DIRAC OPERATORS, SHELL INTERACTIONS AND DISCONTINUOUS GAUGE FUNCTIONS ACROSS THE BOUNDARY

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Abstract. Given a bounded smooth domain $\Omega \subset \mathbb{R}^3$, we explore the relation between couplings of the free Dirac operator $-i\alpha\cdot\nabla + m\beta$ with pure electrostatic shell potentials $\lambda\delta_{\partial\Omega}$ ($\lambda \in \mathbb{R}$) and some perturbations of those potentials given by the normal vector field N on the shell $\partial\Omega$, namely $\{\lambda_e + \lambda_n(\alpha\cdot N)\}\delta_{\partial\Omega}$ (λ_e, $\lambda_n \in \mathbb{R}$). Under the appropiate change of parameters, the couplings with perturbed and unperturbed electrostatic shell potentials yield unitary equivalent self-adjoint operators. The proof relies on the construction of an explicit family of unitary operators that is well adapted to the study of shell interactions, and fits within the framework of gauge theory. A generalization of such unitary operators also allow us to deal with the self-adjointness of couplings of $-i\alpha\cdot\nabla + m\beta$ with some shell potentials of magnetic type, namely $\lambda(\alpha\cdot N)\delta_{\partial\Omega}$ with $\lambda \in \mathcal{C}^1(\partial\Omega)$.

1. Introduction

The main purpose of this paper is to explore the relation between couplings of the free Dirac operator with pure electrostatic shell potentials and some concrete perturbations of those potentials given by the normal vector field on the shell where the formers are defined. The main result in this article states that, under the appropiate change of parameters, the couplings with perturbed and unperturbed electrostatic shell potentials yield unitary equivalent self-ajoint operators. This is proven by constructing an explicit family of simple unitary operators that relates both couplings. A generalization of such unitary operators also allow us to deal with the self-adjointness of couplings of the free Dirac operator with some regular shell potentials of magnetic type.

The free Dirac operator in $\mathbb{R}^3$ is defined by $H = -i\alpha\cdot\nabla + m\beta$, where $\alpha = (\alpha_1, \alpha_2, \alpha_3)$,

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

compose the family of *Pauli matrices*. Note that H acts on functions $\varphi : \mathbb{R}^3 \to \mathbb{C}^4$. Throughout this article we assume $m > 0$.

The shell where the potentials are defined corresponds to the boundary of a bounded smooth domain $\Omega \subset \mathbb{R}^3$. Let σ and N be the surface measure and outward unit normal vector field on $\partial\Omega$, respectively. For convenience of notation, we set $\Omega_+ = \Omega$ and $\Omega_- = \mathbb{R}^3 \setminus \overline{\Omega}$, so $\partial\Omega = \partial\Omega_\pm$. Given $\lambda \in \mathbb{R}$ and $\varphi : \mathbb{R}^3 \to \mathbb{C}^4$, the electrostatic shell potential V_λ applied to φ is formally defined as

$$V_\lambda\varphi = \lambda\frac{\varphi_+ + \varphi_-}{2}\sigma,$$

2010 *Mathematics Subject Classification.* Primary 81Q10, Secondary 35Q40.

Key words and phrases. Dirac operator, shell potential, unitary equivalence.

Mas was supported by the *Juan de la Cierva* program JCI2012-14073 and the spanish funding projects MTM2011-27739 and MTM2014-52402.

where $\varphi_\pm$ denote the boundary values of φ (whenever they exist in a reasonable sense) when one approaches to $\partial\Omega$ from $\Omega_\pm$. Therefore, V_λ maps functions defined in $\mathbb{R}^3$ to vector measures of the form $f\sigma$ with $f : \partial\Omega \to \mathbb{C}^4$. In particular, one can interpret $V_\lambda\varphi$ as the distribution $\lambda\varphi\delta_{\partial\Omega}$ when acting on functions φ which have a well-defined trace on $\partial\Omega$, where $\delta_{\partial\Omega}$ denotes the Dirac-delta distribution on $\partial\Omega$. The self-adjoint character of $H + V_\lambda$ was already treated in [2], although previous results in the case that $\partial\Omega$ is a sphere or, much more in general, viewing $H + V_\lambda$ as a particular instance of singular perturbations of self-adjoint operators were obtained in [6] and [8], respectively.

The perturbed electrostatic shell potentials mentioned before are given, for $\lambda_e, \lambda_n \in \mathbb{R}$, by shell potentials of the type

$$V_{\lambda_e,\lambda_n}\varphi = \{\lambda_e + \lambda_n(\alpha \cdot N)\}\frac{\varphi_+ + \varphi_-}{2}\sigma.$$

From the previous definitions, $V_\lambda = V_{\lambda,0}$. The self-adjoint character of $H + V_{\lambda_e,\lambda_n}$ can be also dealt with the results in [8] but, for the reader's convenience, in this article we include the construction of this self-adjoint operator.

The main purpose of this note is to show that, in general, the spectral study of $H + V_{\lambda_e,\lambda_n}$ can be reduced to the one of $H + V_\lambda$ for some properly chosen $\lambda \in \mathbb{R}$ related to λ_e and λ_n. This reduction relies on the fact that there exists a unitary equivalence between these two operators. Moreover, we show the explicit connection between λ_e, λ_n and λ which, indeed, is independent of the underlying domain Ω. As a consequence of this unitary equivalence, all the results about existence of pure point spectrum in $(-m, m)$ for $H + V_\lambda$ obtained in [3] as well as the isoperimetric-type inequality for electrostatic shell potentials shown in [4] can be transferred to the perturbed case $H + V_{\lambda_e,\lambda_n}$, once they are properly restated in terms of λ_e and λ_n. As a byproduct, the isospectral transformation

$$H + V_\lambda \longleftrightarrow H + V_{-4/\lambda} \tag{2}$$

obtained in [3] shows up as a particular example of the construction developed here.

Most of the results in this article fit within the framework of *gauge transformations*, but where the gauge functions are discontinuous across $\partial\Omega$. More precisely, since the function $\eta = \lambda_n\chi_{\Omega_-}$ is constant in $\Omega_\pm$ and satisfies $\eta_- = \lambda_n$ and $\eta_+ = 0$ on $\partial\Omega$, where $\eta_\pm$ denote the boundary values of η when we approach to $\partial\Omega$ from $\Omega_\pm$, then

$$\nabla\eta = \lambda_n N\sigma \quad \text{and} \quad \alpha \cdot \nabla\eta = \lambda_n(\alpha \cdot N)\sigma.$$

But $\nabla \times (\lambda_n N\sigma) = \nabla \times \nabla\eta = 0$ in the sense of distributions, and thus $\lambda_n(\alpha \cdot N)\sigma$ corresponds to a (discontinuous across the boundary) change of gauge in the Dirac operator. However, at the end of the article, we also deal with the self-adjoint character of shell interactions of the form

$$(H + \mathcal{V}_\lambda)\varphi = H\varphi + \lambda(\alpha \cdot N)\frac{\varphi_+ + \varphi_-}{2}\sigma \tag{3}$$

for $\lambda \in \mathcal{C}^1(\partial\Omega)$, which can be interpreted as a magnetic shell interaction in the normal direction in case that λ is non-constant (we wrote $\mathcal{V}_\lambda$ instead of $V_{0,\lambda}$ to make distinction between the non-constant and constant case, respectively).

Regarding the structure and the concrete contents of the article, in Section 2 we recall some preliminary facts, all of them extracted from [2], which deal with a general construction of self-adjoint shell interactions for Dirac operators (see Therorem 2.1) as well as the boundary behaviour on $\partial\Omega$ of the functions in the domain of definition of those operators (see Lemma 2.2). In Section 3 we introduce a family of unitary operators that, when applied to the shell interactions presented in Section 2, allow us to generate a collection of unitary equivalent operators whose description in the terms of Section 2 is also given (see Lemma 3.1). The construction of these unitary maps is based on the one developed in the proof of [5, Theorem 3.6].

Section 4 contains the main applications of the abstact results developed in the previous sections. First, in Theorem 4.1 we provide an explicit description of the domain of definition where $H+V_{\lambda_e,\lambda_n}$ is self-adjoint. Then, in Theorem 4.3 we present all the possible unitary equivalent self-adjoint operators $H+V_{\lambda_e',\lambda_n'}$ that we can obtain (with the method developed in Section 3) from a given self-adjoint one $H+V_{\lambda_e,\lambda_n}$ and which can be described in the same terms as the former. In the subsequent corollaries we explore the scope of Theorem 4.3. For the reader's convenience, those corollaries are stated below somewhat informally (in particular, we omit the description of the domains where the couplings are defined, which are detailed in Section 4). Theorems 1.1, 1.2 and 1.3 correspond to Corollaries 4.4, 4.5 and 4.6, respectively.

Theorem 1.1. *Let $\lambda_e,\lambda_n\in\mathbb{R}$ be such that $\lambda_e^2-\lambda_n^2\neq 0,4$. Then*

$$H+V_{\lambda_e,\lambda_n} \text{ and } H+V_{-4\lambda_e/(\lambda_e^2-\lambda_n^2),4\lambda_n/(\lambda_e^2-\lambda_n^2)}$$

are unitary equivalent self-adjoint operators.

If we choose $\lambda_n=0$ in Theorem 1.1, we get the isospectral relation (2).

Theorem 1.2. *Let $\lambda_e,\lambda_n\in\mathbb{R}$ be such that $\lambda_e\neq 0$ and $\lambda_e^2-\lambda_n^2=-4$. Then*

$$H+V_{\lambda_e,\lambda_n} \text{ and } H+V_{(\pm 2\lambda_n-4)/\lambda_e,0}$$

are unitary equivalent self-adjoint operators.

This theorem may be seen as a particular instance of the following one (if we do not pay attention to the assumptions on λ_e and λ_n, it would correspond to $\theta=\pm\pi/2$), but we stated it separately because its proof and conclusion are simpler.

Theorem 1.3. *Let $\lambda_e,\lambda_n\in\mathbb{R}\setminus\{0\}$ be such that $|\lambda_e^2-\lambda_n^2|\neq 0,4$,*

$$\lambda_e^2-\lambda_n^2+2\lambda_e\neq 4 \text{ and } \lambda_e^2-\lambda_n^2-2\lambda_e\neq 4. \tag{4}$$

Then there exists $\theta\in\mathbb{R}$ such that

$$H+V_{\lambda_e,\lambda_n} \text{ and } H+V_{\left(2\lambda_n\frac{1+\cos\theta}{\sin\theta}-4\right)/\lambda_e,0}$$

are unitary equivalent self-adjoint operators.

Concerning the assumptions in the theorems above, let us mention that $\lambda_e^2-\lambda_n^2\neq 0,4$ is the only requirement that we need to show that $H+V_{\lambda_e,\lambda_n}$ is self-adjoint and to construct a unitary equivalent operator which can be understood as a coupling of H with a pure electrostatic shell potential $V_{\lambda,0}$ for some $\lambda\in\mathbb{R}$ given by Theorems 1.2 and 1.3. The extra assumption (4) is only used to describe this new operator in the same vein as $H+V_{\lambda_e,\lambda_n}$ (and not by simply using the unitary transformations, that is, by defining it just as $U^{-1}(H+V_{\lambda_e,\lambda_n})U$ for some unitary map U). In Figure 1, the black curves correspond to the points $(\lambda_e,\lambda_n)\in\mathbb{R}^2$ such that $\lambda_e^2-\lambda_n^2=0$ or $\lambda_e^2-\lambda_n^2=4$ and the red curves represent the points such that (4) does not hold.

A final remark regarding the above-mentioned results is in order. Since we are mainly interested on couplings with non-trivial electrostatic shell potentials, some of the results in this paper assume that $\lambda_e\neq 0$. The case of unitary equivalence between the free Dirac operator and its shell interactions with potentials of the type V_{0,λ_n} must be treated separately. However, similar arguments to the ones in this article and in [2] work in that case (for instance, one should use [2, Theorem 2.11(i)] with $\Lambda\equiv 0$ instead of [2, Theorem 2.11(iii)] to

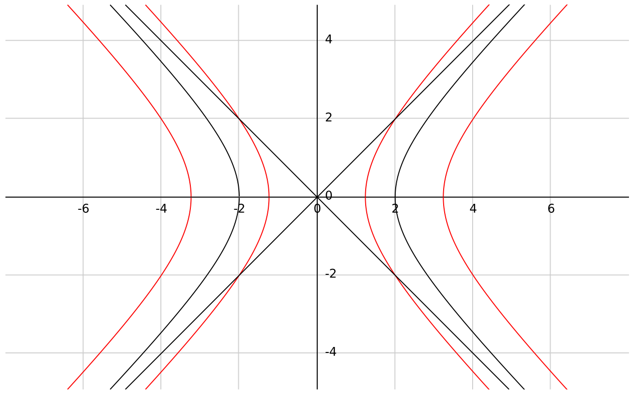

FIGURE 1. Picture of some of the assumptions on $(\lambda_e, \lambda_n) \in \mathbb{R}^2$.

define $H + V_0 \equiv H$ in Theorem 2.1 below). For shortness sake, we don't carry on the study of this particular case in this note.

Finally, in Section 5 we give an explicit construction of a self-adjoint operator that realizes the coupling given by (3), first in the case that $\lambda \in \mathcal{C}^1(\partial\Omega)$ does not vanish on $\partial\Omega$ (see Proposition 5.1), and then in the general case (see Theorem 5.3).

Acknowledgment

The author gratefully acknowledges Eric Séré for useful conversations while preparing this article during a short stay at Université Paris-Dauphine, as well as the facilities provided by the center.

2. Preliminaries

This article relies on [2, 3], so we assume that the reader is familiar with the notation, methods and results in there. However, in this section we recall some basics of those articles for the reader's convenience.

A fundamental solution of H is given by

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

i.e., $H\phi = \delta_0$ in the sense of distributions, where δ_0 denotes the Dirac measure centered at the origin. This fundamental solution is the first key ingredient for the developements below.

We denote by μ the Lebesgue measure in $\mathbb{R}^3$ and by σ the surface measure on $\partial\Omega$. We define the auxiliar space of locally finite $\mathbb{C}^4$-valued Borel measures

$$\mathcal{X} = \left\{G\mu + g\sigma : G \in L^2(\mu)^4,\, g \in L^2(\sigma)^4\right\},$$

where, as usual, $L^2(\nu)^4 = \left\{f : \mathbb{R}^3 \to \mathbb{C}^4 \ \nu\text{-measurable} : \int |f|^2\, d\nu < \infty\right\}$ for a given positive Borel measure ν in $\mathbb{R}^3$. In what follows we use a nonstandard notation, Φ, to define the convolution of measures in $\mathcal{X}$ with the fundamental solution of H, ϕ. Capital letters, as F or G, in the argument of Φ denote elements of $L^2(\mu)^4$, and the lowercase letters, as f or g, denote elements in $L^2(\sigma)^4$. Despite that this notation is nonstandard, it is very convenient in order to shorten the forthcoming computations.

Given $G\mu + g\sigma \in \mathcal{X}$, we define

$$\Phi(G + g) = \phi * G\mu + \phi * g\sigma \in L^2(\mu)^4,$$

where, for a given locally finite $\mathbb{C}^4$-valued Borel measure ν in $\mathbb{R}^3$ and $x \in \mathbb{R}^3$, we have set $\phi * \nu(x) = \int \phi(x-y)\,d\nu(y)$ whenever the integral makes sense. One can check that $H(\Phi(G+g)) = G\mu + g\sigma$ in the sense of distributions. This allows us to define a "generic" potential V acting on functions $\varphi = \Phi(G+g)$ for $G\mu + g\sigma \in \mathcal{X}$ by $V(\varphi) = -g\sigma$, so that $(H+V)(\varphi) = G\mu$ in the sense of distributions. Recall that $G \in L^2(\mu)^4$ and $g \in L^2(\sigma)^4$ so, under this setting, we make the following abuse of notation:

$$\begin{aligned} &\text{For } \varphi = \Phi(G+g) \text{ with } G+g \in \mathcal{X}, \text{ set } V(\varphi) = -g \in L^2(\sigma)^4.\\ &\text{Then } H\varphi = G+g \in \mathcal{X} \text{ and } (H+V)\varphi = G \in L^2(\mu)^4. \end{aligned} \tag{5}$$

That is, we omit the underlying measures μ and σ associated to G and g, respectively, in the distributional relations stated in (5). In particular, we have $\Phi(\mathcal{X}) \subset L^2(\mu)^4$ and $H+V : \Phi(\mathcal{X}) \to L^2(\mu)^4$. This abuse of notation will be systematically used throughout the article.

We also make use of the trace operator as follows. For $G \in \mathcal{C}_c^\infty(\mathbb{R}^3)^4$, one defines the trace on $\partial\Omega$ by $\mathrm{t}_{\partial\Omega}(G) = G\chi_{\partial\Omega}$. Then, $\mathrm{t}_{\partial\Omega}$ extends to a bounded linear operator $\mathrm{t}_\sigma : W^{1,2}(\mu)^4 \to L^2(\sigma)^4$, where $W^{1,2}(\mu)^4$ denotes the Sobolev space of $\mathbb{C}^4$-valued functions such that all its components have all its derivatives up to first order in $L^2(\mu)$. Since $\Phi(G) \in W^{1,2}(\mu)^4$ for all $G \in L^2(\mu)^4$, we can define

$$\Phi_\sigma G = \mathrm{t}_\sigma(\Phi(G)) \in L^2(\sigma)^4.$$

That Φ, V and Φ_σ are well defined and satisfy the above-mentioned properties is justified in [2, Section 2.3].

From the comments above and following [2], we are ready to construct domains where $H+V$ is self-adjoint. This is done with the help of auxiliar operators. More precisely, given a linear operator Λ bounded in $L^2(\sigma)^4$, set

$$\begin{aligned} &D(T_\Lambda) = \{\Phi(G+g) : G+g \in \mathcal{X},\ \Phi_\sigma G = \Lambda g\} \subset L^2(\mu)^4,\\ &T_\Lambda = H+V : D(T_\Lambda) \to L^2(\mu)^4, \text{ where } V \text{ is as in (5).} \end{aligned} \tag{6}$$

The following theorem, which is a direct application of [2, Theorem 2.11(iii)], shows that T_Λ given by (6) is self-adjoint under some assumptions on Λ.

Theorem 2.1. *Let T_Λ be as in* (6). *If Λ is self-adjoint,* Range(Λ) *is closed in $L^2(\sigma)^4$ and $\{\Phi(g) : g \in \mathrm{Ker}(\Lambda)\}$ is closed in $L^2(\mu)^4$, then T_Λ is self-adjoint. In particular, if Λ is self-adjoint and Fredholm, then T_Λ is self-adjoint.*

The next lemma describes the traces on $\partial\Omega$ of functions $\varphi \in \Phi(\mathcal{X})$, and it will be used in the sequel (see [2, Lemma 3.3] for a proof).

Lemma 2.2. *Given $\varphi = \Phi(G+g)$ with $G+g \in \mathcal{X}$ and $x \in \partial\Omega$, set*

$$\varphi_\pm(x) = \Phi_\sigma G(x) + \lim_{\Omega_\pm \ni y \xrightarrow{nt} x} \Phi(g)(y) \quad \text{and}$$
$$C_\sigma g(x) = \lim_{\epsilon \searrow 0} \int_{|x-z|>\epsilon} \phi(x-z) g(z)\,d\sigma(z),$$

where $\Omega_\pm \ni y \xrightarrow{nt} x$ means that $y \in \Omega_\pm$ tends to $x \in \partial\Omega$ non-tangentially. Then, $\varphi_\pm$ are well defined σ-a.e. on $\partial\Omega$, C_σ is bounded and self-adjoint in $L^2(\sigma)^4$ and, furthermore,

(i) $\varphi_\pm = \Phi_\sigma G + \left(\mp \frac{i}{2}(\alpha \cdot N) + C_\sigma\right) g \in L^2(\sigma)^4$,
(ii) $(C_\sigma(\alpha \cdot N))^2 = -\frac{1}{4}$.

Finally, recall that $(\alpha \cdot x)(\alpha \cdot x) = |x|^2$ for all $x \in \mathbb{R}^3$, thus $(\alpha \cdot N)^2 = 1$. Besides, the algebraic properties of the α_j's and β also yield $\beta(\alpha \cdot N) = (\alpha \cdot N)\beta = 0$. These are two basic facts that will also be used in what follows.

3. Unitary equivalence

Given T_Λ as in (6), we are going to construct a family of unitary equivalent operators parametrized by the complex numbers with unit modulus. Given $z\in\mathbb{C}$ with $|z|=1$, define the operator $U_z : L^2(\mu)^4\to L^2(\mu)^4$ by

$$U_z\varphi=(\chi_{\Omega_+}+\overline{z}\chi_{\Omega_-})\varphi,$$

where $\chi_{\Omega_\pm}$ denotes the characteristic function of $\Omega_\pm$. We see that $(U_z)^*=U_{\overline{z}}$ and $U_zU_{\overline{z}}=U_{\overline{z}}U_z=1$, so U is unitary. Given T_Λ as in (6), set

$$(T_\Lambda)_z=U_{\overline{z}}T_\Lambda U_z \quad \text{defined on} \quad D((T_\Lambda)_z)=U_{\overline{z}}D(T_\Lambda). \tag{7}$$

Then T_Λ and $(T_\Lambda)_z$ are unitary equivalent operators. For the applications below, we want to find a description of $(T_\Lambda)_z$ and $D((T_\Lambda)_z)$ similar to the one of T_Λ and $D(T_\Lambda)$ in (6). This is precisely the purpose of the following lemma.

Lemma 3.1. *Let T_Λ be as in (6) and, for $z\in\mathbb{C}$ with $|z|=1$, let $(T_\Lambda)_z$ be the unitary equivalent operator given by (7). If there exists a linear operator Λ_z bounded in $L^2(\sigma)^4$ such that the pair (Λ,Λ_z) satisfies*

$$\Lambda_z\Big(\frac{1+z}{2}+(1-z)i(\alpha\cdot N)(\Lambda+C_\sigma)\Big)=\Big(\frac{1+z}{2}-(1-z)iC_\sigma(\alpha\cdot N)\Big)\Lambda \tag{8}$$

for C_σ as in Lemma 2.2*, then $(T_\Lambda)_z\subset T_{\Lambda_z}$, where T_{Λ_z} is defined by (6).*

Proof. Let $\varphi=\Phi(G+g)\in D(T_\Lambda)$. Reasoning as in the proof of [3, Lemma 5.1] and, more precisely, applying Φ to [3, equation (5.4)], we see that

$$\chi_{\Omega_\pm}\varphi=\Phi\Big(\chi_{\Omega_\pm}G+\Big(\frac{1}{2}\pm i(\alpha\cdot N)(\Lambda+C_\sigma)\Big)g\Big),$$

which, from the definition of $U_{\overline{z}}$, easily implies that

$$U_{\overline{z}}\varphi=\Phi\Big(U_{\overline{z}}G+\Big(\frac{1+z}{2}+(1-z)i(\alpha\cdot N)(\Lambda+C_\sigma)\Big)g\Big), \tag{9}$$

and then, using (5), $(H+V)U_{\overline{z}}\varphi=U_{\overline{z}}G$. Moreover, by (7) we see that $U_{\overline{z}}\varphi\in D((T_\Lambda)_z)$ and, in view of (6), (5) and (9), we get

$$(T_\Lambda)_zU_{\overline{z}}\varphi=U_{\overline{z}}T_\Lambda U_zU_{\overline{z}}\varphi=U_{\overline{z}}T_\Lambda\varphi=U_{\overline{z}}(H+V)\varphi=U_{\overline{z}}G=(H+V)U_{\overline{z}}\varphi. \tag{10}$$

Combining [3, equation (5.3)] with the fact that $\Phi_\sigma G=\Lambda g$ by (6), we deduce that

$$\Phi_\sigma(\chi_{\Omega_\pm}G)=\Big(\frac{1}{2}\mp iC_\sigma(\alpha\cdot N)\Big)\Lambda g,$$

and hence

$$\Phi_\sigma(U_{\overline{z}}G)=\Phi_\sigma(\chi_{\Omega_+}G)+z\Phi_\sigma(\chi_{\Omega_-}G)=\Big(\frac{1+z}{2}-(1-z)iC_\sigma(\alpha\cdot N)\Big)\Lambda g. \tag{11}$$

Finally, assume that (8) holds for some Λ_z bounded in $L^2(\sigma)^4$. Then, by setting

$$F=U_{\overline{z}}G\in L^2(\mu)^4 \quad\text{and}\quad f=\Big(\frac{1+z}{2}+(1-z)i(\alpha\cdot N)(\Lambda+C_\sigma)\Big)g\in L^2(\sigma)^4,$$

a combination of (9), (11) and (8) shows that

$$D((T_\Lambda)_z)\subset\big\{\Phi(F+f):F+f\in\mathcal{X},\,\Phi_\sigma F=\Lambda_z f\big\},$$

and (10) gives $(T_\Lambda)_z=H+V$ on $D((T_\Lambda)_z)$. Using (6), these last conclusions mean that $(T_\Lambda)_z\subset T_{\Lambda_z}$, and the lemma is proved. □

4. Electrostatic shell potentials and gauge transformations

In this section we study the unitary equivalence developed in Section 3 applied to couplings of H with the perturbed and unperturbed electrostatic shell potentials associated to $\partial\Omega$ which were presented in the introduction. As a first step, we deal with the self-adjoint character of such concrete couplings via the following theorem.

Theorem 4.1. *Given $\lambda_e, \lambda_n \in \mathbb{R}$ such that $\lambda_e^2 - \lambda_n^2 \neq 0, 4$ and C_σ as in* Lemma 2.2*, set*

$$\Lambda_{\lambda_e,\lambda_n} = \frac{\lambda_n(\alpha \cdot N) - \lambda_e}{\lambda_e^2 - \lambda_n^2} - C_\sigma. \tag{12}$$

Then $T_{\Lambda_{\lambda_e,\lambda_n}}$ given by (6) *is self-adjoint and $T_{\Lambda_{\lambda_e,\lambda_n}} = H + V_{\lambda_e,\lambda_n}$ on $D(T_{\Lambda_{\lambda_e,\lambda_n}})$, where V_{λ_e,λ_n} is defined, for $\varphi \in \Phi(\mathcal{X})$ and $\varphi_\pm$ as in* Lemma 2.2*, by*

$$V_{\lambda_e,\lambda_n}\varphi = \{\lambda_e + \lambda_n(\alpha \cdot N)\}\frac{\varphi_+ + \varphi_-}{2}. \tag{13}$$

Note that we are omitting the underlying measure σ in the definition of V_{λ_e,λ_n} in (13), as we already did in (5) for the generic potential V. We will keep this abuse of notation in the definition of all shell potentials appearing throughout the article.

Proof. We first prove that $V = V_{\lambda_e,\lambda_n}$ on $D(T_{\Lambda_{\lambda_e,\lambda_n}})$, which would imply that $T_{\Lambda_{\lambda_e,\lambda_n}} = H + V_{\lambda_e,\lambda_n}$ on $D(T_{\Lambda_{\lambda_e,\lambda_n}})$. Let $\varphi = \Phi(G+g) \in D(T_{\Lambda_{\lambda_e,\lambda_n}})$. Then $\varphi_\pm = \Phi_\sigma G + (\mp\frac{i}{2}(\alpha\cdot N) + C_\sigma)g$ by Lemma 2.2(i), which yields

$$\frac{\varphi_+ + \varphi_-}{2} = \Phi_\sigma G + C_\sigma g.$$

Recall that $\Phi_\sigma G = \Lambda_{\lambda_e,\lambda_n} g$ by (6), hence

$$\begin{aligned} V_{\lambda_e,\lambda_n}\varphi &= \{\lambda_e + \lambda_n(\alpha \cdot N)\}(\Phi_\sigma G + C_\sigma g) \\ &= \{\lambda_e + \lambda_n(\alpha \cdot N)\}\frac{\lambda_n(\alpha \cdot N) - \lambda_e}{\lambda_e^2 - \lambda_n^2}\, g = -g = V\varphi, \end{aligned}$$

by (5), and we are done.

The first statement in the theorem follows by Theorem 2.1, as far as we check that $\Lambda_{\lambda_e,\lambda_n}$ is self-adjoint and Fredholm. Since $\lambda_e, \lambda_n \in \mathbb{R}$, the self-adjointness of $\Lambda_{\lambda_e,\lambda_n}$ follows from the one of C_σ and $\alpha \cdot N$. It remains to show that $\Lambda_{\lambda_e,\lambda_n}$ is Fredholm if $\lambda_e^2 - \lambda_n^2 \neq 4$, which follows by arguments similar to the ones in the proof of [3, Theorem 5.5]. Set

$$\Lambda_\pm = \frac{\mp\lambda_n(\alpha \cdot N) + \lambda_e}{\lambda_e^2 - \lambda_n^2} \pm C_\sigma.$$

Note that $C_\sigma^2 = C_\sigma(\alpha\cdot N)(\alpha\cdot N)C_\sigma = C_\sigma(\alpha\cdot N)\{C_\sigma, \alpha\cdot N\} + 1/4$ by Lemma 2.2(ii), where $\{C_\sigma, \alpha\cdot N\}$ denotes the anticommutator $C_\sigma(\alpha\cdot N) + (\alpha\cdot N)C_\sigma$, so we get

$$\Lambda_+\Lambda_- = \frac{1}{\lambda_e^2 - \lambda_n^2} - \frac{1}{4} + \left(\frac{\lambda_n}{\lambda_e^2 - \lambda_n^2} - C_\sigma(\alpha\cdot N)\right)\{C_\sigma, \alpha\cdot N\}.$$

Since $\partial\Omega$ is smooth, $\{C_\sigma, \alpha\cdot N\}$ is a compact operator in $L^2(\sigma)^4$ by [2, Lemma 3.5]. Hence, $\Lambda_-\Lambda_+ = \Lambda_+\Lambda_-$ is Fredholm for $\lambda_e^2 - \lambda_n^2 \neq 4$, and thus $\Lambda_\pm$ are also Fredholm operators by [1, Theorem 1.46(iii)]. Since $\Lambda_{\lambda_e,\lambda_n} = -\Lambda_+$, we get that $\Lambda_{\lambda_e,\lambda_n}$ is Fredholm, and the proof of the theorem is complete thanks to Theorem 2.1. □

Lemma 4.2. *Let $\lambda_e, \lambda_n \in \mathbb{R}$ be such that $\lambda_e^2 - \lambda_n^2 \neq 0$. If $\theta \in \mathbb{R}$ is such that*

$$\frac{1}{2}(\lambda_e^2 - \lambda_n^2 + 4)(1 + \cos\theta) - 4 + 2\lambda_n \sin\theta \neq 0, \tag{14}$$

then the pair $(\Lambda_{\lambda_e,\lambda_n},(\Lambda_{\lambda_e,\lambda_n})_z)$ *satisfies* (8)*, where* $z=e^{i\theta}$*,* $\Lambda_{\lambda_e,\lambda_n}$ *is defined by* (12) *and*

$$(\Lambda_{\lambda_e,\lambda_n})_z=\frac{\big(\lambda_n\cos\theta-\frac{1}{4}(\lambda_e^2-\lambda_n^2+4)\sin\theta\big)(\alpha\cdot N)-\lambda_e}{\frac{1}{2}(\lambda_e^2-\lambda_n^2+4)(1+\cos\theta)-4+2\lambda_n\sin\theta}-C_\sigma. \tag{15}$$

Proof. For shortness sake, set

$$\lambda_1=\frac{-\lambda_e}{\lambda_e^2-\lambda_n^2}\quad\text{and}\quad\lambda_2=\frac{\lambda_n}{\lambda_e^2-\lambda_n^2},\quad\text{so}\quad\lambda_1^2-\lambda_2^2=\frac{1}{\lambda_e^2-\lambda_n^2}.$$

Then $\Lambda_{\lambda_e,\lambda_n}=\lambda_1+\lambda_2(\alpha\cdot N)-C_\sigma$. We are going to find the formula for $(\Lambda_{\lambda_e,\lambda_n})_z$ by working with the pair $(\Lambda_{\lambda_e,\lambda_n},(\Lambda_{\lambda_e,\lambda_n})_z)$ in (8). On one hand,

$$\begin{aligned}\frac{1+z}{2}+(1-z)i(\alpha\cdot N)(\Lambda_{\lambda_e,\lambda_n}+C_\sigma)&=\frac{1+z}{2}+(1-z)i(\alpha\cdot N)(\lambda_1+\lambda_2(\alpha\cdot N))\\&=\frac{1+z}{2}+\lambda_2(1-z)i+\lambda_1(1-z)i(\alpha\cdot N).\end{aligned}\tag{16}$$

On the other hand, using Lemma 2.2(*ii*),

$$\begin{aligned}&\Big(\frac{1+z}{2}-(1-z)iC_\sigma(\alpha\cdot N)\Big)\Lambda_{\lambda_e,\lambda_n}\\&\quad=\Big(\frac{1+z}{2}-(1-z)iC_\sigma(\alpha\cdot N)\Big)(\lambda_1+\lambda_2(\alpha\cdot N)-C_\sigma)\\&\quad=\lambda_1\frac{1+z}{2}+\Big(\lambda_2\frac{1+z}{2}-\frac{1-z}{4}i\Big)(\alpha\cdot N)\\&\qquad-\lambda_1(1-z)iC_\sigma(\alpha\cdot N)-\Big(\frac{1+z}{2}+\lambda_2(1-z)i\Big)C_\sigma.\end{aligned}\tag{17}$$

Note also that

$$\begin{aligned}&\Big(\frac{1+z}{2}+\lambda_2(1-z)i+\lambda_1(1-z)i(\alpha\cdot N)\Big)\Big(\frac{1+z}{2}+\lambda_2(1-z)i-\lambda_1(1-z)i(\alpha\cdot N)\Big)\\&\qquad=\frac{(1+z)^2}{4}+(\lambda_1^2-\lambda_2^2)(1-z)^2+\lambda_2(1-z^2)i.\end{aligned}\tag{18}$$

If we apply the operator $\frac{1+z}{2}+\lambda_2(1-z)i-\lambda_1(1-z)i(\alpha\cdot N)$ from the right in (8) to the pair $(\Lambda_{\lambda_e,\lambda_n},(\Lambda_{\lambda_e,\lambda_n})_z)$, using (16), (18) and (17), we deduce that

$$\begin{aligned}&\Big(\frac{(1+z)^2}{4}+(\lambda_1^2-\lambda_2^2)(1-z)^2+\lambda_2(1-z^2)i\Big)(\Lambda_{\lambda_e,\lambda_n})_z\\&\quad=\Big\{\lambda_1\frac{1+z}{2}+\Big(\lambda_2\frac{1+z}{2}-\frac{1-z}{4}i\Big)(\alpha\cdot N)-\lambda_1(1-z)iC_\sigma(\alpha\cdot N)\\&\qquad-\Big(\frac{1+z}{2}+\lambda_2(1-z)i\Big)C_\sigma\Big\}\Big\{\frac{1+z}{2}+\lambda_2(1-z)i-\lambda_1(1-z)i(\alpha\cdot N)\Big\}\\&\quad=\lambda_1z+\Big\{\Big(\lambda_2^2-\lambda_1^2-\frac{1}{4}\Big)\frac{1-z^2}{2}i+\lambda_2\frac{1+z^2}{2}\Big\}(\alpha\cdot N)\\&\qquad-\Big(\frac{(1+z)^2}{4}+(\lambda_1^2-\lambda_2^2)(1-z)^2+\lambda_2(1-z^2)i\Big)C_\sigma.\end{aligned}\tag{19}$$

Since $|z| = 1$, we can divide (19) by z to get

$$\begin{aligned}
&\left(\frac{(1+z)^2}{4z} + (\lambda_1^2 - \lambda_2^2)\frac{(1-z)^2}{z} + \lambda_2\frac{1-z^2}{z}i\right)(\Lambda_{\lambda_e,\lambda_n})_z \\
&\qquad = \lambda_1 + \left\{\left(\lambda_2^2 - \lambda_1^2 - \frac{1}{4}\right)\frac{1-z^2}{2z}i + \lambda_2\frac{1+z^2}{2z}\right\}(\alpha\cdot N) \\
&\qquad\quad - \left(\frac{(1+z)^2}{4z} + (\lambda_1^2 - \lambda_2^2)\frac{(1-z)^2}{z} + \lambda_2\frac{1-z^2}{z}i\right)C_\sigma.
\end{aligned} \tag{20}$$

For $z = e^{i\theta}$ with $\theta \in \mathbb{R}$, we easily see that

$$\frac{(1\pm z)^2}{z} = 2(\cos\theta \pm 1), \qquad \frac{1-z^2}{z}i = 2\sin\theta, \qquad \frac{1+z^2}{z} = 2\cos\theta.$$

Therefore, (20) is equivalent to

$$\begin{aligned}
&\left\{1 + 2(\cos\theta - 1)\left(\lambda_1^2 - \lambda_2^2 + \frac{1}{4}\right) + 2\lambda_2\sin\theta\right\}(\Lambda_{\lambda_e,\lambda_n})_z \\
&\qquad = \lambda_1 + \left\{\lambda_2\cos\theta - \left(\lambda_1^2 - \lambda_2^2 + \frac{1}{4}\right)\sin\theta\right\}(\alpha\cdot N) \\
&\qquad\quad - \left\{1 + 2(\cos\theta - 1)\left(\lambda_1^2 - \lambda_2^2 + \frac{1}{4}\right) + 2\lambda_2\sin\theta\right\}C_\sigma
\end{aligned}$$

which, in terms of λ_e and λ_n (using that $\lambda_e^2 - \lambda_n^2 \neq 0$), corresponds to

$$\begin{aligned}
&\left\{\frac{1}{2}(\lambda_e^2 - \lambda_n^2 + 4)(1+\cos\theta) - 4 + 2\lambda_n\sin\theta\right\}(\Lambda_{\lambda_e,\lambda_n})_z \\
&\qquad = -\lambda_e + \left\{\lambda_n\cos\theta - \frac{1}{4}(\lambda_e^2 - \lambda_n^2 + 4)\sin\theta\right\}(\alpha\cdot N) \\
&\qquad\quad - \left\{\frac{1}{2}(\lambda_e^2 - \lambda_n^2 + 4)(1+\cos\theta) - 4 + 2\lambda_n\sin\theta\right\}C_\sigma,
\end{aligned} \tag{21}$$

The lemma follows by (21) and (14) because all the computations above can be reverted if $\lambda_e^2 - \lambda_n^2 \neq 0$ and (14) holds. □

Note that, from (15), $(\Lambda_{\lambda_e,\lambda_n})_1 = \Lambda_{\lambda_e,\lambda_n}$ for all $\lambda_e^2 - \lambda_n^2 \neq 0$. Of course, this comes as no surprise because $(T_{\Lambda_{\lambda_e,\lambda_n}})_1 = T_{\Lambda_{\lambda_e,\lambda_n}}$ by (7), since $U_1 = 1$.

Theorem 4.3. *Given $\lambda_e, \lambda_n, \theta \in \mathbb{R}$ set*

$$\begin{aligned}
\gamma &= \frac{1}{2}(\lambda_e^2 - \lambda_n^2 + 4)(1+\cos\theta) - 4 + 2\lambda_n\sin\theta, \\
\lambda_n' &= \lambda_n\cos\theta - \frac{1}{4}(\lambda_e^2 - \lambda_n^2 + 4)\sin\theta.
\end{aligned} \tag{22}$$

Assume that $\lambda_e^2 - \lambda_n^2 \neq 0, 4$, that $\gamma \neq 0$ and that $\lambda_e^2 - \lambda_n'^2 \neq 0, \gamma^2/4$. Then

$$T_{\Lambda_{\lambda_e,\lambda_n}} \text{ and } T_{\Lambda_{\gamma\lambda_e/(\lambda_e^2-\lambda_n'^2),\gamma\lambda_n'/(\lambda_e^2-\lambda_n'^2)}}, \text{ both defined by (6) and (12),}$$

are unitary equivalent self-adjoint operators. Moreover,

$$\begin{aligned}
T_{\Lambda_{\lambda_e,\lambda_n}} &= H + V_{\lambda_e,\lambda_n} \text{ and} \\
T_{\Lambda_{\gamma\lambda_e/(\lambda_e^2-\lambda_n'^2),\gamma\lambda_n'/(\lambda_e^2-\lambda_n'^2)}} &= H + V_{\gamma\lambda_e/(\lambda_e^2-\lambda_n'^2),\gamma\lambda_n'/(\lambda_e^2-\lambda_n'^2)}
\end{aligned}$$

on $D\big(T_{\Lambda_{\lambda_e,\lambda_n}}\big)$ *and* $D\big(T_{\Lambda_{\gamma\lambda_e/(\lambda_e^2-\lambda_n'^2),\gamma\lambda_n'/(\lambda_e^2-\lambda_n'^2)}}\big)$*, respectively, where*

$$V_{\lambda_e,\lambda_n} \text{ and } V_{\gamma\lambda_e/(\lambda_e^2-\lambda_n'^2),\gamma\lambda_n'/(\lambda_e^2-\lambda_n'^2)} \text{ are defined by (13).}$$

Proof. The theorem follows by a combination of Theorem 4.1 and Lemmata 4.2 and 3.1. On one hand, since $\lambda_e^2-\lambda_n^2\neq 0,4$, from Theorem 4.1 we see that $T_{\Lambda_{\lambda_e,\lambda_n}}$ is self-adjoint and $T_{\Lambda_{\lambda_e,\lambda_n}} = H + V_{\lambda_e,\lambda_n}$ on $D(T_{\Lambda_{\lambda_e,\lambda_n}})$.

On the other hand, that $\gamma\neq 0$ means that (14) holds. Hence, Lemma 4.2 shows that the pair $(\Lambda_{\lambda_e,\lambda_n},(\Lambda_{\lambda_e,\lambda_n})_z)$ satisfies (8), where $z=e^{i\theta}$ and $(\Lambda_{\lambda_e,\lambda_n})_z$ is defined by (15). Since $\lambda_e^2-\lambda_n'^2\neq 0$, we can set

$$\lambda_1=\frac{\gamma\lambda_e}{\lambda_e^2-\lambda_n'^2}\quad\text{and}\quad \lambda_2=\frac{\gamma\lambda_n'}{\lambda_e^2-\lambda_n'^2},\quad\text{so}\quad \lambda_1^2-\lambda_2^2=\frac{\gamma^2}{\lambda_e^2-\lambda_n'^2}.$$

Then, from (15), (22) and (12), we easily get

$$\begin{aligned}(\Lambda_{\lambda_e,\lambda_n})_z &= \frac{\lambda_n'(\alpha\cdot N)-\lambda_e}{\gamma}-C_\sigma=\frac{\lambda_2(\alpha\cdot N)-\lambda_1}{\lambda_1^2-\lambda_2^2}-C_\sigma\\ &=\Lambda_{\lambda_1,\lambda_2}=\Lambda_{\gamma\lambda_e/(\lambda_e^2-\lambda_n'^2),\gamma\lambda_n'/(\lambda_e^2-\lambda_n'^2)}.\end{aligned}$$

Now, since the pair $(\Lambda_{\lambda_e,\lambda_n},(\Lambda_{\lambda_e,\lambda_n})_z)$ satisfies (8), Lemma 3.1 yields that

$$(T_{\Lambda_{\lambda_e,\lambda_n}})_z\subset T_{(\Lambda_{\lambda_e,\lambda_n})_z}=T_{\Lambda_{\gamma\lambda_e/(\lambda_e^2-\lambda_n'^2),\gamma\lambda_n'/(\lambda_e^2-\lambda_n'^2)}}.$$

Besides, Theorem 4.1 shows that $T_{\Lambda_{\gamma\lambda_e/(\lambda_e^2-\lambda_n'^2),\gamma\lambda_n'/(\lambda_e^2-\lambda_n'^2)}}$ is self-adjoint whenever

$$\Big(\frac{\gamma\lambda_e}{\lambda_e^2-\lambda_n'^2}\Big)^2-\Big(\frac{\gamma\lambda_n'}{\lambda_e^2-\lambda_n'^2}\Big)^2\neq 0,4,$$

and this last relation holds if $\gamma\neq 0$ and $\lambda_e^2-\lambda_n'^2\neq 0,\gamma^2/4$. In conclusion, from the assumptions in the statement of the theorem, we have proven that

$$(T_{\Lambda_{\lambda_e,\lambda_n}})_z\subset T_{\Lambda_{\gamma\lambda_e/(\lambda_e^2-\lambda_n'^2),\gamma\lambda_n'/(\lambda_e^2-\lambda_n'^2)}}$$

and that both operators are self-adjoint (the first one due to the fact that, by construction, it is unitary equivalent to $T_{\Lambda_{\lambda_e,\lambda_n}}$, which is self-adjoint). Therefore, both operators coincide, and thus $T_{\Lambda_{\lambda_e,\lambda_n}}$ and $T_{\Lambda_{\gamma\lambda_e/(\lambda_e^2-\lambda_n'^2),\gamma\lambda_n'/(\lambda_e^2-\lambda_n'^2)}}$ are unitary equivalent, as claimed. Finally, that

$$T_{\Lambda_{\gamma\lambda_e/(\lambda_e^2-\lambda_n'^2),\gamma\lambda_n'/(\lambda_e^2-\lambda_n'^2)}}=H+V_{\gamma\lambda_e/(\lambda_e^2-\lambda_n'^2),\gamma\lambda_n'/(\lambda_e^2-\lambda_n'^2)}$$

on $D\big(T_{\Lambda_{\gamma\lambda_e/(\lambda_e^2-\lambda_n'^2),\gamma\lambda_n'/(\lambda_e^2-\lambda_n'^2)}}\big)$ is also given by Theorem 4.1. □

The following corollaries are the applications of Theorem 4.3 mentioned in the introduction. Theorems 1.1, 1.2 and 1.3 correspond to informal statemets of Corollaries 4.4, 4.5 and 4.6, respectively.

Corollary 4.4. *Let* $\lambda_e,\lambda_n\in\mathbb{R}$ *be such that* $\lambda_e^2-\lambda_n^2\neq 0,4$*. Then*

$$T_{\Lambda_{\lambda_e,\lambda_n}} \text{ and } T_{\Lambda_{-4\lambda_e/(\lambda_e^2-\lambda_n^2),4\lambda_n/(\lambda_e^2-\lambda_n^2)}}, \text{ both defined by (6) and (12),}$$

are unitary equivalent self-adjoint operators. Moreover, $T_{\Lambda_{\lambda_e,\lambda_n}}=H+V_{\lambda_e,\lambda_n}$ *and*

$$T_{\Lambda_{-4\lambda_e/(\lambda_e^2-\lambda_n^2),4\lambda_n/(\lambda_e^2-\lambda_n^2)}}=H+V_{-4\lambda_e/(\lambda_e^2-\lambda_n^2),4\lambda_n/(\lambda_e^2-\lambda_n^2)}$$

on $D(T_{\Lambda_{\cdot,\cdot}})$*, where* $V_{\cdot,\cdot}$ *is given by* (13).

Proof. Apply Theorem 4.3 taking $\theta=\pi$. □

In particular, from Corollary 4.4 we get that $H+V_{\lambda,0}$ and $H+V_{-4/\lambda,0}$ (defined on $D(T_{\Lambda_{\lambda,0}})$ and $D(T_{\Lambda_{-4/\lambda,0}})$, respectively) are unitary equivalent self-adjoint operators for all $\lambda^2 \neq 0, 4$, which strengthens the first conclusion in [3, Theorem 3.3]. As a byproduct, we also get that $H + V_{0,\lambda}$ and $H + V_{0,-4/\lambda}$ are unitary equivalent self-adjoint operators for all $\lambda \neq 0$.

Corollary 4.5. *Let $\lambda_e, \lambda_n \in \mathbb{R}$ be such that $\lambda_e \neq 0$ and $\lambda_e^2 - \lambda_n^2 = -4$. Then*

$$T_{\Lambda_{\lambda_e,\lambda_n}} \text{ and } T_{\Lambda_{(\pm 2\lambda_n - 4)/\lambda_e,0}}, \text{ all of them defined by (6) and (12),}$$

are unitary equivalent self-adjoint operators. Moreover, $T_{\Lambda_{\lambda_e,\lambda_n}} = H + V_{\lambda_e,\lambda_n}$ and

$$T_{\Lambda_{(\pm 2\lambda_n - 4)/\lambda_e,0}} = H + V_{(\pm 2\lambda_n - 4)/\lambda_e,0}$$

on $D(T_{\Lambda_{\cdot,\cdot}})$, where $V_{\cdot,\cdot}$ is given by (13).

Proof. Apply Theorem 4.3 taking $\theta = \pm\pi/2$. □

Corollary 4.6. *Let $\lambda_e, \lambda_n \in \mathbb{R} \setminus \{0\}$ be such that $|\lambda_e^2 - \lambda_n^2| \neq 0, 4$. Assume that*

$$\lambda_e^2 - \lambda_n^2 + 2\lambda_e \neq 4 \quad \text{and} \quad \lambda_e^2 - \lambda_n^2 - 2\lambda_e \neq 4. \tag{23}$$

Then, there exists $\theta \in \mathbb{R}$ so that

$$\begin{aligned} &\tan\theta = \frac{4\lambda_n}{\lambda_e^2 - \lambda_n^2 + 4}, \quad \text{and} \\ &\cos\theta \neq \frac{16 - (\lambda_e^2 - \lambda_n^2)^2}{16 + (\lambda_e^2 - \lambda_n^2)^2 + 8(\lambda_e^2 + \lambda_n^2)}, \frac{16 - (\lambda_e^2 - \lambda_n^2)^2 \pm 4\lambda_e(\lambda_e^2 - \lambda_n^2 + 4)}{16 + (\lambda_e^2 - \lambda_n^2)^2 + 8(\lambda_e^2 + \lambda_n^2)}. \end{aligned} \tag{24}$$

For any $\theta \in \mathbb{R}$ as in (24),

$$T_{\Lambda_{\lambda_e,\lambda_n}} \text{ and } T_{\Lambda_{\left(2\lambda_n \frac{1+\cos\theta}{\sin\theta} - 4\right)/\lambda_e,0}}, \text{ both defined by (6) and (12),}$$

are unitary equivalent self-adjoint operators. Moreover, $T_{\Lambda_{\lambda_e,\lambda_n}} = H + V_{\lambda_e,\lambda_n}$ and

$$T_{\Lambda_{\left(2\lambda_n \frac{1+\cos\theta}{\sin\theta} - 4\right)/\lambda_e,0}} = H + V_{\left(2\lambda_n \frac{1+\cos\theta}{\sin\theta} - 4\right)/\lambda_e,0}$$

on $D(T_{\Lambda_{\cdot,\cdot}})$, where $V_{\cdot,\cdot}$ is given by (13).

Proof. This is also a consequence of Theorem 4.3. More precisely, a (tedious) computation shows that if $\lambda_e, \lambda_n \in \mathbb{R} \setminus \{0\}$ satisfy $|\lambda_e^2 - \lambda_n^2| \neq 0, 4$ and if there exists $\theta \in \mathbb{R}$ such that (24) holds, then the assuptions in the statement of Theorem 4.3 are fulfilled, and $\lambda_n' = 0$ in (22). We leave the details of this part for the reader.

We impose (23) to show the existence of a $\theta \in \mathbb{R}$ which satisfies (24). To see this, set

$$p = 16 - (\lambda_e^2 - \lambda_n^2)^2 \quad \text{and} \quad q = 4\lambda_e(\lambda_e^2 - \lambda_n^2 + 4).$$

Note that $p, q \neq 0$ by assumption, thus $|p+q| \neq |p-q|$. If $|p \pm q| = |p|$ then we must have

$$\begin{aligned} 0 = \pm q + 2p &= \pm 4\lambda_e(\lambda_e^2 - \lambda_n^2 + 4) + 32 - 2(\lambda_e^2 - \lambda_n^2)^2 \\ &= \pm 4\lambda_e(\lambda_e^2 - \lambda_n^2 + 4) - 2(\lambda_e^2 - \lambda_n^2 + 4)(\lambda_e^2 - \lambda_n^2 - 4), \end{aligned}$$

which is equivalent to $0 = \pm 2\lambda_e - (\lambda_e^2 - \lambda_n^2 - 4)$ because $\lambda_e^2 - \lambda_n^2 \neq -4$ by assumption. Hence, $|p \pm q| \neq |p|$ if (23) holds. That is, under the assumptions of the corollary, we have seen that

$$p - q,\ p \text{ and } p + q \text{ have different absolute value each other.} \tag{25}$$

Now, let $\theta \in \mathbb{R}$ be such that $\tan\theta = 4\lambda_n/(\lambda_e^2 - \lambda_n^2 + 4)$. If θ fulfills (24) then we are done. If not, it means that $\cos\theta$ coincides with one of the three terms on the right hand side of the second condition in (24). But then, by (25), it is enough to pick $\theta + \pi$ instead of θ, since $\tan(\theta + \pi) = \tan\theta$ but $\cos(\theta + \pi) = -\cos\theta$, and so $\theta + \pi$ fulfills (24). □

5. Magnetic shell potentials

This section concerns the construction of shell interactions for the free Dirac operator with regular potentials on $\partial\Omega$ of magnetic type.

Proposition 5.1. *Let $\lambda:\partial\Omega\to\mathbb{R}$ be of class $\mathcal{C}^1(\partial\Omega)$ and such that $\lambda(x)\neq 0$ for all $x\in\partial\Omega$. Set*

$$\Lambda_\lambda=-\frac{1}{\lambda}(\alpha\cdot N)-C_\sigma, \tag{26}$$

where C_σ is as in Lemma 2.2*. Then T_{Λ_λ} given by* (6) *is self-adjoint and $T_{\Lambda_\lambda}=H+\mathcal{V}_\lambda$ on $D(T_{\Lambda_\lambda})$, where $\mathcal{V}_\lambda$ is defined, for $\varphi\in\Phi(\mathcal{X})$ and $\varphi_\pm$ as in* Lemma 2.2*, by*

$$\mathcal{V}_\lambda\varphi=\lambda(\alpha\cdot N)\frac{\varphi_++\varphi_-}{2}. \tag{27}$$

Proof. The proof follows exactly the same lines as the one of Theorem 4.1. To see that $V=\mathcal{V}_\lambda$ on $D(T_{\Lambda_\lambda})$, let $\varphi=\Phi(G+g)\in D(T_{\Lambda_\lambda})$. Then $\varphi_\pm=\Phi_\sigma G+(\mp\frac{i}{2}(\alpha\cdot N)+C_\sigma)g$ by Lemma 2.2(i), which yields $\varphi_++\varphi_-=2(\Phi_\sigma G+C_\sigma g)$. Recall that $\Phi_\sigma G=\Lambda_\lambda g$ by (6), hence

$$\mathcal{V}_\lambda\varphi=\lambda(\alpha\cdot N)(\Phi_\sigma G+C_\sigma g)=-\lambda(\alpha\cdot N)\frac{1}{\lambda}(\alpha\cdot N)g=-g=V\varphi,$$

where we used (5) in the last equality above.

Since λ is continuous on the compact set $\partial\Omega$ and $\lambda(x)\neq 0$ for all $x\in\partial\Omega$, there exists $\epsilon>0$ such that

$$\epsilon\leq\lambda(x)^2\leq 1/\epsilon\quad\text{for all } x\in\partial\Omega. \tag{28}$$

Hence Λ_λ is a bounded operator in $L^2(\sigma)^2$. The first statement in the proposition follows by Theorem 2.1, as far as we check that Λ_λ is self-adjoint and Fredholm. Since λ is real-valued, the self-adjointness of Λ_λ follows from the one of C_σ and $\alpha\cdot N$. Regarding the Fredholm character, recall that

$$C_\sigma^2=C_\sigma(\alpha\cdot N)\{C_\sigma,\alpha\cdot N\}+1/4$$

by Lemma 2.2(ii), where $\{C_\sigma,\alpha\cdot N\}=C_\sigma(\alpha\cdot N)+(\alpha\cdot N)C_\sigma$. Then

$$\begin{aligned}\Lambda_\lambda^2&=\frac{1}{\lambda^2}+C_\sigma^2+\left\{\frac{1}{\lambda}(\alpha\cdot N),C_\sigma\right\}\\&=\frac{1}{\lambda^2}+\frac{1}{4}+C_\sigma(\alpha\cdot N)\{C_\sigma,\alpha\cdot N\}+\left\{\frac{1}{\lambda}(\alpha\cdot N),C_\sigma\right\}.\end{aligned} \tag{29}$$

By (28), $1/\lambda^2+1/4$ is bounded and invertible in $L^2(\sigma)^4$. Besides, $\{C_\sigma,\alpha\cdot N\}$ is compact in $L^2(\sigma)^4$ by [2, Lemma 3.5] because $\partial\Omega$ is smooth. The compactness of $\{\frac{1}{\lambda}(\alpha\cdot N),C_\sigma\}$ follows similarly. More precisely, arguing as in the proof of [2, Lemma 3.5] one shows that $\{\frac{1}{\lambda}(\alpha\cdot N),C_\sigma\}g(x)=\lim_{\epsilon\searrow 0}\int_{|x-z|>\epsilon}K(x,z)g(z)\,d\sigma(z)$ for all $g\in L^2(\sigma)^4$, where

$$K(x,z)=\phi(x-z)\,\alpha\cdot\left(\frac{N(z)}{\lambda(z)}-\frac{N(x)}{\lambda(x)}\right)+\frac{ie^{-m|x-z|}}{2\pi|x-z|^3}\,(1+m|x-z|)\left(\frac{N(x)}{\lambda(x)}\cdot(x-z)\right).$$

The smoothness of $\partial\Omega$ and λ guarantee that $K(x,z)=O(|x-z|^{-1})$ for $|x-z|\to 0$, which yields the compactness of $\{\frac{1}{\lambda}(\alpha\cdot N),C_\sigma\}$ because $\partial\Omega$ is bounded. Therefore, from (29) we see that Λ_λ^2 is Fredholm, and thus Λ_λ is also Fredholm by [1, Theorem 1.46(iii)]. The proof of the proposition is complete thanks to Theorem 2.1. □

Remark 5.2. The reader may realize that less regularity on $\partial\Omega$ and λ can be assumed to get the same conclusions of Proposition 5.1. For instance, $N/\lambda \in \mathcal{C}^\alpha(\partial\Omega)$ with $\alpha > 0$ would suffice, and even less. However, we don't want to look for optimal regularity assumptions to avoid technicalities.

The purpose of the following theorem is to get rid of the non-vanishing assumption of λ in Proposition 5.1. In order to do so, we use a generalization of the unitary transformations introduced at the beginning of Section 3:

$$\text{Given } \theta : \mathbb{R}^3 \to \mathbb{R}, \text{ define } U_\theta : L^2(\mu)^4 \to L^2(\mu)^4 \text{ by } U_\theta\varphi = e^{-i\theta\chi_{\Omega_-}}\varphi.$$

Theorem 5.3. *Let $\lambda : \mathbb{R}^3 \to \mathbb{R}$ be a compactly supported function of class $\mathcal{C}^1(\mathbb{R}^3)$ and let $\lambda_{\partial\Omega}$ denote its restriction to $\partial\Omega$. Let $M > 0$ be such that $\lambda_{\partial\Omega}(x) + M > 0$ for all $x \in \partial\Omega$ and let $\theta : \mathbb{R}^3 \to \mathbb{R}$ of class $\mathcal{C}^1(\mathbb{R}^3)$ so that*

$$e^{i\theta} = \frac{(\lambda + 2i)(\lambda + M - 2i)}{(\lambda - 2i)(\lambda + M + 2i)}. \tag{30}$$

Then, the operator

$$\big(T_{\Lambda_{\lambda_{\partial\Omega}+M}}\big)_\theta = U_\theta^* T_{\Lambda_{\lambda_{\partial\Omega}+M}} U_\theta + \chi_{\Omega_-}(\alpha \cdot \nabla\theta) \tag{31}$$

defined on $U_\theta^* D\big(T_{\Lambda_{\lambda_{\partial\Omega}+M}}\big)$ is self-adjoint, where $\Lambda_{\lambda_{\partial\Omega}+M}$ and $T_{\Lambda_{\lambda_{\partial\Omega}+M}}$ are given by (26) *and* (6)*, respectively. Moreover,*

$$\big(T_{\Lambda_{\lambda_{\partial\Omega}+M}}\big)_\theta = H + \mathcal{V}_{\lambda_{\partial\Omega}} \text{ on } U_\theta^* D\big(T_{\Lambda_{\lambda_{\partial\Omega}+M}}\big), \tag{32}$$

where $\mathcal{V}_{\lambda_{\partial\Omega}}$ is given by (27)*.*

Proof. The existence of M in the statement of the theorem follows from the fact that $\lambda_{\partial\Omega}$ is continuous on the compact set $\partial\Omega$, and the existence of θ is a consequence of the fact that the term on the right hand side of (30) is a complex-valued function of modulus 1. Furthermore, we can take θ so that it inherits the regularity of λ. To see this, note that

$$\frac{(\lambda(x) + 2i)(\lambda(x) + M - 2i)}{(\lambda(x) - 2i)(\lambda(x) + M + 2i)} \neq 1$$

for all $x \in \mathbb{R}^3$ because $t \mapsto (t+2i)/(t-2i)$ is injective from $\mathbb{R}$ to the unit circle in $\mathbb{R}^2$, $M > 0$ and λ can not take the values $\pm\infty$. Hence, there exists a well defined principal value of the argument of the points given by the right hand side of (30) which is as smooth as λ (thanks to the holomorphicity of the corresponding branch of the complex logarithm).

Since $\lambda_{\partial\Omega} + M > 0$ in $\partial\Omega$, from Proposition 5.1 we deduce that $T_{\Lambda_{\lambda_{\partial\Omega}+M}}$ is self-adjoint and $T_{\Lambda_{\lambda_{\partial\Omega}+M}} = H + \mathcal{V}_{\lambda_{\partial\Omega}+M}$ on $D\big(T_{\Lambda_{\lambda_{\partial\Omega}+M}}\big)$, where $\mathcal{V}_{\lambda_{\partial\Omega}+M}$ is given by (27). In particular, $\mathcal{V}_{\lambda_{\partial\Omega}+M} = V$ on $D\big(T_{\Lambda_{\lambda_{\partial\Omega}+M}}\big)$, for V as in (5). Furthermore, thanks to Lemma 2.2(i) this means that if $\varphi = \Phi(G+g) \in D\big(T_{\Lambda_{\lambda_{\partial\Omega}+M}}\big)$ then

$$i(\alpha \cdot N)(\varphi_- - \varphi_+) = -g = V\varphi = \mathcal{V}_{\lambda_{\partial\Omega}+M}\varphi = (\lambda_{\partial\Omega} + M)(\alpha \cdot N)\frac{\varphi_+ + \varphi_-}{2},$$

and therefore, using that $\lambda_{\partial\Omega} + M$ is real-valued, we get

$$\varphi_- = \frac{2i + \lambda_{\partial\Omega} + M}{2i - \lambda_{\partial\Omega} - M}\varphi_+. \tag{33}$$

The operator $U_\theta^* T_{\Lambda_{\lambda_{\partial\Omega}+M}} U_\theta$ defined on $U_\theta^* D\big(T_{\Lambda_{\lambda_{\partial\Omega}+M}}\big)$ is unitary equivalent to $T_{\Lambda_{\lambda_{\partial\Omega}+M}}$, thus it is self-adjoint. Since $\chi_{\Omega_-}(\alpha \cdot \nabla\theta)$ is a bounded and symmetric operator in $L^2(\mu)^4$ (because $\nabla\theta$ is continuous and compactly supported due to the fact that $\lambda \in \mathcal{C}_c^1(\mathbb{R}^3)$), an application of the Kato-Rellich theorem (see [7, Theorem X.12], for example) finally shows that the operator $\big(T_{\Lambda_{\lambda_{\partial\Omega}+M}}\big)_\theta$ defined on $U_\theta^* D\big(T_{\Lambda_{\lambda_{\partial\Omega}+M}}\big)$ by (31) is also self-adjoint.

To conclude the proof of the theorem, it only remains to show that (32) holds. Let $\psi \in U_\theta^* D\big(T_{\Lambda_{\lambda_{\partial\Omega}+M}}\big)$, so $\psi = e^{i\theta\chi_{\Omega_-}}\varphi$ for some $\varphi \in D\big(T_{\Lambda_{\lambda_{\partial\Omega}+M}}\big)$. First, note that

$$U_\theta^* T_{\Lambda_{\lambda_{\partial\Omega}+M}} U_\theta \psi = U_\theta^* T_{\Lambda_{\lambda_{\partial\Omega}+M}} \varphi = U_\theta^* (\chi_{\Omega_+} H\varphi + \chi_{\Omega_-} H\varphi), \tag{34}$$

where we denoted by $\chi_{\Omega_+} H\varphi + \chi_{\Omega_-} H\varphi$ the absolutely continuous part of the distribution $H\varphi$ (it corresponds to G when we write $\varphi = \Phi(G+g)$). Using the distributional equation [3, (5.2)], we see that

$$\begin{aligned}(H+\mathcal{V}_{\lambda_{\partial\Omega}})\psi &= (H+\mathcal{V}_{\lambda_{\partial\Omega}})e^{i\theta\chi_{\Omega_-}}\varphi = H\big(e^{i\theta\chi_{\Omega_-}}\varphi\big) + \lambda_{\partial\Omega}(\alpha\cdot N)\frac{\varphi_+ + e^{i\theta}\varphi_-}{2}\\ &= \chi_{\Omega_+} H\varphi + \chi_{\Omega_-}(e^{i\theta}H(\varphi) + (\alpha\cdot\nabla\theta)e^{i\theta}\varphi)\\ &\quad - i(\alpha\cdot N)(e^{i\theta}\varphi_- - \varphi_+) + \lambda_{\partial\Omega}(\alpha\cdot N)\frac{\varphi_+ + e^{i\theta}\varphi_-}{2}\\ &= U_\theta^*(\chi_{\Omega_+} H\varphi + \chi_{\Omega_-} H\varphi) + \chi_{\Omega_-}(\alpha\cdot\nabla\theta)e^{i\theta}\varphi\\ &\quad + (\alpha\cdot N)\Big\{\Big(\frac{\lambda_{\partial\Omega}}{2} - i\Big)e^{i\theta}\varphi_- + \Big(\frac{\lambda_{\partial\Omega}}{2} + i\Big)\varphi_+\Big\}.\end{aligned} \tag{35}$$

From (33) and (30) we obtain

$$\Big(\frac{\lambda_{\partial\Omega}}{2} - i\Big)e^{i\theta}\varphi_- + \Big(\frac{\lambda_{\partial\Omega}}{2} + i\Big)\varphi_+ = \Big\{\Big(\frac{\lambda_{\partial\Omega}}{2} - i\Big)e^{i\theta}\frac{2i+\lambda_{\partial\Omega}+M}{2i-\lambda_{\partial\Omega}-M} + \Big(\frac{\lambda_{\partial\Omega}}{2} + i\Big)\Big\}\varphi_+ = 0,$$

and then (35), (34) and (31) yield

$$\begin{aligned}(H+\mathcal{V}_{\lambda_{\partial\Omega}})\psi &= U_\theta^*(\chi_{\Omega_+} H\varphi + \chi_{\Omega_-} H\varphi) + \chi_{\Omega_-}(\alpha\cdot\nabla\theta)e^{i\theta}\varphi\\ &= U_\theta^* T_{\Lambda_{\lambda_{\partial\Omega}+M}} U_\theta\psi + \chi_{\Omega_-}(\alpha\cdot\nabla\theta)\psi = \big(T_{\Lambda_{\lambda_{\partial\Omega}+M}}\big)_\theta\psi\end{aligned}$$

for all $\psi \in U_\theta^* D\big(T_{\Lambda_{\lambda_{\partial\Omega}+M}}\big)$. The proof of the theorem is complete. □

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