrm{MIT}}(z) r_{\Omega_i} f||_{L^2(\Sigma)^4} + \left|\left| \mathscr{A}_m^i \Gamma_- r_{\Omega_e} R_M(z) f \right|\right|_{L^2(\Sigma)^4} \\ &\lesssim ||R_{\mathrm{MIT}}(z) r_{\Omega_i} f||_{H^{1/2}(\Omega_i)^4} + ||\Gamma_- r_{\Omega_e} R_M(z) f||_{L^2(\Sigma)^4} \\ &\lesssim ||f||_{L^2(\mathbb{R}^3)^4} + ||\Gamma_- r_{\Omega_e} R_M(z) f||_{L^2(\Sigma)^4}, \end{aligned} \tag{4.6.5}$$

where the boundedness of $\mathscr{A}_m^i$ and the trace theorem were used in the last inequalities.

Let $\varphi \in H^1(\mathbb{R}^3)^4$, then a integration by parts yields that

$$\begin{aligned}||H_M\varphi||^2_{L^2(\mathbb{R}^3)^4} =& ||\nabla\varphi||^2_{L^2(\mathbb{R}^3)^4} + m^2\,||\varphi||^2_{L^2(\Omega_i)^4} + (M+m)^2\,||\varphi||^2_{L^2(\Omega_e)^4}\\ &+ M\,||P_- t_\Sigma\varphi||^2_{L^2(\Sigma)^4} - M\,||P_+ t_\Sigma\varphi||^2_{L^2(\Sigma)^4}\,.\end{aligned} \tag{4.6.6}$$

From this and Lemma 4.6.1 it follows that there exist $C, M_3 > 0$ such that, for all $M > M_3$ it holds that

$$||H_M\varphi||^2_{L^2(\mathbb{R}^3)^4} \geqslant 2mM\,||\varphi||^2_{L^2(\Omega_e)^4} + 2(M-C)\,||P_- t_\Sigma\varphi||^2_{L^2(\Sigma)^4} - C\,||P_+ t_\Sigma\varphi||^2_{L^2(\Sigma)^4}\,. \tag{4.6.7}$$

Now, similar arguments to those of the proof of Lemma 4.5.1 yield that

$$\begin{aligned}\|(H_M - z)\varphi\|^2_{L^2(\mathbb{R}^3)^4} \geqslant& \frac{1}{2}\|H_M\varphi\|^2_{L^2(\mathbb{R}^3)^4} + (|\mathrm{Im}(z)|^2 - |\mathrm{Re}(z)|^2)\|\varphi\|^2_{L^2(\mathbb{R}^3)^4}\\ \geqslant& mM\,||\varphi||^2_{L^2(\Omega_e)^4} + (M-C)\,||P_- t_\Sigma\varphi||^2_{L^2(\Sigma)^4} - \frac{C}{2}\,||P_+ t_\Sigma\varphi||^2_{L^2(\Sigma)^4}\\ &+ \Big(|\mathrm{Im}(z)|^2 - |\mathrm{Re}(z)|^2\Big)\,\|\varphi\|^2_{L^2(\mathbb{R}^3)^4}\end{aligned}$$

Thus, with the substitution $\varphi = R_M(z)f$ and taking $M_0 > \sup\{M_2, M_3\}$ such that $M_0 > |\mathrm{Re}(z)|^2/m$, we get

$$\begin{aligned}M\,||\Gamma_- r_{\Omega_e} R_M(z)f||^2_{L^2(\Sigma)^4} \lesssim& ||f||^2_{L^2(\mathbb{R}^3)^4} + ||\Gamma_+ r_{\Omega_i} R_M(z)f||_{L^2(\Sigma)^4}\\ &+ |\mathrm{Re}(z)|^2\,||r_{\Omega_i} R_M(z)f||^2_{L^2(\Omega_i)^4}\,.\end{aligned}$$

Now, observe that from the first equation in (4.6.1) we have

$$||r_{\Omega_i} R_M(z)f||^2_{L^2(\Omega_i)^4} \lesssim ||f||^2_{L^2(\mathbb{R}^3)^4} + ||\Gamma_- r_{\Omega_e} R_M(z)f||^2_{L^2(\Omega_e)^4}\,,$$

and thus

$$\begin{aligned}M\,||\Gamma_- r_{\Omega_e} R_M(z)f||^2_{L^2(\Sigma)^4} \lesssim& ||f||^2_{L^2(\mathbb{R}^3)^4} + ||\Gamma_+ r_{\Omega_i} R_M(z)f||_{L^2(\Sigma)^4}\\ &+ |\mathrm{Re}(z)|^2\,||\Gamma_- r_{\Omega_e} R_M(z)f||^2_{L^2(\Omega_e)^4}\,.\end{aligned}$$

Therefore, (4.6.4) follows by combining the last inequality and (4.6.5), and this completes the proof of the proposition. ☐

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