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A POINCARÉ–STEKLOV MAP FOR THE MIT BAG MODEL

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The purpose of this paper is to introduce and study Poincaré–Steklov (PS) operators associated to the Dirac operator D_m with the so-called MIT bag boundary condition. In a domain $\Omega \subset \mathbb{R}^3$, for a complex number z and for U_z a solution of $(D_m - z)U_z = 0$, the associated PS operator maps the value of $\Gamma_- U_z$ — the MIT bag boundary value of U_z — to $\Gamma_+ U_z$, where $\Gamma_\pm$ are projections along the boundary $\partial\Omega$ and $(\Gamma_- + \Gamma_+) = t_{\partial\Omega}$ is the trace operator on $\partial\Omega$.

In the first part of this paper, we show that the PS operator is a zeroth-order pseudodifferential operator and give its principal symbol. In the second part, we study the PS operator when the mass m is large, we prove that it fits into the framework of $1/m$-pseudodifferential operators, and we derive some important properties, especially its semiclassical principal symbol. Subsequently, we apply these results to establish a Krein-type resolvent formula for the Dirac operator $H_M = D_m + M\beta 1_{\mathbb{R}^3\setminus\overline{\Omega}}$ for large masses $M > 0$ in terms of the resolvent of the MIT bag operator on Ω. With its help, the large coupling convergence with a convergence rate of $\mathcal{O}(M^{-1})$ is shown.

1. Introduction

Motivation. Boundary integral operators have played a key role in the study of many boundary value problems for partial differential equations arising in various areas of mathematical physics, such as electromagnetism, elasticity, and potential theory. In particular, they are used as a tool for proving the existence of solutions as well as for their construction by means of integral equation methods; see, e.g., [Fabes et al. 1978; Jerison and Kenig 1981a; 1981b; Verchota 1984].

The study of boundary integral operators has also been the motivation for the development of various tools and branches of mathematics, e.g., Fredholm theory and singular integral and pseudodifferential operators. Moreover, it turned out that the functional analytic and spectral properties of some of these

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operators are strongly related to the regularity and geometric properties of surfaces; see for example [Hofmann et al. 2009; 2010]. A typical and well-known example which occurs in many applications is the Dirichlet-to-Neumann (DtN) operator. In the classical setting of a bounded domain $\Omega \subset \mathbb{R}^d$ with a smooth boundary, the DtN operator, $\mathcal{N}$, is defined by

$$\mathcal{N} : H^{1/2}(\partial\Omega) \to H^{-1/2}(\partial\Omega), \quad g \mapsto \mathcal{N} g = \Gamma_N U(g),$$

where $U(g)$ is the harmonic extension of g (i.e., $\Delta U(g) = 0$ in Ω and $\Gamma_D U = g$ on $\partial\Omega$). Here Γ_D and Γ_N denote the Dirichlet and the Neumann traces, respectively. In this setting, it is well known that the DtN operator fits into the framework of pseudodifferential operators; see, e.g., [Taylor 1996]. Moreover, from the point of view of the spectral theory, several geometric properties of the eigenvalue problem for the DtN operator (such as isoperimetric inequalities, spectral asymptotics, and geometric invariants) are closely related to the theory of minimal surfaces [Fraser and Schoen 2016] as well as the problem of determining a complete Riemannian manifold with boundary from the Cauchy data of harmonic functions; see [Lassas et al. 2003] (see also the survey [Girouard and Polterovich 2017] for further details).

The main goal of this paper is to introduce a Poincaré–Steklov map for the Dirac operator (i.e., an analogue of the DtN map for the Laplace operator) and to study its (semiclassical) pseudodifferential properties. Our main motivation for considering this operator is that it arises naturally in the study of the well-known Dirac operator with the MIT bag boundary condition, $H_{\mathrm{MIT}}(m)$, defined rigorously below.

Description of main results. In order to give a rigorous definition of the operator we are dealing with in this paper and to go more into details, we need to introduce some notation. Given $m > 0$, the free Dirac operator D_m on $\mathbb{R}^3$ is defined by $D_m := -i\alpha \cdot \nabla + m\beta$, where

$$\alpha_j = \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix} \text{ for } j = 1, 2, 3, \quad \beta = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}, \quad I_2 := \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$
$$\text{and} \quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

are the family of Dirac and Pauli matrices. We use the notation $\alpha \cdot x = \sum_{j=1}^3 \alpha_j x_j$ for $x = (x_1, x_2, x_3) \in \mathbb{R}^3$. We refer to the Appendix, where we recall some important properties of Dirac matrices for the convenience of the reader. We recall that D_m is self-adjoint in $L^2(\mathbb{R}^3)^4$ with $\mathrm{dom}(D_m) = H^1(\mathbb{R}^3)^4$ (see, e.g., [Thaller 1992, Section 1.4]), and for the spectrum and the continuous spectrum, we have

$$\mathrm{Sp}(D_m) = \mathrm{Sp}_{\mathrm{cont}}(D_m) = (-\infty, -m] \cup [m, +\infty).$$

Let $\Omega \subset \mathbb{R}^3$ be a domain with a compact smooth boundary $\partial\Omega$, let n be the outward unit normal to Ω, and let $\Gamma_\pm$ and $P_\pm$ be the trace mappings and the orthogonal projections, respectively, defined by

$$\Gamma_\pm = P_\pm \Gamma_D : H^1(\Omega)^4 \to P_\pm H^{1/2}(\partial\Omega)^4 \qquad \text{and} \qquad P_\pm := \tfrac{1}{2}(I_4 \mp i\beta(\alpha \cdot n(x))), \quad x \in \partial\Omega.$$

In the present paper, we investigate the specific case of the Poincaré–Steklov (PS for short) operator, $\mathscr{A}_m$, defined by

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

where z belongs to the resolvent set of the MIT bag operator on Ω (i.e., $z \in \rho(H_{\mathrm{MIT}}(m))$) and $U_z \in H^1(\Omega)^4$ is the unique solution to the elliptic boundary problem

$$\begin{cases} (D_m - z)U_z = 0 & \text{in } \Omega, \\ \Gamma_- U_z = g & \text{on } \partial\Omega. \end{cases} \tag{1-1}$$

Here and also in what follows, z or any complex number stands for zI, with I the identity.

We point out that, in the R-matrix theory and the embedding method for the Dirac equation, similar operators linking on $\partial\Omega$ values of the upper and lower components of the spinor wave functions have been studied in [Agranovich 2001; Agranovich and Rozenblum 2004; Bielski and Szmytkowski 2006; Szmytkowski 1998]. There it corresponds to a different boundary condition (the trace of the upper/lower components) which is not necessarily elliptic. As far as we know, such operators for the MIT bag boundary condition have not been studied yet.

Let us now briefly describe the content of the present paper. Our results are mainly concerned with the pseudodifferential properties of $\mathscr{A}_m$ and their applications. Thus, our first goal is to show that $\mathscr{A}_m$ fits into the framework of pseudodifferential operators. In Section 4, we show that, when the mass m is fixed and $z \in \rho(D_m)$, the Poincaré–Steklov operator $\mathscr{A}_m$ is a classical homogeneous pseudodifferential operator of order 0, and that

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

where $S = \frac{1}{2} i (\alpha \wedge \alpha)$ is the spin angular momentum, $\nabla_{\partial\Omega}$ and $\Delta_{\partial\Omega}$ are the surface gradient and the Laplace–Beltrami operator on $\partial\Omega$ (equipped with the Riemann metric induced by the Euclidean one in $\mathbb{R}^3$), respectively, and $\operatorname{Op} \mathcal{S}^{-1}$ is the classical class of pseudodifferential operators of order -1 (see Theorem 4.5 for details). For $D_{\partial\Omega}$ — the extrinsically defined Dirac operator introduced in Section 2D — we also have

$$\mathscr{A}_m = D_{\partial\Omega} (-\Delta_{\partial\Omega})^{-1/2} P_- \mod \operatorname{Op} \mathcal{S}^{-1}(\partial\Omega).$$

The proof of the above result is based on the fact that we have an explicit solution of the system (1-1) for any $z \in \rho(D_m)$, and in this case the PS operator takes the following layer potential form:

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

where $\mathscr{C}_{z,m}$ is the Cauchy operator associated with $(D_m - z)$ defined on $\partial\Omega$ in the principal value sense (see Section 2B for the precise definition). So the starting point of the proof is to analyze the pseudodifferential properties of the Cauchy operator. In this sense, we show that $2\mathscr{C}_{z,m}$ is equal, modulo $\operatorname{Op} \mathcal{S}^{-1}(\partial\Omega)$, to $\alpha \cdot (\nabla_{\partial\Omega} (-\Delta_{\partial\Omega})^{-1/2})$. Using this, the explicit layer potential description of $\mathscr{A}_m$, and the symbol calculus, we then prove that $\mathscr{A}_m$ is a pseudodifferential operator and catch its principal symbol (see Theorem 4.5).

The above strategy allows us to capture the pseudodifferential character of $\mathscr{A}_m$, but unfortunately it does not allow us to trace the dependence on the parameter m, and it also imposes a restriction on the spectral parameter 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 5, we address the m-dependence of the pseudodifferential properties of $\mathscr{A}_m$ for any $z \in \rho(H_{\mathrm{MIT}}(m))$. Since we are mainly concerned with large masses m in our application, we treat this problem from the semiclassical point of view, where $h = 1/m \in (0, 1]$ is the semiclassical parameter. In fact, we show in Theorem 5.1 that $\mathscr{A}_{1/h}$ admits a semiclassical approximation, and that

$$\mathscr{A}_{1/h} = \frac{h D_{\partial\Omega}}{\sqrt{-h^2 \Delta_{\partial\Omega} + I} + I} P_- \mod h \operatorname{Op}^h \mathcal{S}^{-1}(\partial\Omega).$$

The main idea of the proof is to use the system (1-1) instead of the explicit formula (1-2), 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 (1-1) of the form

$$U^h(\tilde{x}, x_3) = \operatorname{Op}^h(A^h(\cdot\,,\cdot\,, x_3))g = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} A^h(\tilde{x}, h\xi, x_3) e^{iy\cdot\xi} \hat{g}(\xi)\,\mathrm{d}\xi, \qquad (\tilde{x}, x_3) \in \mathbb{R}^2 \times [0, \infty),$$

where A^h belongs to a specific symbol class and has the asymptotic expansion

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

The second step is to show that, when applying the trace mapping Γ_+ to the pullback of $U^h(\cdot\,, 0)$, it coincides locally with $\mathscr{A}_{1/h}$ modulo a regularizing and negligible operator. At this point, the properties of the MIT bag operator become crucial, in particular the regularization property of its resolvent which allows us to achieve this second step, as we will see in Section 5. The MIT bag operator on Ω is the Dirac operator on $L^2(\Omega)^4$ defined by

$$H_{\mathrm{MIT}}(m)\psi = D_m\psi \quad \text{for all } \psi \in \operatorname{dom}(H_{\mathrm{MIT}}(m)) := \{\psi \in H^1(\Omega)^4 : \Gamma_-\psi = 0 \text{ on } \partial\Omega\}.$$

It is well known that $(H_{\mathrm{MIT}}(m), \operatorname{dom}(H_{\mathrm{MIT}}(m))$ is self-adjoint when Ω is smooth; see, e.g., [Ourmières-Bonafos and Vega 2018]. In Section 3, we briefly discuss the basic spectral properties of $H_{\mathrm{MIT}}(m)$, when Ω is a domain with compact Lipschitz boundary (see Theorem 3.1). Moreover, in Theorem 3.4 we establish regularity results concerning the regularization property of the resolvent and the Sobolev regularity of the eigenfunctions of H_{MIT}. In particular, we prove that $(H_{\mathrm{MIT}}(m) - z)^{-1}$ is bounded from $H^n(\Omega)^4$ into $H^{n+1}(\Omega)^4 \cap \operatorname{dom}(H_{\mathrm{MIT}}(m))$ for all $n \geqslant 1$.

Motivated by the natural way in which the PS operator is related to the MIT bag operator and to illustrate its usefulness, we consider in Section 6 the large mass problem for the self-adjoint Dirac operator $H_M = D_m + M\beta 1_{\mathcal{U}}$, where $\mathcal{U} = \mathbb{R}^3 \setminus \overline{\Omega}$. Indeed, it is known that, in the limit $M \to \infty$, every eigenvalue of $H_{\mathrm{MIT}}(m)$ is a limit of eigenvalues of H_M; see [Arrizabalaga et al. 2019; Moroianu et al. 2020] (see also [Barbaroux et al. 2019; Benhellal 2019; Stockmeyer and Vugalter 2019] for the two-dimensional setting). Moreover, it is shown in [Barbaroux et al. 2019; Benhellal 2019] that the two-dimensional analogue of H_M converges to the two-dimensional analogue of $H_{\mathrm{MIT}}(m)$ in the norm resolvent sense with a convergence rate of $\mathcal{O}(M^{-1/2})$.

The main goal of Section 6 is to address the following question: Let $M_0 > 0$ be large enough and fix $M \geqslant M_0$ and $z \in \rho(H_{\mathrm{MIT}}(m)) \cap \rho(H_M)$. Given $f \in L^2(\mathbb{R}^3)^4$ such that $f = 0$ in $\mathbb{R}^3 \setminus \overline{\Omega}$ and $U \in H^1(\mathbb{R}^3)^4$, what is the boundary value problem on Ω whose solutions closely approximate those of $(D_m + M\beta 1_{\mathbb{R}^3\setminus\overline{\Omega}} - z)U = f$?

It is worth noting that the answer to this question becomes trivial if one establishes an explicit formula for the resolvent of H_M. Having in mind the connection between the Dirac operators H_M and $H_{\mathrm{MIT}}(m)$, this leads us to address the following question: *for M sufficiently large, is it possible to relate the resolvents of H_M and H_{MIT} via a Krein-type resolvent formula*? In Theorem 6.2, which is the main result of Section 6, we establish a Krein-type resolvent formula for H_M in terms of the resolvent of $H_{\mathrm{MIT}}(m)$. The key point to establish this result is to treat the elliptic problem $(H_M - z)U = f \in L^2(\mathbb{R}^3)^4$ as a transmission problem (where $\Gamma_\pm U_{|\Omega} = \Gamma_\pm U_{|\mathbb{R}^3\setminus\Omega}$ are the transmission conditions) and to use the semiclassical properties of the Poincaré–Steklov operators in order to invert the auxiliary operator $\Psi_M(z)$ acting on the boundary $\partial\Omega$ (see Theorem 6.2 for the precise definition). In addition, we prove an adapted Birman–Schwinger principle relating the eigenvalues of H_M in the gap $(-(m+M), m+M)$ with a spectral property of $\Psi_M(z)$. With their help, we show in Corollary 6.5 that the restriction of U on Ω satisfies the elliptic problem

$$\begin{cases} (D_m - z)U_{|\Omega} = f & \text{in } \Omega, \\ \Gamma_- U_{|\Omega} = \mathscr{B}_M \Gamma_+ R_{\mathrm{MIT}}(z) f & \text{on } \partial\Omega, \\ \Gamma_+ U_{|\Omega} = \Gamma_+ R_{\mathrm{MIT}}(z) f + \mathscr{A}_m \Gamma_- v & \text{on } \partial\Omega, \end{cases}$$

where $\mathscr{B}_M$ is a semiclassical pseudodifferential operator of order 0. Here, the semiclassical parameter is $1/M$. Moreover, we show that the convergence of H_M to $H_{\mathrm{MIT}}(m)$ in the norm resolvent sense indeed holds with a convergence rate of $\mathcal{O}(M^{-1})$, which improves previous works; see Proposition 6.9. The most important ingredient in proving these results is the use of the Krein formula relating the resolvents of H_M and $H_{\mathrm{MIT}}(m)$, as well as regularity estimates for the PS operators (see Proposition 6.4) and layer potential operators (see Lemma 6.10 for details).

Organization of the paper. The paper is organized as follows. Sections 2 and 3 are devoted to preliminaries for the sake of completeness and self-containedness of the paper. In Section 2, we set up some notation, and we recall some basic properties of boundary integral operators associated with $(D_m - z)$. Section 3 is devoted to the study of the MIT bag operator, where we gather its basic properties in Theorem 3.1 and we establish the regularization property of its resolvent in Theorem 3.4. In Section 4 we establish Theorem 4.5, proving that the PS operator is a classical pseudodifferential operator. Then, in Section 5, we study the PS operator from the point of view of semiclassical pseudodifferential operators, the main result being Theorem 5.1. Finally, Section 6 is devoted to the study of the large mass problem for the operator H_M. There, we prove Theorem 6.2 regarding the Krein-type resolvent formula and we solve the large mass problem, and we prove Proposition 6.9 on the resolvent convergence.

2. Preliminaries

In this section we gather some well-known results about boundary integral operators. We also recall some properties of symbol classes and their associated pseudodifferential operators. Before proceeding further, however, we need to introduce some notation that we will use in what follows.

2A. ***Notations.*** Throughout this paper we will write $a \lesssim b$ if there is $C > 0$ such that $a \leqslant Cb$. As usual, the letter C stands for some constant which may change its value at different occurrences.

For a bounded or unbounded Lipschitz domain $\Omega \subset \mathbb{R}^3$, we write $\partial\Omega$ for its boundary, and we denote by n and σ the outward-pointing normal to Ω and the surface measure on $\partial\Omega$, respectively. By $L^2(\mathbb{R}^3)^4 := L^2(\mathbb{R}^3; \mathbb{C}^4)$ and $L^2(\Omega)^4 := L^2(\Omega, \mathbb{C}^4)$, we denote the usual L^2-space over $\mathbb{R}^3$ and Ω, respectively, and we let $r_\Omega : L^2(\mathbb{R}^3)^4 \to L^2(\Omega)^4$ be the restriction operator on Ω and $e_\Omega : L^2(\Omega)^4 \to L^2(\mathbb{R}^3)^4$ be its adjoint operator, i.e., the extension by zero outside of Ω.

For a function $u \in L^2(\mathbb{R}^d)$, its Fourier transform is defined by the formula

$$\hat{u}(\xi) = \int_{\mathbb{R}^d} e^{-ix\cdot\xi} u(x)\,\mathrm{d}x \quad \text{for all } \xi \in \mathbb{R}^d.$$

For $s \in [0, 1]$, we define the usual Sobolev space $H^s(\mathbb{R}^d)^4$ as

$$H^s(\mathbb{R}^d)^4 := \left\{ u \in L^2(\mathbb{R}^d)^4 : \int_{\mathbb{R}^d} (1 + |\xi|^2)^s |\hat{u}(\xi)|^2 \,\mathrm{d}\xi < \infty \right\},$$

and we shall designate by $H^s(\Omega)^4$ the standard L^2-based Sobolev space of order s. We denote the usual L^2-space over $\partial\Omega$ by $L^2(\partial\Omega)^4 := L^2(\partial\Omega, \mathrm{d}\sigma)^4$. If Ω is a C^2-smooth domain with compact boundary $\partial\Omega$, then the Sobolev space of order $s \in (0, 1]$ along the boundary, $H^s(\partial\Omega)^4$, is defined using a local coordinate representation on the surface $\partial\Omega$. As usual, we use the symbol $H^{-s}(\partial\Omega)^4$ to denote the dual space of $H^s(\partial\Omega)^4$. We denote by $t_{\partial\Omega} : H^1(\Omega)^4 \to H^{1/2}(\partial\Omega)^4$ the classical trace operator, and by $\mathcal{E}_\Omega : H^{1/2}(\partial\Omega)^4 \to H^1(\Omega)^4$ the extension operator, that is,

$$t_{\partial\Omega}\mathcal{E}_\Omega[f] = f \quad \text{for all } f \in H^{1/2}(\partial\Omega)^4.$$

Throughout the current paper, we denote by $P_\pm$ the orthogonal projections defined by

$$P_\pm := \tfrac{1}{2}(I_4 \mp i\beta(\alpha \cdot n(x))), \quad x \in \partial\Omega. \tag{2-1}$$

We use the symbol $H(\alpha, \Omega)$ for the Dirac–Sobolev space on a smooth domain Ω defined as

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

which is a Hilbert space (see [Ourmières-Bonafos and Vega 2018, Section 2.3]) endowed with the scalar product

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

We also recall that the trace operator $t_{\partial\Omega}$ extends into a continuous map $t_{\partial\Omega} : H(\alpha, \Omega) \to H^{-1/2}(\partial\Omega)^4$. Moreover, if $v \in H(\alpha, \Omega)$ and $t_{\partial\Omega} v \in H^{1/2}(\partial\Omega)^4$, then $v \in H^1(\Omega)^4$; see [Ourmières-Bonafos and Vega 2018, Propositions 2.1 and 2.16].

2B. ***Boundary integral operators.*** The aim of this part is to introduce boundary integral operators associated with the fundamental solution of the free Dirac operator D_m and to summarize some of their well-known properties.

For $z \in \rho(D_m)$, with the convention that $\operatorname{Im}\sqrt{z^2 - m^2} > 0$, the fundamental solution of $(D_m - z)$ is

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

We define the potential operator $\Phi^{\Omega}_{z,m} : L^2(\partial\Omega)^4 \to L^2(\Omega)^4$ by

$$\Phi^{\Omega}_{z,m}[g](x) = \int_{\partial\Omega} \phi^z_m(x-y)g(y)\,\mathrm{d}\sigma(y) \quad \text{for all } x \in \Omega \tag{2-4}$$

and the Cauchy operator $\mathscr{C}_{z,m} : L^2(\partial\Omega)^4 \to L^2(\partial\Omega)^4$ as the singular integral operator acting as

$$\mathscr{C}_{z,m}[f](x) = \lim_{\rho\searrow 0} \int_{|x-y|>\rho} \phi^z_m(x-y)f(y)\,\mathrm{d}\sigma(y) \quad \text{for } \sigma\text{-a.e. } x \in \partial\Omega,\ \ f \in L^2(\partial\Omega)^4. \tag{2-5}$$

It is well known that $\Phi^{\Omega}_{z,m}$ and $\mathscr{C}_{z,m}$ are bounded and everywhere defined (see, for instance, [Arrizabalaga et al. 2014, Section 2]) and that

$$((\alpha\cdot n)\mathscr{C}_{z,m})^2 = (\mathscr{C}_{z,m}(\alpha\cdot n))^2 = -\tfrac{1}{4} \quad \text{for all } z \in \rho(D_m) \tag{2-6}$$

holds in $L^2(\partial\Omega)^4$; see [Arrizabalaga et al. 2015, Lemma 2.2]. In particular, the inverse

$$\mathscr{C}^{-1}_{z,m} = -4(\alpha\cdot n)\mathscr{C}_{z,m}(\alpha\cdot n)$$

exists and is bounded and everywhere defined. Since we have $\phi^z_m(y-x)^* = \phi^{\bar{z}}_m(x-y)$ for all $z \in \rho(D_m)$, it follows that $\mathscr{C}^*_{z,m}$ and $\mathscr{C}_{\bar{z},m}$ are equal as operators in $L^2(\partial\Omega)^4$. In particular, $\mathscr{C}_{z,m}$ is self-adjoint in $L^2(\partial\Omega)^4$ for all $z \in (-m, m)$.

Next, recall that the trace of the single layer operator S_z associated with the Helmholtz operator $(-\Delta + m^2 - z^2)I_4$ is defined, for every $f \in L^2(\partial\Omega)^4$ and $z \in \rho(D_m)$, by

$$S_z[f](x) := \int_{\partial\Omega} \frac{e^{i\sqrt{z^2-m^2}|x-y|}}{4\pi|x-y|} f(y)\,\mathrm{d}\sigma(y) \quad \text{for } x \in \partial\Omega.$$

It is well known that S_z is bounded from $L^2(\partial\Omega)^4$ into $H^{1/2}(\partial\Omega)^4$ and it is a positive operator in $L^2(\partial\Omega)^4$ for all $z \in (-m, m)$; see [Arrizabalaga et al. 2015, Lemma 4.2]. Now we define the operator Λ^z_m by

$$\Lambda^z_m = \tfrac{1}{2}\beta + \mathscr{C}_{z,m} \qquad \text{for all } z \in \rho(D_m),$$

which is clearly a bounded operator from $L^2(\partial\Omega)^4$ into itself.

In the next lemma we collect the main properties of the operators $\Phi^{\Omega}_{z,m}$, $\mathscr{C}_{z,m}$, and Λ^z_m.

Lemma 2.1. *Assume that Ω is C^2-smooth. Given $z \in \rho(D_m)$, let $\Phi^{\Omega}_{z,m}$, $\mathscr{C}_{z,m}$, and Λ^z_m be as above. Then the following hold*:

(i) *The operator $\Phi^{\Omega}_{z,m}$ is bounded from $H^{1/2}(\partial\Omega)^4$ to $H^1(\Omega)^4$ and extends into a bounded operator from $H^{-1/2}(\partial\Omega)^4$ to $H(\alpha, \Omega)$. Moreover,*

$$t_{\partial\Omega}\Phi^{\Omega}_{z,m}[f] = \left(-\tfrac{1}{2}i(\alpha\cdot n) + \mathscr{C}_{z,m}\right)[f] \quad \textit{for all } f \in H^{1/2}(\partial\Omega)^4. \tag{2-7}$$

(ii) *The operator $\mathscr{C}_{z,m}$ gives rise to a bounded operator $\mathscr{C}_{z,m} : H^{1/2}(\partial\Omega)^4 \to H^{1/2}(\partial\Omega)^4$.*

(iii) *The operator $\Lambda^z_m : H^{1/2}(\partial\Omega)^4 \to H^{1/2}(\partial\Omega)^4$ is bounded invertible for all $z \in \rho(D_m)$.*

Proof. (i) The proof of the boundedness of $\Phi^{\Omega}_{z,m}$ from $H^{1/2}(\partial\Omega)^4$ into $H^1(\Omega)^4$ is contained in [Behrndt and Holzmann 2020, Proposition 4.2], and the jump formula (2-7) is proved in [Arrizabalaga et al. 2014, Lemma 3.3] in terms of the nontangential limit which coincides (almost everywhere in $\partial\Omega$) with the trace operator for functions in $H^1(\Omega)^4$. The boundedness of $\Phi^{\Omega}_{z,m}$ from $H^{-1/2}(\partial\Omega)^4$ to $H(\alpha,\Omega)$ is established in [Ourmières-Bonafos and Vega 2018, Theorem 2.2].

Since n is smooth, it is clear from (i) that $\mathscr{C}_{z,m}$ is bounded from $H^{1/2}(\partial\Omega)^4$ into itself, which proves (ii). As consequence we also obtain that Λ^z_m is bounded from $H^{1/2}(\partial\Omega)^4$ into itself. Now, the invertibility of Λ^z_m in $H^{1/2}(\partial\Omega)^4$ for $z\in\mathbb{C}\setminus\mathbb{R}$ is shown in [Behrndt et al. 2019, Lemma 3.3 (iii)]; see also [Behrndt et al. 2020, Lemma 3.12]. To complete the proof of (iii), note that if $f\in L^2(\partial\Omega)^4$ is such that $\Lambda^z_m[f]\in H^{1/2}(\partial\Omega)^4$, then a simple computation shows that

$$H^{1/2}(\partial\Omega)^4 \ni (\Lambda^z_m)^2[f]=\big(\tfrac{1}{4}+(\mathscr{C}_{z,m})^2+(m+z\beta)S_z\big)[f],$$

which means that $f\in H^{1/2}(\partial\Omega)^4$. From the above computation, we see that Λ^z_m is invertible from $H^{1/2}(\partial\Omega)^4$ into itself for all $z\in(-m,m)$, since $((\mathscr{C}_{z,m})^2+(m+z\beta)S_z)$ is a positive operator. □

Remark 2.2. Note that if Ω is a Lipschitz domain with a compact boundary, then, for all $z\in\rho(D_m)$, the operators $\mathscr{C}_{z,m}$ and Λ^z_m are bounded from $L^2(\partial\Omega)^4$ into itself (see, e.g, [Arrizabalaga et al. 2014, Lemma 3.3]), and since Λ^z_m is an injective Fredholm operator (see the proof of [Benhellal 2022a, Theorem 4.5]), it follows that it is also invertible in $L^2(\partial\Omega)^4$. Note also that, thanks to [Behrndt et al. 2021, Lemmas 5.1 and 5.2], we know the mapping $\Phi^{\Omega}_{z,m}$ defined by (2-4) is bounded from $L^2(\partial\Omega)^4$ to $H^{1/2}(\Omega)^4$, $t_{\partial\Omega}\Phi^{\Omega}_{z,m}[g]\in L^2(\partial\Omega)^4$, and the formula (2-7) still holds true for all $g\in L^2(\partial\Omega)^4$.

2C. ***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 $S^m(\mathbb{R}^d\times\mathbb{R}^d)$ 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

$$|\partial^\alpha_x\,\partial^\beta_\xi a(x,\xi)|\leqslant C_{\alpha\beta}(1+|\xi|^2)^{m-|\beta|}\quad\text{for all } (x,\xi)\in\mathbb{R}^d\times\mathbb{R}^d,\ \text{for all } \alpha\in\mathbb{N}^d,\ \text{for all } \beta\in\mathbb{N}^d.$$

Let $\mathscr{S}(\mathbb{R}^d)$ be the Schwartz class of functions. Then, for each $a\in S^m(\mathbb{R}^d\times\mathbb{R}^d)$ and any $h\in(0,1]$, we associate to it a semiclassical pseudodifferential operator $\mathrm{Op}^h(a):\mathscr{S}(\mathbb{R}^d)^4\to\mathscr{S}(\mathbb{R}^d)^4$ via the standard formula

$$\mathrm{Op}^h(a)u(x)=\frac{1}{(2\pi)^d}\int_{\mathbb{R}^d}e^{i\xi\cdot x}a(x,h\xi)\hat{u}(\xi)\,d\xi\quad\text{for all } u\in\mathscr{S}(\mathbb{R}^d)^4.$$

If $a\in S^0(\mathbb{R}^d\times\mathbb{R}^d)$, then the Calderón–Vaillancourt theorem (see, e.g., [Calderón and Vaillancourt 1972]) yields that $\mathrm{Op}^h(a)$ extends to a bounded operator from $L^2(\mathbb{R}^d)^4$ into itself, and there exists $C, N_C>0$ such that

$$\|\mathrm{Op}^h(a)\|_{L^2\to L^2}\leqslant C\max_{|\alpha+\beta|\leqslant N_C}\|\partial^\alpha_x\,\partial^\beta_\xi a\|_{L^\infty}.\tag{2-8}$$

By definition, a semiclassical pseudodifferential operator $\mathrm{Op}^h(a)$, with $a\in S^0(\mathbb{R}^d\times\mathbb{R}^d)$, can also be considered as a classical pseudodifferential operator $\mathrm{Op}^1(a_h)$, with $a_h=a(x,h\xi)$, which is bounded with respect to $h \in (0, h_0)$, where $h_0 > 0$ is fixed. Thus the Calderón–Vaillancourt theorem also provides the boundedness of these operators in Sobolev spaces $H^s(\mathbb{R}^d)^4 = \langle D_x \rangle^{-s} L^2(\mathbb{R}^d)^4$, where $\langle D_x \rangle = \sqrt{-\Delta + I}$. Indeed, we have

$$\|\mathrm{Op}^1(a_h)\|_{H^s \to H^s} = \|\langle D_x \rangle^s \,\mathrm{Op}^1(a_h) \langle D_x \rangle^{-s}\|_{L^2 \to L^2}, \tag{2-9}$$

and since $\langle D_x \rangle^s \,\mathrm{Op}^1(a_h) \langle D_x \rangle^{-s}$ is a classical pseudodifferential operator with a uniformly bounded symbol in $\mathcal{S}^0$, we deduce that $\mathrm{Op}^h(a)$ is uniformly bounded with respect to h from H^s into itself.

Consider a C^∞-smooth domain $\Omega \subset \mathbb{R}^3$ with a compact boundary $\Sigma = \partial\Omega$. Then Σ is a 2-dimensional parametrized surface, which, in the sense of differential geometry, can also be viewed as a smooth 2-dimensional manifold immersed into $\mathbb{R}^3$. Thus Σ can be covered by an atlas (i.e., a collection of smooth charts)

$$\mathbb{A} = \{(U_j, V_j, \varphi_j) : j \in \{1, \dots, N\}\}, \quad \text{where } N \in \mathbb{N}^*.$$

That is

$$\Sigma = \bigcup_{j=1}^{N} U_j,$$

and for each $j \in \{1, \dots, N\}$, we have that 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^∞-diffeomorphism. Moreover, by the definition of a smooth manifold, if $U_j \cap U_k \neq \varnothing$ then

$$\varphi_k \circ (\varphi_j)^{-1} \in C^\infty(\varphi_j(U_j \cap U_k); \varphi_k(U_j \cap U_k)).$$

As usual, the pullback $(\varphi_j^{-1})^*$ and the pushforward φ_j^* are defined 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 2012, Part 4], we define pseudodifferential operators on the boundary Σ as follows.

Definition 2.3. 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 $\mathscr{A} \in \mathrm{Op}^h \mathcal{S}^m(\Sigma)$, if,

(1) for every chart (U_j, V_j, φ_j), there exists a symbol $a \in \mathcal{S}^m$ such that

$$\psi_1 \mathscr{A}(\psi_2 u) = \psi_1 \varphi_j^* \,\mathrm{Op}^h(a) (\varphi_j^{-1})^* (\psi_2 u)$$

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 $\mathrm{supp}(\psi_1) \cap \mathrm{supp}(\psi_2) = \varnothing$ 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 reduces to a local study on local charts, we recall below the specific local coordinates and surface geometry notation used in the rest of the paper.

We always fix an open set $U \subset \Sigma$, and we let $\chi : V \to \mathbb{R}$ be a C^∞-function (where $V \subset \mathbb{R}^2$ is open) such that its graph coincides with U. Here and in the following, we omit the possible composition with a rotation that allows this, since changes of variables take h-pseudodifferential operators to h-pseudodifferential operators modulo smoothing operators and leave the principal symbol invariant. 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 following forms:

$$\mathrm{I} = g_{11}\, \mathrm{d}\tilde{x}_1^2 + 2g_{12}\, \mathrm{d}\tilde{x}_1\, \mathrm{d}\tilde{x}_2 + g_{22}\, \mathrm{d}\tilde{x}_2^2,$$

$$G(\tilde{x}) = (g_{jk}(\tilde{x})) = \begin{pmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{pmatrix}(\tilde{x}) := \begin{pmatrix} 1+|\partial_1\chi|^2 & \partial_1\chi\, \partial_2\chi \\ \partial_1\chi\, \partial_2\chi & 1+|\partial_2\chi|^2 \end{pmatrix}(\tilde{x}).$$

As $G(\tilde{x})$ is symmetric, it follows that it is diagonalizable by an orthogonal matrix. Indeed, let

$$Q(\tilde{x}) := \begin{pmatrix} \dfrac{|\partial_2\chi|}{|\nabla\chi|} & \dfrac{\partial_1\chi\, \partial_2\chi}{|\partial_2\chi||\nabla\chi|} \\ -\dfrac{\partial_1\chi\, \partial_2\chi}{|\partial_2\chi||\nabla\chi|} & \dfrac{|\partial_2\chi|}{|\nabla\chi|} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & g^{-1/2} \end{pmatrix}(\tilde{x}), \tag{2-10}$$

where g stands for the determinant of G. Then, it is straightforward to check that

$$Q^{\mathrm{T}} G Q(\tilde{x}) = I_2, \quad Q Q^{\mathrm{T}}(\tilde{x}) = G(\tilde{x})^{-1} =: (g^{jk}(\tilde{x})), \quad \det(Q) = \det(Q^{\mathrm{T}}) = g^{-1/2}. \tag{2-11}$$

2D. ***Operators on the boundary $\Sigma = \partial\Omega$.*** As above, we consider $\Sigma = \partial\Omega$ the boundary of a smooth bounded domain Ω. On Σ equipped with the Riemann metric induced by the Euclidean one in $\mathbb{R}^3$, we consider the Laplace–Beltrami operator $-\Delta_\Sigma$ and the surface gradient $\nabla_\Sigma = \nabla - n(n\cdot\nabla)$, where n is the unit normal to the surface pointing outside Ω. Note that, for (e_1, e_2) an orthonormal basis of the tangent space, $\nabla_\Sigma = e_1\nabla_{e_1} + e_2\nabla_{e_2}$, where ∇_{e_j} stands for the tangential derivative in the direction e_j. With the notation of the previous section, in local coordinates, $-\Delta_\Sigma$ and ∇_Σ are pseudodifferential operators with respective principal symbols

$$p_{-\Delta_\Sigma}(\tilde{x}, \xi) = \langle G(\tilde{x})^{-1}\xi, \xi\rangle, \qquad p_{\nabla_\Sigma}(\tilde{x}, \xi) = \xi_G := \begin{pmatrix} G(\tilde{x})^{-1}\xi \\ \langle \nabla\chi(\tilde{x}), G(\tilde{x})^{-1}\xi\rangle \end{pmatrix}. \tag{2-12}$$

Let us now introduce D_Σ, the extrinsically defined Dirac operator. To any $x \in \mathbb{R}^3$ we associate the matrix $\alpha(x) = \alpha \cdot x$, where $\alpha = (\alpha_1, \alpha_2, \alpha_3)$. For H_1, the mean curvature of Σ, D_Σ, is given by

$$D_\Sigma = -\alpha(n)\alpha(\nabla_\Sigma) + \tfrac{1}{2} H_1$$

(for more details see [Moroianu et al. 2020, Appendix B]). It is a pseudodifferential operator with principal symbol

$$p_{D_\Sigma}(\tilde{x}, \xi) = -i\alpha(n^\varphi(\tilde{x}))\alpha(\xi_G),$$

where $n^\varphi = \varphi^* n$. We now define the spin angular momentum S as

$$S \cdot X = -\gamma_5(\alpha\cdot X) \quad \text{for all } X \in \mathbb{R}^3, \qquad \text{where } \gamma_5 := -i\alpha_1\alpha_2\alpha_3 = \begin{pmatrix} 0 & I_2 \\ I_2 & 0 \end{pmatrix}. \tag{2-13}$$

Using properties (A-1) and (A-2) and the fact that $n \cdot \xi_G = 0$, we then have

$$p_{D_\Sigma}(\tilde{x}, \xi) = -i\alpha \cdot n^\varphi(\tilde{x})\alpha \cdot \xi_G = S \cdot (\xi_G \wedge n^\varphi(\tilde{x})).$$

Moreover, for $\bar{\xi} := \binom{\xi}{0}$, we have $\bar{\xi} = \xi_G + (\bar{\xi} \cdot n^\varphi)n^\varphi$. Thus, in local coordinates, the principal symbol of D_Σ is also

$$p_{D_\Sigma}(\tilde{x}, \xi) = S \cdot (\bar{\xi} \wedge n^\varphi(\tilde{x})). \tag{2-14}$$

Let us also point out the relationship between the principal symbols of Δ_Σ and D_Σ:

$$|\bar{\xi} \wedge n^\varphi(\tilde{x})|^2 = \langle G(\tilde{x})^{-1}\xi, \xi\rangle. \tag{2-15}$$

3. Basic properties of the MIT bag model

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.

Let $\mathcal{U} \subset \mathbb{R}^3$ be a Lipschitz domain with a compact boundary $\partial\mathcal{U}$. Then, for $m > 0$, the Dirac operator with the MIT bag boundary condition on $\mathcal{U}$, $(H_{\mathrm{MIT}}(m), \mathrm{dom}(H_{\mathrm{MIT}}(m)))$, or simply the MIT bag operator, is defined on the domain

$$\mathrm{dom}(H_{\mathrm{MIT}}(m)) := \{\psi \in H^{1/2}(\mathcal{U})^4 : (\alpha \cdot \nabla)\psi \in L^2(\mathcal{U})^4 \text{ and } P_- t_{\partial\mathcal{U}}\psi = 0 \text{ on } \partial\mathcal{U}\}$$

by $H_{\mathrm{MIT}}(m)\psi = D_m\psi$ for all $\psi \in \mathrm{dom}(H_{\mathrm{MIT}}(m))$ and where the boundary condition holds in $L^2(\partial\mathcal{U})^4$. Here $P_\pm$ are the orthogonal projections defined by (2-1).

The following theorem gathers the basic properties of the MIT bag operator. We mention that some of these properties are well known in the case of smooth domains; see, e.g., [Arrizabalaga et al. 2017; 2019; 2023; Behrndt et al. 2020; Ourmières-Bonafos and Vega 2018].

Theorem 3.1. *The operator* $(H_{\mathrm{MIT}}(m), \mathrm{dom}(H_{\mathrm{MIT}}(m)))$ *is self-adjoint, and we have*

$$(H_{\mathrm{MIT}}(m) - z)^{-1} = r_{\mathcal{U}}(D_m - z)^{-1}e_{\mathcal{U}} - \Phi^{\mathcal{U}}_{z,m}(\Lambda^z_m)^{-1} t_{\partial\mathcal{U}}(D_m - z)^{-1}e_{\mathcal{U}} \quad \text{for all } z \in \rho(D_m). \tag{3-1}$$

Moreover, the following statements hold:

(i) *If* $\mathcal{U}$ *is bounded, then* $\mathrm{Sp}(H_{\mathrm{MIT}}(m)) = \mathrm{Sp}_{\mathrm{disc}}(H_{\mathrm{MIT}}(m)) \subset \mathbb{R} \setminus [-m, m]$.

(ii) *If* $\mathcal{U}$ *is unbounded, then* $\mathrm{Sp}(H_{\mathrm{MIT}}(m)) = \mathrm{Sp}_{\mathrm{ess}}(H_{\mathrm{MIT}}(m)) = (-\infty, -m] \cup [m, +\infty)$. *Moreover, if* $\mathcal{U}$ *is connected, then* $\mathrm{Sp}(H_{\mathrm{MIT}}(m))$ *is purely continuous.*

(iii) *Let* $z \in \rho(H_{\mathrm{MIT}}(m))$ *be such that* $2|z| < m$. *Then, for all* $f \in L^2(\mathcal{U})^4$,

$$\|(H_{\mathrm{MIT}}(m) - z)^{-1} f\|_{L^2(\mathcal{U})^4} \lesssim \frac{1}{m}\|f\|_{L^2(\mathcal{U})^4}.$$

Proof. Let $\varphi, \psi \in \mathrm{dom}(H_{\mathrm{MIT}}(m))$. Then by density arguments we get the Green formula

$$\langle(-i\alpha \cdot \nabla)\varphi, \psi\rangle_{L^2(\mathcal{U})^4} - \langle\varphi, (-i\alpha \cdot \nabla)\psi\rangle_{L^2(\mathcal{U})^4} = \langle(-i\alpha \cdot n)t_{\partial\mathcal{U}}\varphi, t_{\partial\mathcal{U}}\psi\rangle_{L^2(\partial\mathcal{U})^4}. \tag{3-2}$$

Since $P_- t_{\partial\mathcal{U}}\varphi = P_- t_{\partial\mathcal{U}}\psi = 0$ and $P_\pm(\alpha\cdot n) = (\alpha\cdot n)P_\mp$ (see Lemma A.3), it follows that

$$\langle(-i\alpha\cdot\nabla)\varphi,\psi\rangle_{L^2(\mathcal{U})^4} - \langle\varphi,(-i\alpha\cdot\nabla)\psi\rangle_{L^2(\mathcal{U})^4} = \langle P_+(-i\alpha\cdot n)P_+ t_{\partial\mathcal{U}}\varphi, P_+ t_{\partial\mathcal{U}}\psi\rangle_{L^2(\partial\mathcal{U})^4} = 0.$$

Consequently, we obtain

$$\begin{aligned}\langle H_{\mathrm{MIT}}(m)\varphi,\psi\rangle_{L^2(\mathcal{U})^4} - \langle\varphi, H_{\mathrm{MIT}}(m)\psi\rangle_{L^2(\mathcal{U})^4} &= \langle D_m\varphi,\psi\rangle_{L^2(\mathcal{U})^4} - \langle\varphi, D_m\psi\rangle_{L^2(\mathcal{U})^4}\\ &= \langle(-i\alpha\cdot\nabla)\varphi,\psi\rangle_{L^2(\mathcal{U})^4} - \langle\varphi,(-i\alpha\cdot\nabla)\psi\rangle_{L^2(\mathcal{U})^4} = 0.\end{aligned}$$

Therefore $(H_{\mathrm{MIT}}(m), \mathrm{dom}(H_{\mathrm{MIT}}(m)))$ is symmetric. Now, thanks to [Benhellal 2022a, Proposition 4.3], we know that the MIT bag operator defined on the domain

$$\mathscr{D} = \{\psi = u + \Phi^{\mathcal{U}}_{0,m}[g],\ u\in H^1(\mathcal{U})^4,\ g\in L^2(\partial\mathcal{U})^4 : P_- t_{\partial\mathcal{U}}\psi = 0 \text{ on } \partial\mathcal{U}\} \tag{3-3}$$

by $H_{\mathrm{MIT}}(m)(u + \Phi^{\mathcal{U}}_{0,m}[g]) = D_m u$ for all $(u + \Phi^{\mathcal{U}}_{0,m}[g]) \in \mathscr{D}$ is a self-adjoint operator. Since $H_{\mathrm{MIT}}(m)$ is symmetric on $\mathrm{dom}(H_{\mathrm{MIT}}(m))$, we can deduce that $\mathrm{dom}(H_{\mathrm{MIT}}(m)) \subset \mathscr{D}$. Now, from Remark 2.2, we also get that $\mathscr{D} \subset \mathrm{dom}(H_{\mathrm{MIT}}(m))$, which proves the equality $\mathscr{D} = \mathrm{dom}(H_{\mathrm{MIT}}(m))$, and thus that $(H_{\mathrm{MIT}}(m), \mathrm{dom}(H_{\mathrm{MIT}}(m)))$ is self-adjoint. Next, we check the resolvent formula (3-1). Let $f\in L^2(\mathcal{U})^4$ and $z\in\rho(D_m)$, and set

$$\psi = r_{\mathcal{U}}(D_m - z)^{-1}e_{\mathcal{U}} f - \Phi^{\mathcal{U}}_{z,m}(\Lambda^z_m)^{-1} t_{\partial\mathcal{U}}(D_m - z)^{-1} e_{\mathcal{U}} f.$$

Since $(D_m - z)^{-1}e_{\mathcal{U}}$ is bounded from $L^2(\mathcal{U})^4$ into $H^1(\mathbb{R}^3)^4$ and $(\Lambda^z_m)^{-1}$ is well defined by Remark 2.2, it follows that

$$u := r_{\mathcal{U}}(D_m - z)^{-1}e_{\mathcal{U}} f \in H^1(\mathcal{U})^4 \quad\text{and}\quad g := -(\Lambda^z_m)^{-1} t_{\partial\mathcal{U}}(D_m - z)^{-1}e_{\mathcal{U}} f \in L^2(\partial\mathcal{U})^4,$$

which gives that $\psi\in H^{1/2}(\mathcal{U})^4$ and that $(\alpha\cdot\nabla)\psi\in L^2(\mathcal{U})^4$. Next, using Lemma 2.1(i) and Remark 2.2, we easily get

$$\begin{aligned} t_{\partial\mathcal{U}}\psi &= t_{\partial\mathcal{U}}(D_m - z)^{-1}e_{\mathcal{U}} f + \left(\tfrac12 i(\alpha\cdot n) - \mathscr{C}_{z,m}\right)\left(\tfrac12\beta + \mathscr{C}_{z,m}\right)^{-1} t_{\partial\mathcal{U}}(D_m - z)^{-1}e_{\mathcal{U}} f\\ &= P_+\beta(\Lambda^z_m)^{-1} t_{\partial\mathcal{U}}(D_m - z)^{-1}e_{\mathcal{U}} f,\end{aligned}$$

thus $P_- t_{\partial\mathcal{U}}\psi = 0$ on $\partial\mathcal{U}$, which means that $\psi\in\mathrm{dom}(H_{\mathrm{MIT}}(m))$. Since $(D_m - z)\Phi^{\mathcal{U}}_{z,m}[g] = 0$ in $\mathcal{U}$, it follows that $(H_{\mathrm{MIT}}(m) - z)\psi = f$, and formula (3-1) is proved.

We are now 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 (3-2) yields

$$\|H_{\mathrm{MIT}}(m)\psi\|^2_{L^2(\mathcal{U})^4} = \|(\alpha\cdot\nabla)\psi\|^2_{L^2(\mathcal{U})^4} + m^2\|\psi\|^2_{L^2(\mathcal{U})^4} + m\|P_+ t_{\partial\mathcal{U}}\psi\|^2_{L^2(\partial\mathcal{U})^4}. \tag{3-4}$$

Thus $\|H_{\mathrm{MIT}}(m)\psi\|^2_{L^2(\mathcal{U})^4} \geqslant m^2\|\psi\|^2_{L^2(\mathcal{U})^4}$, which yields $\mathrm{Sp}(H_{\mathrm{MIT}}(m)) \subset (-\infty,-m]\cup[m,+\infty)$. Note that this can be seen immediately from (3-1). 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 $\mathcal{U}$. Then, from (3-4), we have

$$\|(-i\alpha\cdot\nabla)\psi\|^2_{L^2(\mathcal{U})^4} + m\|P_+ t_{\partial\mathcal{U}}\psi\|^2_{L^2(\partial\mathcal{U})^4} = 0.$$

Since $m > 0$, it follows that $P_+ t_{\partial\mathcal{U}}\psi = 0$ and thus that $t_{\partial\mathcal{U}}\psi = 0$. Using this and the above equation, an integration by parts (using density arguments) gives

$$\|\nabla\psi\|_{L^2(\mathcal{U})^4} = \|(-i\alpha\cdot\nabla)\psi\|_{L^2(\mathcal{U})^4} = 0.$$

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 $\mathcal{U}$ is bounded, then the above considerations and the fact that $\mathrm{dom}(H_{\mathrm{MIT}}(m)) \subset H^{1/2}(\mathcal{U})^4$ is compactly embedded in $L^2(\mathcal{U})^4$ yield $\mathrm{Sp}(H_{\mathrm{MIT}}(m)) = \mathrm{Sp}_{\mathrm{disc}}(H_{\mathrm{MIT}}(m)) \subset \mathbb{R}\setminus[-m, m]$, which shows assertion (i).

To finish the proof of (ii), suppose $\mathcal{U}$ is unbounded. We first show $(-\infty, -m]\cup[m, +\infty)$ is contained in $\mathrm{Sp}_{\mathrm{ess}}(H_{\mathrm{MIT}}(m))$ by constructing Weyl sequences as in the case of half-space; see [Benhellal 2022b, Theorem 4.1]. As $\mathcal{U}$ is unbounded, 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 $\mathcal{U}$ and $\mathbb{R}^3 \setminus \overline{\mathcal{U}} \subset B(0, R_1)$. 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 $\varphi : \mathbb{R}^3 \to \mathbb{C}^4$ by

$$\varphi(\bar{x}, x_3) = \left(\frac{\xi_1 - i\xi_2}{\lambda - m}, 0, 0, 1\right)^t e^{i\xi\cdot\bar{x}}, \quad \text{with } \bar{x} = (x_1, x_2).$$

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

$$\varphi_n(\bar{x}, x_3) = n^{-3/2}\varphi(\bar{x}, x_3)\eta(\bar{x}/n)\chi(x_3/n) \quad \text{for } (\bar{x}, x_3) \in \mathcal{U}.$$

Then, it is easy to check that $\varphi_n \in H_0^1(\mathcal{U}) \subset \mathrm{dom}(H_{\mathrm{MIT}}(m))$, $(\varphi_n)_{n\in\mathbb{N}^\star}$ converges weakly to zero, and

$$\|\varphi_n\|^2_{L^2(\mathcal{U})^4} = \frac{2\lambda}{\lambda - m}\|\eta\|^2_{L^2(\mathbb{R}^2)}\|\chi\|^2_{L^2(\mathbb{R})} > 0, \qquad \frac{\|(D_m - \lambda)\varphi_n\|_{L^2(\mathcal{U})^4}}{\|\varphi_n\|_{L^2(\mathcal{U})^4}} \xrightarrow[n\to\infty]{} 0;$$

for more details see the proof of [Benhellal 2022b, Theorem 4.1]. Therefore, Weyl's criterion yields

$$(-\infty, -m)\cup(m, +\infty) \subset \mathrm{Sp}_{\mathrm{ess}}(H_{\mathrm{MIT}}(m)).$$

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 $\mathcal{U}$ is connected, then using the same arguments as in the proof of [Arrizabalaga et al. 2015, Theorem 3.7] (i.e., using Rellich's lemma and the unique continuation property), one can verify 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 (3-4) yields that $\|H_{\mathrm{MIT}}(m)\psi\|^2_{L^2(\Omega)^4} \geqslant m^2\|\psi\|^2_{L^2(\Omega)^4}$, and thus

$$m\|\psi\|_{L^2(\mathcal{U})^4} \leqslant \|H_{\mathrm{MIT}}(m)\psi\|_{L^2(\mathcal{U})^4} \leqslant \|(H_{\mathrm{MIT}}(m) - z)\psi\|_{L^2(\mathcal{U})^4} + |z|\|\psi\|_{L^2(\mathcal{U})^4}.$$

Therefore, for $2|z| < m$ with $z \in \rho(H_{\mathrm{MIT}}(m))$, we get that $\|\psi\|_{L^2(\mathcal{U})^4} \leqslant 2m^{-1}\|(H_{\mathrm{MIT}}(m) - z)\psi\|_{L^2(\mathcal{U})^4}$. Thus, (iii) follows by taking $\psi = (H_{\mathrm{MIT}}(m) - z)^{-1} f$. □

Remark 3.2. We mention that the above statement on the self-adjointness can also be deduced from [Behrndt et al. 2021, Theorem 5.4]. We also mention that the MIT bag operator defined on the domain $\mathscr{D}$ given by (3-3) is still self-adjoint for less regular domains; see [Benhellal 2022a] for more details.

Remark 3.3. Note that if $\mathcal{U}$ is in the class of Hölder's domains $C^{1,\omega}$, with $\omega \in \left(\frac{1}{2}, 1\right)$, then $H_{\mathrm{MIT}}(m)$ is self-adjoint and $\mathrm{dom}(H_{\mathrm{MIT}}(m)) := \{\psi \in H^1(\mathcal{U})^4 : P_- t_{\partial\mathcal{U}}\psi = 0 \text{ on } \partial\mathcal{U}\}$; see [Benhellal 2022a, Theorem 4.3] for example.

Now we establish regularity results concerning the regularization property of the resolvent and the Sobolev regularity of the eigenfunctions of $H_{\mathrm{MIT}}(m)$. The first statement of the following theorem will be crucial in Section 5 when studying the semiclassical pseudodifferential properties of the Poincaré–Steklov operator.

Theorem 3.4. *Let $k \geqslant 1$ be an integer and assume that $\mathcal{U}$ is C^{2+k}-smooth. Then the following statements hold*:

(i) *The mapping $(H_{\mathrm{MIT}}(m)-z)^{-1} : H^k(\mathcal{U})^4 \to H^{k+1}(\mathcal{U})^4 \cap \mathrm{dom}(H_{\mathrm{MIT}}(m))$ is well defined and bounded for all $m > 0$ and all $z \in \rho(H_{\mathrm{MIT}}(m))$. Moreover, for any compact set $K \subset \mathbb{C}$, there exist $m_0, C > 0$ such that, for all $m \geqslant m_0$ and $z \in K$,*

$$\|(H_{\mathrm{MIT}}(m) - z)^{-1}\|_{H^{k-1}(\mathcal{U})^4 \to H^k(\mathcal{U})^4} \leq C m^{k-1}.$$

(ii) *If ϕ is an eigenfunction associated with an eigenvalue $z \in \mathrm{Sp}(H_{\mathrm{MIT}}(m))$, i.e., $(H_{\mathrm{MIT}}(m) - z)\phi = 0$, then $\phi \in H^{1+k}(\mathcal{U})^4$. In particular, if $\mathcal{U}$ is C^∞-smooth, then $\phi \in C^\infty(\mathcal{U})^4$.*

To prove this theorem we need the following classical regularity result.

Proposition 3.5. *Let k be a nonnegative integer. Assume that $\mathcal{U}$ is C^{3+k}-smooth and $u \in H^1(\mathcal{U})$. If u solves the Neumann problem*

$$-\Delta u = f \in H^k(\mathcal{U}) \quad \textit{and} \quad \partial_n u = g \in H^{1/2+k}(\partial\mathcal{U}),$$

then $u \in H^{2+k}(\mathcal{U})$.

Proof. First, assume that $k = 0$. As $\mathcal{U}$ is C^3-smooth we know the Neumann trace $\partial_n : H^2(\mathcal{U}) \to H^{1/2}(\partial\mathcal{U})$ is surjective. Thus, there is $G \in H^2(\mathcal{U})$ such that $\partial_n G = g$ in $\partial\mathcal{U}$. Note that the function $\tilde{u} = u - G$ satisfies the homogeneous Neumann problem

$$-\Delta\tilde{u} = f + \Delta G \quad \text{in } \mathcal{U} \qquad \text{and} \qquad \partial_n \tilde{u} = 0 \quad \text{on } \partial\mathcal{U}.$$

Therefore, $\tilde{u} \in H^2(\mathcal{U})$ by [Mikhailov 1978, Theorem 5, p. 217], which implies that $u \in H^2(\mathcal{U})$, and this proves the result for $k = 0$. If $k \geqslant 1$, then the result follows by [Grisvard 1985, Theorem 2.5.1.1]. ☐

Proof of Theorem 3.4. We prove the theorem 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 $\mathcal{U}$, with $f = (f_1, f_2)^\top \in H^1(\mathcal{U})^4$. By assumption we have $(\Delta + m^2 - z^2)\phi = (D_m + z) f$ in $\mathcal{D}'(\mathcal{U})^4$, and then also in $L^2(\mathcal{U})^4$. We next prove that $\partial_n\phi \in H^{1/2}(\partial\mathcal{U})^4$. To this end, consider $\mathcal{U}_\epsilon := \{x \in \mathbb{R}^3 : \mathrm{dist}(x, \partial\mathcal{U}) < \epsilon\}$ for $\epsilon > 0$. Then, for $\delta > 0$ small enough and $0 < \epsilon \leqslant \delta$, the mapping $\Psi : \partial\mathcal{U} \times (-\epsilon, \epsilon) \to \mathcal{U}_\epsilon$, defined by

$$\Psi(x_{\partial\mathcal{U}}, t) = x_{\partial\mathcal{U}} + t n(x_{\partial\mathcal{U}}), \qquad x_{\partial\mathcal{U}} \in \partial\mathcal{U}, \quad t \in (-\epsilon, \epsilon), \tag{3-5}$$

is a C^2-diffeomorphism and $\mathcal{U}_\epsilon := \{x + t n(x) : x \in \partial\mathcal{U}, t \in (-\epsilon, \epsilon)\}$.

Let $\widetilde{P}_- : L^2(\mathcal{U}_\epsilon \cap \mathcal{U})^4 \to L^2(\mathcal{U}_\epsilon \cap \mathcal{U})^4$ be the bounded operator defined by

$$\widetilde{P}_-\varphi(\Psi(x,t)) = \tfrac{1}{2}(1 + i\beta(\alpha \cdot n(x)))\varphi(\Psi(x,t)), \quad \Psi(x,t) \in \mathcal{U}_\epsilon \cap \mathcal{U}.$$

Let $x^0_{\partial\mathcal{U}}$ be an arbitrary point on the boundary $\partial\mathcal{U}$, fix $0 < r < \frac{1}{2}\epsilon$, and let $\zeta : \mathbb{R}^3 \to [0,1]$ be a C^∞-smooth and compactly supported function such that $\zeta = 1$ on $B(x^0_{\partial\mathcal{U}}, r)$ and $\zeta = 0$ on $\mathbb{R}^3 \setminus B(x^0_{\partial\mathcal{U}}, 2r)$. We claim that $\widetilde{P}_-\zeta\phi$ satisfies the elliptic problem

$$\begin{cases} -\Delta(\widetilde{P}_-\zeta\phi) = g & \text{in } \mathcal{U}, \\ t_{\partial\mathcal{U}}(\widetilde{P}_-\zeta\phi) = 0 & \text{on } \partial\mathcal{U}, \end{cases}$$

with $g \in L^2(\mathcal{U})^4$. Indeed, set $\mathcal{B}(x) = i\beta(\alpha \cdot n(x))$ for $x \in \partial\mathcal{U}$, and observe that

$$(D_m - z)(\widetilde{P}_-\zeta\phi) = \big(\widetilde{P}_-\zeta f + \tfrac{1}{2}[D_m, \zeta]\phi\big) + \tfrac{1}{2}[D_m, \zeta\mathcal{B}]\phi =: I(\phi, f) + \tfrac{1}{2}[D_m, \zeta\mathcal{B}]\phi.$$

Since n is C^2-smooth, ζ is an infinitely differentiable scalar function, and $\phi, f \in H^1(\mathcal{U})^4$, it is clear that $I(\phi, f) \in H^1(\mathcal{U})^4$ and $[D_m, \zeta\mathcal{B}]\phi \in L^2(\mathcal{U})^4$. Now, applying $(D_m + z)$ to the above equation yields $-\Delta(\widetilde{P}_-\zeta\phi) = g$, with

$$g := (z^2 - m^2)\widetilde{P}_-\zeta\phi + (D_m + z)I(\phi, f) + \tfrac{1}{2}z[D_m, \zeta\mathcal{B}]\phi + \tfrac{1}{2}D_m[D_m, \zeta\mathcal{B}]\phi.$$

As before, it is clear that the first three terms are square integrable. Next, observe that

$$D_0[D_0, \zeta\mathcal{B}]\phi = \{D_0, [D_0, \zeta\mathcal{B}]\}\phi - [D_0, \zeta\mathcal{B}]D_0\phi = [-\Delta, \zeta\mathcal{B}]\phi - [D_0, \zeta\mathcal{B}]((D_m - z)\phi - (m\beta - z)\phi),$$

where $\{A, B\} =: AB + BA$ is the anticommutator bracket. Using this, the smoothness assumption on n, the facts that $(D_m - z)\phi = f \in H^1(\mathcal{U})^4$ and that $[D_0, \zeta\mathcal{B}]$ and $[-\Delta, \zeta\mathcal{B}]$ are first-order differential operators, we easily see that $D_0[D_0, \zeta\mathcal{B}]\phi \in L^2(\mathcal{U})^4$. Hence, $D_m[D_m, \zeta\mathcal{B}]\phi$ is square integrable, which means that $g \in L^2(\mathcal{U})^4$. As $P_- t_{\partial\mathcal{U}}\phi = 0$ and $t_{\partial\mathcal{U}}(\widetilde{P}_-\zeta\phi) = t_{\partial\mathcal{U}}\zeta P_- t_{\partial\mathcal{U}}\phi = 0$ on $\partial\mathcal{U}$, by [Gilbarg and Trudinger 1983, Theorem 8.12], it follows that $\widetilde{P}_-\zeta\phi \in H^2(\mathcal{U}_\epsilon \cap \mathcal{U})^4$, which implies

$$\zeta(\phi_1 + i(\sigma \cdot n)\phi_2) \in H^2(B(x^0_{\partial\mathcal{U}}, 2r) \cap \mathcal{U})^2 \quad \text{and} \quad \zeta(-i(\sigma \cdot n)\phi_1 + \phi_2) \in H^2(B(x^0_{\partial\mathcal{U}}, 2r) \cap \mathcal{U})^2.$$

Consequently, we get

$$\phi_1 + i(\sigma \cdot n)\phi_2 \in H^2(B(x^0_{\partial\mathcal{U}}, r) \cap \mathcal{U})^2 \quad \text{and} \quad -i(\sigma \cdot n)\phi_1 + \phi_2 \in H^2(B(x^0_{\partial\mathcal{U}}, r) \cap \mathcal{U})^2. \tag{3-6}$$

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 $H^1(\mathcal{U})^2$, it follows from (3-6) that

$$(\sigma \cdot \nabla)\phi_j \in H^1(B(x^0_{\partial\mathcal{U}}, r))^2 \quad \text{and} \quad (\sigma \cdot \nabla)(\sigma \cdot n)\phi_j \in H^1(B(x^0_{\partial\mathcal{U}}, r))^2, \quad j = 1, 2.$$

Using this and the fact that n is C^2-smooth, we easily get

$$(\sigma \cdot n)(\sigma \cdot \nabla)\phi_j + (\sigma \cdot \nabla)(\sigma \cdot n)\phi_j = (n \cdot \nabla)\phi_j + F_j \in H^1(B(x^0_{\partial\mathcal{U}}, r))^2,$$

with $F_j \in H^1(B(x^0_{\partial\mathcal{U}}, r) \cap \mathcal{U})^2$. As a consequence, we get $(n \cdot \nabla)\phi_j \in H^1(B(x^0_{\partial\mathcal{U}}, r) \cap \mathcal{U})^2$. Since this holds true for all $x^0_{\partial\mathcal{U}} \in \partial\mathcal{U}$, using the compactness of $\partial\mathcal{U}$, it follows that $\partial_n\phi \in H^{1/2}(\partial\mathcal{U})^4$. Therefore, Proposition 3.5 yields $\phi \in H^2(\mathcal{U})^4$.

Next, assume $k \geqslant 2$, $\mathcal{U}$ is C^{2+k}-smooth, and ϕ, $f \in H^k(\mathcal{U})^4$. Since n is C^{1+k}-smooth and Ψ defined by (3-5) is a C^{1+k}-diffeomorphism, following the same arguments as above we then conclude that $\partial_n\phi \in H^{k-1/2}(\partial\mathcal{U})^4$. Note also that $-\Delta\phi = (z^2 - m^2)\phi + (D_m - z)f \in H^{k-1}(\mathcal{U})^4$. Therefore, thanks to Proposition 3.5, we conclude that $\phi \in H^{k+1}(\mathcal{U})^4$, which proves the first statement of (i).

Now, the second statement of (i) is a consequence of the first one, Theorem 3.1(iii), and the Gårding-type inequality

$$\|\varphi\|^2_{H^{k+1}(\mathcal{U})^4} \lesssim \|\varphi\|^2_{H^k(\mathcal{U})^4} + \|D_0\varphi\|^2_{H^k(\mathcal{U})^4}, \tag{3-7}$$

which holds for any $\varphi \in \operatorname{dom}(H_{\mathrm{MIT}}(m)) \cap H^{k+1}(\mathcal{U})^4$, $k \in \mathbb{N}$. Indeed, suppose for instance that (3-7) holds true. Fix a compact set $K \subset \mathbb{C}$, and let $z \in K$. Note that if $z \in \rho(H_{\mathrm{MIT}}(m))$ then, for $\psi \in H^k(\mathcal{U})^4$, $k \geq 0$, we have

$$\|D_0(H_{\mathrm{MIT}}(m) - z)^{-1}\psi\|_{H^k(\mathcal{U})^4} \leq \|\psi\|_{H^k(\mathcal{U})^4} + (m + |z|)\|(H_{\mathrm{MIT}}(m) - z)^{-1}\psi\|_{H^k(\mathcal{U})^4}. \tag{3-8}$$

Let us also remark that Theorem 3.1(iii) gives that there is $m_0 > 0$ such that $z \in \rho(H_{\mathrm{MIT}}(m))$ for any $m \geq m_0$ and, for any $\psi \in H^k(\mathcal{U})^4$, $k \geq 0$,

$$\|D_0(H_{\mathrm{MIT}}(m) - z)^{-1}\psi\|_{L^2(\mathcal{U})^4} \lesssim \|\psi\|_{L^2(\mathcal{U})^4} \leq \|\psi\|_{H^k(\mathcal{U})^4}. \tag{3-9}$$

Hence, by iterating the Gårding inequality and taking into account (3-8) and (3-9), we get

$$\|D_0(H_{\mathrm{MIT}}(m) - z)^{-1}\psi\|_{H^k(\mathcal{U})^4} \lesssim m^k\|\psi\|_{H^k(\mathcal{U})^4},$$

and the conclusion follows by applying again the Gårding inequality. We now return to the proof of (3-7). Let $\varphi \in \operatorname{dom}(H_{\mathrm{MIT}}(m))$. Then [Arrizabalaga et al. 2017, Theorem 1.5] yields

$$\|D_0\varphi\|^2_{L^2(\mathcal{U})^4} = \|\nabla\varphi\|^2_{L^2(\mathcal{U})^4} + \int_{\partial\mathcal{U}} H_1|t_{\partial\mathcal{U}}\varphi|^2\, d\sigma, \tag{3-10}$$

where we recall that $H_1(x)$ is the mean curvature at $x \in \partial\mathcal{U}$. Recall that, for any $\epsilon > 0$, there is $C_\epsilon > 0$ such that

$$\|t_{\partial\mathcal{U}}\varphi\|_{L^2(\partial\mathcal{U})^4} \leq \epsilon\|\nabla\varphi\|^2_{L^2(\mathcal{U})^4} + C_\epsilon\|\varphi\|^2_{L^2(\mathcal{U})^4} \quad \text{for all } \varphi \in H^1(\mathcal{U})^4;$$

see [Barbaroux et al. 2019, Remark 1]. Using this inequality with ϵ sufficiently small and estimating (3-10) we get, for all $\varphi \in H^1(\mathcal{U})^4$,

$$\|\varphi\|^2_{H^1(\mathcal{U})^4} = \|\varphi\|^2_{L^2(\mathcal{U})^4} + \|\nabla\varphi\|^2_{L^2(\mathcal{U})^4} \lesssim \|\varphi\|^2_{L^2(\mathcal{U})^4} + \|D_0\varphi\|^2_{L^2(\mathcal{U})^4},$$

which shows (3-7) for $k = 0$. Note that by local arguments one has

$$\|\varphi\|^2_{H^{k+1}(\mathcal{U})^4} \lesssim \|\varphi\|^2_{L^2(\mathcal{U})^4} + \sum_j \|\partial_j\varphi\|^2_{H^k(\mathcal{U})^4},$$

and since $[\partial_j, D_0] = 0$, (3-7) easily follows by induction for any $k \geq 1$.

Finally, the proof of the first statement of (ii) follows the same lines as the one of (i). In particular, if $\mathcal{U}$ is C^∞-smooth, we then get $\phi \in H^{k+1}(\mathcal{U})^4$ for any $k \geqslant 0$, which implies that ϕ is infinitely differentiable in $\mathcal{U}$, and the theorem is proved. □

Remark 3.6. Note that the estimate in Theorem 3.4(i) is certainly not sharp, but it will be enough for our purposes.

4. Poincaré–Steklov operators as pseudodifferential operators

The main purpose of this section is to introduce the Poincaré–Steklov operator $\mathscr{A}_m$ associated with the MIT bag 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, and let $P_\pm$ be as in (2-1). Let us start by giving the rigorous definition of the Poincaré–Steklov operator, which is the main subject of this paper.

Definition 4.1 (PS operator). Let $z \in \rho(H_{\mathrm{MIT}}(m))$ 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

$$\begin{cases} (D_m - z)U_z = 0 & \text{in } \Omega, \\ P_- t_\Sigma U_z = g & \text{on } \Sigma. \end{cases} \tag{4-1}$$

That is, $E_m^\Omega(z)g$ is the unique function in $H^1(\Omega)^4$ satisfying the equations $(D_m - z)E_m^\Omega(z)g = 0$ in Ω and $P_- t_\Sigma E_m^\Omega(z)g = g$ on Σ. Then, the Poincaré–Steklov (PS) operator $\mathscr{A}_m : P_- H^{1/2}(\Sigma)^4 \to P_+ H^{1/2}(\Sigma)^4$ associated with the system (4-1) 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 Section 2B. Then, the following proposition justifies the existence and the uniqueness of the solution to the elliptic problem (4-1), and gives in particular the explicit formula of the PS operator in terms of the operator $(\Lambda_m^z)^{-1}$ when $z \in \rho(D_m)$. The second assertion of the proposition will be particularly important in Section 5 when studying the PS operator from the semiclassical point of view. In the last statement, we use the notation $\mathscr{A}_m(z)$ to highlight the dependence on the parameter $z \in \rho(H_{\mathrm{MIT}}(m))$.

Proposition 4.2. *For any $z \in \rho(H_{\mathrm{MIT}}(m))$ and $g \in P_- H^{1/2}(\Sigma)^4$, the elliptic problem (4-1) has a unique solution $E_m^\Omega(z)[g] \in H^1(\Omega)^4$. Moreover, the following hold:*

(i) $(E_m^\Omega(z))^* = -\beta P_+ t_\Sigma (H_{\mathrm{MIT}}(m) - \bar{z})^{-1}$.

(ii) *For any compact set $K \subset \mathbb{C}$, there is $m_0 > 0$ such that, for all $m \geqslant m_0$, we have $K \subset \rho(H_{\mathrm{MIT}}(m))$ and, for all $z \in K$, we have*

$$\|E_m^\Omega(z)g\|_{L^2(\Omega)^4} \lesssim \frac{1}{\sqrt{m}} \|g\|_{L^2(\Sigma)^4} \quad \textit{for all } g \in P_- H^{1/2}(\Sigma)^4.$$

(iii) *If $z \in \rho(D_m)$, then $E_m^\Omega(z)$ and $\mathscr{A}_m$ are explicitly given by*

$$E_m^\Omega(z) = \Phi_{z,m}^\Omega (\Lambda_m^z)^{-1} P_- \quad \textit{and} \quad \mathscr{A}_m = -P_+ \beta (\Lambda_m^z)^{-1} P_-. \tag{4-2}$$

(iv) *Let $z \in \rho(H_{\mathrm{MIT}}(m))$, and let $E_m^\Omega(z)$ be as above. Then, for any $\xi \in \rho(H_{\mathrm{MIT}}(m))$, the operator $E_m^\Omega(\xi)$ has the representation*

$$E_m^\Omega(\xi) = (I_4 + (\xi - z)(H_{\mathrm{MIT}}(m) - \xi)^{-1})E_m^\Omega(z). \tag{4-3}$$

In particular, we have

$$\mathscr{A}_m(\xi) - \mathscr{A}_m(z) = (z-\xi)\beta(E_m^\Omega(\bar{\xi}))^* E_m^\Omega(z). \tag{4-4}$$

(v) *For any $z \in \rho(H_{\mathrm{MIT}}(m))$, the operator $E_m^\Omega(z)$ extends into a bounded operator from $P_- H^{-1/2}(\Sigma)^4$ to $H(\alpha, \Omega)$.*

Proof. We first show that the boundary value problem (4-1) has a unique solution. For this, assume that u_1 and u_2 are both solutions of (4-1). Then $(D_m - z)(u_1 - u_2) = 0$ in Ω and $P_- t_\Sigma(u_1 - u_2) = 0$ on Σ. Thus, $(u_1 - u_2) \in \mathrm{dom}(H_{\mathrm{MIT}}(m))$ holds by Remark 3.3, and since $H_{\mathrm{MIT}}(m)$ is injective by Theorem 3.1 it follows that $u_1 = u_2$, which proves the uniqueness. Next, observe that the function

$$v_g = \mathcal{E}_\Omega(P_- g) - (H_{\mathrm{MIT}}(m) - z)^{-1}(D_m - z)\mathcal{E}_\Omega(P_- g)$$

is a solution to (4-1). Indeed, we have $\mathcal{E}_\Omega(P_- g) \in H^1(\Omega)^4$ 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 (4-1) is unique, it follows that v_g is independent of the extension operator $\mathcal{E}_\Omega$, and hence there is a unique solution in $H^1(\Omega)^4$ to the elliptic problem (4-1).

Let us show the assertion (i). Let $\psi \in P_- H^{1/2}(\Sigma)^4$ and $f \in L^2(\Omega)^4$. Then, using Green's formula and the fact that $P_+(-i\alpha \cdot n) = (-i\alpha \cdot n)P_- = -\beta P_-$, we get

$$\begin{aligned}
&\langle E_m^\Omega(z)\psi, f\rangle_{L^2(\Omega)^4} \\
&\quad = \langle E_m^\Omega(z)\psi, (H_{\mathrm{MIT}}(m) - \bar{z})(H_{\mathrm{MIT}}(m) - \bar{z})^{-1} f\rangle_{L^2(\Omega)^4} \\
&\quad = \langle E_m^\Omega(z)\psi, (D_m - \bar{z})(H_{\mathrm{MIT}}(m) - \bar{z})^{-1} f\rangle_{L^2(\Omega)^4} \\
&\quad = \langle (D_m - z)E_m^\Omega(z)\psi, (H_{\mathrm{MIT}}(m) - \bar{z})^{-1} f\rangle_{L^2(\Omega)^4} + \langle (-i\alpha \cdot n)t_\Sigma E_m^\Omega(z)\psi, t_\Sigma(H_{\mathrm{MIT}}(m) - \bar{z})^{-1} f\rangle_{L^2(\Sigma)^4} \\
&\quad = \langle (-i\alpha \cdot n)P_- t_\Sigma E_m^\Omega(z)\psi, P_+ t_\Sigma(H_{\mathrm{MIT}}(m) - \bar{z})^{-1} f\rangle_{L^2(\Sigma)^4} \\
&\quad = \langle \psi, -\beta P_+ t_\Sigma(H_{\mathrm{MIT}}(m) - \bar{z})^{-1} f\rangle_{L^2(\Sigma)^4},
\end{aligned}$$

which gives that $-\beta P_+ t_\Sigma(H_{\mathrm{MIT}}(m) - \bar{z})^{-1}$ is the adjoint of $E_m^\Omega(z)$ and proves (i).

Now we are going to show assertion (ii). So, let K be a compact set of $\mathbb{C}$, and note that, for all $m > \sup\{|\mathrm{Re}(z)| : z \in K\}$, we have 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 Green's formula yields

$$\begin{aligned}
0 &= \|(D_m - z)v\|^2_{L^2(\Omega)^4} \\
&= \|(i\alpha \cdot \nabla - z)v\|^2_{L^2(\Omega)^4} + m^2\|v\|^2_{L^2(\Omega)^4} + m(\langle -i(\alpha \cdot n)t_\Sigma v, \beta t_\Sigma v\rangle_{L^2(\Sigma)^4} - 2\,\mathrm{Re}(z)\langle v, \beta v\rangle_{L^2(\Omega)^4}).
\end{aligned} \tag{4-5}$$

Observe that

$$\langle -i(\alpha \cdot n)t_\Sigma v, \beta t_\Sigma v\rangle_{L^2(\Sigma)^4} = \langle (P_+ - P_-)t_\Sigma v, t_\Sigma v\rangle_{L^2(\Sigma)^4} = \|P_+ t_\Sigma v\|^2_{L^2(\Sigma)^4} - \|P_- t_\Sigma v\|^2_{L^2(\Sigma)^4}.$$

Since $P_- t_\Sigma v = g$ and $P_+ t_\Sigma v = \mathscr{A}_m(g)$ hold by definition and

$$-\mathrm{Re}(z)\langle v, \beta v\rangle_{L^2(\Omega)^4} \geqslant -|\mathrm{Re}(z)|\,\|v\|^2_{L^2(\Omega)^4}$$

holds by the Cauchy–Schwarz inequality, it follows from (4-5) 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

$$\|\mathscr{A}_m(g)\|^2_{L^2(\Sigma)^4} + \tfrac{1}{2}m\|v\|^2_{L^2(\Omega)^4} \leqslant \|g\|^2_{L^2(\Sigma)^4}$$

for any $m \geqslant m_0$, which proves the desired estimate for $E^\Omega_m(z)$.

Let us now show the assertion (iii). 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 2.1. Since ϕ^z_m is a fundamental solution of $(D_m - z)$,

$$(D_m - z)\Phi^\Omega_{z,m}(\Lambda^z_m)^{-1}[g] = 0 \quad \text{in } L^2(\Omega)^4 \qquad \text{for all } g \in H^{1/2}(\Sigma)^4.$$

Now, observe that if $g \in P_- H^{1/2}(\Sigma)^4$, then a direct application of the identity (2-7) yields

$$t_\Sigma \Phi^\Omega_{z,m}(\Lambda^z_m)^{-1}[g] = \bigl(-\tfrac{1}{2}i(\alpha\cdot n) + \mathscr{C}_{z,m}\bigr)(\Lambda^z_m)^{-1}[g] = g - P_+\beta(\Lambda^z_m)^{-1}[g].$$

Consequently, we get

$$P_- t_\Sigma \Phi^\Omega_{z,m}(\Lambda^z_m)^{-1}[g] = g \quad \text{and} \quad P_+ t_\Sigma \Phi^\Omega_{z,m}(\Lambda^z_m)^{-1}[g] = -P_+\beta(\Lambda^z_m)^{-1}[g],$$

which means that $E^\Omega_m(z)[g] = \Phi^\Omega_{z,m}(\Lambda^z_m)^{-1}[g]$ is the unique solution to the boundary value problem (4-1) and proves the identity $\mathscr{A}_m = -P_+\beta(\Lambda^z_m)^{-1}P_-$.

We now prove assertion (iv). Fix $z, \xi \in \rho(H_{\mathrm{MIT}}(m))$, and let $g \in P_- H^{1/2}(\Sigma)^4$. Then, by the definition of $E^\Omega_m(z)$, we have

$$\begin{aligned}(D_m - \xi)(1 + (\xi - z)&(H_{\mathrm{MIT}}(m) - \xi)^{-1})E^\Omega_m(z)g \\ &= (D_m - z)E^\Omega_m(z)g - (\xi - z)E^\Omega_m(z)g + (\xi - z)(D_m - \xi)(H_{\mathrm{MIT}}(m) - \xi)^{-1}E^\Omega_m(z)g \\ &= (\xi - z)E^\Omega_m(z)g - (\xi - z)E^\Omega_m(z)g = 0.\end{aligned}$$

Since $(H_{\mathrm{MIT}}(m) - \xi)^{-1}E^\Omega_m(z)g \in \mathrm{dom}(H_{\mathrm{MIT}}(m))$, and hence $P_- t_\Sigma(H_{\mathrm{MIT}}(m) - \xi)^{-1}E^\Omega_m(z)g = 0$, it follows that $P_- t_\Sigma(1 + (\xi - z)(H_{\mathrm{MIT}}(m) - \xi)^{-1})E^\Omega_m(z)g = P_- t_\Sigma E^\Omega_m(z)g = g$, which prove identity (4-3). Now, (4-4) follows by applying $P_+ t_\Sigma$ to the representation (4-3) and using assertion (i).

It remains to prove item (v). We first consider the case $z \in \rho(D_m)$. For $z \in \rho(H_{\mathrm{MIT}}(m)) \setminus \rho(D_m)$, the claim follows by the representation formula (4-3). Fix $z \in \rho(D_m)$, and recall that the operators $\mathscr{C}_{z,m}$ and Λ^z_m are bounded invertible in $H^{1/2}(\Sigma)^4$ by Lemma 2.1(ii)–(iii) and (2-6). Since $\mathscr{C}^*_{z,m} = \mathscr{C}_{\bar{z},m}$, by duality it follows that Λ^z_m admits a bounded and everywhere defined inverse in $H^{-1/2}(\Sigma)^4$. This together with Lemma 2.1(i) and item (iii) of this proposition show that $E^\Omega_m(z)$ admits a continuous extension from $P_- H^{-1/2}(\Sigma)^4$ to $H(\alpha, \Omega)$. This completes the proof of the proposition. □

Remark 4.3. 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

$$\sup_{m \geqslant m_1} \|\mathscr{A}_m\|_{P_- H^{1/2}(\Sigma)^4 \to P_+ L^2(\Sigma)^4} \lesssim 1.$$

Remark 4.4. Thanks to Theorem 3.1 and Remark 2.2, if Ω is a Lipschitz domain, then $E_m^{\Omega}(z)$ is the unique solution in $H^{1/2}(\Omega)^4$ to the system (4-1) 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 4.1 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 (4-2) and the symbol calculus to obtain the principal symbol of $\mathscr{A}_m$.

Recall the definition of ϕ_m^z from (2-3), and observe that

$$\phi_m^z(x-y) = k^z(x-y) + w(x-y),$$

where

$$k^z(x-y) = \frac{e^{i\sqrt{z^2-m^2}|x-y|}}{4\pi|x-y|}\left(z + m\beta + \sqrt{z^2-m^2}\alpha\cdot\frac{x-y}{|x-y|}\right) + i\frac{e^{i\sqrt{z^2-m^2}|x-y|}-1}{4\pi|x-y|^3}\alpha\cdot(x-y),$$
$$w(x-y) = \frac{i}{4\pi|x-y|^3}\alpha\cdot(x-y).$$

Using this, it follows that

$$\begin{aligned}\mathscr{C}_{z,m}[f](x) &= \lim_{\rho\searrow 0}\int_{|x-y|>\rho} w(x-y)f(y)\,\mathrm{d}\sigma(y) + \int_\Sigma k^z(x-y)f(y)\,\mathrm{d}\sigma(y)\\ &= W[f](x) + K[f](x).\end{aligned} \tag{4-6}$$

As $|k^z(x-y)| = \mathcal{O}(|x-y|^{-1})$ when $|x-y|\to 0$, using the standard layer potential techniques (see, e.g., [Taylor 2000, Chapter 3, Section 4] and [Taylor 1996, Chapter 7, Section 11]), it is not hard to prove that the integral operator K gives rise to a pseudodifferential operator of order -1, i.e., $K \in \mathrm{Op}\,\mathcal{S}^{-1}(\Sigma)$. Thus, we can (formally) write

$$\mathscr{C}_{z,m} = W \mod \mathrm{Op}\,\mathcal{S}^{-1}(\Sigma), \tag{4-7}$$

which means that the 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 [Ando et al. 2019; Miyanishi 2022; Miyanishi and Rozenblum 2019].

Theorem 4.5. *Let $\mathscr{C}_{z,m}$ be as in (2-5), W as in (4-6), and $\mathscr{A}_m$ as in Definition 4.1. Then $\mathscr{C}_{z,m}$, W and $\mathscr{A}_m$ are homogeneous pseudodifferential operators of order* 0, *and we have*

$$\mathscr{C}_{z,m} = \frac{1}{2}\alpha\cdot\frac{\nabla_\Sigma}{\sqrt{-\Delta_\Sigma}} \mod \mathrm{Op}\,\mathcal{S}^{-1}(\Sigma),$$
$$\mathscr{A}_m = \frac{1}{\sqrt{-\Delta_\Sigma}}S\cdot(\nabla_\Sigma\wedge n)P_- \mod \mathrm{Op}\,\mathcal{S}^{-1}(\Sigma) = \frac{D_\Sigma}{\sqrt{-\Delta_\Sigma}}P_- \mod \mathrm{Op}\,\mathcal{S}^{-1}(\Sigma).$$

Proof. We first deal with the operator W. Let $\psi_k : \Sigma \to \mathbb{R}$, $k = 1, 2$, be a C^∞-smooth function. Clearly, if $\operatorname{supp}(\psi_2) \cap \operatorname{supp}(\psi_1) = \varnothing$, 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 Section 2C, and recall the definition of the first fundamental form I and the metric tensor $G(\tilde{x})$. That is, up to a rotation, for all $x \in U$, we have $x = \varphi(\tilde{x}) = (\tilde{x}, \chi(\tilde{x}))$ with $\tilde{x} \in V$, where the graph of $\chi : V \to \mathbb{R}$ coincides with U. Notice that if we assume that ψ_k is compactly supported with $\operatorname{supp}(\psi_k) \subset U$, then, in this setting, the operator $\psi_2 W \psi_1$ has the form

$$\begin{aligned}\psi_2 W[\psi_1 f](x) &= \psi_2(x)\,\text{p.v.}\int_V i\alpha \cdot \frac{\varphi(\tilde{x}) - \varphi(\tilde{y})}{4\pi|\varphi(\tilde{x}) - \varphi(\tilde{y})|^3}\psi_1(\varphi(\tilde{y}))f(\varphi(\tilde{y}))\sqrt{g(\tilde{y})}\,\mathrm{d}\tilde{y}\\ &= \psi_2(x)\sqrt{g(\tilde{x})}\,\text{p.v.}\int_V i\alpha \cdot \frac{\varphi(\tilde{x}) - \varphi(\tilde{y})}{4\pi|\varphi(\tilde{x}) - \varphi(\tilde{y})|^3}\psi_1(\varphi(\tilde{y}))f(\varphi(\tilde{y}))\,\mathrm{d}\tilde{y}\\ &\qquad + \psi_2(x)\int_V i\alpha \cdot \frac{\varphi(\tilde{x}) - \varphi(\tilde{y})}{4\pi|\varphi(\tilde{x}) - \varphi(\tilde{y})|^3} f(\varphi(\tilde{y}))(\sqrt{g(\tilde{y})} - \sqrt{g(\tilde{x})})\,\mathrm{d}\tilde{y},\end{aligned} \tag{4-8}$$

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 (4-8) has a nonsingular kernel and does not require us to write it as an integral operator in the principal value sense. Thus, a simple computation using Taylor's formula shows

$$|x - y|^2 = |\varphi(\tilde{x}) - \varphi(\tilde{y})|^2 = \langle \tilde{x} - \tilde{y}, G(\tilde{x})(\tilde{x} - \tilde{y})\rangle(1 + \mathcal{O}|\tilde{x} - \tilde{y}|),$$

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

$$\frac{x_j - y_j}{|x - y|^3} = \begin{cases} \dfrac{\tilde{x}_j - \tilde{y}_j}{\langle \tilde{x} - \tilde{y}, G(\tilde{x})(\tilde{x} - \tilde{y})\rangle^{3/2}} + (\tilde{x}_j - \tilde{y}_j)k_1(\tilde{x}, \tilde{y}) & \text{for } j = 1, 2,\\ \dfrac{\langle \nabla\chi, \tilde{x} - \tilde{y}\rangle}{\langle \tilde{x} - \tilde{y}, G(\tilde{x})(\tilde{x} - \tilde{y})\rangle^{3/2}} + k_2(\tilde{x}, \tilde{y}) & \text{for } j = 3,\end{cases}$$

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

$$\alpha \cdot \left(\frac{x - y}{|x - y|^3}\right) = \alpha \cdot \frac{(\tilde{x} - \tilde{y}, \langle \nabla\chi, \tilde{x} - \tilde{y}\rangle)}{\langle \tilde{x} - \tilde{y}, G(\tilde{x})(\tilde{x} - \tilde{y})\rangle^{3/2}} + \mathcal{O}(|\tilde{x} - \tilde{y}|^{-1}).$$

Combining the above computations and (4-8), we deduce that

$$\begin{aligned}&\psi_2 W[\psi_1 f](x)\\ &\quad = \psi_2(x)\sqrt{g(\tilde{x})}\,\text{p.v.}\int_V i\alpha \frac{(\tilde{x} - \tilde{y}, \langle \nabla\chi, \tilde{x} - \tilde{y}\rangle)}{4\pi\langle \tilde{x} - \tilde{y}, G(\tilde{x})(\tilde{x} - \tilde{y})\rangle^{3/2}} f(\varphi(\tilde{y}))\,\mathrm{d}\tilde{y} + \psi_2(x)L[\psi_1 f](x),\end{aligned} \tag{4-9}$$

where L is an integral operator with a kernel $l(x, y)$ satisfying

$$|l(x, y)| = \mathcal{O}(|x-y|^{-1}) \quad \text{when } |x-y| \to 0.$$

Thus, similar arguments as the ones in [Taylor 1996, Chapter 7, Section 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, for $(\tilde{x}, \tau) \in \mathbb{R}^2 \times \mathbb{R}^2 \setminus \{0\}$,

$$r_k(\tilde{x}, \tau) = \frac{\tau_k}{\langle \tau, G(\tilde{x})\tau \rangle^{3/2}}.$$

Then the standard formula connecting a pseudodifferential operator and its symbol yields

$$R_k[h](\tilde{x}) = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2}\int_{\mathbb{R}^2} e^{i(\tilde{x}-\tilde{y})\cdot\xi} q_k(\tilde{x}, \xi) h(\tilde{y}) \, \mathrm{d}\xi \, \mathrm{d}\tilde{y},$$

where

$$q_k(\tilde{x}, \xi) = \frac{i\sqrt{g(\tilde{x})}}{4\pi} \int_{\mathbb{R}^2} e^{-i\omega\cdot\xi} r_k(\tilde{x}, \omega) \, \mathrm{d}\omega.$$

Recall the definition of Q from (2-10) and set $\omega = Q(\tilde{x})\tau$. Also recall that

$$\int_{\mathbb{R}^2} e^{-i\omega\cdot\xi} \frac{\omega_k}{|\omega|^3} \, \mathrm{d}\omega = -2\pi i \frac{\xi_k}{|\xi|}, \quad k = 1, 2. \tag{4-10}$$

Thus, the above change of variables together with the properties (2-11) and (4-10) yield

$$q_k(\tilde{x}, \xi) = \frac{i}{4\pi} \int_{\mathbb{R}^2} e^{-i(Q(\tilde{x})\tau)\cdot\xi} \frac{(Q(\tilde{x})\tau)_k}{|\tau|^3} \, \mathrm{d}\tau = \frac{(G^{-1}(\tilde{x})\xi)_k}{2\langle G^{-1}(\tilde{x})\xi, \xi\rangle^{1/2}} = \frac{g_{k1}\xi_1 + g_{k2}\xi_2}{2\langle G^{-1}(\tilde{x})\xi, \xi\rangle^{1/2}},$$

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. From the above observation and (4-9) it follows that

$$\psi_2 W \psi_1 = \psi_2 \alpha \cdot (R_1, R_2, \partial_1\chi(\tilde{x})R_1 + \partial_2\chi(\tilde{x})R_2)\psi_1 + \psi_2 L \psi_1.$$

Since L is a pseudodifferential operator of order -1, we deduce that W is a homogeneous pseudodifferential operator of order 0, and exploiting (2-12), we obtain

$$W = \frac{1}{2}\alpha \cdot \frac{\nabla_\Sigma}{\sqrt{-\Delta_\Sigma}} \mod \operatorname{Op}\mathcal{S}^{-1}(\Sigma). \tag{4-11}$$

Thanks to (4-7) and (4-11), 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

$$\frac{1}{2}\left(\beta + \alpha \cdot \frac{\nabla_\Sigma}{\sqrt{-\Delta_\Sigma}}\right)^2 = I_4 \tag{4-12}$$

and, as $\mathscr{A}_m$ is given by the formula

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

using (4-12) 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

$$q_{\mathscr{A}_m}(\tilde{x},\xi) = -P_+\beta\left(\beta + \alpha\cdot\left(\frac{\xi_G}{\langle G^{-1}\xi,\xi\rangle^{1/2}}\right)\right)P_- + p(\tilde{x},\xi),$$

where $p \in \mathcal{S}^{-1}(\Sigma)$ and ξ_G defined in (2-12) is the principal symbol of ∇_Σ. Therefore, we get

$$q_{\mathscr{A}_m}(\tilde{x},\xi) = -P_+\beta\alpha\cdot\xi_G\langle G^{-1}\xi,\xi\rangle^{-1/2}P_- + p(\tilde{x},\xi).$$

Hence, using the fact that $P_\pm$ are projectors and Lemma A.3, we obtain

$$q_{\mathscr{A}_m}(\tilde{x},\xi) = -i\alpha\cdot n^{\varphi}(\tilde{x})\alpha\cdot\xi_G\langle G^{-1}\xi,\xi\rangle^{-1/2}P_- + p(\tilde{x},\xi).$$

Finally, from results of Section 2D, we deduce

$$q_{\mathscr{A}_m}(\tilde{x},\xi) = S\cdot\left(\frac{\xi_G\wedge n^{\varphi}(\tilde{x})}{\langle G^{-1}\xi,\xi\rangle}\right)P_- + p(\tilde{x},\xi)$$

and

$$\mathscr{A}_m = \frac{D_\Sigma}{\sqrt{-\Delta_\Sigma}}P_- \mod \operatorname{Op}\mathcal{S}^{-1}(\Sigma) = \frac{1}{\sqrt{-\Delta_\Sigma}}S\cdot(\nabla_\Sigma\wedge n)P_- \mod \operatorname{Op}\mathcal{S}^{-1}(\Sigma).$$

This satisfies the claim that $\mathscr{A}_m$ is a homogeneous pseudodifferential operator of order 0 and completes the proof of the theorem. □

5. Approximation of the Poincaré–Steklov operators for large masses

The technique used in the last section allows us to treat the layer potential operator $\mathscr{A}_m$ as a 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 an 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 (4-1) instead of the layer potential formula of $\mathscr{A}_m$. Roughly speaking, we will look for a local approximate formula for the solution of (4-1). 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 $\Sigma := \partial\Omega$. Next, we introduce the semiclassical parameter $h = m^{-1} \in (0, 1]$, and we set $\mathscr{A}^h := \mathscr{A}_m$. The following theorem is the main result of this section; it ensures that $\mathscr{A}^h$ is an h-pseudodifferential operator of order 0 and gives its semiclassical principal symbol.

Theorem 5.1. *Let $h \in (0, 1]$ and $z \in \rho(H_{\mathrm{MIT}}(m))$, and let $\mathscr{A}^h$ be as above. Then, for any $N \in \mathbb{N}$, there exists an h-pseudodifferential operator of order* 0, $\mathscr{A}^h_N \in \operatorname{Op}^h\mathcal{S}^0(\Sigma)$, *such that, for h sufficiently small and any $0 \le l \le N + \frac{1}{2}$,*

$$\|\mathscr{A}^h - \mathscr{A}^h_N\|_{H^{1/2}(\Sigma)\to H^{N+3/2-l}(\Sigma)} = \mathcal{O}(h^{2l-1/2}),$$

and

$$\mathscr{A}^h_N = \frac{hD_\Sigma}{\sqrt{-h^2\Delta_\Sigma + I} + I}P_- \mod h\operatorname{Op}^h\mathcal{S}^{-1}(\Sigma).$$

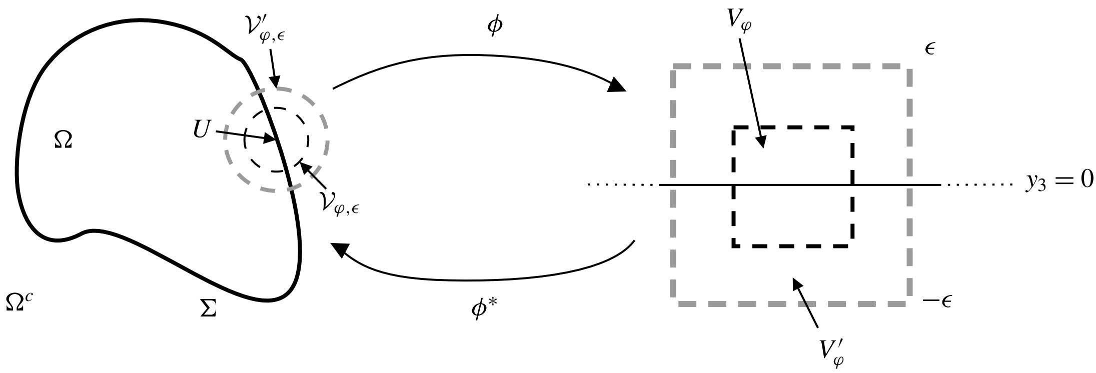

Figure 1. Change of coordinates

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 previously, without loss of generality, we consider only the case where U_φ is the graph of a smooth function χ, and we assume that Ω corresponds locally to the side $x_3 > \chi(x_1, x_2)$ (see Figure 1). Then, for

$$U_\varphi = \{(x_1, x_2, \chi(x_1, x_2)) : (x_1, x_2) \in V_\varphi\}, \quad \varphi((x_1, x_2, \chi(x_1, x_2)) = (x_1, x_2),$$
$$\mathcal{V}_{\varphi,\varepsilon} := \{(y_1, y_2, y_3 + \chi(y_1, y_2)) : (y_1, y_2, y_3) \in V_\varphi \times (0, \varepsilon)\} \subset \Omega,$$

with ε sufficiently small, we have the homeomorphism

$$\phi : \mathcal{V}_{\varphi,\varepsilon} \to V_\varphi \times (0, \varepsilon), \quad (x_1, x_2, x_3) \mapsto (x_1, x_2, x_3 - \chi(x_1, x_2)).$$

Then the pullback

$$\phi^* : C^\infty(V_\varphi \times (0, \varepsilon)) \to C^\infty(\mathcal{V}_{\varphi,\varepsilon}), \quad v \mapsto \phi^* v := v \circ \phi$$

transforms the differential operator D_m restricted on $\mathcal{V}_{\varphi,\varepsilon}$ into the following operator on $V_\varphi \times (0, \varepsilon)$:

$$\begin{aligned}\widetilde{D}^\varphi_m := (\phi^{-1})^* D_m (\phi)^* &= -i(\alpha_1 \partial_{y_1} + \alpha_2 \partial_{y_2} - (\alpha_1 \partial_{x_1}\chi + \alpha_2 \partial_{x_2}\chi - \alpha_3)\partial_{y_3}) + m\beta \\ &= -i(\alpha_1 \partial_{y_1} + \alpha_2 \partial_{y_2}) + \sqrt{1 + |\nabla\chi|^2}(i\alpha \cdot n^\varphi)(\tilde{y})\partial_{y_3} + m\beta,\end{aligned}$$

where $\tilde{y} = (y_1, y_2)$ and $n^\varphi = (\varphi^{-1})^* n$ is the pullback of the outward-pointing normal to Ω restricted on V_φ:

$$n^\varphi(\tilde{y}) = \frac{1}{\sqrt{1 + |\nabla\chi|^2}} \begin{pmatrix} \partial_{x_1}\chi \\ \partial_{x_2}\chi \\ -1 \end{pmatrix} (y_1, y_2).$$

For the projectors $P_\pm$, we have

$$P^\varphi_\pm := (\varphi^{-1})^* P_\pm (\varphi)^* = \tfrac{1}{2}(I_4 \mp i\beta\alpha \cdot n^\varphi(\tilde{y})).$$

Thus, in the variable $y \in V_\varphi \times (0, \varepsilon)$, equation (4-1) becomes

$$\begin{cases} (\widetilde{D}^\varphi_m - z)u = 0 & \text{in } V_\varphi \times (0, \varepsilon), \\ \Gamma^\varphi_- u = g^\varphi = g \circ \varphi^{-1} & \text{on } V_\varphi \times \{0\}, \end{cases} \tag{5-1}$$

where $\Gamma^\varphi_\pm = P^\varphi_\pm t_{\{y_3=0\}}$.

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 (5-1) becomes

$$\begin{cases}\partial_{y_3}u=\dfrac{i\alpha\cdot n^\varphi(\tilde y)}{\sqrt{1+|\nabla\chi(\tilde y)|^2}}(-i\alpha_1\partial_{y_1}-i\alpha_2\partial_{y_2}+m\beta-z)u & \text{in } V_\varphi\times(0,\varepsilon),\\ \Gamma_-^\varphi u=g^\varphi & \text{on } V_\varphi\times\{0\}.\end{cases}\tag{5-2}$$

Let us now introduce the matrix-valued symbols

$$L_0(\tilde y,\xi):=\frac{i\alpha\cdot n^\varphi(\tilde y)}{\sqrt{1+|\nabla\chi(\tilde y)|^2}}(\alpha\cdot\xi+\beta),\quad L_1(\tilde y):=\frac{-iz\alpha\cdot n^\varphi(\tilde y)}{\sqrt{1+|\nabla\chi(\tilde y)|^2}},\tag{5-3}$$

with $\xi=(\xi_1,\xi_2)$ identified with $(\xi_1,\xi_2,0)$. Then, for $h=m^{-1}$, (5-2) is equivalent to

$$\begin{cases}h\,\partial_{y_3}u=L_0(\tilde y,hD_{\tilde y})u+hL_1(\tilde y)u & \text{in } V_\varphi\times(0,\varepsilon),\\ \Gamma_-^\varphi u=g^\varphi & \text{on } V_\varphi\times\{0\}.\end{cases}\tag{5-4}$$

Before constructing an approximate solution of the system (5-4), let us give some properties of L_0.

5A. *Properties of L_0.* The following proposition will be used in the sequel; it gathers some useful spectral properties of the matrix-valued symbol $L_0(\tilde y,\xi)$ introduced in (5-3). The spectral properties of $l_0(n,\xi)=i(\alpha\cdot n)(\alpha\cdot\xi+\beta)$ given in Proposition A.2 (from the Appendix) provides the following properties for

$$L_0(\tilde y,\xi)=\frac{1}{\sqrt{1+|\nabla\chi(\tilde y)|^2}}l_0(n^\varphi(\tilde y),\xi).$$

Proposition 5.2. *Let $L_0(\tilde y,\xi)$ be as in (5-3). Then we have*

$$\begin{aligned}L_0(\tilde y,\xi)&=\frac{1}{\sqrt{1+|\nabla\chi(\tilde y)|^2}}(i\xi\cdot n^\varphi(\tilde y)+S\cdot(n^\varphi(\tilde y)\wedge\xi)-i\beta(\alpha\cdot n^\varphi(\tilde y)))\\&=i\xi\cdot\tilde n^\varphi(\tilde y)+\frac{\lambda(\tilde y,\xi)}{\sqrt{1+|\nabla\chi(\tilde y)|^2}}\Pi_+(\tilde y,\xi)-\frac{\lambda(\tilde y,\xi)}{\sqrt{1+|\nabla\chi(\tilde y)|^2}}\Pi_-(\tilde y,\xi),\end{aligned}$$

where

$$\begin{aligned}\lambda(\tilde y,\xi)&:=\sqrt{|n^\varphi(\tilde y)\wedge\xi|^2+1}=\sqrt{\langle G(\tilde y)^{-1}\xi,\xi\rangle+1},\\ \tilde n^\varphi(\tilde y)&:=\frac{1}{\sqrt{1+|\nabla\chi|^2}}n^\varphi(\tilde y),\\ \Pi_\pm(\tilde y,\xi)&:=\frac12\left(I_4\pm\frac{S\cdot(n^\varphi(\tilde y)\wedge\xi)-i\beta(\alpha\cdot n^\varphi(\tilde y))}{\lambda(\tilde y,\xi)}\right),\end{aligned}\tag{5-5}$$

with G the induced metric defined in Section 2C.

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 two, which are given by

$$\rho_\pm(\tilde y,\xi)=\frac{in^\varphi(\tilde y)\cdot\xi\pm\lambda(\tilde y,\xi)}{\sqrt{1+|\nabla\chi|^2}},\tag{5-6}$$

and for which there exists $c > 0$ such that

$$\frac{(\rho_+ - \rho_-)(\tilde{y}, \xi)}{2} = \pm \operatorname{Re} \rho_\pm(\tilde{y}, \xi) > c\langle \xi \rangle \tag{5-7}$$

uniformly with respect to $\tilde{y}$. Moreover, $\Pi_\pm(\tilde{y}, \xi)$, the projections onto $\operatorname{Kr}(L_0(\tilde{y}, \xi) - \rho_\pm(\tilde{y}, \xi) I_4)$, belong to the symbol class $\mathcal{S}^0$ and satisfy

$$P^\varphi_\pm \Pi_\pm(\tilde{y}, \xi) P^\varphi_\pm = k^\varphi_+(\tilde{y}, \xi) P^\varphi_\pm \quad \text{and} \quad P^\varphi_\pm \Pi_\mp(\tilde{y}, \xi) P^\varphi_\mp = \mp \Theta^\varphi(\tilde{y}, \xi) P^\varphi_\mp, \tag{5-8}$$

with

$$k^\varphi_\pm(\tilde{y}, \xi) = \frac{1}{2}\left(1 \pm \frac{1}{\lambda(\tilde{y}, \xi)}\right), \quad \Theta^\varphi(\tilde{y}, \xi) = \frac{1}{2\lambda(\tilde{y}, \xi)}(S \cdot (n^\varphi(\tilde{y}) \wedge \xi)). \tag{5-9}$$

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 5.3. Thanks to property (5-8), a 4×4-matrix A is uniquely determined by $P^\varphi_- A$ and $\Pi_+ A$, and we have

$$A = P^\varphi_- A + P^\varphi_+ A = P^\varphi_- A + \frac{1}{k^\varphi_+} P^\varphi_+ \Pi_+ P^\varphi_+ A = \left(I - \frac{P^\varphi_+ \Pi_+}{k^\varphi_+}\right) P^\varphi_- A + \frac{P^\varphi_+}{k^\varphi_+} \Pi_+ A.$$

Proof of Proposition 5.2. By definition it is clear that $L_0(\tilde{y}, \xi)$ belongs to the symbol class $\mathcal{S}^1$, and all the formulas follow from those of $l_0(n, \xi)$ proved in the Appendix (see Proposition A.2 and Lemma A.3), mainly taking $n = n^\varphi(\tilde{y})$ and multiplying by $1/\sqrt{1 + |\nabla\chi(\tilde{y})|^2}$. Next, using (2-15),

$$\pm \operatorname{Re} \rho_\pm(\tilde{y}, \xi) = \frac{\sqrt{|n^\varphi \wedge \xi|^2 + 1}}{\sqrt{1 + |\nabla\chi|^2}} = \frac{\sqrt{\langle G(\tilde{y})^{-1}\xi, \xi\rangle + 1}}{\sqrt{1 + |\nabla\chi|^2}} \geqslant c(1 + |\xi|),$$

which gives (5-7) and shows that $\rho_\pm$ are elliptic in $\mathcal{S}^1$. Consequently, we also get that $L_0(\tilde{y}, \xi)$ is elliptic in $\mathcal{S}^1$ and that the functions $\Pi_\pm$, k^φ_+, $(k^\varphi_+)^{-1}$ and Θ^φ belong to the symbol class $\mathcal{S}^0$. □

5B. ***Semiclassical parametrix for the boundary problem.*** In this section, we construct the approximate solution of the system (1-1) mentioned in the introduction. For simplicity of notation, in the sequel we will use y and $P_\pm$ instead of $\tilde{y}$ and $P^\varphi_\pm$, respectively.

We are going to construct a local approximate solution of the first order system

$$\begin{cases} h\,\partial_\tau u^h = L_0(y, hD_y)u^h + hL_1(y)u^h & \text{in } \mathbb{R}^2 \times (0, +\infty), \\ P_- u^h = f & \text{on } \mathbb{R}^2 \times \{0\}. \end{cases}$$

To be precise, we will look for a solution u^h in the form

$$u^h(y, \tau) = \operatorname{Op}^h(A^h(\cdot, \cdot, \tau)) f = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} A^h(y, h\xi, \tau) e^{iy\cdot\xi} \hat{f}(\xi)\, d\xi, \tag{5-10}$$

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

$$T^h(y, \xi, \tau) = h(\partial_\tau A)(y, \xi, \tau) - L_0(y, \xi)A(y, \xi, \tau) - h(L_1(y)A(y, \xi, \tau) - i\,\partial_\xi L_0(y, \xi)\cdot\partial_y A(y, \xi, \tau)).$$

Here we exploited the particular form of L_1 (independent of ξ) and of L_0 (first order polynomial in ξ).

Then we look for A_0 satisfying

$$\begin{cases} h\,\partial_\tau A_0(y, \xi, \tau) = L_0(y, \xi)A_0(y, \xi, \tau), \\ P_-(y)A_0(y, \xi, \tau) = P_-(y), \end{cases} \tag{5-11}$$

and, for $j \geq 1$,

$$\begin{cases} h\,\partial_\tau A_j(y, \xi, \tau) = L_0(y, \xi)A_j(y, \xi, \tau) + L_1(y)A_{j-1}(y, \xi, \tau) - i\,\partial_\xi L_0(y, \xi)\cdot\partial_y A_{j-1}(y, \xi, \tau), \\ P_-(y)A_j(y, \xi, \tau) = 0. \end{cases} \tag{5-12}$$

Let us introduce a class of parametrized symbols in which we will construct the family A_j:

$$\mathcal{P}_h^m := \{b(\cdot\,, \cdot\,, \tau) \in \mathcal{S}^m : \forall (k, l) \in \mathbb{N}^2,\ \tau^k\,\partial_\tau^l b(\cdot\,, \cdot\,, \tau) \in h^{k-l}\mathcal{S}^{m-k+l}\}, \quad m \in \mathbb{Z}.$$

More precisely, $b \in \mathcal{P}_h^m$ means that, for all $(k, l) \in \mathbb{N}^2$, the function $(\tau, h) \mapsto (h^{-1}\tau)^k (h\,\partial_\tau)^l b(\cdot\,, \cdot\,, \tau)$ is uniformly bounded with respect to $(\tau, h) \in (0, +\infty) \times (0, 1)$ in $\mathcal{S}^{m-k+l}$.

Proposition 5.4. *There exists $A_0 \in \mathcal{P}_h^0$ a solution of (5-11) given by*

$$A_0(y, \xi, \tau) = \frac{\Pi_-(y, \xi)P_-(y)}{k_+^\varphi(y, \xi)} e^{h^{-1}\tau\rho_-(y,\xi)}.$$

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

$$e^{h^{-1}\tau L_0(y,\xi)} = e^{h^{-1}\tau\rho_-(y,\xi)}\Pi_-(y, \xi) + e^{h^{-1}\tau\rho_+(y,\xi)}\Pi_+(y, \xi). \tag{5-13}$$

It follows from (5-7) 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 5.3, we deduce that

$$A_0(y, \xi, 0) = P_-(y) - \frac{P_+\Pi_+P_-}{k_+^\varphi}(y, \xi) = P_-(y) + \frac{P_+\Pi_-P_-}{k_+^\varphi}(y, \xi) = \frac{\Pi_-P_-}{k_+^\varphi}(y, \xi).$$

The properties of ρ_-, Π_-, P_-, and k_+ given in Proposition 5.2, imply that $(k_+^\varphi)^{-1}\Pi_-P_- \in \mathcal{S}^0$ and that $e^{h^{-1}\tau\rho_-(y,\xi)} \in \mathcal{P}_h^0$. This concludes the proof of Proposition 5.4. ☐

For the other terms A_j, $j \geq 1$, we have the following.

Proposition 5.5. *Let A_0 be defined by Proposition 5.4. Then, for any $j \geq 1$, there exists $A_j \in h^j\mathcal{P}_h^{-j}$ a solution of (5-12) which has the form*

$$A_j(y, \xi, \tau) = e^{h^{-1}\tau\rho_-(y,\xi)} \sum_{k=0}^{2j} (h^{-1}\tau\langle\xi\rangle)^k B_{j,k}(y, \xi), \tag{5-14}$$

with $B_{j,k} \in h^j\mathcal{S}^{-j}$.

Proof. Let us prove the result by induction. Thanks to Proposition 5.4, the claimed property holds for $j=0$. Now, assume that there exists $A_j \in h^j \mathcal{P}_h^{-j}$, a solution of (5-12) 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 $h\,\partial_\tau A_{j+1} = L_0 A_{j+1} + L_1 A_j - i\,\partial_\xi L_0 \cdot \partial_y A_j$, for A_{j+1} we have

$$A_{j+1} = e^{h^{-1}\tau L_0} A_{j+1}{}_{|\tau=0} + e^{h^{-1}\tau L_0} \int_0^\tau e^{-h^{-1}sL_0}(L_1 A_j - i\,\partial_\xi L_0 \cdot \partial_y A_j)\,\mathrm{d}s, \tag{5-15}$$

where $L_1 A_j$ has still the form (5-14), and we have

$$\partial_y A_j = e^{h^{-1}\tau\rho_-}(h^{-1}\tau\,\partial_y\rho_- + \partial_y)\sum_{k=0}^{2j}(h^{-1}\tau\langle\xi\rangle)^k B_{j,k}.$$

Thus, thanks to the properties of ρ_- and $B_{j,k}$, the quantity $(L_1 A_j - i\,\partial_\xi L_0 \cdot \partial_y A_j)(y,\xi,s)$ has the form

$$e^{h^{-1}s\rho_-(y,\xi)}\sum_{k=0}^{2j+1}(h^{-1}s\langle\xi\rangle)^k \widetilde{B}_{j,k}(y,\xi), \tag{5-16}$$

with $\widetilde{B}_{j,k} \in h^j \mathcal{S}^{-j}$. So, using the decomposition (5-13), for the second term of the right-hand side of (5-15), we have

$$e^{h^{-1}\tau L_0}\int_0^\tau e^{-h^{-1}sL_0}(L_1 A_j - i\,\partial_\xi L_0 \cdot \partial_y A_j)\,\mathrm{d}s = e^{h^{-1}\tau\rho_-}\Pi_- I_-^j(\tau) + e^{h^{-1}\tau\rho_+}\Pi_+ I_+^j(\tau) \tag{5-17}$$

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

$$I_-^j(\tau) = \sum_{k=0}^{2j+1}(h^{-1}\tau\langle\xi\rangle)^{k+1}\frac{h\langle\xi\rangle^{-1}}{k+1}\widetilde{B}_{j,k}. \tag{5-18}$$

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 form

$$e^{\tau^h\rho_+}\Pi_+ I_+^j(\tau) = \Pi_+\sum_{k=0}^{2j+1}\frac{h\langle\xi\rangle^k}{(\rho_- - \rho_+)^{k+1}}\widetilde{B}_{j,k}(e^{\tau^h\rho_-}P_k(\tau^h(\rho_- - \rho_+)) - e^{\tau^h\rho_+}P_k(0)), \tag{5-19}$$

where $\tau^h := h^{-1}\tau$. Thus, combining (5-18) and (5-19) with (5-15), (5-17) and (5-13) yields

$$A_{j+1} = e^{h^{-1}\tau\rho_+}(\Pi_+ A_{j+1}{}_{|\tau=0} - \widetilde{B}_{j+1}^+) + e^{h^{-1}\tau\rho_-}\Bigg(\Pi_- A_{j+1}{}_{|\tau=0} + \sum_{k=0}^{2(j+1)}(h^{-1}\tau\langle\xi\rangle)^k \widetilde{B}_{j+1,k}^-\Bigg),$$

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 $\Pi_- \in \mathcal{S}^0$, of $h\langle\xi\rangle^{-1}$ (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

$$\Pi_+ A_{j+1}(y,\xi,0) = \widetilde{B}^{+}_{j+1}(y,\xi).$$

Then, thanks to Remark 5.3, the boundary condition $P_-(y)A_{j+1}(y,\xi,0) = 0$ gives

$$A_{j+1}(y,\xi,0) = \frac{P_+\Pi_+}{k_+^{\varphi}} \widetilde{B}^{+}_{j+1}(y,\xi).$$

Finally, we have

$$A_{j+1}(y,\xi,\tau) = e^{h^{-1}\tau\rho_-(y,\xi)}\left(\frac{\Pi_- P_+\Pi_+}{k_+^{\varphi}} \widetilde{B}^{+}_{j+1}(y,\xi) + \sum_{k=0}^{2(j+1)} (h^{-1}\tau\langle\xi\rangle)^k \widetilde{B}^{-}_{j+1,k}(y,\xi)\right),$$

and Proposition 5.5 is proven with

$$B_{j+1,0} = \frac{\Pi_- P_+\Pi_+}{k_+^{\varphi}} \widetilde{B}^{+}_{j+1} + \widetilde{B}^{-}_{j+1,0},$$

and, for $k \geq 1$, $B_{j+1,k} = \widetilde{B}^{-}_{j+1,k}$. □

Remark 5.6. The computation of each term $B_{j,0}$ can be done recursively, but this leads to complicated calculations. For example $B_{1,0}$ has the form

$$B_{1,0}(y,\xi) = h\left[\Pi_+ a_0 + \frac{\Pi_- P_+\Pi_+ a_0}{k_+^{\varphi}}\right]\left(\frac{(z + i\alpha\cdot\partial_y)}{2\lambda} + \frac{i\alpha\cdot\partial_y\rho_-}{4\lambda^2}\right)\Pi_- A_0(y,\xi),$$

with $a_0(\tilde{y}) = i\alpha\cdot\tilde{n}^{\varphi}(\tilde{y})$.

Thanks to the relation (5-10), to any $A^h \in \mathcal{P}^0_h$ we can 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 (2-8)), and in the variable $\tau \in (0,+\infty)$, it is essentially multiplication by an L^∞-function. Moreover, for A_j of the form (5-14), we have the following mapping property which captures the Sobolev space regularity.

Proposition 5.7. *Let A_j, $j \geq 0$, be of the form (5-14). Then, for any $s \geq -j-\frac{1}{2}$, the operator $\mathcal{A}_j$ defined by*

$$\mathcal{A}_j : f \mapsto (\mathcal{A}_j f)(y,y_3) = \frac{1}{(2\pi)^2}\int_{\mathbb{R}^2} A_j(y,h\xi,y_3)e^{iy\cdot\xi}\hat{f}(\xi)\,d\xi$$

gives rise to a bounded operator from $H^s(\mathbb{R}^2)$ into $H^{s+j+1/2}(\mathbb{R}^2 \times (0,+\infty))$. Moreover, for any $l \in \left[0, j+\frac{1}{2}\right]$ we have

$$\|\mathcal{A}_j\|_{H^s \to H^{s+j+1/2-l}} = \mathcal{O}(h^{l-|s|}). \tag{5-20}$$

Proof. First, let us prove the result for $s = k - j - \frac{1}{2},\ k \in \mathbb{N}$, between the semiclassical Sobolev spaces

$$H^s_{\mathrm{scl}}(\mathbb{R}^2) := \langle hD_y\rangle^{-s} L^2(\mathbb{R}^2),$$
$$H^k_{\mathrm{scl}}(\mathbb{R}^2 \times (0,+\infty)) := \{u \in L^2 : \langle hD_y\rangle^{k_1}(h\,\partial_{y_3})^{k_2} u \in L^2 \text{ for } (k_1,k_2) \in \mathbb{N}^2,\ k_1 + k_2 = k\},$$

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

$$\|\mathcal{A}_j f\|^2_{H^k_{\mathrm{scl}}(\mathbb{R}^2\times(0,+\infty))} = \sum_{k_1+k_2=k} \|\langle hD_y\rangle^{k_1}(h\,\partial_{y_3})^{k_2}\mathcal{A}_j f\|^2_{L^2(\mathbb{R}^2\times(0,+\infty))}$$
$$= \sum_{k_1+k_2=k} \int_0^{+\infty} \|\langle hD_y\rangle^{k_1}(h\,\partial_{y_3})^{k_2}(\mathcal{A}_j f)(\,\cdot\,, y_3)\|^2_{L^2(\mathbb{R}^2)}\, dy_3. \tag{5-21}$$

Thanks to the ellipticity property (5-7), for A_j given by Proposition 5.5, we have

$$(h\,\partial_{y_3})^{k_2} A_j(y,\xi,y_3) = h^j b_j(y,\xi;y_3) e^{-h^{-1}y_3 c\langle\xi\rangle/2}\langle\xi\rangle^{k_2-j},$$

with b_j satisfying the following: for any $(\alpha,\beta) \in \mathbb{N}^2 \times \mathbb{N}^2$ there exists $C_{\alpha,\beta} > 0$ such that

$$|\partial_y^\alpha \partial_\xi^\beta b_j(y,\xi;y_3)| \le C_{\alpha,\beta} \quad \text{for all } (y,\xi;y_3) \in \mathbb{R}^2 \times \mathbb{R}^2 \times (0,+\infty).$$

Consequently, thanks to the Calderón–Vaillancourt theorem (see (2-8)), we can write

$$\langle hD_y\rangle^{k_1}(h\,\partial_{y_3})^{k_2}\mathcal{A}_j = h^j \mathcal{B}_j(y_3)\langle hD_y\rangle^{k_1+k_2-j} e^{-h^{-1}y_3 c\langle hD_y\rangle/2},$$

with $(\mathcal{B}_j(y_3))_{y_3>0}$ a family of bounded operators on $L^2(\mathbb{R}^2)$, uniformly bounded with respect to $y_3 > 0$. Then, for $f \in H^s(\mathbb{R}^2)^4$, we have

$$\|\langle hD_y\rangle^{k_1}(h\,\partial_{y_3})^{k_2}(\mathcal{A}_j f)(\,\cdot\,,y_3)\|^2_{L^2(\mathbb{R}^2)} \lesssim h^j \|\langle hD_y\rangle^{k_1+k_2-j} e^{-h^{-1}y_3 c\langle hD_y\rangle/2} f\|^2_{L^2(\mathbb{R}^2)},$$

and from (5-21) we deduce that

$$\|\mathcal{A}_j f\|^2_{H^k_{\mathrm{scl}}(\mathbb{R}^2\times(0,+\infty))} \lesssim h^{2j+1}\|\langle hD_y\rangle^{k-j-1/2} f\|^2_{L^2(\mathbb{R}^2)} = h^{2j+1}\|f\|^2_{H^{k-j-1/2}_{\mathrm{scl}}(\mathbb{R}^2)},$$

where we used that, for any $l \in \mathbb{N}$ and $f \in H^{l-1/2}_{\mathrm{scl}}(\mathbb{R}^2)$,

$$\|\langle hD_y\rangle^l e^{-h^{-1}y_3 c\langle hD_y\rangle/2} f\|^2_{L^2(\mathbb{R}^2)} = \langle e^{-h^{-1}y_3 c\langle hD_y\rangle}\langle hD_y\rangle^l f, \langle hD_y\rangle^l f\rangle_{L^2}$$
$$= -\frac{h}{c}\frac{\partial}{\partial_{y_3}}\langle e^{-h^{-1}y_3 c\langle hD_y\rangle}\langle hD_y\rangle^{l-1} f, \langle hD_y\rangle^l f\rangle_{L^2}.$$

By interpolation arguments we thus deduce that, for any $j \in \mathbb{N}$ and $s \ge -j - \frac{1}{2}$,

$$\|\mathcal{A}_j\|_{H^s_{\mathrm{scl}} \to H^{s+j+1/2}_{\mathrm{scl}}} = \mathcal{O}(h^{j+1/2}).$$

This means that, for $\bar{y} := (y, y_3)$,

$$\|\langle hD_{\bar{y}}\rangle^{s+j+1/2}\mathcal{A}_j\langle hD_y\rangle^{-s}\|_{L^2(\mathbb{R}^2)\to L^2(\mathbb{R}^2\times(0,+\infty))} = \mathcal{O}(h^{j+1/2}). \tag{5-22}$$

In order to prove (5-20) (in *classical* Sobolev spaces), let us estimate $\langle D_{\bar{y}}\rangle^{s+j+1/2-l}\mathcal{A}_j\langle D_y\rangle^{-s}$ from $L^2(\mathbb{R}^2)$ into $L^2(\mathbb{R}^2\times(0,+\infty))$. The inequalities, for all $\xi\in\mathbb{R}^d$, $d=2,3$, and $h\in(0,1)$,

$$1\le\langle\xi\rangle\le h^{-1}\langle h\xi\rangle,\quad \langle\xi\rangle^{-1}\le\langle h\xi\rangle^{-1},\quad \langle\xi\rangle^{-1}\le 1$$

imply, for $j+\frac{1}{2}\ge l$, $s_+=\max(s,0)$, and $s_-=s-s_+$, the estimates

$$\langle\xi\rangle^{s+j+1/2-l}\le h^{-j-1/2+l}h^{-s_+}\langle h\xi\rangle^{s+j+1/2},\quad \langle\xi\rangle^{-s}\le h^{s_-}\langle h\xi\rangle^{-s}.$$

We deduce

$$\|\langle D_{\bar{y}}\rangle^{s+j+1/2-l}\mathcal{A}_j\langle D_y\rangle^{-s}\|_{L^2\to L^2}\lesssim h^{-j-1/2+l}h^{-s_+}h^{s_-}\|\langle hD_{\bar{y}}\rangle^{s+j+1/2}\mathcal{A}_j\langle hD_y\rangle^{-s}\|_{L^2\to L^2}.$$

Then estimate (5-20) follows from (5-22) using $s_+-s_-=|s|$. □

Proposition 5.8. *Let $f\in H^s(\mathbb{R}^2)$ and A_j, $j\ge 0$, be as in Propositions 5.4 and 5.5. Then, for any $N\ge -s-\frac{1}{2}$, the function $u_N^h=\sum_{j=0}^N h^j\mathcal{A}_jf$ satisfies*

$$\begin{cases} h\,\partial_\tau u_N^h-L_0(y,hD_y)u_N^h-hL_1(y)u_N^h=h^{N+1}\mathcal{R}_N^hf & \text{in } \mathbb{R}^2\times(0,+\infty),\\ P_-u_N^h=f & \text{on } \mathbb{R}^2\times\{0\},\end{cases}\tag{5-23}$$

with

$$\mathcal{R}_N^h: f\mapsto\frac{-1}{(2\pi)^2}\int_{\mathbb{R}^2}(L_1A_N-i\,\partial_\xi L_0\cdot\partial_yA_N)(y,h\xi,\tau)e^{iy\cdot\xi}\hat{f}(\xi)\,d\xi$$

a bounded operator from $H^s(\mathbb{R}^2)$ into $H^{s+N+1/2}(\mathbb{R}^2\times(0,+\infty))$ satisfying, for any $l\in\left[0,N+\frac{1}{2}\right]$,

$$\|\mathcal{R}_N^h\|_{H^s\to H^{s+N+1/2-l}}=\mathcal{O}(h^{l-|s|}).\tag{5-24}$$

Proof. By construction of the sequence $(A_j)_{j\in\{0,\dots,N-1\}}$, we have the system (5-23) with

$$\mathcal{R}_N^h=\mathrm{Op}^h(r_N^h(\cdot,\cdot,\tau))\quad\text{and}\quad r_N^h(y,\xi,\tau)=-(L_1A_N-i\,\partial_\xi L_0\cdot\partial_yA_N)(y,\xi,\tau)$$

(see the beginning of Section 5B). As in the proof of Proposition 5.5, r_N^h has the form (5-16) (with $j=N$). Then, as in the proof of Proposition 5.7 we obtain the estimate (5-24). □

5C. *Proof of Theorem 5.1.* In this section, we apply the above construction in order to prove Theorem 5.1.

Let $g\in P_-H^{1/2}(\partial\Omega)^4$, let $(U_\varphi,V_\varphi,\varphi)$ be a chart of the atlas $\mathbb{A}$, and let $\psi_1,\psi_2\in C_0^\infty(U_\varphi)$. 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

$$\begin{cases}(\widetilde{D}_m^\varphi-z)u_N^h=h^{N+1}\mathcal{R}_N^hf & \text{in } \mathbb{R}^2\times(0,\varepsilon),\\ \Gamma_-u_N^h=f & \text{on } \mathbb{R}^2\times\{0\},\end{cases}$$

with $u_N^h=\sum_{j=0}^N h^j\mathcal{A}_jf$ (see Proposition 5.7) and $\mathcal{R}_N^hf\in H^{N+1}(\mathbb{R}^2\times(0,\varepsilon))$ with norm in H^{N+1-l}, $l\in\left[0,N+\frac{1}{2}\right]$, bounded by $\mathcal{O}(h^{l-1/2})$. Consequently, $v_N^h:=\phi^*u_N^h$, defined on $\mathcal{V}_{\varphi,\varepsilon}$, satisfies

$$\begin{cases}(D_m-z)v_N^h=h^{N+1}\phi^*(\mathcal{R}_N^hf) & \text{in } \mathcal{V}_{\varphi,\varepsilon},\\ \Gamma_-v_N^h=\psi_2g & \text{on } U_\varphi.\end{cases}$$

Now, let $E_m^\Omega(z)[\psi_2 g] \in H^1(\Omega)^4$ be as in Definition 4.1. Since $\Gamma_- v_N^h = \Gamma_- E_m^\Omega(z)[\psi_2 g] = \psi_2 g$, the following equality holds in $\mathcal{V}_{\varphi,\varepsilon}$:

$$v_N^h - E_m^\Omega(z)[\psi_2 g] = h^{N+1}(H_{\mathrm{MIT}}(m) - z)^{-1}\phi^*(\mathcal{R}_N^h(\varphi^{-1})^*(\psi_2 g)).$$

From this, we deduce that

$$\psi_1 \mathscr{A}_m \psi_2(g) := \psi_1 \Gamma_+ E_m^\Omega(z)[\psi_2 g] = \psi_1 \Gamma_+ v_N^h - h^{N+1}\psi_1 \Gamma_+ (H_{\mathrm{MIT}} - z)^{-1}\phi^*(\mathcal{R}_N^h(\varphi^{-1})^*(\psi_2 g)).$$

Since $\phi \restriction_{U_\varphi} = \varphi$, for any $u \in H^1(V_\varphi \times (0,\varepsilon))^4$, we have that

$$\Gamma_+ \phi^*(u) = \varphi^*(P_+ u \restriction_{V_\varphi \times \{0\}}), \quad \psi_1 \Gamma_+ v_N^h = \psi_1 \varphi^* \operatorname{Op}^h(a_N^h)(\varphi^{-1})^* \psi_2 g,$$

with

$$a_N^h(\tilde{y}, \xi) = \sum_{j=0}^N h^j P_+ A_j(y, \xi, 0) = \sum_{j=0}^N h^j P_+ B_{j,0}(y, \xi),$$

where $B_{j,0} \in h^j \mathcal{S}^{-j}$ are introduced in Proposition 5.5. Thus, from Proposition 5.4, 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 property (5-8) it is equal to

$$-\Theta^\varphi P_-(y, \xi) = \frac{S \cdot (\xi \wedge n^\varphi(y))}{\sqrt{\langle G(y)^{-1}\xi, \xi\rangle + 1} + 1} P_-(y, \xi).$$

We conclude the proof of Theorem 5.1 from results of Section 2D and by proving the following lemma which is a consequence of the above considerations, the regularity estimates from Theorem 3.1(iii), Theorem 3.4(i), and Proposition 4.2.

Lemma 5.9. *Let $\psi_1, \psi_2 \in C^\infty(\Sigma)$ be such that* $\operatorname{supp}(\psi_1) \cap \operatorname{supp}(\psi_2) = \varnothing$. *Then, for $m_0 > 0$ sufficiently large, $m \geqslant m_0$, and for any $(k, N) \in \mathbb{N}^* \times \mathbb{N}^*$,*

$$\|\psi_1 \mathscr{A}_m \psi_2\|_{P_- H^{1/2}(\Sigma)^4 \to P_+ H^k(\Sigma)^4} = \mathcal{O}(m^{-N}).$$

Proof. Let $\psi_1, \psi_2 \in C^\infty(\Sigma)$ with disjoint supports. Thanks to Theorem 3.1(iii) and Theorem 3.4(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, for $g \in P_- H^{1/2}(\Sigma)^4$,

$$\|(\psi_1 \mathscr{A}_m \psi_2) g\|_{P_+ H^{N_2+1/2}(\Sigma)^4} \le \frac{C_{N_1,N_2}}{\sqrt{m}} (\Pi_{i=0}^{N_2} \|(H_{\mathrm{MIT}}(m) - z)^{-1}\|_{H^i(\Omega)^4 \to H^{i+1}(\Omega)^4}) \times \|(H_{\mathrm{MIT}}(m) - z)^{-1}\|_{L^2(\Omega)^4 \to L^2(\Omega)^4}^{N_1} \|g\|_{P_- H^{1/2}(\Sigma)^4}. \tag{5-25}$$

For this, let us introduce $\Phi_1 \in C_0^\infty(\bar{\Omega})$ such that $\Phi_1 = 1$ near $\operatorname{supp}(\psi_1)$ and $\Phi_1 = 0$ near $\operatorname{supp}(\psi_2)$. Thus for $g \in P_- H^{1/2}(\Sigma)^4$ and $E_m^\Omega(z)[\psi_2 g] \in H^1(\Omega)$ as in Definition 4.1, the function $u_{1,2} := \Phi_1 E_m^\Omega(z)[\psi_2 g]$ satisfies

$$\begin{cases} (D_m - z) u_{1,2} = [D_0, \Phi_1] E_m^\Omega(z)[\psi_2 g] & \text{in } \Omega, \\ \Gamma_- u_{1,2} = \Phi_{1|_\Sigma} \psi_2 g = 0 & \text{on } \Sigma. \end{cases}$$

Then, $u_{1,2} = (H_{\mathrm{MIT}}(m) - z)^{-1}[D_0, \Phi_1]E_m^\Omega(z)[\psi_2 g]$, and, for any $\widetilde{\Phi}_1 \in C_0^\infty(\overline{\Omega})$ equal to 1 near $\operatorname{supp}(\psi_1)$, 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 $\operatorname{supp}(\widetilde{\Phi}_1)$, both functions $\widetilde{\Phi}_1$ and $[D_0, \Phi_1]$ have disjoint supports, and we can then apply the telescopic formula

$$\widetilde{\Phi}_1 (H_{\mathrm{MIT}}(m) - z)^{-1}(1 - \chi_1) = \widetilde{\Phi}_1 (H_{\mathrm{MIT}}(m) - z)^{-1}[D_0, \chi_J] \cdots (H_{\mathrm{MIT}}(m) - z)^{-1}[D_0, \chi_2] \\ \times (H_{\mathrm{MIT}}(m) - z)^{-1}(1 - \chi_1)$$

for $(\chi_i)_{1 \le i \le J}$ a family of compactly supported smooth functions such that $\widetilde{\Phi}_1 \prec \chi_J \prec \chi_{J-1} \prec \cdots \prec \chi_1 \prec \Phi_1$, $J = N_1 + N_2$. 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 J cutoff resolvents of $H_{\mathrm{MIT}}(m)$. Now, by Proposition 4.2, we have

$$\| E_m^\Omega(z)[\psi_2 g] \|_{L^2(\Omega)^4} \lesssim \frac{1}{\sqrt{m}} \| g \|_{L^2(\Sigma)^4}.$$

Thus, using the continuity of Γ_+ from $H^{N_2+1}(\Omega)$ to $H^{N_2+1/2}(\Sigma)$, we then get the estimation (5-25), finishing the proof of the lemma taking $N_2 = k$ and N_1 such that $N_1 \ge N + \frac{1}{2}N_2(N_2 - 1)$. □

Remark 5.10. Note that, for any $m > 0$ and $z \in \rho(H_{\mathrm{MIT}}(m))$, the parametrix we have constructed for $\mathscr{A}_m$ is valid from the classical pseudodifferential point of view. Actually, Lemma 5.9 is the only result where the assumption that m is big enough has been assumed, and it is exclusively required to ensure 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 5.9 still ensures that away from the diagonal $\mathscr{A}_m$ is regularizing. Consequently, we deduce that, for any $m > 0$ and $z \in \rho(H_{\mathrm{MIT}}(m))$, the operator $\mathscr{A}_m$ is a homogeneous pseudodifferential operator of order 0, and that

$$\mathscr{A}_m = \frac{D_\Sigma}{\sqrt{-\Delta_\Sigma}} P_- \mod \operatorname{Op} \mathcal{S}^{-1}(\Sigma),$$

which is in accordance with Theorem 4.5.

Remark 5.11. 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

$$a_m(\xi) = -\frac{i\alpha_3(\alpha \cdot \xi - z)}{\sqrt{|\xi|^2 + m^2} + m} P_-.$$

6. Resolvent convergence to the MIT bag model

In the whole section, $\Omega \subset \mathbb{R}^3$ denotes a bounded smooth domain, we set

$$\Omega_i = \Omega, \quad \Omega_e = \mathbb{R}^3 \setminus \overline{\Omega}, \quad \text{and} \quad \Sigma = \partial\Omega,$$

and we let n be the outward (with respect to Ω_i) unit normal vector field on Σ.

Fix $m > 0$, and let $M > 0$. Consider the perturbed Dirac operator

$$H_M \varphi = (D_m + M\beta 1_{\Omega_e})\varphi \quad \text{for all } \varphi \in \operatorname{dom}(H_M) := H^1(\mathbb{R}^3)^4,$$

where 1_{Ω_e} is the characteristic function of Ω_e. Using the Kato–Rellich theorem and Weyl's theorem, it is easy to see that $(H_M, \mathrm{dom}(H_M))$ is self-adjoint and that

$$\mathrm{Sp}_{\mathrm{ess}}(H_M) = (-\infty, -(m+M)] \cup [m+M, +\infty)$$

and

$$\mathrm{Sp}(H_M) \cap (-(m+M), m+M) \text{ is purely discrete.}$$

Now, let $H_{\mathrm{MIT}}(m)$ be the MIT bag operator acting on $L^2(\Omega_i)^4$, that is

$$H_{\mathrm{MIT}}(m)v = D_m v \quad \text{for all } v \in \mathrm{dom}(H_{\mathrm{MIT}}(m)) := \{v \in H^1(\Omega_i)^4 : P_- t_\Sigma v = 0 \text{ on } \Sigma\},$$

where t_Σ and $P_\pm$ are the trace operator and the orthogonal projection from Section 2A.

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 $H_{\mathrm{MIT}}(m)$ holds in the norm resolvent sense with a convergence rate of $\mathcal{O}(1/M)$, which improves the result of [Barbaroux et al. 2019].

Before stating the main results of this section, we need to introduce some notation and definitions. First, we introduce the Dirac auxiliary operator

$$\widetilde{H}_M u = D_{m+M} u \quad \text{for all } u \in \mathrm{dom}(\widetilde{H}_M) := \{u \in H^1(\Omega_e)^4 : P_+ t_\Sigma u = 0 \text{ on } \Sigma\}.$$

Notice that $\widetilde{H}_M$ is the MIT bag operator on Ω_e (the boundary condition is with P_+ because the normal n is incoming for Ω_e). Since Ω_e is unbounded, Theorem 3.1 together with Remark 3.2 imply that $(\widetilde{H}_M, \mathrm{dom}(\widetilde{H}_M))$ is self-adjoint and that

$$\mathrm{Sp}(\widetilde{H}_M) = \mathrm{Sp}_{\mathrm{ess}}(\widetilde{H}_M) = (-\infty, -(m+M)] \cup [m+M, +\infty).$$

In particular, $\rho(H_M) \subset \rho(\widetilde{H}_M))$. Let $z \in \rho(H_{\mathrm{MIT}}(m)) \cap \rho(\widetilde{H}_M)$, $g \in P_- H^{1/2}(\Sigma)^4$, and $h \in P_+ H^{1/2}(\Sigma)^4$. 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 boundary value problem

$$\begin{cases} (D_m - z)v = 0 & \text{in } \Omega_i, \\ P_- t_\Sigma v = g & \text{in } \Sigma. \end{cases} \tag{6-1}$$

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 boundary value problem

$$\begin{cases} (D_{m+M} - z)u = 0 & \text{in } \Omega_e, \\ P_+ t_\Sigma u = h & \text{in } \Sigma. \end{cases} \tag{6-2}$$

Define the Poincaré–Steklov operators associated to the above problems by

$$\mathscr{A}_m^i = P_+ t_\Sigma E_m^{\Omega_i}(z) P_- \quad \text{and} \quad \mathscr{A}_{m+M}^e = P_- t_\Sigma E_{m+M}^{\Omega_e}(z) P_+.$$

Notation 6.1. In the sequel we shall denote by $R_M(z)$, $\widetilde{R}_M(z)$, and $R_{\mathrm{MIT}}(z)$ the resolvent of H_M, $\widetilde{H}_M$, and $H_{\mathrm{MIT}}(m)$, respectively. We also use the notation

- $\Gamma_\pm = P_\pm t_\Sigma$ and $\Gamma = \Gamma_+ r_{\Omega_i} + \Gamma_- r_{\Omega_e}$,
- $E_M(z) = e_{\Omega_i} E_m^{\Omega_i}(z) P_- + e_{\Omega_e} E_{m+M}^{\Omega_e}(z) P_+$,
- $\widetilde{R}_{\mathrm{MIT}}(z) = e_{\Omega_i} R_{\mathrm{MIT}}(z) r_{\Omega_i} + e_{\Omega_e} \widetilde{R}_M(z) r_{\Omega_e}$.

With these notations in hand, we can state the main results of this section. The following theorem is the main tool to show the large coupling convergence with a rate of convergence of $\mathcal{O}(1/M)$.

Theorem 6.2. *There is $M_0 > 0$ such that, for all $M > M_0$ and all $z \in \rho(H_{\text{MIT}}(m)) \cap \rho(H_M)$, the operator $\Psi_M(z) := (I - \mathscr{A}_m^i - \mathscr{A}_{m+M}^e)$ is bounded invertible in $H^{1/2}(\Sigma)^4$, the inverse is given by*

$$\Psi_M^{-1}(z) = (I_4 - \mathscr{A}_m^i \mathscr{A}_{m+M}^e - \mathscr{A}_{m+M}^e \mathscr{A}_m^i)^{-1}(I + \mathscr{A}_m^i + \mathscr{A}_{m+M}^e),$$

and the following resolvent formula holds:

$$R_M(z) = \widetilde{R}_{\text{MIT}}(z) + E_M(z)\Psi_M^{-1}(z)\Gamma\widetilde{R}_{\text{MIT}}(z). \tag{6-3}$$

Remark 6.3. By Proposition 4.2(i), we have that

$$(E_m^{\Omega_i}(z))^* = -\beta\Gamma_+ R_{\text{MIT}}(\bar{z}) \quad \text{and} \quad (E_{m+M}^{\Omega_e}(z))^* = -\beta\Gamma_- \widetilde{R}_M(\bar{z})$$

for any $z \in \rho(H_{\text{MIT}}(m)) \cap \rho(H_M)$. Thus, the resolvent formula (6-3) can be written in the form

$$R_M(z) = \widetilde{R}_{\text{MIT}}(z) - (\beta\Gamma\widetilde{R}_{\text{MIT}}(\bar{z}))^* \Psi_M^{-1}(z)\Gamma\widetilde{R}_{\text{MIT}}(z).$$

Before going through the proof of Theorem 6.2, 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 $\mathscr{A}_{m+M}^e$.

Proposition 6.4. *Let $\mathscr{A}_m^i$ and $\mathscr{A}_{m+M}^e$ be as above. Then, there is $M_0 > 0$ such that, for every $M > M_0$ and all $z \in \rho(H_{\text{MIT}}(m)) \cap \rho(H_M)$, the following hold*:

(i) *For any $s \in \mathbb{R}$, the operator $\Xi_M(z) : H^s(\Sigma)^4 \to H^s(\Sigma)^4$ defined by*

$$\Xi_M(z) = (I_4 - \mathscr{A}_m^i \mathscr{A}_{m+M}^e - \mathscr{A}_{m+M}^e \mathscr{A}_m^i)^{-1} \tag{6-4}$$

is everywhere defined and uniformly bounded with respect to M.

(ii) *The Poincaré–Steklov operator, $\mathscr{A}_{m+M}^e$, satisfies the estimate*

$$\|\mathscr{A}_{m+M}^e\|_{P_+ H^{s+1}(\Sigma)^4 \to P_- H^s(\Sigma)^4} \lesssim M^{-1} \quad \text{for all } s \in \mathbb{R}.$$

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. Indeed, fix $z \in \rho(H_{\text{MIT}}(m)) \cap \rho(H_M)$ and set $h = \tau^{-1}$. Then, from Theorem 4.5 and Remark 5.10, 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, $\mathscr{A}_m^i \in \text{Op}^h \mathcal{S}^0(\Sigma)$, and, in local coordinates, its semiclassical principal symbol is given by

$$p_{h,\mathscr{A}_m^i}(x, \xi) = \frac{S \cdot (\xi \wedge n(x)) P_-}{|\xi \wedge n(x)|},$$

where we identify $\xi \in \mathbb{R}^2$ with $\bar{\xi} = (\xi_1, \xi_2, 0)^t \in \mathbb{R}^3$, and, for $x = \varphi(\tilde{x}) \in \Sigma$, we let $n(x)$ stand for $n^\varphi(\tilde{x})$. Similarly, thanks to Theorem 5.1, for h_0 sufficiently small (and hence M_0 big enough) and all $h < h_0$, we also know that $\mathscr{A}^e_{m+M}$ is a h-pseudodifferential operator and that

$$\mathscr{A}^e_{m+M} \in \mathrm{Op}^h \mathcal{S}^0(\Sigma), \quad p_{h,\mathscr{A}^e_{m+M}}(x,\xi) = -\frac{S\cdot(\xi\wedge n(x))P_+}{\sqrt{|\xi\wedge n(x)|^2+1}+1}.$$

Therefore, the symbol calculus yields, for all $h < h_0$, that $(I_4 - \mathscr{A}^i_m \mathscr{A}^e_{m+M} - \mathscr{A}^e_{m+M}\mathscr{A}^i_m)$ is a $1/\tau$-pseudodifferential operator of order 0. Now, Lemmas A.3 and A.1 yield

$$\frac{S\cdot(\xi\wedge n(x))P_\pm S\cdot(\xi\wedge n(x))P_\mp}{|\xi\wedge n(x)|(\sqrt{|\xi\wedge n(x)|^2+1}+1)} = \frac{|\xi\wedge n(x)|P_\mp}{\sqrt{|\xi\wedge n(x)|^2+1}+1}.$$

Thus

$$\begin{aligned} I_4 - p_{h,\mathscr{A}^i_m}(x,\xi)p_{h,\mathscr{A}^e_{m+M}}(x,\xi) - p_{h,\mathscr{A}^e_{m+M}}(x,\xi)p_{h,\mathscr{A}^i_m}(x,\xi) \\ = I_4 + \frac{|\xi\wedge n(x)|}{\sqrt{|\xi\wedge n(x)|^2+1}+1} = \frac{\sqrt{|\xi\wedge n(x)|^2+1}+1+|\xi\wedge n(x)|}{\sqrt{|\xi\wedge n(x)|^2+1}+1} \gtrsim 1. \end{aligned}$$

From this, we deduce that $(I_4 - \mathscr{A}^i_m \mathscr{A}^e_{m+M} - \mathscr{A}^e_{m+M}\mathscr{A}^i_m)$ is elliptic in $\mathrm{Op}^h \mathcal{S}^0(\Sigma)$. Thus, $\Xi_M(z) \in \mathrm{Op}^h \mathcal{S}^0(\Sigma)$, 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 an h-pseudodifferential operator of order 0, it follows from the Calderón–Vaillancourt theorem (see (2-9)) that $\Xi_M(z) : H^s(\Sigma)^4 \to H^s(\Sigma)^4$ is well defined and uniformly bounded with respect to M for any $s \in \mathbb{R}$ proving assertion (i) of the theorem.

The proof of assertion (ii) exploits also the Calderón–Vaillancourt theorem which shows that, for any $s \in \mathbb{R}$, any operator in $h\,\mathrm{Op}^h \mathcal{S}^0(\Sigma)$ is uniformly bounded by $\mathcal{O}(h)$, with respect to $h = \tau^{-1} \in (0,1)$, from $H^{s+1}(\Sigma)^4$ into $H^s(\Sigma)^4$ (see (2-9)). Thus, for any $s \in \mathbb{R}$,

$$\Big\| \mathscr{A}^e_\tau - \frac{1}{\tau} D_\Sigma(\sqrt{-\tau^{-2}\Delta_\Sigma + I} + I)^{-1} P_+ \Big\|_{H^{s+1}(\Sigma)^4 \to H^s(\Sigma)^4} \lesssim \tau^{-1},$$

uniformly with respect to τ large enough. Then we conclude the proof of assertion (ii) by using that $(\sqrt{-\tau^{-2}\Delta_\Sigma + I} + I)^{-1}$ is uniformly bounded from $H^{s+1}(\Sigma)^4$ into itself and that D_Σ is bounded from $H^{s+1}(\Sigma)^4$ into $H^s(\Sigma)^4$ (as a first order differential operator). □

We can now give the proof of Theorem 6.2.

Proof of Theorem 6.2. Let M_0 be as in Proposition 6.4 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 system

$$\begin{cases} (D_m - z)v = f & \text{in } \Omega_i, \\ (D_{m+M} - z)u = f & \text{in } \Omega_e, \\ P_- t_\Sigma v = P_- t_\Sigma u & \text{on } \Sigma, \\ P_+ t_\Sigma v = P_+ t_\Sigma u & \text{on } \Sigma. \end{cases}$$

Since $E_m^{\Omega_i}(z)$ and $E_{m+M}^{\Omega_e}(z)$ give the unique solution to the boundary value problem (6-1) and (6-2), respectively, and

$$\Gamma_- R_{\mathrm{MIT}}(z) r_{\Omega_i} f = 0 \quad \text{and} \quad \Gamma_+ \widetilde{R}_M(z) r_{\Omega_e} f = 0,$$

if we let

$$\varphi = \Gamma_- u \quad \text{and} \quad \psi = \Gamma_+ v,$$

then it is easy to check that

$$\begin{cases} v = R_{\mathrm{MIT}}(z) r_{\Omega_i} f + E_m^{\Omega_i}(z)\varphi, \\ u = \widetilde{R}_M(z) r_{\Omega_e} f + E_{m+M}^{\Omega_e}(z)\psi. \end{cases} \tag{6-5}$$

Hence, to get an explicit formula for $R_M(z)$, it remains to find the unknowns φ and ψ. For this, note that from (6-5) we have

$$\begin{cases} \psi = \Gamma_+ r_{\Omega_i} R_M(z) f = \Gamma_+ R_{\mathrm{MIT}}(z) r_{\Omega_i} f + \Gamma_+ E_m^{\Omega_i}(z)[\varphi], \\ \varphi = \Gamma_- r_{\Omega_e} R_M(z) f = \Gamma_- \widetilde{R}_M(z) r_{\Omega_e} f + \Gamma_- E_{m+M}^{\Omega_e}(z)[\psi]. \end{cases} \tag{6-6}$$

Substituting the values of ψ and φ (from (6-6)) into the system (6-5), we obtain

$$\begin{aligned} R_M(z) &= e_{\Omega_i} R_{\mathrm{MIT}}(z) r_{\Omega_i} + e_{\Omega_e} \widetilde{R}_M(z) r_{\Omega_e} + (e_{\Omega_i} E_m^{\Omega_i}(z) \Gamma_- r_{\Omega_e} + e_{\Omega_e} E_{m+M}^{\Omega_e}(z) \Gamma_+ r_{\Omega_i}) R_M(z) \\ &= \widetilde{R}_{\mathrm{MIT}}(z) + E_M(z) \Gamma R_M(z). \end{aligned} \tag{6-7}$$

Note that, by definition of the Poincaré–Steklov operators, (6-6) is equivalent to

$$\begin{cases} \psi = \Gamma_+ R_{\mathrm{MIT}}(z) r_{\Omega_i} f + \mathscr{A}_m^i(\varphi), \\ \varphi = \Gamma_- \widetilde{R}_M(z) r_{\Omega_e} f + \mathscr{A}_{m+M}^e(\psi). \end{cases} \tag{6-8}$$

Thus, applying Γ to the identity (6-7) yields

$$\Gamma \widetilde{R}_{\mathrm{MIT}}(z) = (I - \mathscr{A}_m^i - \mathscr{A}_{m+M}^e) \Gamma R_M(z) = \Psi_M(z) \Gamma R_M(z).$$

Now, we apply $(I + \mathscr{A}_m^i + \mathscr{A}_{m+M}^e)$ to the last identity and get

$$(I + \mathscr{A}_m^i + \mathscr{A}_{m+M}^e) \Gamma \widetilde{R}_{\mathrm{MIT}}(z) = (I - \mathscr{A}_m^i \mathscr{A}_{m+M}^e - \mathscr{A}_{m+M}^e \mathscr{A}_m^i) \Gamma R_M(z) =: (\Xi_M(z))^{-1} \Gamma R_M(z),$$

where $\Xi_M(z)$ is given by (6-4). Then, thanks to Proposition 6.4, 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

$$\Psi_M^{-1} = \Xi_M(z)(I + \mathscr{A}_m^i + \mathscr{A}_{m+M}^e).$$

From this, it follows that

$$\Gamma R_M(z) = \Psi_M^{-1}(z) \Gamma \widetilde{R}_{\mathrm{MIT}}(z).$$

Substituting this into formula (6-7) yields

$$R_M(z) = \widetilde{R}_{\mathrm{MIT}}(z) + E_M(z) \Psi_M^{-1}(z) \Gamma \widetilde{R}_{\mathrm{MIT}}(z),$$

which achieves the proof of the theorem. □

As an immediate consequence of Theorem 6.2 and Proposition 6.4 we have the following.

Corollary 6.5. *There is $M_0 > 0$ such that, for every $M > M_0$ and all $z \in \rho(H_{\mathrm{MIT}}(m)) \cap \rho(H_M)$, the operators $\Xi^{\pm}_M(z) : P_{\pm}H^s(\Sigma)^4 \to P_{\pm}H^s(\Sigma)^4$ defined by*

$$\Xi^{+}_M(z) = (I - \mathscr{A}^i_m \mathscr{A}^e_{m+M})^{-1} \quad \textit{and} \quad \Xi^{-}_M(z) = (I - \mathscr{A}^e_{m+M} \mathscr{A}^i_m)^{-1}$$

are everywhere defined and bounded for any $s \in \mathbb{R}$, and

$$\| \Xi^{\pm}_M(z) \|_{P_{\pm}H^s(\Sigma)^4 \to P_{\pm}H^s(\Sigma)^4} \lesssim 1$$

uniformly with respect to $M > M_0$.

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 boundary value problem

$$\begin{cases} (D_m - z) r_{\Omega_i} v = f & \textit{in } \Omega_i, \\ \Gamma_- v = \Xi^{-}_M(z) \mathscr{A}^e_{m+M} \Gamma_+ R_{\mathrm{MIT}}(z) f & \textit{on } \Sigma, \\ \Gamma_+ v = \Gamma_+ R_{\mathrm{MIT}}(z) f + \mathscr{A}^i_m \Gamma_- v & \textit{on } \Sigma. \end{cases} \tag{6-9}$$

Proof. We first note that $\Xi^{\pm}_M(z) = P_{\pm} \Xi_M(z) P_{\pm}$. Thus, the first statement follows immediately from Proposition 6.4 . Now, let $f \in L^2(\Omega_i)^4$, and suppose that $v \in H^1(\mathbb{R}^3)^4$ 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

$$\varphi = P_- t_\Sigma v \quad \text{and} \quad \psi = P_+ t_\Sigma v,$$

then, from (6-8), we easily get

$$\varphi = \Xi^{-}_M(z) \mathscr{A}^e_{m+M} \Gamma_+ R_{\mathrm{MIT}}(z) f \quad \text{and} \quad \psi = \Gamma_+ R_{\mathrm{MIT}}(z) f + \mathscr{A}^i_m \varphi,$$

which means that $r_{\Omega_i} v$ satisfies (6-9). □

Remark 6.6. Notice, from (6-8) and Corollary 6.5, we have

$$\begin{pmatrix} \Gamma_+ r_{\Omega_i} R_M(z) f \\ \Gamma_- r_{\Omega_e} R_M(z) f \end{pmatrix} = \begin{pmatrix} \Xi^{+}_M(z) & 0 \\ 0 & \Xi^{-}_M(z) \end{pmatrix} \begin{pmatrix} I_4 & \mathscr{A}^i_m \\ \mathscr{A}^e_{m+M} & I_4 \end{pmatrix} \begin{pmatrix} \Gamma_+ R_{\mathrm{MIT}}(z) r_{\Omega_i} f \\ \Gamma_- \widetilde{R}_M(z) r_{\Omega_e} f \end{pmatrix}.$$

With this observation, we remark that the resolvent formula (6-3) can also be written in the following matrix form:

$$\begin{pmatrix} r_{\Omega_i} R_M(z) \\ r_{\Omega_e} R_M(z) \end{pmatrix} = \begin{pmatrix} R_{\mathrm{MIT}}(z) r_{\Omega_i} \\ \widetilde{R}_M(z) r_{\Omega_e} \end{pmatrix} + \begin{pmatrix} E^{\Omega_i}_m(z) \Xi^{-}_M(z) \mathscr{A}^e_{m+M} & E^{\Omega_i}_m(z) \Xi^{-}_M(z) \\ E^{\Omega_e}_{m+M}(z) \Xi^{+}_M(z) & E^{\Omega_e}_{m+M}(z) \Xi^{+}_M(z) \mathscr{A}^i_m \end{pmatrix} \begin{pmatrix} \Gamma_+ R_{\mathrm{MIT}}(z) r_{\Omega_i} \\ \Gamma_- \widetilde{R}_M(z) r_{\Omega_e} \end{pmatrix}.$$

An inspection of the proof of Theorem 6.2 shows that, for any $M > 0$, $z \in \rho(H_{\mathrm{MIT}}(m)) \cap \rho(H_M)$, and $f \in L^2(\mathbb{R}^3)^4$, one has

$$\Gamma \widetilde{R}_{\mathrm{MIT}}(z) f = \Psi_M(z) \Gamma R_M(z) f. \tag{6-10}$$

When f runs through the whole space $L^2(\mathbb{R}^3)^4$, then the values of $\Gamma \widetilde{R}_{\mathrm{MIT}}(z) f$ and $\Gamma R_M(z) f$ cover the whole space $H^{1/2}(\Sigma)^4$, which means that $\mathrm{Rn}(\Psi_M(z)) = H^{1/2}(\Sigma)^4$. Hence, if one proves that $\mathrm{Kr}(\Psi_M(z)) = \{0\}$, then $\Psi_M(z)$ would be boundedly invertible in $H^{1/2}(\Sigma)^4$, and thus (6-3) holds without restriction on $M > 0$. The following theorem provides a Birman–Schwinger-type principle relating $\mathrm{Kr}(H_M - z)$ with $\mathrm{Kr}(\Psi_M(z))$ and allows us to recover the resolvent formula (6-3) for any $M > 0$.

Theorem 6.7. *Let $M > 0$, and let Ψ_M be as in Theorem 6.2. Then, the following hold*:

(i) *For any $a \in (-(m+M), m+M) \cap \rho(H_{\mathrm{MIT}}(m))$, we have $a \in \mathrm{Sp}_p(H_M) \Leftrightarrow 0 \in \mathrm{Sp}_p(\Psi_M(a))$ and*

$$\mathrm{Kr}(H_M - a) = \{E_M(a)g : g \in \mathrm{Kr}(\Psi_M(a))\}.$$

In particular, $\dim \mathrm{Kr}(H_M - a) = \dim \mathrm{Kr}(\Psi_M(a))$ *for all $a \in (-(m+M), m+M) \cap \rho(H_{\mathrm{MIT}}(m))$.*

(ii) *The operator $\Psi_M(z)$ is boundedly invertible in $H^{1/2}(\Sigma)^4$ for all $z \in \rho(H_{\mathrm{MIT}}(m)) \cap \rho(H_M)$, and the following resolvent formula holds*:

$$R_M(z) = \widetilde{R}_{\mathrm{MIT}}(z) + E_M(z)\Psi_M^{-1}(z)\Gamma\widetilde{R}_{\mathrm{MIT}}(z). \tag{6-11}$$

Proof. (i) Let us first prove the implication ($\Rightarrow$). Let $a \in (-(m+M), m+M) \cap \rho(H_{\mathrm{MIT}}(m))$ 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 (6-1) for $z = a$ with $g = \Gamma_-\varphi$, and φ_- solves the system (6-2) 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

$$(I_4 + \mathscr{A}_m^i)\Gamma_-\varphi =: t_\Sigma\varphi_+ = t_\Sigma\varphi = t_\Sigma\varphi_- := (I_4 + \mathscr{A}_{m+M}^e)\Gamma_+\varphi,$$

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 $\mathrm{Kr}(H_M - a) \subset \{E_M(a)g : g \in \mathrm{Kr}(\Psi_M(a))\}$.

Now, we turn to the proof of the implication ($\Leftarrow$). Let $a \in (-(m+M), m+M) \cap \rho(H_{\mathrm{MIT}}(m))$ 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

$$(P_- + \mathscr{A}_m^i)g = (P_+ + \mathscr{A}_{m+M}^e)g. \tag{6-12}$$

Since $a \in (-(m+M), m+M) \cap \rho(H_{\mathrm{MIT}}(m))$, 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. Hence, it remains to show that $\varphi \in H^1(\mathbb{R}^3)^4$. For this, observe that, by (6-12), we have

$$t_\Sigma E_m^{\Omega_i}(a)P_-g = (P_- + \mathscr{A}_m^i)g = (P_+ + \mathscr{A}_{m+M}^e)g = t_\Sigma E_{m+M}^{\Omega_e}(a)P_+g.$$

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 φ satisfies the equation $(H_M - a)\varphi = 0$. Therefore, $a \in \mathrm{Sp}_p(H_M)$, and the inclusion $\{E_M(a)g : g \in \mathrm{Kr}(\Psi_M(a))\} \subset \mathrm{Kr}(H_M - a)$ holds, which completes the proof of (i).

(ii) Let $z \in \rho(H_{\mathrm{MIT}}(m)) \cap \rho(H_M)$, and note that the self-adjointness of H_M together with assertion (i) imply that $\mathrm{Kr}(\Psi_M(z)) = \{0\}$, as otherwise $\mathrm{Kr}(H_M - z) \neq \{0\}$. Since $\mathrm{Rn}(\Psi_M(z)) = H^{1/2}(\Sigma)^4$ holds for all $z \in \rho(H_{\mathrm{MIT}}(m)) \cap \rho(H_M)$, it follows that $\Psi_M(z)$ admits a bounded and everywhere defined inverse in $H^{1/2}(\Sigma)^4$. Therefore, (6-10) yields $\Gamma R_M(z) = \Psi_M^{-1}(z)\Gamma\widetilde{R}_{\mathrm{MIT}}(z)$, and the resolvent formula (6-11) follows from this and (6-7). $\square$

Remark 6.8. Note the different nature of Theorems 6.2 and 6.7: the second ensures the invertibility of Ψ_M and yields the resolvent formula (6-11) without assumption, while the first is based on a largeness assumption that allows us (thanks to the semiclassical properties of PS operators) to obtain the explicit formula of the operator $(\Psi_M)^{-1}$. Note that in Theorem 6.7 we do not know a priori whether $(\Psi_M)^{-1}$ is uniformly bounded when M is large, and hence (6-11) is not suitable for studying the large coupling convergence.

In the next proposition we prove the norm convergence of $R_M(z)$ toward $R_{\mathrm{MIT}}(z)$ and estimate the rate of convergence.

Proposition 6.9. *For any compact set $K \subset \rho(H_{\mathrm{MIT}}(m))$, there is $M_0 > 0$ such that, for all $M > M_0$, we have $K \subset \rho(H_M)$ 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*

$$R_M(z) = e_{\Omega_i} R_{\mathrm{MIT}}(z) r_{\Omega_i} + \frac{1}{M}(K_M(z) + L_M(z)), \tag{6-13}$$

where $K_M(z), L_M(z) : L^2(\mathbb{R}^3)^4 \to L^2(\mathbb{R}^3)^4$ are uniformly bounded with respect to M and satisfy

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

In particular,

$$\| R_M(z) - e_{\Omega_i} R_{\mathrm{MIT}}(z) r_{\Omega_i} \|_{L^2(\mathbb{R}^3)^4 \to L^2(\mathbb{R}^3)^4} = \mathcal{O}\Big(\frac{1}{M}\Big). \tag{6-14}$$

Before giving the proof, we need the following estimates.

Lemma 6.10. *Let $K \subset \mathbb{C}$ be a compact set. Then, there is $M_0 > 0$ such that, for all $M > M_0$, we have $K \subset \rho(\widetilde{H}_M)$ and, for every $z \in K$, the following estimates hold:*

$$\|\widetilde{R}_M(z) f\|_{L^2(\Omega_e)^4} + \frac{1}{\sqrt{M}} \|\Gamma_- \widetilde{R}_M(z) f\|_{L^2(\Sigma)^4} \lesssim \frac{1}{M} \|f\|_{L^2(\Omega_e)^4} \quad \text{for all } f \in L^2(\Omega_e)^4,$$

$$\|\Gamma_- \widetilde{R}_M(z) f\|_{H^{-1/2}(\Sigma)^4} \lesssim \frac{1}{M} \|f\|_{L^2(\Omega_e)^4} \quad \text{for all } f \in L^2(\Omega_e)^4,$$

$$\|E^{\Omega_e}_{m+M}(z)\psi\|_{L^2(\Omega_e)^4} \lesssim \frac{1}{\sqrt{M}} \|\psi\|_{L^2(\Sigma)^4} \quad \text{for all } \psi \in P_+ L^2(\Sigma)^4,$$

$$\|E^{\Omega_e}_{m+M}(z)\psi\|_{L^2(\Omega_e)^4} \lesssim \frac{1}{M} \|\psi\|_{H^{1/2}(\Sigma)^4} \quad \text{for all } \psi \in P_+ H^{1/2}(\Sigma)^4.$$

Proof. Fix a compact set $K \subset \mathbb{C}$, and note that, for $M_1 > \sup_{z \in K}\{|\mathrm{Re}(z)| - m\}$, we have $K \subset \rho(D_{m+M_1})$, 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, let $z \in K$, and assume that $M > M_1$. Let $\varphi \in \mathrm{dom}(\widetilde{H}_M)$. Then a straightforward application of Green's formula yields

$$\|\widetilde{H}_M \varphi\|^2_{L^2(\Omega_e)^4} = \|(\alpha \cdot \nabla)\varphi\|^2_{L^2(\Omega_e)^4} + (m+M)^2 \|\varphi\|^2_{L^2(\Omega_e)^4} + (m+M)\|P_- t_\Sigma \varphi\|^2_{L^2(\Sigma)^4}.$$

Using this and the Cauchy–Schwarz inequality we obtain

$$\begin{aligned} \|(\widetilde{H}_M - z)\varphi\|^2_{L^2(\Omega_e)^4} &= \|\widetilde{H}_M \varphi\|^2_{L^2(\Omega_e)^4} + |z|^2 \|\varphi\|^2_{L^2(\Omega_e)^4} - 2\,\mathrm{Re}(z) \langle \widetilde{H}_M \varphi, \varphi \rangle_{L^2(\Omega_e)^4} \\ &\geqslant \|\widetilde{H}_M \varphi\|^2_{L^2(\Omega_e)^4} + |z|^2 \|\varphi\|^2_{L^2(\Omega_e)^4} - \tfrac{1}{2} \|\widetilde{H}_M \varphi\|^2_{L^2(\Omega_e)^4} - 2|\mathrm{Re}(z)|^2 \|\varphi\|^2_{L^2(\Omega_e)^4} \\ &\geqslant \big(\tfrac{1}{2}(m+M)^2 + |\mathrm{Im}(z)|^2 - |\mathrm{Re}(z)|^2\big) \|\varphi\|^2_{L^2(\Omega_e)^4} + \tfrac{1}{2} M \|P_- t_\Sigma \varphi\|^2_{L^2(\Sigma)^4}. \end{aligned}$$

Therefore, taking $\widetilde{R}_M(z)f=\varphi$ and $M\geqslant M_2\geqslant \sup_{z\in K}\{\sqrt{|\mathrm{Re}(z)|^2-|\mathrm{Im}(z)|^2}-m\}$, we obtain the inequality

$$\|\widetilde{R}_M(z)f\|_{L^2(\Omega_e)^4}+\frac{1}{\sqrt{M}}\|\Gamma_-\widetilde{R}_M(z)f\|_{L^2(\Sigma)^4}\lesssim\frac{1}{M}\|f\|_{L^2(\Omega_e)^4}.$$

Since Γ_- is bounded from $L^2(\Omega_e)^4$ into $H^{-1/2}(\Sigma)^4$, it follows from the above inequality that

$$\|\Gamma_-\widetilde{R}_M(z)f\|_{H^{-1/2}(\Sigma)^4}\lesssim\|\Gamma_-\|_{L^2(\Omega_e)^4\to H^{-1/2}(\Sigma)^4}\|\widetilde{R}_M(z)f\|_{L^2(\Omega_e)^4}\lesssim\frac{1}{M}\|f\|_{L^2(\Omega_e)^4}$$

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 4.2, we have

$$\|\psi\|^2_{L^2(\Sigma)^4}\geqslant(m+M)\|E^{\Omega_e}_{m+M}(z)\psi\|^2_{L^2(\Omega_e)^4}-2|\mathrm{Re}(z)|\|E^{\Omega_e}_{m+M}(z)\psi\|^2_{L^2(\Omega_e)^4}.$$

Thus, for any $M\geqslant M_3\geqslant\sup_{z\in K}\{4|\mathrm{Re}(z)|-m\}$, we get

$$M\|E^{\Omega_e}_{m+M}(z)\psi\|^2_{L^2(\Omega_e)^4}\leqslant 2\|\psi\|^2_{L^2(\Sigma)^4},$$

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 4.2. Indeed, from Proposition 4.2(ii), we know that $\beta\Gamma_-\widetilde{R}_M(\bar z)$ is the adjoint of the operator $E^{\Omega_e}_{m+M}(z):P_+H^{1/2}(\Sigma)^4\to L^2(\Omega_e)^4$. Using this and the estimate fulfilled by $\Gamma_-\widetilde{R}_M(\bar z)$, we obtain

$$\begin{aligned}|\langle f,E^{\Omega_e}_{m+M}(z)\psi\rangle_{L^2(\Omega_e)^4}|&=|\langle\Gamma_-\widetilde{R}_M(\bar z)f,\beta\psi\rangle_{H^{-1/2}(\Sigma)^4,H^{1/2}(\Sigma)^4}|\\&\leqslant\|\Gamma_-\widetilde{R}_M(z)f\|_{H^{-1/2}(\Sigma)^4}\|\psi\|_{H^{1/2}(\Sigma)^4}\lesssim\frac{1}{M}\|f\|_{L^2(\Omega_e)^4}\|\psi\|_{H^{1/2}(\Sigma)^4}.\end{aligned}$$

Since this is true for all $f\in L^2(\Omega_e)^4$, by duality arguments, it follows that

$$\|E^{\Omega_e}_{m+M}(z)\psi\|_{L^2(\Omega_e)^4}\lesssim\frac{1}{M}\|\psi\|_{H^{1/2}(\Sigma)^4}\quad\text{for all }\psi\in P_+H^{1/2}(\Sigma)^4,$$

which proves the last inequality. Hence, the lemma follows by taking $M_0=\max\{M_1,M_2,M_3\}$. □

Proof of Proposition 6.9. We first show (6-14) for some $M_0'>0$ and any $z\in\mathbb{C}\setminus\mathbb{R}$. So, let us 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 6.2 and Remark 6.6, we know that there is $M_0'>0$ such that, for all $M>M_0'$,

$$\begin{aligned}&\|(R_M(z)-e_{\Omega_i}R_{\mathrm{MIT}}(z)r_{\Omega_i})f\|_{L^2(\mathbb{R}^3)^4}\\&\quad\leqslant\|E^{\Omega_i}_m(z)\Xi^-_M(z)\mathscr{A}^e_{m+M}\Gamma_+R_{\mathrm{MIT}}(z)r_{\Omega_i}f\|_{L^2(\Omega_i)^4}+\|E^{\Omega_i}_m(z)\Xi^-_M(z)\Gamma_-\widetilde{R}_M(z)r_{\Omega_e}f\|_{L^2(\Omega_i)^4}\\&\qquad+\|E^{\Omega_e}_{m+M}(z)\Xi^+_M(z)\Gamma_+R_{\mathrm{MIT}}(z)r_{\Omega_i}f\|_{L^2(\Omega_e)^4}+\|E^{\Omega_e}_{m+M}(z)\Xi^+_M(z)\mathscr{A}^i_m\Gamma_-\widetilde{R}_M(z)r_{\Omega_e}f\|_{L^2(\Omega_e)^4}\\&\qquad+\|\widetilde{R}_M(z)r_{\Omega_e}f\|_{L^2(\Omega_e)^4}\\&\quad=:J_1+J_2+J_3+J_4+J_5.\end{aligned}$$

From Lemma 6.10 we immediately get $J_5\lesssim M^{-1}\|f\|$. Now notice 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 (2-2)) are bounded operators and do not depend on M. Moreover, thanks to Corollary 6.5, we know that, for all $s \in \mathbb{R}$, there is $C > 0$ independent of M such that

$$\|\Xi_M^{\pm}(z)\|_{P_\pm H^s(\Sigma)^4 \to P_\pm H^s(\Sigma)^4} \leqslant C.$$

Using this and the above observation, for $j \in \{1, 2, 3, 4\}$, we can estimate J_k as follows:

$$\begin{aligned}
J_1 &\lesssim \|E_m^{\Omega_i}(z)\|_{P_- H^{-1/2}(\Sigma)^4 \to L^2(\Omega_i)^4} \|\mathscr{A}_{m+M}^e\|_{H^{1/2}(\Sigma)^4 \to H^{-1/2}(\Sigma)^4} \|\Gamma_+ R_{\mathrm{MIT}}(z) r_{\Omega_i} f\|_{H^{1/2}(\Sigma)^4},\\
J_2 &\lesssim \|E_m^{\Omega_i}(z)\|_{H^{-1/2}(\Sigma)^4 \to L^2(\Omega_i)^4} \|\Gamma_- \widetilde{R}_M(z) r_{\Omega_e} f\|_{H^{-1/2}(\Sigma)^4},\\
J_3 &\lesssim \|E_{m+M}^{\Omega_e}(z)\|_{H^{1/2}(\Sigma)^4 \to L^2(\Omega_e)^4} \|\Gamma_+ R_{\mathrm{MIT}}(z) r_{\Omega_i} f\|_{H^{1/2}(\Sigma)^4},\\
J_4 &\lesssim \|E_{m+M}^{\Omega_e}(z)\|_{L^2(\Sigma)^4 \to L^2(\Omega_e)^4} \|\mathscr{A}_m^i\|_{L^2(\Sigma)^4 \to L^2(\Sigma)^4} \|\Gamma_- \widetilde{R}_M(z) r_{\Omega_e} f\|_{L^2(\Sigma)^4}.
\end{aligned}$$

Therefore, Proposition 6.4(ii) together with Lemma 6.10 yield

$$J_k \lesssim \frac{1}{M} \|f\|_{L^2(\mathbb{R}^3)^4} \quad \text{for any } j \in \{1, 2, 3, 4\}.$$

Thus, we obtain the estimate

$$\|(R_M(z) - e_{\Omega_i} R_{\mathrm{MIT}}(z) r_{\Omega_i}) f\|_{L^2(\mathbb{R}^3)^4} \leqslant \frac{C}{M} \|f\|_{L^2(\mathbb{R}^3)^4}. \tag{6-15}$$

Moreover, the asymptotic expansion (6-13) holds with

$$L_M(z) = M\big(e_{\Omega_e} \widetilde{R}_M(z) r_{\Omega_e} + e_{\Omega_i} E_m^{\Omega_i}(z) \Xi_M^-(z) \mathscr{A}_{m+M}^e \Gamma_+ R_{\mathrm{MIT}}(z) r_{\Omega_i} + e_{\Omega_e} E_{m+M}^{\Omega_e}(z) \Xi_M^+(z) \mathscr{A}_m^i \Gamma_- \widetilde{R}_M(z) r_{\Omega_e}\big),$$

and

$$K_M(z) = M\big(e_{\Omega_i} E_m^{\Omega_i}(z) \Xi_M^-(z) \Gamma_- \widetilde{R}_M(z) r_{\Omega_e} + e_{\Omega_e} E_{m+M}^{\Omega_e}(z) \Xi_M^+(z) \Gamma_+ R_{\mathrm{MIT}}(z) r_{\Omega_i}\big),$$

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 (6-15) holds true for every $z \in \mathbb{C} \setminus \mathbb{R}$, for any fixed compact subset $K \subset \rho(H_{\mathrm{MIT}}(m))$, one can show by arguments similar to those in the proof of [Barbaroux et al. 2019, Lemma A.1] that there is $M_0 > M_0'$ such that $K \subset \rho(H_M)$. The proposition follows from the same arguments as before. □

6A. *Comments and further remarks.* In this part we discuss possible generalizations of our results and comment on the usefulness of the pseudodifferential properties of the Poincaré–Steklov operators.

(1) First note that all the results in this article which are proved without the use of the (semi) classical properties of the Poincaré–Steklov operator are valid when Σ is just $C^{1,\omega}$-smooth with $\omega \in \left(\frac{1}{2}, 1\right)$, and can also be generalized without difficulty to the case of local deformation of the plane $\mathbb{R}^2 \times \{0\}$ (see [Benhellal 2022b] where the self-adjointness of $H_{\mathrm{MIT}}(m)$ and the regularity properties of $\Phi_{z,m}^{\Omega}$, $\mathscr{C}_{z,m}$, and Λ_m^z were shown for this case). We mention, however, that in the latter case the spectrum of the MIT bag operator is equal to that of the free Dirac operator; see [Benhellal 2022b, Theorem 4.1].

(2) It should also be noted that there are several boundary conditions that lead to self-adjoint realizations of the Dirac operator on domains (see, e.g., [Arrizabalaga et al. 2023; Behrndt et al. 2020; Benhellal 2022a]) and for which the associated PS operators can be analyzed in a similar way as for the MIT

bag model. In particular, one can consider the PS operator $\mathscr{B}_m(z)$ associated with the self-adjoint Dirac operator

$$\widetilde{H}_{\mathrm{MIT}}(m)v = D_m v \quad \text{for all } v \in \mathrm{dom}(\widetilde{H}_{\mathrm{MIT}}(m)) := \{v \in H^1(\Omega_i)^4 : P_+ t_\Sigma v = 0 \text{ on } \Sigma\}.$$

According to the previous considerations, this operator can be viewed as an analogue of the Neumann-to-Dirichlet map for the Dirac operator. Moreover, the same arguments as in the proof of Theorem 4.5 show that

$$\mathscr{B}_m(z) = \frac{1}{\sqrt{-\Delta_\Sigma}} S \cdot (\nabla_\Sigma \wedge n) P_+ \mod \mathrm{Op}\,\mathcal{S}^{-1}(\Sigma) = \frac{D_\Sigma}{\sqrt{-\Delta_\Sigma}} P_+ \mod \mathrm{Op}\,\mathcal{S}^{-1}(\Sigma)$$

for all $z \in \rho(D_m) \cap \rho(\widetilde{H}_{\mathrm{MIT}}(m))$.

(3) As already mentioned in the introduction, in [Barbaroux et al. 2019], it was shown that (in the two-dimensional massless case) the norm resolvent convergence of H_M to $H_{\mathrm{MIT}}(m)$ holds with a convergence rate of $M^{-1/2}$. Their proof is based on two main ingredients: the first is a resolvent identity (see [Barbaroux et al. 2019, Lemma 2.2] for the exact formula), and the second is the inequality

$$\|\Gamma_- R_M(z) f\|_{L^2(\Sigma)^4} \lesssim \frac{1}{\sqrt{M}} \|f\|_{L^2(\mathbb{R}^3)^4}, \tag{6-16}$$

which is a consequence of the lower bound

$$\|\nabla\psi\|^2_{L^2(\Omega_e)^4} + M^2\|\psi\|^2_{L^2(\Omega_e)^4} \geqslant (M - C)\|t_\Sigma\psi\|^2_{L^2(\Sigma)^4},$$

which holds for all $\psi \in H^1(\mathbb{R}^3)^4$ and M large enough (see [Stockmeyer and Vugalter 2019, Lemma 4] for the proof in the two-dimensional case, and [Arrizabalaga et al. 2019, Proposition 2.1(i)] for the three-dimensional case). Note that the resolvent formula (6-7) together with (6-16) yield the same result. Indeed, from (6-6) and (6-16), we easily get the inequality

$$\|\Gamma_+ R_M(z) f\|_{L^2(\Sigma)^4} \lesssim \|f\|_{L^2(\mathbb{R}^3)^4}.$$

This together with (6-7) and Lemma 6.10 yield

$$\begin{aligned}
&\|(R_M(z) - e_{\Omega_i} R_{\mathrm{MIT}}(z) r_{\Omega_i}) f\|_{L^2(\mathbb{R}^3)^4} \\
&\qquad \leqslant \|E_m^{\Omega_i}(z)\Gamma_- r_{\Omega_e} R_M(z) f\|_{L^2(\Omega_i)^4} + \|\widetilde{R}_M(z) r_{\Omega_e} f\|_{L^2(\Omega_e)^4} + \|E_{m+M}^{\Omega_e}(z)\Gamma_+ r_{\Omega_i} R_M(z) f\|_{L^2(\Omega_e)^4} \\
&\qquad \lesssim \frac{1}{\sqrt{M}} \|f\|_{L^2(\mathbb{R}^3)^4}.
\end{aligned}$$

(4) Finally, let us point out that a first order asymptotic expansion of the eigenvalues of H_M in terms of the eigenvalues of $H_{\mathrm{MIT}}(m)$ was established in [Arrizabalaga et al. 2019] when $M \to \infty$. In their proof, the authors used the min-max characterization and optimization techniques. Note that it is also possible to obtain such a result using the properties of the PS operator, the Krein formula from Theorem 6.2, and the finite-dimensional perturbation theory (see [Kato 1966] for example); see, e.g., [Benhellal 2019; Bruneau and Carbou 2002] for similar arguments. Note also that the asymptotic expansion of the eigenvalues of H_M depends only on the term $E_m^{\Omega_i}(z)\Xi_M^-(z)\mathscr{A}_{m+M}^e\Gamma_+ R_{\mathrm{MIT}}(z) r_{\Omega_i}$. Indeed, let λ_{MIT} be

an eigenvalue of $H_{\mathrm{MIT}}(m)$ with multiplicity l, and let $(f_1, \dots, f_l)$ be an $L^2(\Omega_i)^4$-orthonormal basis of $\mathrm{Kr}(H_{\mathrm{MIT}}(m) - \lambda_{\mathrm{MIT}} I_4)$. Then, using the explicit resolvent formula from Remark 6.6, we see that

$$\begin{aligned}\langle R_M(z) e_{\Omega_i} f_k, e_{\Omega_i} f_j\rangle_{L^2(\mathbb{R}^3)^4} &= \langle E_m^{\Omega_i}(z)\,\Xi_M^-(z)\mathscr{A}_{m+M}^e \Gamma_+ R_{\mathrm{MIT}}(z) f_k, f_j\rangle_{L^2(\Omega_i)^4}\\ &= \langle \Xi_M^-(z)\mathscr{A}_{m+M}^e \Gamma_+ R_{\mathrm{MIT}}(z) f_k, -\beta\Gamma_+ R_{\mathrm{MIT}}(\bar{z}) f_j\rangle_{L^2(\Sigma)^4}\\ &= \frac{1}{(z-\lambda_{\mathrm{MIT}})^2}\langle \Xi_M^-(z)\mathscr{A}_{m+M}^e \Gamma_+ f_k, -\beta\Gamma_+ f_j\rangle_{L^2(\Sigma)^4},\end{aligned}$$

which means that $E_m^{\Omega_i}(z)\,\Xi_M^-(z)\mathscr{A}_{m+M}^e \Gamma_+ R_{\mathrm{MIT}}(z) r_{\Omega_i}$ is the only term that intervenes in the asymptotic expansion of the eigenvalues of H_M. Besides, recall that the principal symbol of $\Xi_M^-(z)\mathscr{A}_{m+M}^e$ is given by

$$q_M(x,\xi) = -\frac{S\cdot(\xi\wedge n(x))P_+}{\sqrt{|\xi\wedge n(x)|^2 + (m+M)^2} + |\xi\wedge n(x)| + (m+M)},$$

and, for $M > 0$ large enough, one has

$$q_M(x,\xi) = -\frac{1}{2M} S\cdot(\xi\wedge n(x))P_+ \sum_{l=1}^{\infty} \frac{1}{M^{l+1}} p_l(x,\xi)P_+, \qquad p_l \in \mathcal{S}^{-l}.$$

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 $B(\lambda_{\mathrm{MIT}}, \eta)$, with $B(\lambda_{\mathrm{MIT}}, \eta) \cap \mathrm{Sp}(H_{\mathrm{MIT}}(m)) = \{\lambda_{\mathrm{MIT}}\}$) and these eigenvalues admit an asymptotic expansion of the form

$$\lambda_k^M = \lambda_{\mathrm{MIT}} + \frac{1}{M}\mu_k + \sum_{j=2}^{N} \frac{1}{M^j}\mu_k^j + \mathcal{O}(M^{-(N+1)}), \tag{6-17}$$

where $(\mu_k)_{1\leqslant k\leqslant l}$ are the eigenvalues of the matrix $\mathcal{M}$ with coefficients

$$m_{kj} = \tfrac{1}{2}\langle \beta\,\mathrm{Op}(S\cdot(\xi\wedge n(x)))\Gamma_+ f_k, \Gamma_+ f_j\rangle_{L^2(\Sigma)^4}.$$

Appendix: Dirac algebra and applications

In this appendix, we recall the anticommutation relations of Dirac matrices and give formulas used in the paper. Consider the 4×4-Hermitian Dirac matrices α_j, $j = 1, 2, 3$, and β, whose possible representation is given at the beginning of the paper. These Dirac matrices satisfy the anticommutation relations

$$\{\alpha_j, \alpha_k\} = 2\delta_{jk} I_4, \qquad \{\alpha_j, \beta\} = 0, \qquad \beta^2 = I_4, \qquad j,k \in \{1,2,3\}, \tag{A-1}$$

where we recall that $\{\cdot\,,\cdot\}$ is the anticommutator bracket.

Recall the definition of the spin angular momentum S and the matrix γ_5 (see (2-13)), and note that, by (A-1), we have $S = (i\alpha_2\alpha_3, -i\alpha_1\alpha_3, i\alpha_1\alpha_2)$.

Using the anticommutation relations (A-1), we easily get the following identities for all $X, Y \in \mathbb{R}^3$:

$$\begin{aligned} i(\alpha\cdot X)(\alpha\cdot Y) &= iX\cdot Y + S\cdot(X\wedge Y), & [\gamma_5, \alpha\cdot X] &= 0,\\ \{S\cdot X, \alpha\cdot Y\} &= -2(X\cdot Y)\gamma_5, & [S\cdot X, \beta] &= 0.\end{aligned} \tag{A-2}$$

Let us now give some relations we have used for n, a normal vector field to a smooth domain $\Omega \subset \mathbb{R}^3$, and for τ, a tangent vector, in particular for $\tau = n \wedge \xi$, where ξ is a Fourier variable.

Lemma A.1. *Let $n \in \mathbb{R}^3$, and let $\tau \in \mathbb{R}^3$ be such that $\tau \perp n$. Then the following identity holds*:

$$(S \cdot \tau + i(\alpha \cdot n)\beta)^2 = (|\tau|^2 + |n|^2)I_4.$$

Proof. Using the relations (A-1) and (A-2), we get

$$(S \cdot \tau)^2 = \gamma_5(\alpha \cdot \tau)\gamma_5(\alpha \cdot \tau) = (\gamma_5)^2(\alpha \cdot \tau)^2 = |\tau|^2 I_4.$$

Then we have

$$(S \cdot \tau + i(\alpha \cdot n)\beta)^2 = |\tau|^2 I_4 - ((\alpha \cdot n)\beta)^2 + i\{S \cdot \tau, (\alpha \cdot n)\beta\} = (|\tau|^2 + |n|^2)I_4 + i\{S \cdot \tau, (\alpha \cdot n)\beta\},$$

and since $\tau \cdot n = 0$, by (A-2), we obtain

$$\{S \cdot \tau, (\alpha \cdot n)\beta\} = \{S \cdot \tau, \alpha \cdot n\}\beta + \alpha \cdot n[S \cdot \tau, \beta] = 0,$$

and the conclusion follows. □

Proposition A.2. *For $\xi \in \mathbb{R}^3$ and $n \in \mathbb{R}^3$ such that $|n| = 1$, we define the matrix-valued function*

$$l_0(n, \xi) = i(\alpha \cdot n)(\alpha \cdot \xi + \beta).$$

Then $l_0(n, \xi)$ has two eigenvalues given by

$$\rho_\pm(n, \xi) := in \cdot \xi \pm \lambda(n, \xi), \quad \text{with } \lambda(n, \xi) = \sqrt{|n \wedge \xi|^2 + 1}.$$

The associated eigenprojections (*onto* $\mathrm{Kr}(l_0(n, \xi) - \rho_\pm(n, \xi)I_4)$) *are given by*

$$\Pi_\pm(n, \xi) := \frac{1}{2}\left(I_4 \pm \frac{S \cdot (n \wedge \xi) + i(\alpha \cdot n)\beta}{\lambda(n, \xi)}\right).$$

Proof. By applying (A-2) for $(X, Y) = (n, \xi)$, we get

$$l_0(n, \xi) = in \cdot \xi I_4 + S \cdot (n \wedge \xi) + i(\alpha \cdot n)\beta.$$

Thanks to Lemma A.1, the Hermitian matrix $h(n, \xi) := S \cdot (n \wedge \xi) + i(\alpha \cdot n)\beta$ satisfies

$$h(n, \xi)^2 = (|n \wedge \xi|^2 + 1)I_4 = \lambda(n, \xi)^2 I_4.$$

Therefore, $h(n, \xi)$ has the eigenvalues $\pm\lambda(n, \xi)$, and the associated eigenprojections are given by

$$\Pi_\pm(n, \xi) = \frac{1}{2}\left(I_4 \pm \frac{h(n, \xi)}{\lambda(n, \xi)}\right),$$

which proves the claimed results since $l_0(n, \xi) = in \cdot \xi I_4 + h(n, \xi)$. □

Lemma A.3. *Given $n \in \mathbb{R}^3$ such that $|n| = 1$, let $P_\pm = \Pi_\pm(n, 0) = \frac{1}{2}(I_4 \pm i(\alpha \cdot n)\beta)$ be the eigenprojections onto* $\mathrm{Kr}(i(\alpha \cdot n)\beta \mp I_4)$. *The following properties hold*:

(i) *For any $\tau \in \mathbb{R}^3$ such that $\tau \perp n$, we have*

$$P_\pm(S \cdot \tau) = (S \cdot \tau)P_\mp, \quad P_\pm(\alpha \cdot n) = (\alpha \cdot n)P_\mp \quad \text{and} \quad P_\pm\beta = \beta P_\mp.$$

(ii) *For any* $\xi \in \mathbb{R}^3$, *the projections* $\Pi_\pm(n,\xi)$ *defined in Proposition A.2 satisfy*

$$P_\pm \Pi_\pm P_\pm = k_+ P_\pm, \quad P_\mp \Pi_\pm P_\mp = k_- P_\pm \quad \textit{and} \quad P_\pm \Pi_\mp P_\mp = \mp\Theta P_\mp, \tag{A-3}$$

with

$$k_\pm(n,\xi) = \frac{1}{2}\left(1 \pm \frac{1}{\lambda(n,\xi)}\right), \quad \Theta(n,\xi) = \frac{1}{2\lambda(n,\xi)} S\cdot(n\wedge\xi). \tag{A-4}$$

Proof. The relations of (i) follow from (A-2). For the proof of (ii), let us write $\Pi_\pm(n,\xi)$ as

$$\Pi_\pm(n,\xi) = P_\pm \pm \frac{1}{2\lambda(x,\xi)} S\cdot(n\wedge\xi)P_\mp \pm \frac{i}{2}(\alpha\cdot n)\beta\left(\frac{1}{\lambda(n,\xi)} - 1\right).$$

Then, using item (i) of this lemma (with $\tau = n\wedge\xi$) and the fact that $P_\pm i(\alpha\cdot n)\beta = \pm P_\pm$, we get

$$P_\pm\Pi_\pm = P_\pm \pm \frac{1}{2\lambda} S\cdot(n\wedge\xi)P_\mp + \frac{1}{2}\left(\frac{1}{\lambda} - 1\right)P_\pm = k_+ P_\pm \pm \Theta P_\mp,$$
$$P_\mp\Pi_\pm = \pm\frac{1}{2\lambda} S\cdot(n\wedge\xi)P_\pm - \frac{1}{2}\left(\frac{1}{\lambda} - 1\right)P_\mp = k_- P_\mp \pm \Theta P_\pm,$$

with $k_\pm$ and Θ as in (A-4). Hence, (A-3) directly follows from the above formulas and the fact that $P_\pm$ are orthogonal projections. □

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