Rev. Mat. Iberoam. 42 (2026), no. 6, 2377–2402
DOI 10.4171/RMI/1639

MIT bag in non-smooth convex domains

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Abstract. The Dirac operator with MIT bag boundary condition in a bounded convex domain is shown to be always self-adjoint in the H^1-setting. This allows one to show that such operators appear as limits of Dirac operators with large positive mass outside the domain. Similar results were previously known for smooth domains only.

Dedicated to the memory of my doctoral co-advisor Jochen Brüning (*1947–2025*)

1. Introduction

For $n \geq 2$ and $N := 2^{[(n+1)/2]}$, let $\alpha_1, \dots, \alpha_n, \beta$ be pairwise anticommuting Hermitian $N \times N$ matrices with $\alpha_k^2 = \beta^2 = I_N$, where I_N is the $N \times N$ identity matrix (see Appendix A for a possible explicit choice). The Euclidean Dirac operator D_m with a mass $m \in \mathbb{R}$ acts on vector functions $f : \mathbb{R}^n \to \mathbb{C}^N$ by the differential expression

$$D_m f := -\mathrm{i} \sum_{k=1}^{n} \alpha_k \partial_k f + m\beta f, \tag{1.1}$$

and it is a central object in relativistic quantum mechanics, see, e.g., [42].

Now let $\Omega \subset \mathbb{R}^n$ be a bounded domain with sufficiently regular (e.g., Lipschitz) boundary and outer unit normal ν. By the MIT bag operator with mass m in Ω, one means the operator A_m^Ω acting in $L^2(\Omega, \mathbb{C}^N)$ as $f \mapsto D_m f$ on functions f satisfying the MIT bag boundary condition $f = -\mathrm{i}\beta\alpha \cdot \nu f$ on $\partial\Omega$, where we use the notation

$$\alpha \cdot x = \sum_{k=1}^{n} x_k \alpha_k \quad \text{for any } x = (x_1, \dots, x_n) \in \mathbb{R}^n,$$

and denote a function on Ω and its trace on $\partial\Omega$ by the same symbol for the sake of readability. The precise regularity of the functions f in the operator domain guaranteeing "good" properties of A_m^Ω will be discussed below in greater detail.

Mathematics Subject Classification 2020: 35P20 (primary); 81Q05, 35F45, 47B25 (secondary).
Keywords: Dirac operator, boundary condition, convex domain, self-adjointness.

The Dirac operator with the above boundary condition appeared initially in the physics literature [14, 20, 28], in particular, as a model of quark confinement in hadrons. One of the interesting features observed is that the MIT bag operator appears as the limit of Dirac operators in the whole space with a large mass applied outside Ω, see [13], which explains the fact that the MIT bag boundary condition is often referred to as the "infinite mass boundary condition" (and it is usually considered as an analog of the Dirichlet boundary condition for the Laplacian). While the operator has a long history in the physics literature, its mathematically rigorous analysis has become an active area of research only in the last decade. For Ω with smooth boundary and $n \in \{2, 3\}$, several authors [4, 9, 11, 35] have shown that the above operator A_m^Ω is self-adjoint if considered on the domain

$$\{f \in H^1(\Omega, \mathbb{C}^N) : f = -\mathrm{i}\beta\alpha \cdot \nu f \text{ on } \partial\Omega\}. \tag{1.2}$$

As noted in [34], the result holds in any dimension as a corollary of more general results on manifolds with boundaries [5, 6]. Moreover, if one denotes by $E_j(T)$ the j-th eigenvalue of a lower semibounded operator T (assuming the usual numbering in the non-decreasing order with multiplicities counted), for each $j \in \mathbb{N}$, one has

$$E_j\big((A_m^\Omega)^2\big) = \lim_{M\to+\infty} E_j\big((B_{m,M}^\Omega)^2\big), \tag{1.3}$$

where $B_{m,M}^\Omega$ is the Dirac operator in $L^2(\mathbb{R}^n, \mathbb{C}^N)$ with mass m in Ω and mass M in Ω^{c},

$$\begin{aligned} B_{m,M}^\Omega : f \mapsto D_0 f + (m\mathbb{1}_\Omega + M\mathbb{1}_{\Omega^{\mathrm{c}}})\beta f \equiv D_m f + (M-m)\mathbb{1}_{\Omega^{\mathrm{c}}}\beta f,\\ \operatorname{dom} B_{m,M}^\Omega = H^1(\mathbb{R}^n, \mathbb{C}^N), \end{aligned} \tag{1.4}$$

see [41] for $n = 2$, or [3] for $n = 3$, or [34] for arbitrary n. The relation (1.3) is usually viewed as the mathematical expression of the infinite mass limit mentioned above. Note that there are some extensions to unbounded domains [7] and spin manifolds [24], and some estimates for the rate of convergence are available as well [3, 8]. It should be noted that the proofs of the convergence are mainly based on the expression

$$\begin{aligned} \|A_m^\Omega f\|^2_{L^2(\Omega,\mathbb{C}^N)} &= \int_\Omega \big(|\nabla f|^2 + m^2|f|^2\big)\,\mathrm{d}x \\ &\quad + \int_{\partial\Omega}\Big(m + \frac{H}{2}\Big)|f|^2\,\mathrm{d}\mathcal{H}^{n-1}, \quad f \in \operatorname{dom} A_m^\Omega, \end{aligned} \tag{1.5}$$

where $H : x \mapsto \operatorname{tr} \mathrm{d}|_x \nu$ is the mean curvature of $\partial\Omega$ and $\mathcal{H}^{n-1}$ is the $(n-1)$-dimensional Hausdorff measure, and also on the use of tubular coordinates near $\partial\Omega$. Note that the same expression also plays a central role in spectral optimization [1, 2, 16].

While there is a vast literature on boundary value problems for Dirac-type operators on domains/manifolds with smooth boundaries, see, e.g., [5, 6, 15, 17, 26] and references therein, the case of non-smooth boundaries is much less elaborated. The paper [31] studied the self-adjointness of A_m^Ω for the case $n = 2$ when Ω is a polygon, and it was shown that the domain (1.2) leads to a self-adjoint operator if and only if the polygon is convex (more generally, the deficiency indices coincide with the number of concave corners). In [19], it was shown that A_m^Ω is self-adjoint on the domain (1.2) if Ω is a convex circular cone in three dimensions. As shown in [10, 12, 37], for bounded Lipschitz Ω and $n \in \{2,3\}$, the operator A_m^Ω becomes self-adjoint if considered on the larger domain

$$\{f \in H^{1/2}(\Omega,\mathbb{C}^N) : D_m f \in L^2(\Omega,\mathbb{C}^N),\ f = -\mathrm{i}\beta\alpha\cdot\nu f \text{ on } \partial\Omega\},$$

and the paper [43] studied the local regularity of eigenfunctions. It should be noted that the loss of regularity also destroys the proofs for (1.3), as the finiteness of the summands in the crucially important identity (1.5) implicitly means the inclusion $\operatorname{dom} A_m^\Omega \subset H^1(\Omega,\mathbb{C}^N)$. The paper [8] contains an alternative proof of (1.3) for $n = 3$ and smooth Ω with the help of the resolvents, but its main constructions are based on the microlocal analysis, and no obvious extension to non-smooth domains is expected. Overall, to our knowledge, there are no proofs of the asymptotics (1.3) for any non-smooth Ω.

The main goal of the present paper is to show that the above results for smooth Ω can be extended to a large class of non-smooth but *convex* Ω. Note that the convexity is one of the standard assumptions guaranteeing maximal regularity for Laplacians with various boundary conditions, see, e.g., Chapter 3 of [25] for most classical results or [29, 30] for recent developments. Before passing to rigorous formulations, we recall that any bounded convex domain has Lipschitz boundary, see Corollary 1.2.2.3 in [25], hence the usual machineries in Sobolev spaces (embeddings, traces, extension operators) are available. Our central result is as follows.

Theorem 1.1 (Self-adjointness). *Let $\Omega \subset \mathbb{R}^n$ be a bounded convex domain with outer unit normal ν (which is defined a.e. on $\partial\Omega$), and let $m \in \mathbb{R}$. Then the operator*

(1.6) $$A_m^\Omega : f \mapsto D_m f, \quad \operatorname{dom} A_m^\Omega = \{f \in H^1(\Omega,\mathbb{C}^N) : f = -\mathrm{i}\beta\alpha\cdot\nu f \text{ on } \partial\Omega\},$$

is self-adjoint in $L^2(\Omega,\mathbb{C}^N)$ with compact resolvent.

For the subsequent discussion, we assume higher regularity of the boundary.

Definition 1.2. Let $U \subset \mathbb{R}^n$ be a bounded domain with Lipschitz boundary. A point $s \in \partial U$ is called *regular* if U coincides with a C^∞-smooth domain in an open neighborhood of s, otherwise it is called *singular*. One denotes

$$\begin{aligned} \partial_\infty U &:= \{s \in \partial U : s \text{ is regular}\} \quad (\text{the } \textit{regular boundary} \text{ of } U),\\ \partial_0 U &:= \{s \in \partial U : s \text{ is singular}\} \quad (\text{the } \textit{singular boundary} \text{ of } U). \end{aligned}$$

The domain U will be called *piecewise smooth* if its singular boundary is contained in the union of finitely many compact $(n-2)$-dimensional submanifolds of $\mathbb{R}^n$.

We show the following.

Theorem 1.3 (Quadratic form). *Let $\Omega \subset \mathbb{R}^n$ be a bounded convex domain with piecewise smooth boundary and outer unit normal ν (which is defined at least on the regular boundary). Then, for any $f \in \operatorname{dom} A_m^\Omega$, one has*

$$\|A_m^\Omega f\|^2_{L^2(\Omega,\mathbb{C}^N)} = \int_\Omega (|\nabla f|^2 + m^2|f|^2)\,\mathrm{d}x + \int_{\partial\Omega}\Big(m + \frac{H}{2}\Big)|f|^2\,\mathrm{d}\mathcal{H}^{n-1},$$

where $H\colon x \mapsto \operatorname{tr} \mathrm{d}|_x \nu \geq 0$ is the mean curvature defined on the regular boundary of Ω.

By imposing an additional geometric condition, we are finally able to extend (1.3) to a large class of non-smooth domains.

Theorem 1.4 (Infinite mass limit). *Let $\Omega \subset \mathbb{R}^n$ be a bounded convex domain with piecewise smooth boundary, and assume that the mean curvature of the regular boundary is bounded. Then, for any $m \in \mathbb{R}$ and $j \in \mathbb{N}$, one has $E_j\big((A_m^\Omega)^2\big) = \lim_{M\to+\infty} E_j\big((B_{m,M}^\Omega)^2\big)$, where the operator $B_{m,M}^\Omega$ acting in $L^2(\mathbb{R}^n, \mathbb{C}^N)$ is defined by* (1.4).

The assumptions of Theorem 1.4 are satisfied, in particular, if Ω is a bounded convex polyhedron (i.e., a bounded domain obtained as an intersection of halfspaces), or a convex curvilinear polyhedron (i.e., obtained as a diffeomorphic image of a bounded convex polyhedron), or a convex piecewise smooth domain obtained as the intersection of finitely many C^∞-smooth bounded domains. On the other hand, the assumption on the boundedness of the mean curvature excludes, e.g., the three-dimensional domains whose boundary has conical singularities of the form $x_3 = \sqrt{x_1^2 + x_2^2}$. We believe that the assumption on the mean curvature is purely technical, see Remark 5.2 at the end of the paper.

Our proof of Theorem 1.1 is presented in Section 2, and it is based on adaptations of some constructions in Section 3.2 of Grisvard's book [25], for second-order operators. Remark 2.6 indicates possible extensions. In Section 3 we derive some approximation results for Sobolev spaces. This allows one to show the essential self-adjointness of A_m^Ω on smooth functions vanishing near the singular boundary (Lemma 3.6), which is an essential ingredient for the subsequent analysis. In particular, it is used in Section 4 to prove Theorem 1.3 by transferring the results known for the smooth case. Theorem 1.4 is shown in Section 5, and is mainly in the spirit of the analysis of [34], while a more involved choice of test functions is used, and the constructions with tubular coordinates near $\partial\Omega$ (which are now unavailable due to non-smoothness) are replaced by some estimates for Robin Laplacians in exterior domains. The short Appendix A collects a necessary information on the Dirac matrices.

2. Proof of Theorem 1.1 (self-adjointness)

As a starting point let us summarize rigorously some results on smooth domains, see Lemma 2.1 and Proposition A.2 in [34].

Lemma 2.1. *Let $\Omega \subset \mathbb{R}^n$ be a bounded domain with C^∞-smooth boundary and outer unit normal ν, and let $m \in \mathbb{R}$. Then the operator A_m^Ω defined by* (1.6) *is self-adjoint in $L^2(\Omega, \mathbb{C}^N)$, and for any $f \in \operatorname{dom} A_m^\Omega$, one has the identity* (1.5).

As the parameter m only results in adding a bounded symmetric perturbation, it is sufficient to show that the operator

$$A := A_0^\Omega$$

is self-adjoint and has compact resolvent. The integration by parts show that A is symmetric, and its self-adjointness is equivalent to the equalities $\operatorname{ran}(A \pm \mathrm{i}) = L^2(\Omega, \mathbb{C}^N)$. We will show $\operatorname{ran}(A + \mathrm{i}) = L^2(\Omega, \mathbb{C}^N)$, as the other condition is proved completely analogously by adjusting the signs.

Our constructions will be based on the following results of convex analysis, see, e.g., Section 3.4 of [39] and Lemma 3.2.3.2 in [25].

Lemma 2.2. *Let $\Omega \subset \mathbb{R}^n$ be a bounded convex domain. There exist bounded convex C^∞-smooth domains $\Omega_p \subset \mathbb{R}^n$, $p \in \mathbb{N}$, such that $\Omega \subset \Omega_p$ for all p and $d_H(\partial\Omega_p, \partial\Omega) \xrightarrow{p\to\infty} 0$, where d_H stands for the Hausdorff distance. Moreover, one can find open subsets $V_k \subset \mathbb{R}^n$, $k \in \{1,\dots,K\}$, with the following properties*:

- *For each k, there exist Cartesian coordinates $y_1^k,\dots,y_n^k$ in which V_k is a hypercube,*
$$V_k = \{(y_1^k,\dots,y_n^k) : -a_j^k < y_j^k < a_j^k \text{ for all } j \in \{1,\dots,n\}\}, \quad a_j^k > 0.$$
- *For all $p \in \mathbb{N}$ and each $k \in \{1,\dots,K\}$, there exist a Lipschitz function h^k and a C^∞-smooth function h_p^k, defined on*
$$V_k' = \{(y_1^k,\dots,y_{n-1}^k) : -a_j^k < y_j^k < a_j^k \text{ for all } j \in \{1,\dots,n-1\}\},$$
such that
$$h^k(z^k) \le h_p^k(z^k), \quad |h^k(z^k)| \le \frac{a_n^k}{2}, \quad |h_p^k(z^k)| \le \frac{a_n^k}{2} \quad \text{for all } z^k \in V_k',$$
$$\Omega \cap V_k = \{y^k = (z^k, y_n^k) \in V_k : z^k \in V_k',\ y_n^k < h^k(z^k)\},$$
$$\Omega_p \cap V_k = \{y^k = (z^k, y_n^k) \in V_k : z^k \in V_k',\ y_n^k < h_p^k(z^k)\},$$
$$\partial\Omega \cap V_k = \{y^k = (z^k, y_n^k) \in V_k : z^k \in V_k',\ y_n^k = h^k(z^k)\},$$
$$\partial\Omega_p \cap V_k = \{y^k = (z^k, y_n^k) \in V_k : z^k \in V_k',\ y_n^k = h_p^k(z^k)\}.$$
- *We have $\partial\Omega \subset \bigcup_{k=1}^K V_k$ and $\partial\Omega_p \subset \bigcup_{k=1}^K V_k$ for all $p \in \mathbb{N}$.*
- *For each $k \in \{1,\dots,K\}$, one has $h_p^k \to h^k$ as $p \to \infty$ uniformly in V_k'.*
- *There is an $L > 0$ such that $|\nabla h^k(z^k)| \le L$ and $|\nabla h_p^k(z^k)| \le L$ for a.e. $z^k \in V_k'$, all $k \in \{1,\dots,K\}$ and all $p \in \mathbb{N}$.*
- *For each $k \in \{1,\dots,K\}$, one has $\nabla h_p^k(z^k) \to \nabla h^k(z^k)$ as $p \to \infty$ for a.e. $z^k \in V_k'$.*

Let us approximate Ω by bounded convex C^∞-smooth domains Ω_p (with $p \in \mathbb{N}$) as in Lemma 2.2 and consider the associated Dirac operators
$$\widetilde{A}_p := A_0^{\Omega_p},$$
which are self-adjoint in $L^2(\Omega_p, \mathbb{C}^N)$ by Lemma 2.1.

Let $g \in L^2(\Omega, \mathbb{C}^N)$. For each p, denote by $\widetilde{g}_p$ the continuation of g by zero to Ω_p. Then, because of the self-adjointness of $\widetilde{A}_p$, there is a unique $\widetilde{f}_p \in \operatorname{dom} \widetilde{A}_p$ such that $(\widetilde{A}_p + \mathrm{i})\widetilde{f}_p = \widetilde{g}_p$. Let H_p be the mean curvature of $\partial\Omega_p$. Then $H_p \ge 0$ due to convexity of Ω_p, and by Lemma 2.1, we obtain

$$\begin{aligned}
\|g\|^2_{L^2(\Omega,\mathbb{C}^N)} &= \|\widetilde{g}_p\|^2_{L^2(\Omega_p,\mathbb{C}^N)} = \|(\widetilde{A}_p + \mathrm{i})\widetilde{f}_p\|^2_{L^2(\Omega_p,\mathbb{C}^N)} \\
&= \|\widetilde{A}_p\widetilde{f}_p\|^2_{L^2(\Omega_p,\mathbb{C}^N)} + \|\widetilde{f}_p\|^2_{L^2(\Omega_p,\mathbb{C}^N)} \\
&= \int_{\Omega_p} (|\nabla \widetilde{f}_p|^2 + |\widetilde{f}_p|^2)\,\mathrm{d}x + \frac{1}{2}\int_{\partial\Omega_p} H_p |\widetilde{f}_p|^2\,\mathrm{d}\mathcal{H}^{n-1} \\
&\ge \int_{\Omega_p} (|\nabla \widetilde{f}_p|^2 + |\widetilde{f}_p|^2)\,\mathrm{d}x = \|\widetilde{f}_p\|^2_{H^1(\Omega_p,\mathbb{C}^N)}.
\end{aligned} \tag{2.1}$$

Denote by f_p the restriction of $\widetilde{f}_p$ on Ω. Then

$$\|f_p\|_{H^1(\Omega,\mathbb{C}^N)} \le \|\widetilde{f}_p\|_{H^1(\Omega_p,\mathbb{C}^N)} \le \|g\|_{L^2(\Omega,\mathbb{C}^N)}, \tag{2.2}$$

which shows that the sequence $(f_p)_{p\in\mathbb{N}}$ is bounded in $H^1(\Omega,\mathbb{C}^N)$ and, hence, contains a weakly convergent subsequence. To keep the notation simple, we assume (by replacing the initial sequence of Ω_p by the corresponding subsequence) that $f_p \to f$ as $p\to\infty$ weakly in $H^1(\Omega,\mathbb{C}^N)$ for some $f\in H^1(\Omega,\mathbb{C}^N)$. We are going to show that $f\in \operatorname{dom} A$ with $(A+\mathrm{i})f = g$, which will conclude the proof of self-adjointness for A.

Due to the compactness of the embedding $H^1(\Omega,\mathbb{C}^N)\hookrightarrow L^2(\Omega,\mathbb{C}^N)$, we have

$$\|f_p - f\|_{L^2(\Omega,\mathbb{C}^N)} \xrightarrow{p\to\infty} 0. \tag{2.3}$$

Let $\varphi\in C_c^\infty(\Omega,\mathbb{C}^N)$ and let $\widetilde{\varphi}_p$ be its extension by zero on Ω_p. Then $\widetilde{\varphi}_p\in C_c^\infty(\Omega_p,\mathbb{C}^N)\subset \operatorname{dom}\widetilde{A}_p$, and

$$\begin{aligned}\langle g,\varphi\rangle_{L^2(\Omega,\mathbb{C}^N)} &= \langle \widetilde{g}_p,\widetilde{\varphi}_p\rangle_{L^2(\Omega_p,\mathbb{C}^N)} = \langle (\widetilde{A}_p+\mathrm{i})\widetilde{f}_p,\widetilde{\varphi}_p\rangle_{L^2(\Omega_p,\mathbb{C}^N)}\\ &= \langle \widetilde{f}_p,(\widetilde{A}_p-\mathrm{i})\widetilde{\varphi}_p\rangle_{L^2(\Omega_p,\mathbb{C}^N)} = \langle \widetilde{f}_p,(D_0-\mathrm{i})\widetilde{\varphi}_p\rangle_{L^2(\Omega_p,\mathbb{C}^N)}\\ &= \langle f_p,(D_0-\mathrm{i})\varphi\rangle_{L^2(\Omega,\mathbb{C}^N)} \underset{(2.3)}{\xrightarrow{p\to\infty}} \langle f,(D_0-\mathrm{i})\varphi\rangle_{L^2(\Omega,\mathbb{C}^N)}.\end{aligned}$$

Hence,

$$\int_\Omega \langle g(x),\varphi(x)\rangle_{\mathbb{C}^N}\,\mathrm{d}x = \int_\Omega \langle f(x),(D_0-\mathrm{i})\varphi(x)\rangle_{\mathbb{C}^N}\,\mathrm{d}x \quad \text{for all } \varphi\in C_c^\infty(\Omega,\mathbb{C}^N),$$

which means $(D_0+\mathrm{i})f = g$ in $\mathscr{D}'(\Omega,\mathbb{C}^N)$. As $f\in H^1(\Omega,\mathbb{C}^N)$ by construction, it remains to check that f satisfies the required boundary condition.

Let V_k, V_k', h^k, h_p^k and L be as in Lemma 2.2. Let $\nu^k(z^k)$ be the outer unit normal for Ω at the point $(z^k,h^k(z^k))\in V_k\cap\partial\Omega$, and let $\nu_p^k(z^k)$ be the outer unit normal for Ω_p at the point $(z^k,h_p^k(z^k))\in V_k\cap\partial\Omega_p$, i.e.,

$$\nu^k(z^k) = \frac{(-\nabla h^k(z^k),1)}{\sqrt{1+|\nabla h^k(z^k)|^2}} \quad\text{and}\quad \nu_p^k(z^k) = \frac{(-\nabla h_p^k(z^k),1)}{\sqrt{1+|\nabla h_p^k(z^k)|^2}}.$$

In order to show that the function f satisfies the boundary condition, we need to check that for any $k\in\{1,\dots,K\}$, one has

$$\begin{aligned}&\int_{V_k\cap\partial\Omega} |(1+\mathrm{i}\beta\alpha\cdot\nu)f|^2\,\mathrm{d}\mathcal{H}^{n-1}\\ &\qquad\equiv \int_{V_k'} |(1+\mathrm{i}\beta\alpha\cdot\nu^k(z^k))f(z^k,h^k(z^k))|^2\sqrt{1+|\nabla h^k(z^k)|^2}\,\mathrm{d}z^k = 0,\end{aligned}$$

and in view of the bound $|\nabla h^k(z^k)|\le L$, this is equivalent to

$$\int_{V_k'} |(1+\mathrm{i}\beta\alpha\cdot\nu^k(z^k))f(z^k,h^k(z^k))|^2\,\mathrm{d}z^k = 0. \tag{2.4}$$

By construction, the functions $\widetilde{f}_p$ satisfy $(1+\mathrm{i}\beta\alpha\cdot\nu_p)\widetilde{f}_p = 0$ on $\partial\Omega_p$, with ν_p being the unit normal for Ω_p, which means that for any $k\in\{1,\dots,K\}$,

$$\int_{V_k\cap\partial\Omega_p} |(1+\mathrm{i}\beta\alpha\cdot\nu_p)\widetilde{f}_p^{\,2}\,\mathrm{d}\mathcal{H}^{n-1} = 0,$$

hence

$$\int_{V_k'} |(1+\mathrm{i}\beta\alpha\cdot\nu_p^k(z^k))\widetilde{f}_p(z^k,h^k(z^k))|^2\,\mathrm{d}z^k = 0. \tag{2.5}$$

Our goal is to pass to the limit $p\to\infty$ in this last formula in order to obtain the required identities (2.4). As a preparation, let us derive some preliminary estimates.

Lemma 2.3. *For any $F\in H^1(\mathbb{R}^n,\mathbb{C}^N)$ and any $k\in\{1,\dots,K\}$, one has*

$$\int_{V_k'} |F(z^k,h_p^k(z^k)) - F(z^k,h^k(z^k))|^2\,\mathrm{d}z^k \xrightarrow{p\to\infty} 0.$$

Proof. Using the Cauchy–Schwarz inequality, we have

$$\begin{aligned}
\int_{V_k'} |F(z^k,h_p^k(z^k)) - F(z^k,h^k(z^k))|^2\,\mathrm{d}z^k &= \int_{V_k'}\Big|\int_{h^k(z^k)}^{h_p^k(z^k)} \partial_{y_n^k}F(z^k,t)\,\mathrm{d}t\Big|^2\mathrm{d}z^k\\
&\le \int_{V_k'} |h_p^k(z^k)-h^k(z^k)|\int_{h^k(z^k)}^{h_p^k(z^k)} |\partial_{y_n^k}F(z^k,t)|^2\,\mathrm{d}t\,\mathrm{d}z^k\\
&\le \sup_{z^k\in V_k'} |h_p^k(z^k)-h^k(z^k)|\int_{V_k\cap\Omega_p} |\partial_{y_n^k}F|^2\,\mathrm{d}y^k\\
&\le \sup_{z^k\in V_k'} |h_p^k(z^k)-h^k(z^k)|\,\|F\|^2_{H^1(\mathbb{R}^n,\mathbb{C}^N)} \xrightarrow{p\to\infty} 0,
\end{aligned}$$

due to the uniform convergence of h_p^k to h^k on V_k'. ■

Lemma 2.4. *Let $F\in H^1(\mathbb{R}^n,\mathbb{C}^N)$ be a continuation of f on $\mathbb{R}^n$. For any $k\in\{1,\dots,K\}$, one has*

$$\int_{V_k'} |F(z^k,h_p^k(z^k)) - \widetilde{f}_p(z^k,h_p^k(z^k))|^2\,\mathrm{d}z^k \xrightarrow{p\to\infty} 0.$$

Proof. We need to show that

$$\int_{V_k'} |\eta_p(z^k,h_p^k(z^k))|^2\,\mathrm{d}z^k \xrightarrow{p\to\infty} 0 \quad \text{for the functions } \eta_p := F-\widetilde{f}_p \in H^1(\Omega_p).$$

First, remark that due to (2.2), one can find $c>0$ such that

$$\|\eta_p\|_{H^1(\Omega_p,\mathbb{C}^N)} \le c \quad \text{for all } p\in\mathbb{N}. \tag{2.6}$$

Furthermore, by assumption, $\eta_p \to 0$ weakly in $H^1(\Omega)$. Using the boundedness of the trace operator $H^1(\Omega) \to H^{1/2}(\partial\Omega)$ and the compactness of the embedding $H^{1/2}(\partial\Omega) \hookrightarrow L^2(\partial\Omega)$, we obtain

$$\int_{\partial\Omega} |\eta_p|^2 \,\mathrm{d}\mathcal{H}^{n-1} \xrightarrow{p\to\infty} 0,$$

and by combining with

$$\begin{aligned}\int_{V_k'} |\eta_p(z^k, h^k(z^k))|^2 \,\mathrm{d}z^k &\le \frac{1}{\sqrt{1+L^2}} \int_{V_k'} |\eta_p(z^k, h^k(z^k))|^2 \sqrt{1+|\nabla h^k(z^k)|^2}\,\mathrm{d}z^k\\ &= \frac{1}{\sqrt{1+L^2}} \int_{V_k\cap\partial\Omega} |\eta_p|^2 \,\mathrm{d}\mathcal{H}^{n-1} \le \frac{1}{\sqrt{1+L^2}} \int_{\partial\Omega} |\eta_p|^2 \,\mathrm{d}\mathcal{H}^{n-1},\end{aligned}$$

we conclude that

$$\int_{V_k'} |\eta_p(z^k, h^k(z^k))|^2 \,\mathrm{d}z^k \xrightarrow{p\to\infty} 0. \tag{2.7}$$

Now we estimate

$$\begin{aligned}\int_{V_k'} |\eta_p(z^k, h_p^k(z^k))|^2 \,\mathrm{d}z^k &= \int_{V_k'} \Big|\eta_p(z^k, h^k(z^k)) + \int_{h^k(z^k)}^{h_p^k(z^k)} \partial_{y_n^k}\eta_p(z^k,t)\,\mathrm{d}t\Big|^2 \mathrm{d}z^k\\ &\le 2\int_{V_k'} |\eta_p(z^k, h^k(z^k))|\,\mathrm{d}z^k + 2\int_{V_k'} \Big|\int_{h^k(z^k)}^{h_p^k(z^k)} \partial_{y_n^k}\eta_p(z^k,t)\,\mathrm{d}t\Big|^2 \mathrm{d}z^k.\end{aligned}$$

For $p\to\infty$, the first summand on the right-hand side converges to zero by (2.7), and the second summand is easily controlled using the Cauchy–Schwarz inequality:

$$\begin{aligned}\int_{V_k'} \Big|\int_{h^k(z^k)}^{h_p^k(z^k)} \partial_{y_n}\eta_p(z^k,t)\,\mathrm{d}t\Big|^2 \mathrm{d}z^k &\le \int_{V_k'} |h_p^k(z^k) - h^k(z^k)| \int_{h^k(z^k)}^{h_p^k(z^k)} |\partial_{y_n^k}\eta_p(z^k,t)|^2 \,\mathrm{d}t\,\mathrm{d}z^k\\ &\le \sup_{z^k\in V_k'} |h_p^k(z^k) - h^k(z^k)| \int_{V_k\cap\Omega_p} |\partial_{y_n^k}\eta_p|^2 \,\mathrm{d}y^k\\ &\le \sup_{z^k\in V_k'} |h_p^k(z^k) - h^k(z^k)|\, \|\eta_p\|^2_{H^1(V_k\cap\Omega_p)}\\ &\overset{(2.6)}{\le} c^2 \sup_{z^k\in V_k'} |h_p^k(z^k) - h^k(z^k)| \xrightarrow{p\to\infty} 0,\end{aligned}$$

due to the uniform convergence of h_p^k to h^k on V_k'. ∎

Let $k\in\{1,\dots,K\}$ and let $F\in H^1(\mathbb{R}^n,\mathbb{C}^N)$ be an arbitrary continuation of f. Then

$$\|\beta\alpha\cdot\nu^k(z^k)\| \le 1 \quad\text{and}\quad \|\beta\alpha\cdot\nu_p^k(z^k)\| \le 1 \quad \text{for all } p\in\mathbb{N} \text{ and a.e. } z^k\in V_k', \tag{2.8}$$

and

$$\beta\alpha\cdot\nu_p^k(z^k) \xrightarrow{p\to\infty} \beta\alpha\cdot\nu^k(z^k) \quad \text{for a.e. } z^k\in V_k'. \tag{2.9}$$

Using the representation

$$\begin{aligned}(1+\mathrm{i}\beta\alpha\cdot\nu^k(z^k))\,f(z^k,h^k(z^k)) &= (1+\mathrm{i}\beta\alpha\cdot\nu^k(z^k))F(z^k,h^k(z^k))\\ &= (\mathrm{i}\beta\alpha\cdot\nu^k(z^k)-\mathrm{i}\beta\alpha\cdot\nu^k_p(z^k))F(z^k,h^k(z^k))\\ &\quad+(1+\mathrm{i}\beta\alpha\cdot\nu^k_p(z^k))(F(z^k,h^k(z^k))-F(z^k,h^k_p(z^k)))\\ &\quad+(1+\mathrm{i}\beta\alpha\cdot\nu^k_p(z^k))(F(z^k,h^k_p(z^k))-\widetilde{f}_p(z^k,h^k_p(z^k)))\\ &\quad+(1+\mathrm{i}\beta\alpha\cdot\nu^k_p(z^k))\,\widetilde{f}_p(z^k,h^k_p(z^k)),\end{aligned}$$

we obtain

$$\int_{V_k'}|(1+\mathrm{i}\beta\alpha\cdot\nu^k(z^k))\,f(z^k,h^k(z^k))|^2\,\mathrm{d}z^k\le 4(I^1_p+I^2_p+I^3_p+I^4_p), \tag{2.10}$$

where

$$\begin{aligned}I^1_p&:=\int_{V_k'}|(\mathrm{i}\beta\alpha\cdot\nu^k(z^k)-\mathrm{i}\beta\alpha\cdot\nu^k_p(z^k))F(z^k,h^k(z^k))|^2\,\mathrm{d}z^k,\\ I^2_p&:=\int_{V_k'}|(1+\mathrm{i}\beta\alpha\cdot\nu^k_p(z^k))(F(z^k,h^k(z^k))-F(z^k,h^k_p(z^k)))|^2\,\mathrm{d}z^k,\\ I^3_p&:=\int_{V_k'}|(1+\mathrm{i}\beta\alpha\cdot\nu^k_p(z^k))(F(z^k,h^k_p(z^k))-\widetilde{f}_p(z^k,h^k_p(z^k)))|^2\,\mathrm{d}z^k,\\ I^4_p&:=\int_{V_k'}|(1+\mathrm{i}\beta\alpha\cdot\nu^k_p(z^k))\,\widetilde{f}_p(z^k,h^k_p(z^k))|^2\,\mathrm{d}z^k\overset{(2.5)}{=}0.\end{aligned}$$

By virtue of (2.8) and (2.9), the dominated convergence theorem implies that $I^1_p\to 0$ as $p\to\infty$. Using (2.8) again, we estimate

$$\begin{aligned}I^2_p&\le 4\int_{V_k'}|F(z^k,h^k(z^k))-F(z^k,h^k_p(z^k))|^2\,\mathrm{d}z^k\xrightarrow{p\to\infty}0\quad\text{(by Lemma 2.3)},\\ I^3_p&\le 4\int_{V_k'}|F(z^k,h^k_p(z^k))-\widetilde{f}_p(z^k,h^k_p(z^k))|^2\,\mathrm{d}z^k\xrightarrow{p\to\infty}0\quad\text{(by Lemma 2.4)}.\end{aligned}$$

This shows that the right-hand side of (2.10) converges to 0 for $p\to\infty$, hence the left-hand side is zero. The proof of self-adjointness is completed.

For the sake of completeness, we include the following standard assertion.

Lemma 2.5. *The graph norm of A on* dom A *is equivalent to the H^1-norm, and A has compact resolvent.*

Proof. The self-adjointness of A implies that dom A is complete with respect to the graph norm. At the same time, dom A is also complete with respect to the H^1-norm being the kernel of the bounded linear operator $H^1(\mathbb{R}^n,\mathbb{C}^N)\ni f\mapsto(1+\mathrm{i}\beta\alpha\cdot\nu)f|_{\partial\Omega}\in L^2(\partial\Omega)$. The embedding operator (dom A with H^1-norm) $\ni f\mapsto f\in$ (dom A with the graph norm) is obviously bijective and bounded, hence its inverse is bounded due to the closed graph theorem, and this shows that both norms are equivalent. It follows that dom A with the graph norm is continuously embedded into $H^1(\Omega,\mathbb{C}^N)$ and, therefore, compactly embedded in $L^2(\Omega,\mathbb{C}^N)$, which gives the conclusion. ∎

Remark 2.6. One easily sees that the convexity was actually used only to establish a uniform upper bound for the H^1-norms of the functions $\widetilde{f}_p$ in (2.1). In fact, the proof can be adapted to a larger class of domains of Ω as follows. Let us drop the convexity assumption but require instead that Ω can be approximated (in the sense described in Lemma 2.2) by C^∞-smooth domains Ω_p such that the mean curvatures H_p of their boundaries are uniformly bounded from below, $H_p \geq -2m$ for some $m > 0$. Then one can consider the operators $A := A_m^\Omega$ and $\widetilde{A}_p := A_m^{\Omega_p}$. If $g \in L^2(\Omega, \mathbb{C}^N)$ and $\widetilde{g}_p$ are its extensions by zero to Ω_p, then we can find $\widetilde{f}_p \in \operatorname{dom} \widetilde{A}_p$ with $(\widetilde{A}_p + \mathrm{i})\widetilde{f}_p = \widetilde{g}_p$, and (2.1) can be replaced by

$$\begin{aligned}
\|g\|^2_{L^2(\Omega,\mathbb{C}^N)} &= \|\widetilde{g}_p\|^2_{L^2(\Omega_p,\mathbb{C}^N)} = \|(\widetilde{A}_p + \mathrm{i})\widetilde{f}_p\|^2_{L^2(\Omega_p,\mathbb{C}^N)} \\
&= \|\widetilde{A}_p \widetilde{f}_p\|^2_{L^2(\Omega_p,\mathbb{C}^N)} + \|\widetilde{f}_p\|^2_{L^2(\Omega_p,\mathbb{C}^N)} \\
&= \int_{\Omega_p} \big(|\nabla \widetilde{f}_p|^2 + (m^2+1)|\widetilde{f}_p|^2\big)\,\mathrm{d}x + \int_{\partial\Omega_p} \Big(m + \frac{H_p}{2}\Big)|\widetilde{f}_p|^2\,\mathrm{d}\mathcal{H}^{n-1} \\
&\geq \int_{\Omega_p} \big(|\nabla \widetilde{f}_p|^2 + |\widetilde{f}_p|^2\big)\,\mathrm{d}x = \|\widetilde{f}_p\|^2_{H^1(\Omega_p,\mathbb{C}^N)},
\end{aligned}$$

and the rest of the proof remains literally the same, which provides the self-adjointness of A for such Ω. Simple geometric considerations show that for $n = 2$, these observations apply, for example, to curvilinear polygons without concave corners.

Remark 2.7. It would be interesting to understand if the self-adjointness results can be extended to the case when Ω is an unbounded convex domain. The above approach does not seem to be directly applicable. In fact, even if one manages to approximate Ω by smooth convex domains Ω_p, similarly to Lemma 2.2, the self-adjointness of the MIT bag operators on Ω_p is not automatically guaranteed, as all known works require a suitable uniform behavior at infinity, see, e.g., [7, 38] for $n \in \{2, 3\}$ and smooth boundaries, as well as [18] for unbounded polygonal domains with corners. It is unclear if this additional requirement is generally satisfied for the approximating domains Ω_p or some additional assumptions on the behavior of Ω at infinity is needed. Clarifying these geometric aspects goes far beyond the scope of the present paper, and we prefer to postpone the study of the MIT bag operators in unbounded convex domains to future work.

3. Approximations

In this section we establish several approximation results for Sobolev spaces on piecewise smooth domains. The constructions are inspired by [21]. We need first a simple result on the approximation of non-smooth domains by smooth ones.

Lemma 3.1 ("Rounding the corners"). *Let $\Omega \subset \mathbb{R}^n$ be a bounded convex domain. Then, for any open neighborhood $V_0 \subset \mathbb{R}^n$ of its singular boundary $\partial_0\Omega$, one can find a bounded domain $\Omega_0 \subset \mathbb{R}^n$ with C^∞-smooth boundary such that Ω and Ω_0 coincide outside V_0.*

Proof. Without loss of generality assume that $0 \in \Omega$. Then, due to convexity, we can describe Ω using polar coordinates,

$$\Omega = \{r\theta : \theta \in \mathbb{S}^{n-1},\ 0 \leq r < R(\theta)\}, \quad \partial\Omega = \{R(\theta)\theta : \theta \in \mathbb{S}^{n-1}\},$$

with a Lipschitz function $R: \mathbb{S}^{n-1} \to (0,\infty)$ which is C^∞-smooth on the open set

$$S_\infty := \{\theta \in \mathbb{S}^{n-1} : R(\theta)\,\theta \in \partial_\infty\Omega\} \subset \mathbb{S}^{n-1}.$$

Note that $\partial_0\Omega$ is compact and that the Lipschitz map

$$\Pi : \mathbb{R}^n \setminus \{0\} \ni x \mapsto \frac{x}{|x|} \in \mathbb{S}^{n-1}$$

is the inverse of $\theta \mapsto R(\theta)\,\theta$, which means that $S_0 := \mathbb{S}^{n-1} \setminus S_\infty \equiv \Pi(\partial_0\Omega)$ is a compact subset of the open set $\Theta_0 := \Pi(V_0) \subset \mathbb{S}^{n-1}$, and $\{R(\theta)\,\theta : \theta \in S_0\} = \partial_0\Omega \subset V_0$.

We now choose two open neighborhoods Θ_1 and Θ_2 of S_0 in $\mathbb{S}^{n-1}$ such that $\overline{\Theta}_2 \subset \Theta_1$ and $\overline{\Theta}_1 \subset \Theta_0$. Due to compactness of $\overline{\Theta}_1$, there is $\varepsilon > 0$ such that

$$\{r\theta : \theta \in \overline{\Theta}_1,\ |r - R(\theta)| \le \varepsilon\} \subset V_0,$$

and we can choose a C^∞-function $R_1: \Theta_1 \to (0,\infty)$ such that $|R_1(\theta) - R(\theta)| \le \varepsilon$ for all $\theta \in \Theta_1$. Now choose a cut-off function $\chi \in C^\infty(\mathbb{S}^{n-1})$, with $0 \le \chi \le 1$, such that $\operatorname{supp}\chi \subset \Theta_1$ and $\chi = 1$ on Θ_2. Then $R_0 := (1-\chi)R + \chi R_1: \mathbb{S}^{n-1} \to (0,\infty)$ is smooth, and the graphs of $\theta \mapsto R(\theta)\theta$ and $\theta \mapsto R_0(\theta)\theta$ coincide outside V_0. It follows that the domain

$$\Omega_0 := \{r\theta : \theta \in \mathbb{S}^{n-1},\ 0 \le r < R_0(\theta)\}$$

satisfies all the requirements. ∎

The following assertion is Lemma 2.4 in [21] with a reformulation adapted to the subsequent use.

Lemma 3.2. *Let $\chi \in C_c^\infty(\mathbb{R})$, with $0 \le \chi \le 1$, such that* $\operatorname{supp}\chi \in (-1,1)$ *and $\chi = 1$ in an open neighborhood of 0. For $\alpha \in (0,1)$ and $n \in \mathbb{N}$, define the functions*

$$\rho_{\alpha,n} : [0,\infty) \ni t \mapsto \min\{t^\alpha, 1\}(1 - \chi(nt)) \in \mathbb{R}.$$

Then one can choose $\alpha_j \to 0$ and $n_j \to \infty$ as $j \to \infty$ so that the functions

$$\psi_j : \mathbb{R}^2 \ni x \mapsto \rho_{\alpha_j,n_j}(|x|) \in \mathbb{R}$$

satisfy:

(a) *for any j, one has $0 \le \psi_j \le 1$, the function ψ_j vanishes in an open neighborhood of 0 in $\mathbb{R}^2$, and $\psi_j(x) \to 1$ as $j \to \infty$ for all $x \ne 0$,*

(b) *$\|\psi_j f - f\|_{H^1(\mathbb{R}^2)} \to 0$ as $j \to \infty$ for any $f \in H^1(\mathbb{R}^2)$,*

(c) *there is a constant $C > 0$ such that $\|\psi_j f\|_{H^1(\mathbb{R}^2)} \le C\|f\|_{H^1(\mathbb{R}^2)}$ for any $f \in H^1(\mathbb{R}^2)$ and any $j \in \mathbb{N}$.*

Note that [21] only states (b) explicitly. Part (a) follows from the explicit structure of ψ_j, and (c) follows from (b) by virtue of the Banach–Steinhaus theorem.

Lemma 3.3 (Cut-off near a submanifold). *Let $n \ge 2$ and let Γ be a compact $(n-2)$-dimensional submanifold in $\mathbb{R}^n$. For $x \in \mathbb{R}^n$, let $d(x)$ be the distance from x to Γ. Then the functions $\varphi_j := \psi_j \circ d$, with ψ_j from Lemma 3.2, satisfy*

$$\|\varphi_j f - f\|_{H^1(\mathbb{R}^n)} \xrightarrow{j\to\infty} 0 \quad \text{for any } f \in H^1(\mathbb{R}^n). \tag{3.1}$$

In addition, $\varphi_j = 0$ *in an open neighborhood of* Γ*, with* $0 \le \varphi_j \le 1$*, and* $\varphi_j(x) \to 1$ *as* $j \to \infty$ *for any* $x \in \mathbb{R}^n \setminus \Gamma$*.*

Proof. For $r > 0$, denote $B_2(0,r) := \{x \in \mathbb{R}^2 : |x| < r\}$. It is a classical result of differential geometry that for some sufficiently small $\varepsilon > 0$, the ε-neighborhood Γ_ε of Γ admits a tubular neighborhood, see, e.g., Theorem 10.19 in [32]. In the coordinate form, this means that one can cover Γ_ε by finitely many open sets $V_1, \dots, V_L$ such that for any $s \in \Gamma_\ell := V_\ell \cap \Gamma$, one can choose an orthonormal basis $(n_1(s), n_2(s))$ in the normal space to Γ at s, depending smoothly on s, and the maps

$$\Phi_\ell : \Gamma_\ell \times B_2(0,\varepsilon) \ni (s, t_1, t_2) \mapsto s + t_1 n_1(s) + t_2 n_2(s) \in V_\ell,$$

are diffeomorphisms, with $d(\Phi_\ell(s,t_1,t_2)) = \sqrt{t_1^2 + t_2^2} = |t|$, and the map $f \mapsto f \circ \Phi_\ell$ defines an isomorphism between $H^1(V_\ell)$ and $H^1(\Gamma_\ell \times B_2(0,\varepsilon))$. Without loss of generality, we assume that $\varepsilon \in (0,1)$.

Let $f \in H^1(\mathbb{R}^n)$. Note first that, by construction, one has $\varphi_j f = f$ outside Γ_1. Furthermore, for $x \in \Gamma_1 \setminus \Gamma_\varepsilon$ and all sufficiently large j, one has $(\varphi_j f)(x) = d(x)^{\alpha_j} f(x)$, and by using the fact that $\alpha_j \to 0$ and the dominated convergence theorem, we arrive at $\|\varphi_j f - f\|_{L^2(\Gamma_1 \setminus \Gamma_\varepsilon)} \to 0$ as $j \to \infty$. In addition, for the same x, one has

$$\nabla(\varphi_j f)(x) - \nabla f(x) = d(x)^{\alpha_j} \nabla f(x) - \nabla f(x) + \alpha_j \frac{\nabla d(x)}{d(x)^{1-\alpha_j}} f(x),$$

and

$$\int_{\Gamma_1 \setminus \Gamma_\varepsilon} |\nabla(\varphi_j f)(x) - \nabla f|^2 \,\mathrm{d}x \le 2 \int_{\Gamma_1 \setminus \Gamma_\varepsilon} |d^{\alpha_j} \nabla f - \nabla f|^2 \,\mathrm{d}x + 2\alpha_j^2 \int_{\Gamma_1 \setminus \Gamma_\varepsilon} \left| \frac{\nabla d}{d^{1-\alpha_j}} \right|^2 |f|^2 \,\mathrm{d}x.$$

The first summand on the right-hand side of the last inequality converges to zero by the dominated convergence theorem, while for the second summand, we have

$$2\alpha_j^2 \int_{\Gamma_1 \setminus \Gamma_\varepsilon} \left| \frac{\nabla d}{d^{1-\alpha_j}} \right|^2 |f|^2 \,\mathrm{d}x \le \frac{2\alpha_j^2}{\varepsilon^{2(1-\alpha_j)}} \int_{\Gamma_1 \setminus \Gamma_\varepsilon} |f|^2 \mathrm{d}x \xrightarrow{j \to \infty} 0.$$

The above considerations show that $\|\varphi_j f - f\|_{H^1(\mathbb{R}^n \setminus \overline{\Gamma}_\varepsilon)} \to 0$ as $j \to \infty$, and it remains to check $\|\varphi_j f - f\|_{H^1(\Gamma_\varepsilon)} \to 0$ as $j \to \infty$. In view of the preceding discussion, it is sufficient to show that for each $\ell \in \{1, \dots, L\}$, one has

$$\widehat{f}_j \xrightarrow{j \to \infty} \widehat{f} \quad \text{in } H^1(\Gamma_\ell \times B_2(0,\varepsilon)), \qquad \widehat{f}_j := (\varphi_j f) \circ \Phi_\ell, \qquad \widehat{f} := f \circ \Phi_\ell.$$

One has $\widehat{f}_j(s,t) = \psi_j(t) \widehat{f}(s,t)$, in particular, $\nabla_s \widehat{f}_j = \nabla_s \widehat{f}$, and

$$\|\widehat{f}_j - \widehat{f}\|^2_{H^1(\Gamma_\ell \times B_2(0,\varepsilon_0))} = \int_{\Gamma_\ell} \Big(\|\psi_j f(s,\cdot) - f(s,\cdot)\|^2_{H^1(B_2(0,\varepsilon))} + \|\psi_j \nabla_s f(s,\cdot) - \nabla_s f(s,\cdot)\|^2_{L^2(B_2(0,\varepsilon))} \Big) \,\mathrm{d}\mathscr{H}^{n-2}(s).$$

The subintegral expression admits integrable upper bound and converges to 0 for a.e. $s \in \Gamma_\ell$ as $j \to \infty$ by Lemma 3.2, so the whole integral converges to 0 for $j \to \infty$ by the dominated convergence theorem. This completes the proof of (3.1), and the remaining claims on φ_j follow from the properties of ψ_j in Lemma 3.2. ∎

Corollary 3.4. *Let $\Omega \subset \mathbb{R}^n$ be a bounded domain with piecewise smooth boundary. Then one can find functions $\rho_j \in C^\infty(\mathbb{R}^n)$, with $j \in \mathbb{N}$, such that $0 \le \rho_j \le 1$,*

$$\rho_j = 0 \qquad \text{in an open neighborhood of } \partial_0\Omega,$$

$$\rho_j(x) \xrightarrow{j\to\infty} 1 \quad \text{for a.e. } x \in \mathbb{R}^n,$$

$$\rho_j f \xrightarrow{j\to\infty} f \quad \text{in } H^1(\Omega) \text{ for any } f \in H^1(\Omega).$$

Proof. Let $\Gamma_1, \dots, \Gamma_K$ be compact $(n-2)$-dimensional submanifolds whose union contains $\partial_0\Omega$, and denote by $d_k(x)$ the distance from $x \in \mathbb{R}^n$ to Γ_k.

Let $f \in H^1(\Omega)$ and $j \in \mathbb{N}$. Denote $h_0 := f$. Then, for each $k \in \{1, \dots, K\}$, successively use Lemma 3.3 to choose $j_k \ge j$ such that the function $h_k := (\psi_{j_k} \circ d_k)h_{k-1}$ satisfies

$$\|h_k - h_{k-1}\|_{H^1(\Omega)} < \frac{1}{jK}.$$

By construction, one has

$$h_K = \rho_j f, \quad \text{with} \quad \rho_j := \prod_{k=1}^{K} (\psi_{j_k} \circ d_k),$$

and

$$\|\rho_j f - f\|_{H^1(\Omega)} \equiv \|h_K - h_0\|_{H^1(\Omega,\mathbb{C}^N)} \le \sum_{k=1}^{K} \|h_k - h_{k-1}\|_{H^1(\Omega,\mathbb{C}^N)} < K \cdot \frac{1}{jK} = \frac{1}{j}.$$

Hence $\rho_j f \to f$ as $j \to \infty$ in $H^1(\Omega)$. The function $\psi_{j_k} \circ d_k$ vanishes in an open neighborhood of Γ_k, so ρ_j vanishes in the union of these neighborhoods (which is also an open neighborhood of $\partial_0\Omega$). For $j \to \infty$, one has $j_k \to \infty$ for each k, hence $\psi_{j_k} \circ d_k(x) \to 1$ for $x \notin \Gamma_k$, which implies that $\rho_j(x) \to 1$ as $j \to \infty$ for any $x \notin \bigcup_{k=1}^K \Gamma_k$. Finally, the required bound $0 \le \rho_j \le 1$ follows from $0 \le \psi_j \le 1$ (Lemma 3.2). ■

Corollary 3.5. *Let $\Omega \subset \mathbb{R}^n$ be a bounded convex domain with piecewise smooth boundary and $m \in \mathbb{R}$. Then the Dirac operator A_m^Ω is essentially self-adjoint on*

$$\operatorname{dom}_0 A_m^\Omega := \{f \in \operatorname{dom} A_m^\Omega : f = 0 \text{ in an open neighborhood of } \partial_0\Omega\}.$$

Proof. Let ρ_j be as in Corollary 3.4 and $f \in \operatorname{dom} A_m^\Omega$. As the boundary condition for A_m^Ω is invariant under multiplication by smooth scalar functions, one has $\rho_j f \in \operatorname{dom}_0 A_m^\Omega$, with $\rho_j f \to f$ as $j \to \infty$ in $H^1(\Omega, \mathbb{C}^N)$, and the conclusion follows by Lemma 2.5. ■

Lemma 3.6 (Essential self-adjointness on smooth functions). *Let $\Omega \subset \mathbb{R}^n$ be a bounded convex domain with piecewise smooth boundary. Then, for any $m \in \mathbb{R}$, the Dirac operator A_m^Ω is essentially self-adjoint on*

$$\operatorname{dom}_\infty A_m^\Omega := \big\{f \in \operatorname{dom} A_m^\Omega : f \in C^\infty(\overline{\Omega}, \mathbb{C}^N),\; f = 0 \text{ in an open neighborhood of } \partial_0\Omega\big\}.$$

Proof. Let $f \in \operatorname{dom} A_m^\Omega$ and $\varepsilon > 0$. By Corollary 3.5, one can find a function $h \in \operatorname{dom} A_m^\Omega$ which vanishes in an open neighborhood U of $\partial_0\Omega$ and satisfies $\|h - f\|_{H^1(\Omega,\mathbb{C}^N)} < \varepsilon/3$.

Choose bounded open neighborhoods V_0 and V of $\partial_0\Omega$ such that $\overline{V_0} \subset V$ and $\overline{V} \subset U$; then pick a function $\chi \in C_c^\infty(\mathbb{R}^n)$, with $0 \le \chi \le 1$, such that $\operatorname{supp}\chi \subset V$ and $\chi = 1$ in V_0. The map

$$H^{1/2}(\partial\Omega, \mathbb{C}^N) \ni \varphi \mapsto (1 + i\beta\alpha \cdot \nu)(1-\chi)\varphi \in H^{1/2}(\partial\Omega, \mathbb{C}^N)$$

is a bounded linear operator (being a multiplication by a smooth matrix function compactly supported on the regular boundary), and we denote its norm by C_0. Furthermore, it maps the subspace

$$\{\varphi \in H^{1/2}(\partial\Omega, \mathbb{C}^N) : \operatorname{supp}\varphi \subset \partial_\infty\Omega,\ \varphi \in C^\infty(\partial_\infty\Omega, \mathbb{C}^N)\}$$

in itself and, in addition, $(1 + i\beta\alpha \cdot \nu)(1-\chi)\varphi = (1 + i\beta\alpha \cdot \nu)\varphi$ for $\operatorname{supp}\varphi \subset \partial\Omega \setminus V_0$.

Now let Ω_0 be a bounded C^∞-smooth domain which coincides with Ω outside V_0 (see Lemma 3.1). For any $\varphi \in H^{1/2}(\partial\Omega_0)$, there is a unique $F \in H^1(\Omega_0)$ with $\Delta F = 0$ in Ω_0 and $F = \varphi$ on $\partial\Omega_0$, and the associated Poisson operator $\mathcal{E}_0\colon H^{1/2}(\partial\Omega_0) \ni \varphi \mapsto F \in H^1(\Omega_0)$ is bounded with $\mathcal{E}_0(C^\infty(\partial\Omega_0)) \subset C^\infty(\overline{\Omega}_0)$, see Theorem 11.14 in [27]. Note that for any function φ defined on $\partial\Omega$, we can consider $(1-\chi)\varphi$ as a function defined on $\partial\Omega_0$ and vanishing on $V_0 \cap \partial\Omega_0$. Similarly, for any function v_0 on Ω_0, one can consider $(1-\chi)v_0$ as a function on Ω which vanishes in $V_0 \cap \Omega$. With these identifications we conclude that

$$\mathcal{E} : H^{1/2}(\partial\Omega, \mathbb{C}^N) \ni \varphi \mapsto (1-\chi)(\mathcal{E}_0 \otimes I_N)\big((1-\chi)\varphi\big) \in H^1(\Omega, \mathbb{C}^N)$$

is a bounded operator, and we denote by C_1 its norm. Moreover, it maps $C^\infty(\partial\Omega)$ to $C^\infty(\overline{\Omega})$ by construction, and $\mathcal{E}\varphi = \varphi$ on $\partial\Omega$ for any $\varphi \in C^\infty(\partial\Omega)$ with $\varphi = 0$ on $V \cap \partial\Omega$.

Let $\widetilde{h} \in H^1(\mathbb{R}^n, \mathbb{C}^N)$ be an arbitrary continuation of the above h. Consider its convolutions $\widetilde{h}_\varepsilon := \widetilde{h} * \rho_\varepsilon$ with standard mollifiers ρ_ε, and let h_ε be their restrictions to Ω. Then $h_\varepsilon \in C^\infty(\overline{\Omega}, \mathbb{C}^N)$. Having in mind that $h = 0$ in U and that the support of h_ε is contained in the ε-neighborhood of the support of h, we conclude that we can choose ε sufficiently small such that the function $g := h_\varepsilon \in C^\infty(\overline{\Omega}, \mathbb{C}^N)$ satisfies $g = 0$ on $V \cap \Omega$, with

$$\|g - h\|_{H^1(\Omega,\mathbb{C}^N)} < \frac{\varepsilon}{3} \quad \text{and} \quad \|g - h\|_{H^{1/2}(\partial\Omega)} < \frac{\varepsilon}{3C_0C_1}.$$

Consider the function $v := g - \mathcal{E}(1 + i\beta\alpha \cdot \nu)(g|_{\partial\Omega})$. Due to the above considerations, we have $v \in C^\infty(\overline{\Omega}, \mathbb{C}^N)$ with $v = 0$ in V_0, and $(1 + i\beta\alpha \cdot \nu)(v|_{\partial\Omega}) = 0$, i.e., $v \in \operatorname{dom}_\infty A$. In addition, using $(1 + i\beta\alpha \cdot \nu)(h|_{\partial\Omega}) = 0$, we obtain

$$\begin{aligned}
\|v - g\|_{H^1(\Omega,\mathbb{C}^N)} &= \|\mathcal{E}(1 + i\beta\alpha \cdot \nu)(g|_{\partial\Omega})\|_{H^1(\Omega,\mathbb{C}^N)}\\
&\le C_1\|(1 + i\beta\alpha \cdot \nu)(g|_{\partial\Omega})\|_{H^{1/2}(\partial\Omega,\mathbb{C}^N)}\\
&= C_1\|(1 + i\beta\alpha \cdot \nu)(1-\chi)(g|_{\partial\Omega} - h|_{\partial\Omega})\|_{H^{1/2}(\partial\Omega,\mathbb{C}^N)}\\
&\le C_1C_0\|g - h\|_{H^{1/2}(\partial\Omega,\mathbb{C}^N)} < \frac{\varepsilon}{3},
\end{aligned}$$

therefore

$$\begin{aligned}
\|v - f\|_{H^1(\Omega,\mathbb{C}^N)} &\le \|v - g\|_{H^1(\Omega,\mathbb{C}^N)} + \|g - h\|_{H^1(\Omega,\mathbb{C}^N)} + \|h - f\|_{H^1(\Omega,\mathbb{C}^N)}\\
&< \frac{\varepsilon}{3} + \frac{\varepsilon}{3} + \frac{\varepsilon}{3} = \varepsilon,
\end{aligned}$$

and the claims follow due to the arbitrariness of ε. ■

4. Proof of Theorem 1.3 (quadratic form)

As a simple application of the preceding approximations, we show that the formulas for the quadratic forms of A^2_m and $B^2_{m,M}$ previously obtained for smooth Ω are also valid for convex piecewise smooth Ω. The following assertion completes the proof of Theorem 1.3.

Lemma 4.1. *Let $\Omega \subset \mathbb{R}^n$ be a bounded convex domain with piecewise smooth boundary. Then, for any $f \in \operatorname{dom} A^\Omega_m$, one has*

$$\|A^\Omega_m f\|^2_{L^2(\Omega,\mathbb{C}^N)} = \int_\Omega (|\nabla f|^2 + m^2|f|^2)\,\mathrm{d}x + \int_{\partial\Omega} \Big(m + \frac{H}{2}\Big)|f|^2\,\mathrm{d}\mathcal{H}^{n-1},$$

where H is the mean curvature on $\partial_\infty\Omega$.

Proof. Let $f \in \operatorname{dom}_0 A^\Omega_m$ (see Lemma 3.6) vanish in an open neighborhood V_0 of $\partial_0\Omega$. By Lemma 3.1, one can find a bounded C^∞-smooth domain Ω_0 coinciding with Ω outside V_0. Define $f_0\colon \Omega_0 \to \mathbb{C}^N$ by $f_0 := f$ in $\Omega_0 \setminus V_0 \equiv \Omega \setminus V_0$ and $f_0 := 0$ in $\Omega_0 \cap V_0$. Then $f_0 \in \operatorname{dom} A^{\Omega_0}_m$, with

$$\begin{aligned}
\nabla f_0 = \nabla f \ \text{ and } \ A^{\Omega_0}_m f_0 &= A^\Omega_m f && \text{in } \Omega_0 \setminus V_0 \equiv \Omega \setminus V_0,\\
\nabla f_0 = 0 \ \text{ and } \ A^{\Omega_0}_m f_0 &= 0 && \text{in } \Omega_0 \cap V_0,\\
\nabla f = 0 \ \text{ and } \ A^{\Omega}_m f &= 0 && \text{in } \Omega \cap V_0,\\
f_0 &= f && \text{on } \partial\Omega_0 \setminus V_0 \equiv \partial\Omega \setminus V_0,\\
f_0 &= 0 && \text{on } \partial\Omega_0 \cap V,\\
f &= 0 && \text{on } \partial\Omega \cap V.
\end{aligned}$$

In addition, the mean curvature H_0 on $\partial\Omega_0$ satisfies $H_0 = H$ on $\partial\Omega_0 \setminus V_0 \equiv \partial\Omega \setminus V_0$. Hence,

$$\begin{aligned}
\|A^\Omega_m f\|^2_{L^2(\Omega,\mathbb{C}^N)} &= \|A^\Omega_m f\|^2_{L^2(\Omega\setminus V_0,\mathbb{C}^N)} = \|A^{\Omega_0}_m f_0\|^2_{L^2(\Omega_0\setminus V_0,\mathbb{C}^N)} = \|A^{\Omega_0}_m f_0\|^2_{L^2(\Omega_0,\mathbb{C}^N)}\\
&\overset{\text{(by Lemma 2.1)}}{=} \int_{\Omega_0} (|\nabla f_0|^2 + m^2|f_0|^2)\,\mathrm{d}x + \int_{\partial\Omega_0} \Big(m + \frac{H_0}{2}\Big)|f_0|^2\,\mathrm{d}\mathcal{H}^{n-1}\\
&= \int_{\Omega_0\setminus V_0} (|\nabla f_0|^2 + m^2|f_0|^2)\,\mathrm{d}x + \int_{\partial\Omega_0\setminus V_0} \Big(m + \frac{H_0}{2}\Big)|f_0|^2\,\mathrm{d}\mathcal{H}^{n-1}\\
&= \int_{\Omega\setminus V_0} (|\nabla f|^2 + m^2|f|^2)\,\mathrm{d}x + \int_{\partial\Omega\setminus V_0} \Big(m + \frac{H}{2}\Big)|f|^2\,\mathrm{d}\mathcal{H}^{n-1}\\
&= \int_{\Omega} (|\nabla f|^2 + m^2|f|^2)\,\mathrm{d}x + \int_{\partial\Omega} \Big(m + \frac{H}{2}\Big)|f|^2\,\mathrm{d}\mathcal{H}^{n-1}.
\end{aligned}$$

Hence, the required formula holds for all functions in $\operatorname{dom}_0 A^\Omega_m$. Note that H can become unbounded near $\partial_0\Omega$, so some attention is needed when extending to the whole domain.

Let $f \in \operatorname{dom} A^\Omega_m$ and let ρ_j be as in Corollary 3.5 Then, for $f_j := \rho_j f \in \operatorname{dom}_0 A^\Omega_m$,

$$\begin{aligned}
\|A^\Omega_m f\|^2_{L^2(\Omega,\mathbb{C}^N)} &= \lim_{j\to\infty} \|A^\Omega_m f_j\|^2_{L^2(\Omega,\mathbb{C}^N)}\\
&= \lim_{j\to\infty} \Big[\int_\Omega (|\nabla f_j|^2 + m^2|f_j|^2)\,\mathrm{d}x + \int_{\partial\Omega} \Big(m + \frac{H}{2}\Big)|f_j|^2\,\mathrm{d}\mathcal{H}^{n-1}\Big].
\end{aligned}$$

By Corollary 3.5, we have

$$\int_{\Omega}(|\nabla f_j|^2+m^2|f_j|^2)\,\mathrm{d}x \xrightarrow{j\to\infty} \int_{\Omega}(|\nabla f|^2+m^2|f|^2)\,\mathrm{d}x,$$
$$\int_{\partial\Omega} m|f_j|^2\,\mathrm{d}\mathcal{H}^{n-1} \xrightarrow{j\to\infty} \int_{\partial\Omega} m|f|^2\,\mathrm{d}\mathcal{H}^{n-1}.$$

Furthermore, $|f_j|\le|f|$, with $f_j(x)\to f(x)$ as $j\to\infty$ for a.e. x, and Fatou's lemma yields

$$\int_{\partial\Omega}\frac{H}{2}\,|f_j|^2\,\mathrm{d}\mathcal{H}^{n-1} \xrightarrow{j\to\infty} \int_{\partial\Omega}\frac{H}{2}\,|f|^2\,\mathrm{d}\mathcal{H}^{n-1},$$

which concludes the proof. ∎

As a preparation for the next section, we use similar ideas to show an analogous result for the Dirac operator $B^{\Omega}_{m,M}$ on $\mathbb{R}^n$ defined in (1.4).

Lemma 4.2. *Let $\Omega\subset\mathbb{R}^n$ be a bounded convex domain with piecewise smooth boundary and $m, M\in\mathbb{R}$. Then, for all $f\in\operatorname{dom} B^{\Omega}_{m,M}$,*

$$\|B^{\Omega}_{m,M}f\|^2_{L^2(\mathbb{R}^n,\mathbb{C}^N)} = \int_{\Omega}(|\nabla f|^2+m^2|f|^2)\,\mathrm{d}x + \int_{\Omega^c}(|\nabla f|^2+M^2|f|^2)\,\mathrm{d}x + (M-m)\int_{\partial\Omega}(|\mathcal{P}_- f|^2-|\mathcal{P}_+ f|^2)\,\mathrm{d}\mathcal{H}^{n-1}, \tag{4.1}$$

where $\mathcal{P}_\pm(s) := (1\mp \mathrm{i}\beta\alpha\cdot\nu(s))/2$ for $s\in\partial_\infty\Omega$.

Proof. Recall that the formula is already proved for smooth Ω in Lemma 2.3 of [34]. Assume first that $f\in H^1(\mathbb{R}^n,\mathbb{C}^N)$ and that f vanishes in an open neighborhood V_0 of $\partial_0\Omega$. By Lemma 3.1, one can find a bounded C^∞-smooth domain Ω_0 which coincides with Ω outside V_0. Let ν_0 be the outer unit normal on $\partial\Omega_0$ and consider the respective pointwise projectors

$$\mathcal{P}^0_\pm(s) := \frac{1\mp \mathrm{i}\beta\alpha\cdot\nu_0(s)}{2},\quad s\in\partial\Omega_0.$$

Then $\mathcal{P}^0_\pm f=\mathcal{P}_\pm f$ on $\partial\Omega\setminus V_0$. Due to $B^{\Omega}_{m,M}f = B^{\Omega_0}_{m,M}f$, one can use the already known formula for the smooth Ω_0 as follows:

$$\begin{aligned}
\|B^{\Omega}_{m,M}f\|^2_{L^2(\mathbb{R}^n,\mathbb{C}^N)} &= \|B^{\Omega_0}_{m,M}f\|^2_{L^2(\mathbb{R}^n,\mathbb{C}^N)}\\
&= \int_{\Omega_0}(|\nabla f|^2+m^2|f|^2)\,\mathrm{d}x + \int_{\Omega_0^c}(|\nabla f|^2+M^2|f|^2)\,\mathrm{d}x\\
&\quad + (M-m)\int_{\partial\Omega_0}(|\mathcal{P}^0_- f|^2-|\mathcal{P}^0_+ f|^2)\,\mathrm{d}\mathcal{H}^{n-1}\\
&= \int_{\Omega_0\setminus V_0}(|\nabla f|^2+m^2|f|^2)\,\mathrm{d}x + \int_{\Omega_0^c\setminus V_0}(|\nabla f|^2+M^2|f|^2)\,\mathrm{d}x\\
&\quad + (M-m)\int_{\partial\Omega_0\setminus V_0}(|\mathcal{P}^0_- f|^2-|\mathcal{P}^0_+ f|^2)\,\mathrm{d}\mathcal{H}^{n-1}
\end{aligned}$$

$$= \int_{\Omega\setminus V_0} (|\nabla f|^2 + m^2|f|^2)\,\mathrm{d}x + \int_{\Omega^c\setminus V_0} (|\nabla f|^2 + M^2|f|^2)\,\mathrm{d}x$$
$$+ (M-m)\int_{\partial\Omega\setminus V_0} (|\mathcal{P}_- f|^2 - |\mathcal{P}_+ f|^2)\,\mathrm{d}\mathcal{H}^{n-1}$$
$$= \int_{\Omega} (|\nabla f|^2 + m^2|f|^2)\,\mathrm{d}x + \int_{\Omega^c} (|\nabla f|^2 + M^2|f|^2)\,\mathrm{d}x$$
$$+ (M-m)\int_{\partial\Omega} (|\mathcal{P}_- f|^2 - |\mathcal{P}_+ f|^2)\,\mathrm{d}\mathcal{H}^{n-1}.$$

Hence, the required formula holds for the functions vanishing near $\partial_0\Omega$. By Lemma 3.2, the operator $B^{\Omega}_{m,M}$ is essentially self-adjoint on the set of all such functions, which allows one to extend the formula by density to the whole of dom $B^{\Omega}_{m,M}$. ■

5. Proof of Theorem 1.4 (infinite mass limit)

In this section the domain Ω and the mass parameter m in Ω are fixed, and we abbreviate

$$A := A^{\Omega}_m \quad \text{and} \quad B_M := B^{\Omega}_{m,M}.$$

Recall that $\mathrm{dom}_\infty A$ is defined in Lemma 3.6. Let us briefly discuss some geometric ingredients appearing in the constructions below. For each $s \in \partial_\infty\Omega$, the shape operator $W(s)\colon T_s\partial_\infty\Omega \to T_s\partial_\infty\Omega$ is defined by $W(s) := \mathrm{d}|_s\nu$. Its eigenvalues $\kappa_1(s),\dots,\kappa_{n-1}(s)$ are the principal curvatures of the boundary at s. One often uses the Jacobian (with I being the identity operator and $t > 0$)

$$J(s,t) := \det(I + tW(s)) \equiv \prod_{j=1}^{n-1}(1 + t\kappa_j(s)) \equiv 1 + \sum_{k=1}^{n-1} H_k(s)t^k, \tag{5.1}$$

with

$$H_k(s) := \sum_{1\le j_1<\cdots<j_k\le n-1} \kappa_{j_1}(s)\cdots\kappa_{j_k}(s), \quad k \in \{1,\dots,n-1\}.$$

In particular, $H_1 = \kappa_1 + \cdots + \kappa_{n-1} \equiv H$.

5.1. Upper bound

Let $j \in \mathbb{N}$ and denote $E := E_j(A^2)$. Let $\varepsilon > 0$. Then, by Lemma 3.6 and the min-max principle, one can find a j-dimensional subspace $F \subset \mathrm{dom}_\infty A$ such that

$$\max_{f\in F\setminus\{0\}} \frac{\|Af\|^2_{L^2(\Omega,\mathbb{C}^N)}}{\|f\|^2_{L^2(\Omega,\mathbb{C}^N)}} \le E + \varepsilon. \tag{5.2}$$

Due to convexity, the map $S\colon \Omega^c \to \partial\Omega$ given by the rule $|x - S(x)| \le |x - y|$ for any $y \in \partial\Omega$ is a well-defined Lipschitz function. For any $f \in F$, denote by $\widetilde{f}$ its extension to $\mathbb{R}^n$ by

$$\widetilde{f}(x) := f(S(x))e^{-Md(x)}, \quad d(x) := \mathrm{dist}(x,\partial\Omega), \quad x \in \Omega^c,$$

and consider the j-dimensional subspace $\widetilde{F} := \{\widetilde{f} : f \in F\} \subset H^1(\mathbb{R}^n, \mathbb{C}^N)$. Our goal is to show that for some $c > 0$ and all sufficiently large $M > 0$, one has

$$\max_{\widetilde{f}\in\widetilde{F}\setminus\{0\}} \frac{\|B_M \widetilde{f}\|^2_{L^2(\mathbb{R}^n,\mathbb{C}^N)}}{\|\widetilde{f}\|^2_{L^2(\mathbb{R}^n,\mathbb{C}^N)}} \le E + \varepsilon + \frac{c}{M}. \tag{5.3}$$

Then the min-max principle implies first $\limsup_{M\to+\infty} E_j(B_M^2) \le E + \varepsilon$, and due to the arbitrariness of ε, one obtains the upper bound

$$\limsup_{M\to+\infty} E_j(B_M^2) \le E \equiv E_j(A^2). \tag{5.4}$$

Now let us show (5.3). For any $\widetilde{f} \in \widetilde{F}$, one has $\mathcal{P}_+ \widetilde{f} = \widetilde{f}$ and $\mathcal{P}_- \widetilde{f} = 0$, hence, with $f := \widetilde{f}|_\Omega \in F \subset \operatorname{dom}_\infty A$, one can rewrite the expression of Lemma 4.2 in the form

$$\begin{aligned} \|B_M \widetilde{f}\|^2_{L^2(\mathbb{R}^n,\mathbb{C}^N)} &\equiv \int_\Omega (|\nabla f|^2 + m^2|f|^2)\,\mathrm{d}x + \int_{\partial\Omega}\Big(m + \frac{H_1}{2}\Big)|f|^2\,\mathrm{d}\mathcal{H}^{n-1}\\ &\quad + \int_{\Omega^c}(|\nabla \widetilde{f}|^2 + M^2|u|^2)\,\mathrm{d}x - \int_{\partial\Omega}\Big(M + \frac{H_1}{2}\Big)|\widetilde{f}|^2\,\mathrm{d}\mathcal{H}^{n-1}\\ &\equiv \|Af\|^2_{L^2(\Omega,\mathbb{C}^N)} + R_M(\widetilde{f}), \end{aligned} \tag{5.5}$$

where

$$R_M(\widetilde{f}) := \int_{\Omega^c}(|\nabla \widetilde{f}|^2 + M^2|\widetilde{f}|^2)\,\mathrm{d}x - \int_{\partial\Omega}\Big(M + \frac{H_1}{2}\Big)|\widetilde{f}|^2\,\mathrm{d}\mathcal{H}^{n-1}.$$

Let us derive an upper bound for $R_M(\widetilde{f})$ using local coordinates. Note first that one can find a compact subset $K \subset \partial_\infty\Omega$ with $\operatorname{supp} \widetilde{f}|_{\partial\Omega} \subset K$ for all $\widetilde{f} \in \widetilde{F}$, and then $\widetilde{f}(x) = 0$ for all $x \in \Omega^c$ with $S(x) \notin K$. We further choose open subsets $V_1, \dots, V_P \subset \partial_\infty\Omega$ such that $K \subset V_1 \cup \dots \cup V_P$, with each V_p covered by a local chart $\varphi_p\colon \mathbb{R}^{n-1} \supset U_p \to V_p$, and we pick $\chi_p \in C_c^\infty(V_p)$ such that $\chi_1 + \dots + \chi_P = 1$ on K. Then $\chi_1 \circ S + \dots + \chi_P \circ S = 1$ on $\operatorname{supp} \widetilde{f} \cap \Omega^c$ for all $\widetilde{f} \in \widetilde{F}$. Furthermore, the maps

$$\Phi_p : U_p \times (0,\infty) \ni (s,t) \mapsto \varphi_p(s) + t\nu\big(\varphi_p(s)\big) \in \Omega^c$$

are diffeomorphisms satisfying the identities $d(\Phi_p(s,t)) = t$ and $S(\Phi_p(s,t)) = \varphi_p(s)$.

Let $\widetilde{f} \in \widetilde{F}$ and denote $f_p := \widetilde{f} \circ \Phi_p$. Then $f_p(s,t) = f(\varphi_p(s))e^{-Mt}$ for all (s,t), and the partition of unity $\chi_p \circ S$ and a standard change of variables yield

$$\begin{aligned} R_M(\widetilde{f}) &= \sum_{p=1}^P \Big[\int_{\Omega^c}(\chi_p \circ S)(|\nabla \widetilde{f}|^2 + M^2|\widetilde{f}|^2)\,\mathrm{d}x - \int_{\partial\Omega}\chi_p\Big(M + \frac{H_1}{2}\Big)|\widetilde{f}|^2\,\mathrm{d}\mathcal{H}^{n-1}\Big]\\ &= \sum_{p=1}^P \int_{U_p}\chi_p(\varphi_p(s))\Big[\int_0^\infty(\langle\nabla f_p(s,t), G_p(s,t)^{-1}\nabla f_p(s,t)\rangle + M^2|f_p(s,t)|^2)J_p(s,t)\,\mathrm{d}t\\ &\quad - \Big(M + \frac{H_1(\varphi_p(s))}{2}\Big)|f_p(s,0)|^2\Big]\sqrt{\det g_p(s)}\,\mathrm{d}s, \end{aligned}$$

with matrices

$$G_p(s,t) := \begin{pmatrix} \big(\langle (1+tW_p(s))\partial_j\varphi(s), (1+tW_p(s))\partial_k\varphi(s)\rangle\big)_{j,k=1}^{n-1} & 0 \\ 0 & 1 \end{pmatrix},$$

$$g_p(s) := \big(\langle \partial_j\varphi(s), \partial_k\varphi(s)\rangle\big)_{j,k=1}^{n-1}, \quad W_p := W\circ\varphi_p.$$

and Jacobians $J_p(s,t) := J(\varphi_p(s),t)$, see (5.1). As $W_p(s)$ is self-adjoint and its eigenvalues (the principal curvatures) are non-negative due to convexity, the min-max principle implies $G_p(s,t) \ge G_p(s,0) \equiv g_p(s)\oplus 1$, resulting in

$$G_p(s,t)^{-1} \le G_p(s,0)^{-1} \equiv \begin{pmatrix} g_p(s)^{-1} & 0 \\ 0 & 1\end{pmatrix}.$$

Hence,

$$\begin{aligned} R_M(\tilde f) &\le \sum_{p=1}^P \int_{U_p} \chi_p(\varphi_p(s))\Big[\int_0^\infty \big(\langle \nabla_s f_p(s,t), g_p^{-1}(s)\nabla_s f_p(s,t)\rangle + |\partial_t f_p(s,t)|^2 \\ &\quad + M^2|f_p(s,t)|^2\big)J_p(s,t)\,\mathrm{d}t - \Big(M + \frac{H_1(\varphi_p(s))}{2}\Big)|f_p(s,0)|^2\Big]\sqrt{\det g_p(s)}\,\mathrm{d}s \\ &= \sum_{p=1}^P \int_{U_p} \chi_p(\varphi_p(s))\Big[\int_0^\infty \big(\langle \nabla_s f(\varphi_p(s)), g_p^{-1}(s)\nabla_s f(\varphi_p(s))\rangle e^{-2Mt} \\ &\quad + 2M^2|f(\varphi_p(s))|^2 e^{-2Mt}\big)J_p(s,t)\,\mathrm{d}t - \Big(M + \frac{H_1(\varphi_p(s))}{2}\Big)|f(\varphi_p(s))|^2\Big] \\ &\quad \times \sqrt{\det g_p(s)}\,\mathrm{d}s. \end{aligned}$$

A simple direct computation shows that

$$\int_0^\infty e^{-2Mt}\,\mathrm{d}t = \frac{1}{2M}, \quad \int_0^\infty J_p(s,t)e^{-2Mt}\,\mathrm{d}t = \frac{1}{2M} + \sum_{k=1}^{n-1}\frac{k!H_k(\varphi_p(s))}{(2M)^{k+1}},$$

and there is a $C_p > 0$ such that, for all s with $\varphi_p(s) \in \operatorname{supp}\chi_p$ and sufficiently large M, one has

$$\int_0^\infty J_p(s,t)e^{-2Mt}\,\mathrm{d}t \le \frac{1}{2M^2}\Big(M + \frac{H_1(\varphi_p(s))}{2}\Big) + \frac{C_p}{M^3},$$

which results in

$$\begin{aligned} R_M(\tilde f) &\le \sum_{p=1}^P \int_{U_p} \chi_p(\varphi_p(s))\Big[\frac{1}{2M}\langle \nabla_s f(\varphi_p(s)), g_p^{-1}(s)\nabla_s f(\varphi_p(s))\rangle \\ &\quad + \frac{2C_p}{M}|f(\varphi_p(s))|^2\Big]\sqrt{\det g_p(s)}\,\mathrm{d}s \le \frac{C}{M}\|\tilde f\|^2_{H^1(\partial\Omega,\mathbb{C}^N)} \end{aligned}$$

for some constant $C > 0$ independent of $\tilde f$ and M. In addition, one can find another constant $C_1 > 0$ with $\|\tilde f\|^2_{H^1(\partial\Omega,\mathbb{C}^N)} \le C_1\|\tilde f\|^2_{L^2(\mathbb{R}^n,\mathbb{C}^N)}$ for all $\tilde f \in \tilde F$, as $\tilde F$ is finite-dimensional. Hence,

$$R_M(\tilde f) \le \frac{CC_1}{M}\|\tilde f\|^2_{L^2(\mathbb{R}^n,\mathbb{C}^N)} \quad \text{for all } \tilde f \in \tilde F.$$

By inserting this estimate and (5.2) into the representation (5.5), for all $\widetilde{f} \in \widetilde{F} \setminus \{0\}$, we obtain

$$\frac{\|B_M \widetilde{f}\|^2_{L^2(\mathbb{R}^n,\mathbb{C}^N)}}{\|\widetilde{f}\|^2_{L^2(\mathbb{R}^n,\mathbb{C}^N)}} \le \frac{(E+\varepsilon)\|f\|^2_{L^2(\Omega,\mathbb{C}^N)} + \frac{CC_1}{M}\|\widetilde{f}\|^2_{L^2(\mathbb{R}^n,\mathbb{C}^N)}}{\|\widetilde{f}\|^2_{L^2(\mathbb{R}^n,\mathbb{C}^N)}} \le E+\varepsilon+\frac{CC_1}{M},$$

which shows the sought estimate (5.3) with $c := CC_1$.

We make a side remark that the upper bound did not require the boundedness of H.

5.2. Lower bound

We start with a preliminary estimate.

Lemma 5.1. *Let the mean curvature H of $\partial_\infty\Omega$ be bounded. Then, for some $c > 0$, one has*

$$R_\gamma(f) := \int_{\Omega^c} (|\nabla f|^2 + \gamma^2|f|^2)\,\mathrm{d}x - \int_{\partial\Omega}\Big(\gamma + \frac{H}{2}\Big)|f|^2\,\mathrm{d}\mathcal{H}^{n-1} \ge -c\int_{\Omega^c}|f|^2\,\mathrm{d}x$$

for all $f \in H^1(\Omega^c)$ and $\gamma > 0$.

Proof. We adapt some constructions from Theorem 2 in [36]. Denote $\Pi := \partial_\infty\Omega \times (0,\infty)$ and note that the map $\Phi\colon \Pi \ni (s,t) \mapsto s + t\nu(s)$ is a diffeomorphism between Π and $\Phi(\Pi) \subset \Omega^c$. For any $f \in C_c^\infty(\mathbb{R}^n)$, using the standard change of variables, one has

$$\begin{aligned} R_\gamma(f) &\ge \int_{\Phi(\Pi)} (|\nabla f|^2 + \gamma^2|f|^2)\,\mathrm{d}x - \int_{\partial_\infty\Omega}\Big(\gamma + \frac{H}{2}\Big)|f|^2\,\mathrm{d}\mathcal{H}^{n-1} \\ &= \int_{\partial_\infty\Omega}\int_0^\infty (|(\nabla f)(\Phi(s,t))|^2 + \gamma^2|f(\Phi(s,t))|^2)J(s,t)\,\mathrm{d}t\,\mathrm{d}\mathcal{H}^{n-1}(s) \\ &\quad - \gamma\int_{\partial_\infty\Omega}\Big(\gamma + \frac{H_1(s)}{2}\Big)|f(\Phi(s,0))|^2\,\mathrm{d}\mathcal{H}^{n-1}(s), \end{aligned}$$

with J given by (5.1). Furthermore,

$$|(\nabla f)(\Phi(s,t))|^2 \ge |\langle \nu(s), (\nabla f)(\Phi(s,t))\rangle|^2 = \Big|\frac{\partial}{\partial t} f(\Phi(s,t))\Big|^2, \tag{5.6}$$

hence

$$\begin{aligned} R_\gamma(f) \ge R'_\gamma(f) := \int_{\partial_\infty\Omega}\Big[\int_0^\infty (|\partial_t g(s,t)|^2 + \gamma^2|g(s,t)|^2)J(s,t)\,\mathrm{d}t \\ - \Big(\gamma + \frac{H_1}{2}\Big)|g(s,0)|^2\Big]\,\mathrm{d}\mathcal{H}^{n-1}(s), \quad \text{with } g := f\circ\Phi. \end{aligned} \tag{5.7}$$

We further consider the function $h := \sqrt{J}g$. Then

$$\begin{aligned} |\partial_t g|^2 = \Big|\partial_t \frac{h}{\sqrt{J}}\Big|^2 = \Big|\frac{\partial_t h}{\sqrt{J}} - \frac{h\partial_t J}{2J\sqrt{J}}\Big|^2 &= \frac{1}{J}\Big|\partial_t h - \frac{\partial_t J}{2J}h\Big|^2 \\ &= \frac{1}{J}\Big(|\partial_t h|^2 - \frac{\partial_t J}{2J}\partial_t|h|^2 + \Big(\frac{\partial_t J}{2J}\Big)^2|h|^2\Big), \end{aligned}$$

therefore

$$R'_\gamma(f) = \int_{\partial_\infty\Omega}\Big[\int_0^\infty\Big(|\partial_t h|^2 - \frac{\partial_t J}{2J}\partial_t|h|^2 + \Big(\frac{\partial_t J}{2J}\Big)^2|h|^2 + \gamma^2|h|^2\Big)\,\mathrm{d}t - \Big(\gamma + \frac{H_1(s)}{2}\Big)|h(s,0)|^2\Big]\,\mathrm{d}\mathcal{H}^{n-1}(s).$$

Note that

$$\frac{\partial_t J(s,t)}{2J(s,t)} = \frac{1}{2}\,\partial_t \log J(s,t) = \frac{1}{2}\partial_t\sum_{j=1}^{n-1}\log(1+t\kappa_j(s)) = \frac{1}{2}\sum_{j=1}^{n-1}\frac{\kappa_j(s)}{1+t\kappa_j(s)}, \tag{5.8}$$

with

$$\frac{\partial_t J(s,t)}{2J(s,t)}\Big|_{t=0} = \frac{1}{2}H_1(s),$$

and integration by parts yields

$$\begin{aligned}\int_0^\infty\Big(-\frac{\partial_t J(s,t)}{2J(s,t)}\partial_t|h(s,t)|^2\Big)\,\mathrm{d}t &= \Big[-\frac{\partial_t J(s,t)}{2J(s,t)}|h(s,t)|^2\Big]_{t=0}^{t=\infty} + \int_0^\infty \partial_t\Big(\frac{\partial_t J(s,t)}{2J(s,t)}\Big)|h(s,t)|^2\,\mathrm{d}t\\ &= \frac{H_1(s)}{2}\,|h(s,0)|^2 + \int_0^\infty \partial_t\Big(\frac{\partial_t J(s,t)}{2J(s,t)}\Big)|h(s,t)|^2\,\mathrm{d}t.\end{aligned}$$

The substitution into the preceding expression for $R'_\gamma(f)$ gives

$$\begin{aligned}R'_\gamma(f) &= \int_{\partial_\infty\Omega}\Big[\int_0^\infty(|\partial_t h(s,t)|^2 + \gamma^2|h(s,t)|^2)\,\mathrm{d}t - \gamma|h(s,0)|^2\Big]\,\mathrm{d}\mathcal{H}^{n-1}(s)\\ &\quad + \int_{\partial_\infty\Omega}\int_0^\infty\Big(\partial_t\Big(\frac{\partial_t J}{2J}\Big) + \Big(\frac{\partial_t J}{2J}\Big)^2\Big)|h|^2\,\mathrm{d}t\,\mathrm{d}\mathcal{H}^{n-1}.\end{aligned} \tag{5.9}$$

Using

$$\begin{aligned}|h(s,0)|^2 &= -\int_0^\infty \partial_t|h(s,t)|^2\,\mathrm{d}t = -\int_0^\infty 2\,\mathrm{Re}(\overline{\partial_t h(s,t)}\,h(s,t))\,\mathrm{d}t\\ &\le \int_0^\infty 2|\partial_t h(s,t)|\cdot|h(s,t)|\,\mathrm{d}t \le \int_0^\infty\Big(\frac{1}{\gamma}|\partial_t h(s,t)|^2 + \gamma|h(s,t)|^2\Big)\,\mathrm{d}t,\end{aligned}$$

we show that the first integral in (5.9) is always non-negative. To estimate the second integral in (5.9), we use (5.8):

$$\partial_t\Big(\frac{\partial_t J(s,t)}{2J(s,t)}\Big) = -\frac{1}{2}\sum_{j=1}^{n-1}\frac{\kappa_j(s)^2}{(1+t\kappa_j(s))^2} \ge -\frac{n-1}{2}\,H(s)^2,$$

$$\partial_t\Big(\frac{\partial_t J}{2J}\Big) + \Big(\frac{\partial_t J}{2J}\Big)^2 \ge \partial_t\Big(\frac{\partial_t J}{2J}\Big) \ge -c, \quad \text{where} \quad c := \frac{n-1}{2}\|H\|_\infty^2.$$

The substitution into (5.9) gives

$$\begin{aligned} R'_\gamma(f) &\geq -c \int_{\partial_\infty \Omega} \int_0^\infty |h|^2 \,\mathrm{d}t \,\mathrm{d}\mathcal{H}^{n-1}(s) \\ &= -c \int_{\partial_\infty \Omega} \int_0^\infty |f(\Phi(s,t))|^2 J(s,t) \,\mathrm{d}t \,\mathrm{d}\mathcal{H}^{n-1}(s) \\ &= -c \int_{\Phi(\Pi)} |f|^2 \,\mathrm{d}x \geq -c \int_{\Omega^\mathrm{c}} |f|^2 \,\mathrm{d}x, \end{aligned}$$

and using (5.7), we arrive at

$$R_\gamma(f) \geq -c \int_{\Omega^\mathrm{c}} |f|^2 \,\mathrm{d}x \quad \text{for all } f \in C_c^\infty(\mathbb{R}^n),$$

which extends by density to all $f \in H^1(\Omega^\mathrm{c})$. ■

With the lower bound of Lemma 5.1 at hand, the remaining analysis is very close to the constructions in Section 5.3 of [34]. We use the formula (4.1) for $\|B_M f\|^2_{L^2(\mathbb{R}^n,\mathbb{C}^N)}$ to obtain

$$\begin{aligned} &\|B_M f\|^2_{L^2(\mathbb{R}^n,\mathbb{C}^N)} \\ &\quad= \int_\Omega (|\nabla f|^2 + m^2|f|^2) \,\mathrm{d}x \\ &\qquad+ \int_{\partial\Omega} \Big(m - \frac{1}{\sqrt{M}} + \frac{H}{2}\Big)|f|^2 \,\mathrm{d}\mathcal{H}^{n-1} + 2(M-m) \int_{\partial\Omega} |\mathcal{P}_- f|^2 \,\mathrm{d}\mathcal{H}^{n-1} \\ &\qquad+ \Big[\int_{\Omega^\mathrm{c}} (|\nabla f|^2 + M^2|f|^2) \,\mathrm{d}x - \int_{\partial\Omega} \Big(M - \frac{1}{\sqrt{M}} + \frac{H}{2}\Big)|f|^2 \,\mathrm{d}\mathcal{H}^{n-1}\Big] \\ &\quad\geq \int_\Omega (|\nabla f|^2 + m^2|f|^2) \,\mathrm{d}x + \int_{\partial\Omega} \Big(m - \frac{1}{\sqrt{M}} + \frac{H}{2}\Big)|f|^2 \,\mathrm{d}\mathcal{H}^{n-1} \\ &\qquad+ 2(M-m) \int_{\partial\Omega} |\mathcal{P}_- f|^2 \mathrm{d}\mathcal{H}^{n-1} + C_M \int_{\Omega^\mathrm{c}} |f|^2 \mathrm{d}x, \end{aligned}$$

with

$$C_M := 2\sqrt{M} - \frac{1}{M} - c,$$

where the term is the square brackets was estimated from below by Lemma 5.1. Using the Neumann decoupling of Ω and Ω^c along $\partial\Omega$ and the min-max principle, we conclude that for any fixed $j \in \mathbb{N}$ and all $M > 0$, one has

$$E_j(B_M^2) \geq E_j(K_M \oplus C_M I^\mathrm{c}), \tag{5.10}$$

where K_M is the self-adjoint operator with compact resolvent in $L^2(\Omega, \mathbb{C}^N)$ whose sesquilinear form k_M is defined on $\operatorname{dom} k_M := H^1(\Omega, \mathbb{C}^N)$ by

$$\begin{aligned} k_M(f,f) &= \int_\Omega (|\nabla f|^2 + m^2|f|^2) \,\mathrm{d}x \\ &\quad+ \int_{\partial\Omega} \Big(m - \frac{1}{\sqrt{M}} + \frac{H}{2}\Big)|f|^2 \,\mathrm{d}\mathcal{H}^{n-1} + 2(M-m) \int_{\partial\Omega} |\mathcal{P}_- f|^2 \,\mathrm{d}\mathcal{H}^{n-1}, \end{aligned}$$

and I^c is the identity operator in $L^2(\Omega^\mathrm{c}, \mathbb{C}^N)$.

Due to the upper bound (5.4), the eigenvalue $E_j(B_M^2)$ remains bounded for $M \to +\infty$, while $C_M \to +\infty$ as $M \to +\infty$, and (5.10) yields

$$\liminf_{M\to+\infty} E_j(B_M^2) \geq \liminf_{M\to+\infty} E_j(K_M). \tag{5.11}$$

For each $f \in H^1(\Omega, \mathbb{C}^N)$, the function $M \to k_M(f, f)$ is monotonically increasing, with

$$\Big\{f \in \bigcap_{M>0} \operatorname{dom} k_M : \sup_{M>0} k_M(f, f) < \infty\Big\}$$
$$= \{f \in H^1(\Omega, \mathbb{C}^N) : \mathcal{P}_- f = 0 \text{ on } \partial\Omega\} = \operatorname{dom} A,$$

and for any $f \in \operatorname{dom} A$, one has $\lim_{M\to+\infty} k_M(f, f) = \|Af\|^2_{L^2(\Omega,\mathbb{C}^N)}$. Hence, the monotone convergence principle implies $\lim_{M\to+\infty} E_j(K_M) = E_j(A^2)$, see [40, 44] for the general theory or Proposition 7 in [34] for the most adapted formulation. The substitution into (5.11) gives the required lower bound $\liminf_{M\to+\infty} E_j(B_M^2) \geq E_j(A^2)$.

Remark 5.2. While the boundedness of H is explicitly used in Lemma 5.1, we believe that this assumption is technical and can probably be avoided by applying more advanced proof methods. It is implicitly supported by the fact that the boundary integral containing H in the expression for $\|A_m^\Omega f\|^2$ in Theorem 1.3 turns out to be always finite, while H can be unbounded. The proof of Lemma 5.1 does not exploit the tangential derivatives, as they are dropped in the step (5.6). One may expect that these tangential derivatives can actually compensate the unbounded curvature terms (using the idea that a Schrödinger operator with an unbounded negative potential may still remains lower semibounded). Nevertheless, such an improvement would require a very advanced analysis (like a control of unbounded curvatures near the singular boundary), which goes significantly beyond the scope of the present work.

A. Dirac matrices

The most frequently used choices for the Dirac matrices α_k and β entering (1.1) are based on the Pauli matrices

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

For $n = 2$, one has $N = 2$, and the standard choice is $\alpha_k := \sigma_k$ for $k \in \{1, 2\}$ and $\beta := \sigma_3$. For $n = 3$, one has $N = 4$, and one often uses

$$\alpha_k := \begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{pmatrix}, \quad k \in \{1, 2, 3\}, \qquad \beta := \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix},$$

where I_2 is the 2×2 identity matrix. For higher dimensions, one can use various iterative procedures: see, e.g., Chapter 15 of [23] or Appendix E of [22] for a general theory, or Section 2.1 of [33] for a more specific description. We remark that the choice of α_k and β is unique up to similarity transforms and sign changes, as described in the aforementioned references, and all associated Dirac operators are unitarily equivalent to each other.

Funding. The work was partially supported by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation), project 491606144.

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Received September 25, 2025; revised March 23, 2026.

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