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Extension operator for the MIT Bag Model [(*)]

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Abstract. — This paper is devoted to the construction of an extension operator for the MIT bag Dirac operator on a $\mathcal{C}^{2,1}$ bounded open set of $\mathbb{R}^3$ in the spirit of the extension theorems for Sobolev spaces. As an elementary byproduct, we prove that the MIT bag Dirac operator is self-adjoint.

Résumé. — Cet article est consacré à la construction d'un opérateur d'extension pour l'opérateur MIT bag Dirac sur un ouvert borné de classe $\mathcal{C}^{2,1}$ de $\mathbb{R}^3$ dans l'esprit des théorèmes d'extension pour les espaces de Sobolev. L'auto-adjonction de l'opérateur MIT bag Dirac en est une conséquence élémentaire.

1. Introduction

1.1. The MIT bag Dirac operator

In the whole paper, Ω denotes a fixed bounded domain of $\mathbb{R}^3$ with $\mathcal{C}^{2,1}$ boundary. The Planck constant and the velocity of light are assumed to be

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equal to 1. Let us recall the definition of the Dirac operator associated with the energy of a relativistic particle of mass $m \in \mathbb{R}$ and spin $\frac{1}{2}$ (see [12]). The Dirac operator is a first order differential operator, acting on $L^2(\Omega, \mathbb{C}^4)$ in the sense of distributions, defined by

$$H = \alpha \cdot D + m\beta\,, \qquad D = -i\nabla\,, \tag{1.1}$$

where $\alpha = (\alpha_1, \alpha_2, \alpha_3)$, β and γ_5 are the 4×4 Hermitian and unitary matrices given by

$$\beta = \begin{pmatrix} 1_2 & 0 \\ 0 & -1_2 \end{pmatrix}, \quad \gamma_5 = \begin{pmatrix} 0 & 1_2 \\ 1_2 & 0 \end{pmatrix}, \quad \alpha_k = \begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{pmatrix} \quad \text{for } k = 1, 2, 3\,.$$

Here, the Pauli matrices σ_1, σ_2 and σ_3 are defined by

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

and $\alpha \cdot X$ denotes $\sum_{j=1}^3 \alpha_j X_j$ for any $X = (X_1, X_2, X_3)$. Let us now impose the boundary conditions under consideration in this paper and define the associated unbounded operator.

Notation 1.1. — In the following, $\Gamma := \partial\Omega$ and for all $\mathbf{x} \in \Gamma$, $\mathbf{n}(\mathbf{x})$ is the outward-pointing unit normal to the boundary.

Definition 1.2. — *The MIT bag Dirac operator $(H_m^\Omega, \mathrm{Dom}(H_m^\Omega))$ is defined on the domain*

$$\mathrm{Dom}(H_m^\Omega) = \{\psi \in H^1(\Omega, \mathbb{C}^4) \ : \ \mathcal{B}\psi = \psi \ \text{on}\ \Gamma\}\,, \quad \text{with} \quad \mathcal{B} = -i\beta(\alpha \cdot \mathbf{n})\,,$$

by $H_m^\Omega \psi = H\psi$ for all $\psi \in \mathrm{Dom}(H_m^\Omega)$. Note that the trace is well-defined by a classical trace theorem.

Notation 1.3. — We will denote $H = H_m^\Omega$ when there is no risk of confusion. We denote $\langle \cdot , \cdot \rangle$ the $\mathbb{C}^4$ scalar product (antilinear w.r.t. the left argument) and $\langle \cdot , \cdot \rangle_U$ the L^2 scalar product on the set U.

Remark 1.4. — The operator $(H_m^\Omega, \mathrm{Dom}(H_m^\Omega))$ is symmetric (see Lemma A.2) and densely defined.

Remark 1.5. — The operator $\mathcal{B}$ defined for all $\mathbf{x} \in \Gamma$ is a Hermitian matrix which satisfies $\mathcal{B}^2 = 1_4$ so that its spectrum is $\{\pm 1\}$. Both eigenvalues have multiplicity two. Thus, the MIT bag boundary condition imposes the wavefunctions ψ to be eigenvectors of $\mathcal{B}$ associated with the eigenvalues $+1$. This boundary condition is chosen by the physicists [8] so as to get a vanishing normal flow at the bag surface $-i\mathbf{n}\cdot\mathbf{j} = 0$ at the boundary Γ where the current density $\mathbf{j}$ is defined by

$$\mathbf{j} = \langle \psi, \alpha\psi \rangle.$$

Let us now describe our main result.

1.2. Main result

The aim of this paper is to construct a bounded extension operator from the domain of H_m^Ω into $H^1(\mathbb{R}^3)^4$ in the spirit of extension operators for Sobolev spaces (see for instance [6, Section 9.2]). As we will see, a motivation to construct such an operator is to prove self-adjointness. Our main result is the following one.

Theorem 1.6. — *Let Ω be a nonempty, bounded and $\mathcal{C}^{2,1}$ open set in $\mathbb{R}^3$ and $m \in \mathbb{R}$. There exist a constant $C > 0$ and an operator*

$$P : \mathrm{Dom}(H) \to H^1(\mathbb{R}^3)^4$$

such that $P\psi_{|\Omega} = \psi$ and

$$\|P\psi\|^2_{H^1(\mathbb{R}^3)} \leqslant C \left(\|\psi\|^2_{L^2(\Omega)} + \|\alpha \cdot D\psi\|^2_{L^2(\Omega)} \right),$$

for all $\psi \in \mathrm{Dom}(H)$. Moreover, the operator $(H, \mathrm{Dom}(H))$ is self-adjoint.

Remark 1.7. — The proof of Theorem 1.6 relies on the construction of an extension operator

$$P : \mathrm{Dom}(H^\star) \to H^1(\mathbb{R}^3)^4 ,$$

where $H^\star$ is the adjoint of H. Thus,

$$\mathrm{Dom}(H^\star) \subset H^1(\Omega)^4 ,$$

and then the inclusion $\mathrm{Dom}(H^\star) \subset \mathrm{Dom}(H)$ easily follows. Since H is symmetric (see Lemma A.2), we get $\mathrm{Dom}(H^\star) = \mathrm{Dom}(H)$.

Remark 1.8. — Note that the existence of an extension operator

$$P : \mathrm{Dom}(H^\star) \to H^1(\mathbb{R}^3)^4$$

is a necessary condition for H to be self-adjoint. Indeed, if H is self-adjoint, we have the bounded injections:

$$\mathrm{Dom}(H) = \mathrm{Dom}(H^\star) \hookrightarrow H^1(\Omega)^4 \hookrightarrow H^1(\mathbb{R}^3)^4 .$$

To see this, let us recall that, if Ω is $\mathcal{C}^{1,1}$, we have (see [1, Theorem 1.5] and [7, p. 379]):

$$\forall\, \psi \in \mathrm{Dom}(H) , \quad \|\alpha \cdot \nabla\psi\|^2_{L^2(\Omega)} = \|\nabla\psi\|^2_{L^2(\Omega)} + \frac{1}{2} \int_{\partial\Omega} \kappa |\psi|^2 \,\mathrm{d}s , \tag{1.2}$$

where κ is the trace of the Weingarten map. From this formula, we can show that the injection $\mathrm{Dom}(H) = \mathrm{Dom}(H^\star) \hookrightarrow H^1(\Omega)^4$ is bounded. The embedding $H^1(\Omega)^4 \hookrightarrow H^1(\mathbb{R}^3)^4$ is given by the extension theorem for Sobolev spaces (see for instance [9, Theorem 3.9]) which requires $\mathcal{C}^{0,1}$ regularity on Ω.

Remark 1.9. — Observe that, without loss of generality, we can assume that $m = 0$ since the operator βm is bounded (and self-adjoint) from $L^2(\Omega)^4$ into itself so that $\mathrm{Dom}(H^\star)$ is independent of m.

Remark 1.10. — Self-adjointness results have already been obtained in the case of $\mathcal{C}^\infty$-boundaries in [5] through Calderón projections and sophisticated pseudo-differential techniques. In two dimensions, $\mathcal{C}^2$-boundaries are considered in [4] (see also [11]) by using Cauchy kernels and the Riemann mapping theorem. The recent paper [10] tackles the three dimensions case for $\mathcal{C}^2$ boundaries via Calderón projections. The reader may also consult the survey [2] in the context of spin geometry or [3, Theorem 4.11] devoted to the smooth case. Let us also mention that more general local boundary conditions are considered in [4, 5].

2. Proof of the main theorem

We denote by $\mathscr{L}(E, F)$ the set of continuous linear applications from E to F where E and F are Banach spaces. We recall that the domain of H is independent of m:

$$\mathrm{Dom}(H) = \{\psi \in H^1(\Omega)^4,\ \mathcal{B}\psi = \psi \text{ on } \partial\Omega\}\,,$$

and that the domain of the adjoint $H^\star$ is defined by

$$\mathrm{Dom}(H^\star) = \{\psi \in L^2(\Omega)^4,\ L_\psi \in \mathscr{L}(L^2(\Omega)^4, \mathbb{C})\}\,,$$

where

$$L_\psi : \varphi \in \mathrm{Dom}(H) \mapsto \langle \psi, H\varphi\rangle_\Omega \in \mathbb{C}\,.$$

The proof is divided in several steps. First, we construct an extension map on the domain of the adjoint as follows.

Lemma 2.1. — *There exists an operator*

$$P : \mathrm{Dom}(H^\star) \to H^1(\mathbb{R}^3)^4$$

such that $P\psi_{|\Omega} = \psi$ *and*

$$\|P\psi\|^2_{H^1(\mathbb{R}^3)} \leqslant C\left(\|\psi\|^2_{L^2(\Omega)} + \|\alpha \cdot D\psi\|^2_{L^2(\Omega)}\right),$$

for all $\psi \in \mathrm{Dom}(H^\star)$.

We get as a consequence that

$$\mathrm{Dom}(H^\star) \subset H^1(\Omega)^4.$$

The second step in the proof of Theorem 1.6 relies on a study of the boundary conditions satisfied by the functions of $\mathrm{Dom}(H^\star)$.

2.1. Extension operator in the half-space case

In this section, we consider the case when $\Omega = \mathbb{R}^3_+$ and we establish the existence of an extension operator.

Lemma 2.2. — *There exists an operator*

$$P : \mathrm{Dom}(H^\star) \to \{\psi \in L^2(\mathbb{R}^3)^4,\ \alpha \cdot D\psi \in L^2(\mathbb{R}^3)^4\} = H^1(\mathbb{R}^3)^4$$

such that $P\psi_{|\mathbb{R}^3_+} = \psi$ *and*

$$\begin{aligned}\|P\psi\|^2_{H^1(\mathbb{R}^3)} &= \|P\psi\|^2_{L^2(\mathbb{R}^3)} + \|\nabla P\psi\|^2_{L^2(\mathbb{R}^3)}\\ &= 2\left(\|\psi\|^2_{L^2(\mathbb{R}^3_+)} + \|\alpha \cdot D\psi\|^2_{L^2(\mathbb{R}^3_+)}\right).\end{aligned}$$

Proof. — The outward-pointing normal $\mathbf{n}$ is equal to $-e_3 = (0,0,-1)^T$ so that the boundary condition is

$$i\beta\alpha_3\psi = \psi\,,$$

on $\partial\mathbb{R}^3_+$. Let us diagonalize the matrix $i\beta\alpha_3$ appearing in the boundary condition. We introduce the matrix

$$T = \frac{1}{\sqrt{2}}\begin{pmatrix} 1_2 & i1_2 \\ i1_2 & 1_2\end{pmatrix}.$$

We have

$$T\beta T^\star = \begin{pmatrix} 0 & -i1_2 \\ i1_2 & 0\end{pmatrix}, \quad T\alpha_k T^\star = \alpha_k, \quad T(i\beta\alpha_3)T^\star = \begin{pmatrix}\sigma_3 & 0 \\ 0 & -\sigma_3\end{pmatrix} =: \mathcal{B}^0\,.$$

We consider $\widetilde{H} = THT^\star$. The operator $\widetilde{H}$ is defined by $\widetilde{H}\psi = \alpha \cdot D\psi$ for any $\psi \in \mathrm{Dom}(\widetilde{H})$ where

$$\begin{aligned}\mathrm{Dom}(\widetilde{H}) &= \left\{\psi \in H^1(\mathbb{R}^3_+),\ \mathcal{B}^0\psi = \psi,\ \text{on } \partial\mathbb{R}^3_+\right\}\\ &= \left\{\psi \in H^1(\mathbb{R}^3_+),\ \psi^2 = \psi^3 = 0 \text{ on } \partial\mathbb{R}^3_+\right\}\end{aligned} \tag{2.1}$$

and $\psi = (\psi^1, \psi^2, \psi^3, \psi^4)^T$. This unitarily equivalent representation of the Dirac operator is called the *supersymmetric representation* (see [12, Appendix 1.A]). This expression of the domain makes more apparent the fact that the MIT bag boundary condition is intermediary between the Dirichlet and Neumann boundary conditions.

Let us denote by $S : \mathbb{R}^3 \to \mathbb{R}^3$ and $\Pi : \mathbb{R}^3 \to \mathbb{R}^3$ the orthogonal symmetry with respect to $\partial\mathbb{R}^3_+$ and the orthogonal projection on $\partial\mathbb{R}^3_+$. Based on (2.1), we define the extension operator $\widetilde{P}$ for $\psi \in \mathrm{Dom}(\widetilde{H}^\star)$ as follows:

$$\widetilde{P}\psi(x,y,z) = \begin{cases}\psi(x,y,z), & \text{if } z > 0\\ (\psi^1, -\psi^2, -\psi^3, \psi^4)^T(x,y,-z) = \mathcal{B}^0\left(\psi \circ S\right)(x,y,z), & \text{if } z < 0\end{cases}$$

for $(x,y,z)\in\mathbb{R}^3$. In other words, we extend ψ^1,ψ^4 by symmetry and ψ^2,ψ^3 by antisymmetry.

Let us get back to the standard representation and define the extention operator P for $\psi\in\mathcal{D}(H^\star)$ and $(x,y,z)\in\mathbb{R}^3$ as follows :

$$P\psi(x,y,z)=T^\star\widetilde{P}T\psi(x,y,z)=\begin{cases}\psi(x,y,z), & \text{if } z>0,\\ (\mathcal{B}\circ\Pi)\,(\psi\circ S)\,(x,y,z), & \text{if } z<0.\end{cases}$$

Since $\mathcal{B}(s)$ is a unitary transformation of $\mathbb{C}^4$ for any $s\in\partial\mathbb{R}^3_+$, we get that

$$\|P\psi\|^2_{L^2(\mathbb{R}^3)}=2\|\psi\|^2_{L^2(\mathbb{R}^3_+)}.$$

Let us study $\alpha\cdot DP\psi$ in the distributional sense. We have for $\varphi\in\mathcal{D}=\mathcal{C}^\infty_0(\mathbb{R}^3)$ that

$$\begin{aligned}\langle\alpha\cdot DP\psi,\varphi\rangle_{\mathcal{D}'\times\mathcal{D}}&=\langle P\psi,\alpha\cdot D\varphi\rangle_{\mathbb{R}^3}\\&=\langle\psi,\alpha\cdot D\varphi\rangle_{\mathbb{R}^3_+}+\langle(\mathcal{B}\circ\Pi)\,\psi\circ S,\alpha\cdot D\varphi\rangle_{\mathbb{R}^3_-}\end{aligned}$$

where $\langle\,\cdot\,,\cdot\,\rangle_{\mathcal{D}'\times\mathcal{D}}$ is the distributional bracket on $\mathbb{R}^3$. Since $\mathcal{B}$ is Hermitian, commutes with α_1, α_2 and anti-commutes with α_3, we obtain by a change of variables, that

$$\begin{aligned}\langle(\mathcal{B}\circ\Pi)\psi\circ S,\alpha\cdot D\varphi\rangle_{\mathbb{R}^3_-}&=\langle\psi\circ S,(\mathcal{B}\circ\Pi)\,\alpha\cdot D\varphi\rangle_{\mathbb{R}^3_-}\\&=\langle\psi,-i\,(\mathcal{B}\circ\Pi)\,(\alpha_1\partial_x+\alpha_2\partial_y-\alpha_3\partial_z)\,\varphi\circ S\rangle_{\mathbb{R}^3_+}\\&=\langle\psi,\alpha\cdot D\left((\mathcal{B}\circ\Pi)\,\varphi\circ S\right)\rangle_{\mathbb{R}^3_+}.\end{aligned}$$

Hence, we get

$$\langle\alpha\cdot DP\psi,\varphi\rangle_{\mathcal{D}'\times\mathcal{D}}=\langle\psi,\alpha\cdot D\left(\varphi+(\mathcal{B}\circ\Pi)\,\varphi\circ S\right)\rangle_{\mathbb{R}^3_+}.$$

Let us remark that the function $\varphi+(\mathcal{B}\circ\Pi)\,\varphi\circ S$ belongs to $\mathrm{Dom}(H)$. Indeed, we have that

$$(\mathcal{B}\circ\Pi)\left(\varphi+(\mathcal{B}\circ\Pi)\,\varphi\circ S\right)(x,y,0)=\left(\varphi+(\mathcal{B}\circ\Pi)\,\varphi\circ S\right)(x,y,0)$$

for all $(x,y)\in\mathbb{R}^2$. Since $\psi\in\mathrm{Dom}(H^\star)$, by a change of variables, we have that

$$\begin{aligned}\langle\alpha\cdot DP\psi,\varphi\rangle_{\mathcal{D}'\times\mathcal{D}}&=\langle\alpha\cdot D\psi,\left(\varphi+(\mathcal{B}\circ\Pi)\,\varphi\circ S\right)\rangle_{\mathbb{R}^3_+}\\&=\langle\alpha\cdot D\psi,\varphi\rangle_{\mathbb{R}^3_+}+\langle(\mathcal{B}\circ\Pi)\,(\alpha\cdot D\psi)\circ S,\varphi\rangle_{\mathbb{R}^3_-}\,.\end{aligned}$$

Thus, we obtain that in the distributional sense

$$\alpha\cdot DP\psi=\chi_{\mathbb{R}^3_+}\,(\alpha\cdot D\psi)+\chi_{\mathbb{R}^3_-}\,(\mathcal{B}\circ\Pi)\,(\alpha\cdot D\psi)\circ S\in L^2(\mathbb{R}^3)$$

so that

$$\|\nabla P\psi\|^2_{L^2(\mathbb{R}^3)}=\|\alpha\cdot DP\psi\|^2_{L^2(\mathbb{R}^3)}=2\|\alpha\cdot D\psi\|^2_{L^2(\mathbb{R}^3_+)}\,.\qquad\square$$

2.2. Proof of Lemma 2.1

Let us now consider the case of our general Ω. Let us remark that the understanding of the case of the half-space is not sufficient to conclude since curvature effects have to be taken into account (see for instance (1.2)). The proof of Lemma 2.2 will be used as a guideline for the proof of Lemma 2.1.

Proof. — Using a partition of unity and the fact that

$$\{u \in L^2(\mathbb{R}^3)^4 : \ \alpha \cdot Du \in L^2(\mathbb{R}^3)^4\} = H^1(\mathbb{R}^3)^4,$$

we are reduced to study the case of a deformed half-space. Let us recall the standard tubular coordinates near the boundary of Ω :

$$\begin{aligned} \eta : (U \cap \partial\Omega) \times (-T, T) &\longrightarrow U, \\ (\mathbf{x}_0, t) &\longmapsto \mathbf{x}_0 - t\mathbf{n}(\mathbf{x}_0) \end{aligned}$$

where $T > 0$ and U is a suitable bounded open set of $\mathbb{R}^3$. Since Ω is $\mathcal{C}^2$, without loss of generality, we can assume that η is a $\mathcal{C}^1$-diffeomorphism such that

$$\eta((U \cap \partial\Omega) \times (0, T)) = \Omega \cap U\,, \quad \eta((U \cap \partial\Omega) \times \{0\}) = \partial\Omega \cap U\,.$$

The rest of the proof is divided into four steps:

(1) we introduce a bounded extension operator $P : L^2(U \cap \Omega) \to L^2(U)$,

(2) we introduce a map $\widetilde{\alpha}$ which extends the α-matrices on U so that, we have

$$\|\widetilde{\alpha} \cdot DP\psi\|_{L^2(U)} \leqslant C \left(\|\psi\|^2_{L^2(\Omega \cap U)} + \|\alpha \cdot D\psi\|^2_{L^2(\Omega \cap U)} \right),$$

for any function $\psi \in \mathrm{Dom}(H^\star)$ whose support is a compact subset of $U \cap \overline{\Omega}$,

(3) we show that the norm $\|\cdot\|_{\mathcal{V}}$ defined on

$$\mathcal{V} = \{v \in L^2(U),\ \widetilde{\alpha} \cdot Dv \in L^2(U), \operatorname{supp} v \subset\subset U\}$$

by

$$\|v\|^2_{\mathcal{V}} = \|v\|^2_{L^2} + \|\widetilde{\alpha} \cdot Dv\|^2_{L^2}$$

is equivalent to the H^1 norm on $\mathcal{C}^\infty_0(U)$,

(4) we deduce by a density argument that $\mathcal{V} \subset H^1_0(U)$.

Note that the parts of the proof that are almost immediate in the cases of Sobolev spaces have to be studied carefully. Here, the presence of the Dirac matrices introduce some additional difficulties. We tried to stress where the differences occur and where the regularity on Ω is needed.

Step 1. — Let us define the symmetry $\phi_s = \eta\circ S\circ\eta^{-1}$ and the projection $\phi_p = \eta\circ\Pi\circ\eta^{-1}$, where $S : (x,t)\mapsto(x,-t)$ and $\Pi : (x,t)\mapsto(x,0)$. For all $\mathbf{x}_0\in\partial\Omega\cap U$, let us denote by $P(\mathbf{x}_0)$ the matrix of the identity map of $\mathbb{R}^3$ from the canonical basis (e_1,e_2,e_3) to the orthonormal basis $(\epsilon_1(\mathbf{x}_0),\epsilon_2(\mathbf{x}_0),\mathbf{n}(\mathbf{x}_0))$ defined by

$$P(\mathbf{x}_0) = \mathrm{Mat}(\mathrm{Id},(e_1,e_2,e_3),(\epsilon_1(\mathbf{x}_0),\epsilon_2(\mathbf{x}_0),\mathbf{n}(x_0)))\,,$$

where $(\epsilon_1(\mathbf{x}_0),\epsilon_2(\mathbf{x}_0))$ is a basis of the tangent space $T_{\mathbf{x}_0}\partial\Omega$.

Up to taking a smaller T, we have, for all $\mathbf{x}_0\in\partial\Omega\cap U$,

$$\mathrm{jac}\ \phi_s(\mathbf{x}_0) = P(\mathbf{x}_0)^{-1}\begin{pmatrix}1&0&0\\0&1&0\\0&0&-1\end{pmatrix}P(\mathbf{x}_0)\,,$$

and, for all $\mathbf{x}\in U$,

$$\frac{3}{2}\geqslant|\mathrm{jac}\ \phi_s(\mathbf{x})| := |\det\mathrm{jac}\,\phi_s(\mathbf{x})|\geqslant\frac{1}{2}\,. \tag{2.2}$$

Following the idea of the proof of Lemma 2.2, we define the extension operator

$$P : L^2(U\cap\Omega)\to L^2(U)$$

for $\psi\in L^2(U\cap\Omega)$ and $\mathbf{x}\in U$ as follows:

$$P\psi(\mathbf{x}) = \begin{cases}\psi(\mathbf{x}), & \text{if } \mathbf{x}\in U\cap\Omega\,,\\ (\mathcal{B}\circ\phi_p(\mathbf{x}))\,\psi\circ\phi_s(\mathbf{x}), & \text{if } \mathbf{x}\in U\cap\Omega^c.\end{cases}$$

By (2.2) and a change of variables, we get that

$$\|P\psi\|_{L^2(U)}\leqslant C\|\psi\|_{L^2(U\cap\Omega)}\,.$$

Step 2. — Let us *extend* the α-matrices as follows:

$$\widetilde{\alpha}(\mathbf{x}) = \begin{cases}(\alpha_1,\alpha_2,\alpha_3)^T\,, & \text{if } \mathbf{x}\in U\cap\Omega,\\ |\mathrm{jac}\ \phi_s(\mathbf{x})|\mathcal{B} & \\ \quad\circ\,\phi_p(\mathbf{x})\left(\mathrm{jac}\ \phi_s(\phi_s(\mathbf{x}))(\alpha_1,\alpha_2,\alpha_3)^T\right)\mathcal{B}\circ\phi_p(\mathbf{x})\,, & \text{if } \mathbf{x}\in U\cap\Omega^c.\end{cases}$$

Let us remark that $\widetilde{\alpha}(\mathbf{x})$ is a column-vector of three matrices and the above matrix product makes sense as a product in the modulus on the ring of the 4×4 Hermitian matrices. For instance, the first matrix $\widetilde{\alpha}_1(\mathbf{x})$ is given for $\mathbf{x}\in U\cap\Omega^c$ by

$$\widetilde{\alpha}_1(\mathbf{x}) = |\mathrm{jac}\ \phi_s(\mathbf{x})|\mathcal{B}\circ\phi_p(\mathbf{x})\left(\sum_{k=1}^{3}b_{1,k}\alpha_k\right)\mathcal{B}\circ\phi_p(\mathbf{x})$$

where jac $\phi_s(\phi_s(\mathbf{x})) = (b_{i,j})_{i,j=1,3} \in \mathbb{R}^{3\times 3}$. We get for almost every $\mathbf{x}_0 \in \partial\Omega \cap U$ that

$$\begin{aligned}
|\text{jac } \phi_s(\mathbf{x}_0)| \mathcal{B} \circ \phi_p(\mathbf{x}_0) &\left(\text{jac } \phi_s(\phi_s(\mathbf{x}_0))(\alpha_1, \alpha_2, \alpha_3)^T\right) \mathcal{B} \circ \phi_p(\mathbf{x}_0) \\
&= \mathcal{B}(\mathbf{x}_0) \left(P(\mathbf{x}_0)^{-1} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} P(\mathbf{x}_0) \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{pmatrix} \right) \mathcal{B}(\mathbf{x}_0) \\
&= \mathcal{B}(\mathbf{x}_0) \left(P(\mathbf{x}_0)^{-1} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} \alpha \cdot \epsilon_1(\mathbf{x}_0) \\ \alpha \cdot \epsilon_2(\mathbf{x}_0) \\ \alpha \cdot \mathbf{n}(\mathbf{x}_0) \end{pmatrix} \right) \mathcal{B}(\mathbf{x}_0) \\
&= P(\mathbf{x}_0)^{-1} \mathcal{B}(\mathbf{x}_0) \begin{pmatrix} \alpha \cdot \epsilon_1(\mathbf{x}_0) \\ \alpha \cdot \epsilon_2(\mathbf{x}_0) \\ -\alpha \cdot \mathbf{n}(\mathbf{x}_0) \end{pmatrix} \mathcal{B}(\mathbf{x}_0) \\
&= P(\mathbf{x}_0)^{-1} \begin{pmatrix} \alpha \cdot \epsilon_1(\mathbf{x}_0) \\ \alpha \cdot \epsilon_2(\mathbf{x}_0) \\ \alpha \cdot \mathbf{n}(\mathbf{x}_0) \end{pmatrix} = \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{pmatrix}.
\end{aligned}$$

Hence, the application $\widetilde{\alpha}$ is continuous on U. Since it is also a $\mathcal{C}^1$-map on both $\overline{\Omega \cap U}$ and $\overline{\Omega^c \cap U}$, we get that $\widetilde{\alpha}$ is Lipschitzian. This choice for the extension of α is made in order to get

$$\widetilde{\alpha} \cdot DP\psi \in L^2(U),$$

in the sense of distributions. Indeed, since $\widetilde{\alpha}$ is Lipschitz, we get that, for $\varphi \in H_0^1(U)$,

$$\langle \widetilde{\alpha} \cdot DP\psi, \varphi \rangle_{H^{-1}(U) \times H_0^1(U)} = \langle P\psi, \widetilde{\alpha} \cdot D\varphi \rangle_U + \langle P\psi, -i \operatorname{div}(\widetilde{\alpha})\varphi \rangle_{U \cap \Omega^c}.$$

For $\mathbf{x} \in U \cap \Omega$, we also have

$$(\widetilde{\alpha} \cdot \nabla\varphi)(\phi_s(\mathbf{x})) = |\text{jac } \phi_s(\phi_s(\mathbf{x}))| \left(\mathcal{B} \circ \phi_p \alpha \mathcal{B} \circ \phi_p\right) \cdot \nabla \left(\varphi \circ \phi_s\right)(\mathbf{x})$$

and thus

$$\begin{aligned}
(\widetilde{\alpha} \cdot \nabla\varphi)(\phi_s(\mathbf{x})) = &|\text{jac } \phi_s(\phi_s(\mathbf{x}))| \, \mathcal{B} \circ \phi_p \left(\alpha \cdot \nabla \left((\mathcal{B} \circ \phi_p)\varphi \circ \phi_s\right)\right)(\mathbf{x}) \\
&- |\text{jac } \phi_s(\phi_s(\mathbf{x}))| \, \mathcal{B} \circ \phi_p \left(\alpha \cdot \nabla(\mathcal{B} \circ \phi_p)\right) \varphi \circ \phi_s(\mathbf{x}).
\end{aligned}$$

We deduce that

$$\begin{aligned}
\langle P\psi, \widetilde{\alpha} \cdot D\varphi \rangle_{U \cap \Omega^c} = &\langle \psi, \alpha \cdot D \left((\mathcal{B} \circ \phi_p)\, \varphi \circ \phi_s\right) \rangle_{U \cap \Omega} \\
&- \langle \psi, \left(\alpha \cdot D \left(\mathcal{B} \circ \phi_p\right)\right) \varphi \circ \phi_s \rangle_{U \cap \Omega}.
\end{aligned}$$

Since $\psi \in \mathrm{Dom}(H^\star)$ and the function $\varphi + (\mathcal{B}\circ\phi_p)\,\varphi\circ\phi_s : \Omega\cap U \to \mathbb{C}^4$ belongs to $\mathrm{Dom}(H)$ (since ϕ_s and ϕ_p are $\mathcal{C}^1$), we get that

$$\begin{aligned}&\langle \widetilde{\alpha}\cdot DP\psi, \varphi\rangle_{H^{-1}(U)\times H^1_0(U)}\\ &\qquad\qquad = \langle \alpha\cdot D\psi, \varphi + (\mathcal{B}\circ\phi_p)\,\varphi\circ\phi_s\rangle_{U\cap\Omega} + \langle P\psi, R\varphi\rangle_{U\cap\Omega^c}\,,\end{aligned}$$

where $R\in L^\infty(U\cap\Omega^c, \mathbb{C}^{4\times 4})$ is defined by

$$R = -i\ \mathrm{div}(\widetilde{\alpha}) + i|\mathrm{jac}\ \phi_s|\mathcal{B}\circ\phi_p\left(\mathrm{jac}\ \phi_s(\phi_s(\cdot))(\alpha_1,\alpha_2,\alpha_3)^T\right)\cdot\nabla(\mathcal{B}\circ\phi_p)\,.$$

By the Riesz theorem, we get $\widetilde{\alpha}\cdot DP\psi\in L^2(U)$ and

$$\|\widetilde{\alpha}\cdot DP\psi\|_{L^2(U)} \leqslant C\left(\|\psi\|^2_{L^2(\Omega)} + \|\alpha\cdot D\psi\|^2_{L^2(\Omega)}\right),$$

where $C>0$ does not depend on ψ.

Step 3. — Let $\varphi\in\mathcal{C}^\infty_0(U)$, we have

$$\|-i\widetilde{\alpha}\cdot\nabla\varphi\|^2_{L^2(U)} = \langle\varphi, (-i\widetilde{\alpha}\cdot\nabla)^2\varphi\rangle_U - \langle\varphi, \mathrm{div}(\widetilde{\alpha})\,(\widetilde{\alpha}\cdot\nabla\varphi)\rangle_{U\cap\Omega^c}$$

and

$$(-i\widetilde{\alpha}\cdot\nabla)^2 = -\sum_{j,k=1}^3 \widetilde{\alpha}_j\widetilde{\alpha}_k\partial^2_{jk} + (\widetilde{\alpha}_j\partial_j\widetilde{\alpha}_k)\,\partial_k\,.$$

Let us define the matrix-valued function A for all $\mathbf{x}\in U$ by

$$A(\mathbf{x}) = |\mathrm{jac}\ \phi_s(\mathbf{x})|(\mathrm{jac}\ \phi_s(\phi_s(\mathbf{x})))\chi_{U\cap\Omega^c}(\mathbf{x}) + 1_3\chi_{U\cap\Omega}(\mathbf{x}) = (a_{jk}(\mathbf{x}))_{jk}$$

and denote by $A_j(\mathbf{x})$ the j-th line of $A(\mathbf{x})$. We get that, for all $\mathbf{x}\in U$,

$$\begin{aligned}&\widetilde{\alpha}_j(\mathbf{x})\widetilde{\alpha}_k(\mathbf{x})\\ &\quad = \mathcal{B}\circ\phi_p\,(a_{j1}\alpha_1 + a_{j2}\alpha_2 + a_{j3}\alpha_3)\,(a_{k1}\alpha_1 + a_{k2}\alpha_2 + a_{k3}\alpha_3)\,\mathcal{B}\circ\phi_p\\ &\quad = \left(\sum_{l=1}^3 a_{jl}a_{kl}\right)1_4 + \mathcal{B}\circ\phi_p\left(\sum_{1\leqslant l<s\leqslant 3}\alpha_l\alpha_s(a_{jl}a_{ks} - a_{js}a_{kl})\right)\mathcal{B}\circ\phi_p\end{aligned}$$

and

$$\sum_{j,k=1}^3 \widetilde{\alpha}_j\widetilde{\alpha}_k\partial^2_{jk} = 1_4\sum_{j,k=1}^3 A_jA_k^T\partial^2_{jk}\,.$$

Since, $AA^T(\mathbf{x}) = 1_3$ for all $\mathbf{x}\in U\cap\partial\Omega$, we get that $\mathbf{x}\mapsto AA^T(\mathbf{x})$ is a Lipschitz mapping on U and

$$\sum_{j,k=1}^3 \widetilde{\alpha}_j\widetilde{\alpha}_k\partial^2_{jk} = 1_4\ \mathrm{div}\left(AA^T\nabla\right) - 1_4\sum_{j,k=1}^3\left(\partial_jAA^T\right)\partial_k.$$

Integrating by parts yields

$$\begin{aligned}\| -i\widetilde{\alpha}\cdot\nabla\varphi\|^2_{L^2(U)} &\geqslant \|A^T\nabla\varphi\|^2_{L^2(U)} - C\|\varphi\|_{L^2(U)}\|\nabla\varphi\|_{L^2(U)}\\ &\geqslant c\|\nabla\varphi\|^2_{L^2(U)} - C\|\varphi\|_{L^2(U)}\|\nabla\varphi\|_{L^2(U)}\,,\end{aligned}$$

where

$$c = \min\{\inf\ \mathrm{sp}(AA^T(\mathbf{x})),\ \mathbf{x}\in U\}\,.$$

Note that $c>0$ by (2.2). This ensures that the H^1-norm and the $\|\cdot\|_{\mathcal{V}}$-norm are equivalent on $\mathcal{C}_0^\infty(U)$.

Step 4. — Let $v\in\mathcal{V}$ and $(\rho_\varepsilon)_\varepsilon$ a mollifier defined for $\mathbf{x}\in\mathbb{R}^3$ by

$$\rho_\varepsilon(\mathbf{x}) = \frac{1}{\varepsilon^3}\rho_1\left(\frac{\mathbf{x}}{\varepsilon}\right),$$

where $\rho_1\in\mathcal{C}_0^\infty(\mathbb{R}^3)$, supp $\rho_1\subset B(0,1)$, $\rho_1\geqslant 0$ and $\|\rho_1\|_{L^1}=1$. Let us define $v_\varepsilon = v*\rho_\varepsilon$ for any $\varepsilon>0$. There exists $\varepsilon_0>0$ such that for all $\varepsilon\in(0,\varepsilon_0]$, the function v_ε belongs to $\mathcal{C}_0^\infty(U)$. Let us temporarily admit that there exists C independent of v and ε such that

$$\|v_\varepsilon\|_{\mathcal{V}} \leqslant C\|v\|_{\mathcal{V}}. \tag{2.3}$$

Then, Step 3 and the fact that v_ε converges to v in $L^2(U)$ ensure that $\mathcal{V}\subset H_0^1(U)$ and the result follows.

It remains to prove (2.3). There exists a constant $C>0$ such that

$$\|v_\varepsilon\|_{L^2}\leqslant C\|v\|_{L^2}$$

and

$$\begin{aligned}\|\widetilde{\alpha}\cdot Dv_\varepsilon\|_{L^2} &\leqslant \|\widetilde{\alpha}\cdot\nabla v_\varepsilon - (\widetilde{\alpha}\cdot\nabla v)*\rho_\varepsilon\|_{L^2} + \|\left(\widetilde{\alpha}\cdot\nabla v\right)*\rho_\varepsilon\|_{L^2}\\ &\leqslant \|\widetilde{\alpha}\cdot\nabla v_\varepsilon - (\widetilde{\alpha}\cdot\nabla v)*\rho_\varepsilon\|_{L^2} + C\|\widetilde{\alpha}\cdot\nabla v\|_{L^2}\,.\end{aligned}$$

By integration by parts, we get, for $\mathbf{x}\in U$,

$$\begin{aligned}&\widetilde{\alpha}\cdot\nabla v_\varepsilon(\mathbf{x}) - (\widetilde{\alpha}\cdot\nabla v)*\rho_\varepsilon(\mathbf{x})\\ &= \int_{\mathbb{R}^3}\widetilde{\alpha}(\mathbf{x})\cdot(v(\mathbf{y})\nabla\rho_\varepsilon(\mathbf{x}-\mathbf{y}))\,\mathrm{d}\mathbf{y} - \int_{\mathbb{R}^3}\widetilde{\alpha}(\mathbf{y})\cdot\nabla v(\mathbf{y})\rho_\varepsilon(\mathbf{x}-\mathbf{y})\,\mathrm{d}\mathbf{y}\\ &= \int_{\mathbb{R}^3}(\widetilde{\alpha}(\mathbf{x})-\widetilde{\alpha}(\mathbf{y}))\cdot(v(\mathbf{y})\nabla\rho_\varepsilon(\mathbf{x}-\mathbf{y}))\,\mathrm{d}\mathbf{y} + \int_{\mathbb{R}^3}(\mathrm{div}\ \widetilde{\alpha}(\mathbf{y}))\,v(\mathbf{y})\rho_\varepsilon(\mathbf{x}-\mathbf{y})\,\mathrm{d}\mathbf{y}\,,\end{aligned}$$

and by a change of variable

$$\begin{aligned}&\int_{\mathbb{R}^3}(\widetilde{\alpha}(\mathbf{x})-\widetilde{\alpha}(\mathbf{y}))\cdot(v(\mathbf{y})\nabla\rho_\varepsilon(\mathbf{x}-\mathbf{y}))\,\mathrm{d}\mathbf{y}\\ &\qquad= \int_{\mathbb{R}^3}\frac{\widetilde{\alpha}(\mathbf{x})-\widetilde{\alpha}(\mathbf{x}-\varepsilon\mathbf{z})}{\varepsilon}\cdot(v(\mathbf{x}-\varepsilon\mathbf{z})\nabla\rho_1(\mathbf{z}))\,\mathrm{d}\mathbf{z}\,.\end{aligned}$$

Since $\widetilde{\alpha}$ is Lipschitzian, we get that

$$\left\| \int_{\mathbb{R}^3} \frac{\widetilde{\alpha}(\,\cdot\,) - \widetilde{\alpha}(\,\cdot - \varepsilon\mathbf{z})}{\varepsilon} \cdot (v(\,\cdot - \varepsilon\mathbf{z})\nabla\rho_1(\mathbf{z}))\,\mathrm{d}\mathbf{z} \right\|_{L^2} \leqslant C\|v\|_{L^2} \|\,|\cdot|\,|\nabla\rho_1(\,\cdot\,)|\|_{L^1}\,,$$

and

$$\left\| \int_{\mathbb{R}^3} (\mathrm{div}\ \widetilde{\alpha}(\mathbf{y}))\, v(\mathbf{y})\rho_\varepsilon(\cdot - \mathbf{y})\,\mathrm{d}\mathbf{y} \right\|_{L^2} \leqslant C\|v\|_{L^2}\,,$$

so that (2.3) follows. This ends the proof of Lemma 2.1. □

2.3. Proof of the self-adjointness of H

We finally prove the second assertion of the main theorem, which is that the operator $(H, \mathrm{Dom}(H))$ is self-adjoint. Thanks to Lemma 2.1, the set $\mathrm{Dom}(H^\star)$ is included in $H^1(\Omega)^4$. Hence, for any $\psi \in \mathrm{Dom}(H^\star)$, the trace of ψ on the set $\partial\Omega$ is well-defined and belongs to $H^{1/2}(\partial\Omega)^4$. By the definition of $\mathrm{Dom}(H^\star)$ and an integration by parts, we obtain that, for any $\varphi \in \mathrm{Dom}(H)$,

$$0 = \langle \psi, H\varphi\rangle_\Omega - \langle H\psi, \varphi\rangle_\Omega = \langle \psi, -i\alpha\cdot n\varphi\rangle_{\partial\Omega} = \langle \beta\psi, \varphi\rangle_{\partial\Omega}\,.$$

Hence, we have, for almost any $s \in \partial\Omega$,

$$\beta\psi(s) \in \ker(\mathcal{B} - 1_4)^\perp = \ker(\mathcal{B} + 1_4)\,,$$

so that

$$\psi(s) \in \ker(\mathcal{B} - 1_4)\,,$$

and the conclusion follows.

Appendix A. Some elementary properties

Lemma A.1. — *For all $\mathbf{x}, \mathbf{y} \in \mathbb{R}^3$, we have*

$$\begin{gathered}(\alpha\cdot\mathbf{x})(\alpha\cdot\mathbf{y}) = (\mathbf{x}\cdot\mathbf{y})1_4 + i\gamma_5\alpha\cdot(\mathbf{x}\times\mathbf{y})\,,\\ \beta(\alpha\cdot\mathbf{x}) = -(\alpha\cdot\mathbf{x})\beta\,,\quad \beta\gamma_5 = -\gamma_5\beta\,,\\ \gamma_5(\alpha\cdot\mathbf{x}) = (\alpha\cdot\mathbf{x})\gamma_5\,.\end{gathered}$$

Proof. — We refer to [12, Appendix 1.B]. □

In the following lemma, we recall the proof of the symmetry of H.

Lemma A.2. — $(H, \mathrm{Dom}(H))$ *is a symmetric operator.*

Proof. — Since the α-matrices are Hermitian, we have, thanks to the Green–Riemann formula:

$$\forall\, \varphi, \psi \in H^1(\Omega, \mathbb{C}^4)\,, \quad \langle \alpha \cdot D\varphi, \psi\rangle_\Omega = \langle \varphi, \alpha \cdot D\psi\rangle_\Omega + \langle(-i\alpha \cdot \mathbf{n})\varphi, \psi\rangle_{\partial\Omega}\,. \tag{A.1}$$

Now we consider $\psi, \varphi \in \mathrm{Dom}(H)$. By using $\beta^2 = 1_4$ and the boundary condition, we get

$$\langle(-i\alpha \cdot \mathbf{n})\varphi, \psi\rangle_{\partial\Omega} = \langle \beta\varphi, \psi\rangle_{\partial\Omega}\,,$$

so that, we deduce

$$\forall\, \varphi, \psi \in \mathcal{D}(H)\,, \quad \langle \alpha \cdot D\varphi, \psi\rangle_\Omega - \langle \varphi, \alpha \cdot D\psi\rangle_\Omega = \langle \beta\varphi, \psi\rangle_{\partial\Omega}\,. \tag{A.2}$$

The left hand side of (A.2) is a skew-Hermitian expression of (φ, ψ) and the right hand side is Hermitian in (φ, ψ) since β is Hermitian. Thus both sides must be zero. □

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