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Dirichlet-to-Neumann and Neumann-to-Dirichlet embedding methods for bound states of the Dirac equation

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Abstract

The embedding method (Inglesfield J E 1981 *J. Phys. C: Solid State Phys.* **14** 3795) is nowadays widely used for determining properties of bound and continuum eigenstates of the Schrödinger equation. Recently, Crampin (2004 *J. Phys.: Condens. Matter* **16** 8875) extended Inglesfield's formalism to systems described by the Dirac equation. In this paper, we reformulate the embedding method for bound states of Dirac particles in the language of the theory of surface integral operators, which are natural analogues of the Dirichlet-to-Neumann (DtN) and Neumann-to-Dirichlet (NtD) operators used in the non-relativistic theory. A method of constructing kernels of these Dirac counterparts of the DtN and NtD maps from solutions to an analogue of the Steklov (Stekloff) eigenproblem for an exterior Dirac problem is presented. A numerical example illustrating the utility of the DtN/NtD embedding method is provided.

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1. Introduction

In quantum physics, one frequently encounters situations in which an explicit form of a local potential $V(\boldsymbol{r})$ acting on a particle is such that the particle's configuration space, say $\mathbb{R}^3$, may be naturally divided into two disjoint regions, separated by a sufficiently smooth closed surface $\mathcal{S}$. In the finite, simply connected internal domain $\mathcal{V}_I$ the potential $V(\boldsymbol{r})$ is a complicated function of the position vector $\boldsymbol{r}$. To the contrary, in the infinite remainder, $\mathcal{V}_{II} = \mathbb{R}^3 \backslash \overline{\mathcal{V}}_I$, the potential $V(\boldsymbol{r})$ has a form sufficiently simple that solutions to the pertinent time-independent quantum wave equation, subject to the usual condition of sufficiently rapid decaying at spatial infinity,

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may be found with no difficulty, either analytically or at least in a numerical form. In principle, an energy eigenproblem for a Hamiltonian involving a potential belonging to the aforementioned category may be solved numerically by using some of standard global variational techniques, with no attempt to exploit in any way the specific properties of $V(\boldsymbol{r})$ in the external region. Yet, there exist methods capable of solving such particular eigenproblems more efficiently. Among them there is an embedding method, introduced in 1981 by Inglesfield [1] in the context of non-relativistic quantum mechanics.

In [1], Inglesfield pointed out that in the case of a Schrödinger particle bound in a potential belonging to the category described above, after exploiting some techniques of the calculus of variations, it was possible to replace an original energy eigenvalue problem in $\mathbb{R}^3$ by another one in $\mathcal{V}_I$. This new eigenproblem was constituted by the original Schrödinger equation truncated to $\mathcal{V}_I$, augmented by a homogeneous, but nonlocal, boundary condition imposed at $\mathcal{S}$, with both the equation and the boundary condition being eigenvalue dependent. The boundary condition contained an integral operator, called by Inglesfield 'an embedding potential,' which at the surface $\mathcal{S}$ transformed a wavefunction into its normal derivative. A kernel of this operator was constructed from surface parts of all particular asymptotically decaying solutions to the Schrödinger equation in the external region $\mathcal{V}_{II}$ at some energy $\mathcal{E}$. Inglesfield made a conjecture that if $\mathcal{E}$ was a reasonable estimate of some eigenvalue E of the original eigenproblem in $\mathbb{R}^3$, then algebraizing the new eigenproblem, solving, and iterating the procedure with $\mathcal{E}$ replaced by the closest from among eigenvalues found in the preceding step, after an infinite number of iterations one should eventually find E in the resulting spectrum. A numerical illustration provided by Inglesfield showed that the class of problems for which the procedure converges is non-empty and that for some problems, even with a relatively poor initial guess $\mathcal{E}$, only a few iterations were necessary to achieve convergence within a prescribed numerical accuracy. In addition, Inglesfield proved that, after necessary modifications, the embedding method might be also used for computing Green functions for continuum problems.

Since the moment of publication of the above-mentioned paper of Inglesfield, the embedding method has found applications in non-relativistic solid-state physics [2–19] and in molecular theory [20–22]. Moreover, the ideas forming the background of the method were applied by Inglesfield in electromagnetism [23], resulting in a recent application of the technique in the field of photonics [24]. Finally, very recently, Crampin [25] has presented an extension of the embedding method to bound and continuum states of Dirac particles.

In our recent paper [26] on the non-relativistic embedding method, we have pointed out that the embedding potential of Inglesfield is identical with the Dirichlet-to-Neumann (DtN) operator, well known in applied mathematics (cf, e.g. [27] and papers cited therein). In the realm of non-relativistic quantum theory, the DtN operator and its inverse, the Neumann-to-Dirichlet (NtD) operator, were used extensively by one of the present authors in his research on fundamentals of a so-called R-matrix method for scattering of Schrödinger particles [28–32]. Exploiting the experience gained during these studies, and making also use of variational principles admitting the use of discontinuous trial functions [33], in [26] we have been able to put the non-relativistic embedding method on a firm mathematical ground. In particular, we have presented two variants of the method, one based on the use of the DtN operator and the second one employing the NtD operator; also, we have proposed a general procedure for constructing kernels of the DtN and NtD operators from eigensolutions to a so-called Steklov (Stekloff) spectral problem.

In the present work, we are concerned with the embedding method for bound states of Dirac particles. Having of necessity points of contact with the approach described by Crampin [25], in many technical aspects our way of attacking the problem differs from that adopted in [25]. In the latter work, the non-relativistic formalism of Inglesfield [1] has been followed

closely and consequently an extensive use of the Green functions concept has been made. Here, we follow conceptually [26] and base our presentation on a suitably adapted formalism of Dirac counterparts of the DtN and NtD operators, developed by one of us in the context of the R-matrix method for scattering of Dirac particles [29, 30, 32, 34, 35] (for a thorough mathematical investigations of some mathematical aspects of this formalism, the reader is referred to [36–38]).

The structure of the paper is as follows. In section 2 we summarize the relevant results of [33] and present a variational principle for energies of bound states of a Dirac particle, allowing the use of trial functions with a discontinuity at the surface $\mathcal{S}$. Then, in section 3, we introduce the aforementioned analogues of the DtN and NtD operators, associated with an exterior Dirac problem. (Hereafter, we shall be calling these operators simply the (Dirac) DtN and NtD operators. However, one should be aware of some fundamental differences between these operators and their Schrödinger counterparts; for the nature and origins of these differences, cf section 3 of the present work and section III of [26].) We consider also here an auxiliary, non-standard, spectral problem, which is a counterpart of the Steklov eigenproblem exploited in [26]. We demonstrate how 4×4 matrix kernels of the Dirac DtN and NtD operators may be constructed using eigensolutions to this problem. Section 4 is the heart of the paper. Here we show how the variational principle of section 2 and the Dirac DtN operators defined in section 3 may be used to replace the Dirac energy eigenproblem in $\mathbb{R}^3$ by a generalized one in the finite interior domain $\mathcal{V}_I$, with a whole information on the system behaviour in the eliminated exterior region $\mathcal{V}_{II}$ contained in a nonlocal, eigenvalue-dependent boundary condition constraining eigenspinors at the separating interface $\mathcal{S}$. The analogous considerations based on the use of the Dirac NtD operators are very briefly summarized in section 5. In section 6 the eigenproblem derived in section 4 is algebraized. Section 7 is devoted to a thorough discussion of the case when the interior region $\mathcal{V}_I$ is a sphere, while in the exterior region $\mathcal{V}_{II}$ the potential acting on the Dirac particle is spherically symmetric, with its symmetry centre coinciding with the centre of the sphere $\mathcal{V}_I$. In particular, we dilate on simplifications in the explicit forms of relevant Steklov eigenfunctions and in the kernels of the DtN and NtD operators. In addition, we present first-order ordinary differential equations allowing one to compute conveniently Steklov eigenvalues and their derivatives with respect to energy for any potential which is spherically symmetric in $\mathcal{V}_{II}$. The general considerations are illustrated by two examples: one embodying a potential vanishing identically in the external domain and the other involving a potential possessing an asymptotic Coulomb tail. A numerical illustration showing capabilities of the Dirac DtN/NtD embedding methods developed in this work is then provided in section 8. The paper ends with conclusions, forming section 9, followed by an appendix containing some supplementary material.

2. Variational principle for energy allowing the use of discontinuous trial functions

We seek to solve the bound-state energy eigenvalue problem

$$\hat{\mathcal{H}}\Psi(E,\boldsymbol{r}) = E\Psi(E,\boldsymbol{r}) \qquad (\boldsymbol{r} \in \mathbb{R}^3) \tag{2.1}$$

$$\lim_{r\to\infty} r^{3/2}\Psi(E,\boldsymbol{r}) = 0 \tag{2.2}$$

for the Dirac Hamiltonian

$$\hat{\mathcal{H}} = -\mathrm{i}c\hbar\boldsymbol{\alpha}\cdot\boldsymbol{\nabla} + \beta mc^2 + V(\boldsymbol{r}) \tag{2.3}$$

with the Hermitian 4×4 Dirac matrices $\boldsymbol{\alpha}$ and β defined in the usual way [39]. Hereafter, it will be assumed that the potential $V(\boldsymbol{r})$ is real, local, and such that the eigenproblem (2.1) and (2.2) possesses at least one non-trivial solution.

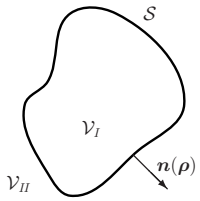

Figure 1. Partitioning of $\mathbb{R}^3$ into the finite domain $\mathcal{V}_I$ and the infinite remainder $\mathcal{V}_{II} = \mathbb{R}^3\backslash\overline{\mathcal{V}}_I$, separated by the surface $\mathcal{S}$; $\boldsymbol{n}(\boldsymbol{\rho})$ is the unit vector normal to the surface $\mathcal{S}$ at the point $\boldsymbol{\rho}$.

Suppose next that the potential $V(\boldsymbol{r})$ has such a particular functional form which suggests in the natural manner to decompose, as depicted in figure 1, the whole space $\mathbb{R}^3$ into two domains: the finite simply-connected volume $\mathcal{V}_I$ and the remainder $\mathcal{V}_{II} = \mathbb{R}^3\backslash\overline{\mathcal{V}}_I$, separated by a sufficiently smooth surface $\mathcal{S}$. (For clarity, hereafter a position vector for any particular point located on $\mathcal{S}$ will be marked using the symbol $\boldsymbol{\rho}$ rather than $\boldsymbol{r}$. A unit vector normal to $\mathcal{S}$ at the point $\boldsymbol{\rho}$, pointing from $\mathcal{V}_I$ to $\mathcal{V}_{II}$, will be denoted by $\boldsymbol{n}(\boldsymbol{\rho})$.) Let us define

$$\Psi_X(E,\boldsymbol{r}) = \Psi(E,\boldsymbol{r}) \qquad (\boldsymbol{r}\in\mathcal{V}_X;\ X = I, II). \tag{2.4}$$

In virtue of equation (2.2), asymptotically one has

$$\lim_{r\to\infty} r^{3/2}\Psi_{II}(E,\boldsymbol{r}) = 0 \tag{2.5}$$

while, since the Dirac equation (2.1) is essentially a system of first-order partial differential equations, at the interface $\mathcal{S}$ the matching condition

$$\Psi_I(E,\boldsymbol{\rho}) = \Psi_{II}(E,\boldsymbol{\rho}) \tag{2.6}$$

holds. (Observe that, strictly speaking, equation (2.6) is a short-hand notation for *four* matching conditions, one for each of the four components of $\Psi_I(E,\boldsymbol{\rho})$ and $\Psi_{II}(E,\boldsymbol{\rho})$.)

In [33], we have shown that once the domain decomposition described above has been carried out, the energy eigenproblem (2.1) and (2.2) appears to be equivalent to the following variational principle:

$$\delta\mathcal{F}[\Psi_I,\Psi_{II}] = 0 \qquad E = \mathcal{F}[\Psi_I,\Psi_{II}] \tag{2.7}$$

with the real functional

$$\begin{aligned}\mathcal{F}[\overline{\Psi}_I,\overline{\Psi}_{II}] = {}& \frac{\langle\overline{\Psi}_I|\hat{\mathcal{H}}\overline{\Psi}_I\rangle_I + \langle\overline{\Psi}_{II}|\hat{\mathcal{H}}\overline{\Psi}_{II}\rangle_{II}}{\langle\overline{\Psi}_I|\overline{\Psi}_I\rangle_I + \langle\overline{\Psi}_{II}|\overline{\Psi}_{II}\rangle_{II}} + c\hbar\frac{\left(a\overline{\Psi}_I + [1-a]\overline{\Psi}_{II}\middle|\mathrm{i}\alpha_\perp^{(+)}\overline{\Psi}_I - \mathrm{i}\alpha_\perp^{(+)}\overline{\Psi}_{II}\right)}{\langle\overline{\Psi}_I|\overline{\Psi}_I\rangle_I + \langle\overline{\Psi}_{II}|\overline{\Psi}_{II}\rangle_{II}} \\ & + c\hbar\frac{\left([1-a^*]\overline{\Psi}_I + a^*\overline{\Psi}_{II}\middle|\mathrm{i}\alpha_\perp^{(-)}\overline{\Psi}_I - \mathrm{i}\alpha_\perp^{(-)}\overline{\Psi}_{II}\right)}{\langle\overline{\Psi}_I|\overline{\Psi}_I\rangle_I + \langle\overline{\Psi}_{II}|\overline{\Psi}_{II}\rangle_{II}}\end{aligned} \tag{2.8}$$

(cf also [40, 41]). Here a is an arbitrary *fixed* complex number which may be chosen at will,

$$\alpha_\perp^{(\pm)}(\boldsymbol{\rho}) = \beta^{(\pm)}\alpha_\perp(\boldsymbol{\rho}) \tag{2.9}$$

where

$$\beta^{(\pm)} = \tfrac{1}{2}(\mathcal{I}\pm\beta) \tag{2.10}$$

($\mathcal{I}$ is the unit 4×4 matrix) and

$$\alpha_\perp(\boldsymbol{\rho}) = \boldsymbol{n}(\boldsymbol{\rho})\cdot\boldsymbol{\alpha} \tag{2.11}$$

while $\langle\,|\,\rangle_X$ and $(\,|\,)$ are volume and surface scalar products defined as

$$\langle\Phi|\Phi'\rangle_X = \int_{\mathcal{V}_X} \mathrm{d}^3\boldsymbol{r}\,\Phi^\dagger(\boldsymbol{r})\Phi'(\boldsymbol{r}) \tag{2.12}$$

and

$$(\Phi|\Phi') = \oint_{\mathcal{S}} \mathrm{d}^2\boldsymbol{\rho}\, \Phi^{\dagger}(\boldsymbol{\rho})\Phi'(\boldsymbol{\rho}) \tag{2.13}$$

respectively ($\mathrm{d}^3\boldsymbol{r}$ is an infinitesimal volume element around the point $\boldsymbol{r}$ and $\mathrm{d}^2\boldsymbol{\rho}$ is an infinitesimal *scalar* element of $\mathcal{S}$ around the point $\boldsymbol{\rho}$). The functions $\overline{\Psi}_I(\boldsymbol{r})$ and $\overline{\Psi}_{II}(\boldsymbol{r})$, the latter subjected to the constraint

$$\lim_{r\to\infty} r^{3/2}\overline{\Psi}_{II}(\boldsymbol{r}) = 0 \tag{2.14}$$

(cf equations (2.2) and (2.5)), are trial estimates of $\Psi_I(E,\boldsymbol{r})$ and $\Psi_{II}(E,\boldsymbol{r})$, respectively.

As opposed to the plain Rayleigh quotient

$$\mathcal{F}^{(\mathrm{R})}[\overline{\Psi}] = \frac{\langle\overline{\Psi}|\hat{\mathcal{H}}\overline{\Psi}\rangle_{\mathbb{R}^3}}{\langle\overline{\Psi}|\overline{\Psi}\rangle_{\mathbb{R}^3}} \tag{2.15}$$

used in the standard variational principle

$$\delta\mathcal{F}^{(\mathrm{R})}[\Psi] = 0 \qquad E = \mathcal{F}^{(\mathrm{R})}[\Psi] \tag{2.16}$$

the functional (2.8) admits the use of trial functions, components of which, being continuous in interiors of $\mathcal{V}_I$ and $\mathcal{V}_{II}$, may experience jumps across the interface $\mathcal{S}$, i.e., such trial functions for which, in general, it holds that

$$\overline{\Psi}_I(\boldsymbol{\rho}) \neq \overline{\Psi}_{II}(\boldsymbol{\rho}). \tag{2.17}$$

(Observe that, for equation (2.17) to be valid, it suffices that only one of the components of $\overline{\Psi}_I(\boldsymbol{\rho})$ does not match with its counterpart in $\overline{\Psi}_{II}(\boldsymbol{\rho})$.) We shall exploit this attribute of the functional (2.8) in sections 4 and 5.

3. DtN and NtD surface integral operators

Let us denote by $\mathcal{D}_{II}(\mathcal{E})$ a set $\{\psi(\mathcal{E},\boldsymbol{r})\}$ of functions which in the outer domain $\mathcal{V}_{II}$ are solutions to the Dirac equation

$$\hat{\mathcal{H}}\psi(\mathcal{E},\boldsymbol{r}) = \mathcal{E}\psi(\mathcal{E},\boldsymbol{r}) \qquad (\boldsymbol{r}\in\mathcal{V}_{II}) \tag{3.1}$$

($\hat{\mathcal{H}}$ is the Hamiltonian (2.3)) at some *fixed* value of the energy parameter $\mathcal{E}\in\mathbb{R}$ (which need *not* be in the spectrum of the eigenproblem (2.1) and (2.2); we recall that this spectrum is sought) and, in addition, obey the asymptotic condition

$$\lim_{r\to\infty} r^{3/2}\psi(\mathcal{E},\boldsymbol{r}) = 0. \tag{3.2}$$

We introduce two linear integral operators $\hat{\mathcal{B}}^{(\pm)}(\mathcal{E})$, possessing the properties

$$\beta^{(\pm)}\hat{\mathcal{B}}^{(\pm)}(\mathcal{E})\beta^{(\pm)} = \hat{\mathcal{B}}^{(\pm)}(\mathcal{E}) \tag{3.3}$$

and such that for any $\psi(\mathcal{E},\boldsymbol{r})\in\mathcal{D}_{II}(\mathcal{E})$ at the separating surface $\mathcal{S}$ it holds that

$$\mathrm{i}\alpha_{\perp}^{(\pm)}(\boldsymbol{\rho})\psi(\mathcal{E},\boldsymbol{\rho}) = \gamma^{(\pm)}\hat{\mathcal{B}}^{(\pm)}(\mathcal{E})\psi(\mathcal{E},\boldsymbol{\rho}) \tag{3.4}$$

where

$$\gamma^{(\pm)} = \pm\left(\frac{\hbar}{2mc}\right)^{\pm 1}. \tag{3.5}$$

In addition, we introduce also two other operators $\hat{\mathcal{R}}^{(\pm)}(\mathcal{E})$, possessing the properties

$$\beta^{(\pm)}\hat{\mathcal{R}}^{(\pm)}(\mathcal{E})\beta^{(\pm)} = \hat{\mathcal{R}}^{(\pm)}(\mathcal{E}) \tag{3.6}$$

(cf equation (3.3)); these operators are generalized inverses of $\hat{\mathcal{B}}^{(\pm)}(\mathcal{E})$ in the sense of

$$\hat{\mathcal{B}}^{(\pm)}(\mathcal{E})\hat{\mathcal{R}}^{(\pm)}(\mathcal{E}) = \hat{\mathcal{R}}^{(\pm)}(\mathcal{E})\hat{\mathcal{B}}^{(\pm)}(\mathcal{E}) = \hat{\mathcal{I}}_{\mathcal{S}}\beta^{(\pm)}. \tag{3.7}$$

Here $\hat{\mathcal{I}}_{\mathcal{S}}$ is the unit operator on $\mathcal{S}$ (its kernel is the surface Dirac delta function $\delta^{(2)}_{\mathcal{S}}(\boldsymbol{\rho}-\boldsymbol{\rho}')$). Rewritten in terms of the operators $\hat{\mathcal{R}}^{(\pm)}(\mathcal{E})$, equation (3.4) becomes

$$\beta^{(\pm)}\psi(\mathcal{E},\boldsymbol{\rho}) = -\gamma^{(\mp)}\hat{\mathcal{R}}^{(\pm)}(\mathcal{E})\mathrm{i}\alpha^{(\pm)}_{\perp}(\boldsymbol{\rho})\psi(\mathcal{E},\boldsymbol{\rho}). \tag{3.8}$$

The operators $\hat{\mathcal{B}}^{(\pm)}(\mathcal{E})$ and $\hat{\mathcal{R}}^{(\pm)}(\mathcal{E})$ are represented by their integral kernels $\mathcal{B}^{(\pm)}(\mathcal{E},\boldsymbol{\rho},\boldsymbol{\rho}')$ and $\mathcal{R}^{(\pm)}(\mathcal{E},\boldsymbol{\rho},\boldsymbol{\rho}')$, respectively. In terms of these kernels, equations (3.4), (3.7) and (3.8) read

$$\mathrm{i}\alpha^{(\pm)}_{\perp}(\boldsymbol{\rho})\psi(\mathcal{E},\boldsymbol{\rho}) = \gamma^{(\pm)}\oint_{\mathcal{S}}\mathrm{d}^2\boldsymbol{\rho}'\,\mathcal{B}^{(\pm)}(\mathcal{E},\boldsymbol{\rho},\boldsymbol{\rho}')\psi(\mathcal{E},\boldsymbol{\rho}') \tag{3.9}$$

$$\begin{aligned}\oint_{\mathcal{S}}\mathrm{d}^2\boldsymbol{\rho}''\,\mathcal{B}^{(\pm)}(\mathcal{E},\boldsymbol{\rho},\boldsymbol{\rho}'')\mathcal{R}^{(\pm)}(\mathcal{E},\boldsymbol{\rho}'',\boldsymbol{\rho}') &= \oint_{\mathcal{S}}\mathrm{d}^2\boldsymbol{\rho}''\,\mathcal{R}^{(\pm)}(\mathcal{E},\boldsymbol{\rho},\boldsymbol{\rho}'')\mathcal{B}^{(\pm)}(\mathcal{E},\boldsymbol{\rho}'',\boldsymbol{\rho}')\\ &= \delta^{(2)}_{\mathcal{S}}(\boldsymbol{\rho}-\boldsymbol{\rho}')\beta^{(\pm)}\end{aligned} \tag{3.10}$$

and

$$\beta^{(\pm)}\psi(\mathcal{E},\boldsymbol{\rho}) = -\gamma^{(\mp)}\oint_{\mathcal{S}}\mathrm{d}^2\boldsymbol{\rho}'\,\mathcal{R}^{(\pm)}(\mathcal{E},\boldsymbol{\rho},\boldsymbol{\rho}')\mathrm{i}\alpha^{(\pm)}_{\perp}(\boldsymbol{\rho}')\psi(\mathcal{E},\boldsymbol{\rho}') \tag{3.11}$$

respectively.

Consider now the following auxiliary spectral problem:

$$\hat{\mathcal{H}}\psi_n(\mathcal{E},\boldsymbol{r}) = \mathcal{E}\psi_n(\mathcal{E},\boldsymbol{r}) \qquad (\boldsymbol{r}\in\mathcal{V}_{II}) \tag{3.12}$$

$$\lim_{r\to\infty} r^{3/2}\psi_n(\mathcal{E},\boldsymbol{r}) = 0 \tag{3.13}$$

$$\mathrm{i}\alpha^{(+)}_{\perp}(\boldsymbol{\rho})\psi_n(\mathcal{E},\boldsymbol{\rho}) = \gamma^{(+)}b_n(\mathcal{E})\beta^{(+)}\psi_n(\mathcal{E},\boldsymbol{\rho}) \qquad (\boldsymbol{\rho}\in\mathcal{S}) \tag{3.14}$$

(cf [30, 32, 34, 35, 42]). Here $\mathcal{E}\in\mathbb{R}$ has the same meaning as hitherto and remains fixed, $b_n(\mathcal{E})$ is an eigenvalue, while $\psi_n(\mathcal{E},\boldsymbol{r})$ is an associated eigenfunction. We emphasize that the problem (3.12)–(3.14) is of a non-standard character because the spectral parameter, $b_n(\mathcal{E})$, appears in the boundary condition rather than (as it happens more frequently) in the differential equation. In physical mathematics, eigenproblems falling into this category are generally known as Steklov, or Steklov–Poincaré, eigenproblems [43–51]; henceforth, we shall be referring to the spectral problem (3.12)–(3.14) using this terminology.

From equations (3.12)–(3.14) one may draw some general inferences about properties of eigensolutions to the Steklov eigenproblem constituted by these equations. Let $\psi_n(\mathcal{E},\boldsymbol{r})$ and $\psi_{n'}(\mathcal{E},\boldsymbol{r})$ be two arbitrary eigenfunctions. Referring to the explicit form of the Dirac Hamiltonian (2.3) and employing the Gauss divergence theorem, together with the asymptotic condition (3.13), we have

$$\langle\hat{\mathcal{H}}\psi_n|\psi_{n'}\rangle_{II} - \langle\psi_n|\hat{\mathcal{H}}\psi_{n'}\rangle_{II} = -c\hbar(\psi_n|\mathrm{i}\alpha_{\perp}\psi_{n'}). \tag{3.15}$$

(The minus sign on the right-hand side of equation (3.15) stems from the fact that, according to the convention introduced in section 2, the unit vector normal to the surface $\mathcal{S}$, i.e., $\boldsymbol{n}(\boldsymbol{\rho})$, points *inward* the volume $\mathcal{V}_{II}$.) Now, invoking equation (3.12) and exploiting the fact that $\mathcal{E}$ is real, we deduce immediately that the left-hand side of equation (3.15) vanishes; consequently, we may write

$$(\psi_n|\mathrm{i}\alpha_{\perp}\psi_{n'}) = 0 \tag{3.16}$$

or equivalently, after utilizing equation (A.1):

$$\left(\psi_n\middle|\left[\mathrm{i}\alpha_\perp^{(+)}+\mathrm{i}\alpha_\perp^{(-)}\right]\psi_{n'}\right)=0. \tag{3.17}$$

Hence, with the aid of the relation (A.3), one obtains

$$\left(\mathrm{i}\alpha_\perp^{(\pm)}\psi_n\middle|\psi_{n'}\right)=\left(\psi_n\middle|\mathrm{i}\alpha_\perp^{(\pm)}\psi_{n'}\right). \tag{3.18}$$

Presume for a while that in equation (3.18) the upper superscripts are chosen. Then, making use of the boundary condition (3.14) and the property (A.4), yields

$$[b_n^*(\mathcal{E})-b_{n'}(\mathcal{E})](\psi_n|\beta^{(+)}\psi_{n'})=0 \tag{3.19}$$

and, in particular,

$$[b_n^*(\mathcal{E})-b_n(\mathcal{E})](\psi_n|\beta^{(+)}\psi_n)=0. \tag{3.20}$$

In what follows, we shall be taking for granted that the Steklov spectrum $\{b_n(\mathcal{E})\}$ is purely discrete and that the surface $\mathcal{S}$ is such that for any eigenfunction $\psi_n(\mathcal{E},\boldsymbol{r})$ the scalar product on the left-hand side of equation (3.20) does not vanish. (The second assumption does not impose any severe restriction since in applications there is always some freedom in choosing $\mathcal{S}$, which one may take advantage of.) With these assumptions in mind, from equation (3.20) one deduces that all eigenvalues to the Steklov eigenproblem (3.12)–(3.14) are real:

$$b_n(\mathcal{E})=b_n^*(\mathcal{E}). \tag{3.21}$$

This, in turn, allows one to infer from equation (3.19) that eigenfunctions belonging to different eigenvalues are orthogonal in the sense of

$$(\psi_n|\beta^{(+)}\psi_{n'})=0 \qquad [b_n(\mathcal{E})\neq b_{n'}(\mathcal{E})]. \tag{3.22}$$

Henceforth, we shall be assuming that *all* eigenfunctions have been orthonormalized in the sense that for *any* two of them it holds that

$$(\psi_n|\beta^{(+)}\psi_{n'})=\delta_{nn'}. \tag{3.23}$$

Moreover, we shall be assuming that the following closure relation holds:

$$\sum_n \beta^{(+)}\psi_n(\mathcal{E},\boldsymbol{\rho})\psi_n^\dagger(\mathcal{E},\boldsymbol{\rho}')\beta^{(+)}=\delta_{\mathcal{S}}^{(2)}(\boldsymbol{\rho}-\boldsymbol{\rho}')\beta^{(+)}. \tag{3.24}$$

It ought to be mentioned here that, after straightforward manipulations exploiting the identities (A.6) and (A.11), the boundary condition (3.14) may be rewritten as

$$\mathrm{i}\alpha_\perp^{(-)}(\boldsymbol{\rho})\psi_n(\mathcal{E},\boldsymbol{\rho})=\gamma^{(-)}b_n^{-1}(\mathcal{E})\beta^{(-)}\psi_n(\mathcal{E},\boldsymbol{\rho}) \tag{3.25}$$

(the reason for factoring out $\gamma^{(+)}$ on the right-hand side of equation (3.14) should be now evident). With the aid of the same identities, equations (3.23) and (3.24) may be cast into the following alternative forms:

$$(\psi_n|\beta^{(-)}\psi_{n'})=(\gamma^{(+)})^2b_n^2(\mathcal{E})\delta_{nn'} \tag{3.26}$$

and

$$(\gamma^{(-)})^2\sum_n \beta^{(-)}\psi_n(\mathcal{E},\boldsymbol{\rho})b_n^{-2}(\mathcal{E})\psi_n^\dagger(\mathcal{E},\boldsymbol{\rho}')\beta^{(-)}=\delta_{\mathcal{S}}^{(2)}(\boldsymbol{\rho}-\boldsymbol{\rho}')\beta^{(-)} \tag{3.27}$$

respectively.

The reason for considering here the Steklov eigenproblem (3.12)–(3.14) is that, on combining equations (3.14) and (3.25) with equations (3.4) and (3.7), one obtains

$$\hat{\mathcal{B}}^{(\pm)}(\mathcal{E})\psi_n(\mathcal{E},\boldsymbol{\rho})=b_n^{\pm1}(\mathcal{E})\beta^{(\pm)}\psi_n(\mathcal{E},\boldsymbol{\rho}) \tag{3.28}$$

$$\hat{\mathcal{R}}^{(\pm)}(\mathcal{E})\psi_n(\mathcal{E},\boldsymbol{\rho})=b_n^{\mp1}(\mathcal{E})\beta^{(\pm)}\psi_n(\mathcal{E},\boldsymbol{\rho}). \tag{3.29}$$

Equations (3.28) and (3.29) are generalized (weighted) eigenequations for the operators $\hat{\mathcal{B}}^{(\pm)}(\mathcal{E})$ and $\hat{\mathcal{R}}^{(\pm)}(\mathcal{E})$, with the weights $\beta^{(\pm)}$. It is seen that eigenvalues to these equations are either the Steklov eigenvalues $\{b_n(\mathcal{E})\}$ (for $\hat{\mathcal{B}}^{(+)}(\mathcal{E})$ and $\hat{\mathcal{R}}^{(-)}(\mathcal{E})$) or their reciprocals $\{b_n^{-1}(\mathcal{E})\}$ (for $\hat{\mathcal{B}}^{(-)}(\mathcal{E})$ and $\hat{\mathcal{R}}^{(+)}(\mathcal{E})$), while associated eigenfunctions are the surface parts $\{\psi_n(\mathcal{E},\boldsymbol{\rho})\}$ of the Steklov eigenfunctions $\{\psi_n(\mathcal{E},\boldsymbol{r})\}$. With these facts in mind, recalling equations (3.3) and (3.6) and the orthogonality relations (3.23) and (3.26), spectral expansions of the kernels $\mathcal{B}^{(\pm)}(\mathcal{E},\boldsymbol{\rho},\boldsymbol{\rho}')$ and $\mathcal{R}^{(\pm)}(\mathcal{E},\boldsymbol{\rho},\boldsymbol{\rho}')$ are found to be

$$\mathcal{B}^{(+)}(\mathcal{E},\boldsymbol{\rho},\boldsymbol{\rho}') = \sum_n \beta^{(+)}\psi_n(\mathcal{E},\boldsymbol{\rho})b_n(\mathcal{E})\psi_n^\dagger(\mathcal{E},\boldsymbol{\rho}')\beta^{(+)} \tag{3.30}$$

$$\mathcal{B}^{(-)}(\mathcal{E},\boldsymbol{\rho},\boldsymbol{\rho}') = (\gamma^{(-)})^2\sum_n \beta^{(-)}\psi_n(\mathcal{E},\boldsymbol{\rho})b_n^{-3}(\mathcal{E})\psi_n^\dagger(\mathcal{E},\boldsymbol{\rho}')\beta^{(-)} \tag{3.31}$$

$$\mathcal{R}^{(+)}(\mathcal{E},\boldsymbol{\rho},\boldsymbol{\rho}') = \sum_n \beta^{(+)}\psi_n(\mathcal{E},\boldsymbol{\rho})b_n^{-1}(\mathcal{E})\psi_n^\dagger(\mathcal{E},\boldsymbol{\rho}')\beta^{(+)} \tag{3.32}$$

$$\mathcal{R}^{(-)}(\mathcal{E},\boldsymbol{\rho},\boldsymbol{\rho}') = (\gamma^{(-)})^2\sum_n \beta^{(-)}\psi_n(\mathcal{E},\boldsymbol{\rho})b_n^{-1}(\mathcal{E})\psi_n^\dagger(\mathcal{E},\boldsymbol{\rho}')\beta^{(-)}. \tag{3.33}$$

From these expansions, it is evident that the four kernels are Hermitian:

$$\mathcal{B}^{(\pm)}(\mathcal{E},\boldsymbol{\rho},\boldsymbol{\rho}') = \mathcal{B}^{(\pm)\dagger}(\mathcal{E},\boldsymbol{\rho}',\boldsymbol{\rho}) \tag{3.34}$$

$$\mathcal{R}^{(\pm)}(\mathcal{E},\boldsymbol{\rho},\boldsymbol{\rho}') = \mathcal{R}^{(\pm)\dagger}(\mathcal{E},\boldsymbol{\rho}',\boldsymbol{\rho}). \tag{3.35}$$

In addition, with the aid of the relationships (A.10) and (A.11), as well as equations (3.14), (3.25) and (3.5), from equations (3.30)–(3.33) one deduces the interesting relationships:

$$\hat{\mathcal{B}}^{(\pm)}(\mathcal{E},\boldsymbol{\rho},\boldsymbol{\rho}') = \alpha_\perp^{(\pm)}(\boldsymbol{\rho})\hat{\mathcal{R}}^{(\mp)}(\mathcal{E},\boldsymbol{\rho},\boldsymbol{\rho}')\alpha_\perp^{(\mp)}(\boldsymbol{\rho}') \tag{3.36}$$

which, in view of later applications, we rewrite also abstractly as

$$\hat{\mathcal{B}}^{(\pm)}(\mathcal{E}) = \alpha_\perp^{(\pm)}\hat{\mathcal{R}}^{(\mp)}(\mathcal{E})\alpha_\perp^{(\mp)}. \tag{3.37}$$

Comparison of the above exposition with the contents of section III of [26] shows that the operators $\hat{\mathcal{B}}^{(\pm)}(\mathcal{E})$ are formal counterparts of the Dirichlet-to-Neumann operator $\hat{\mathcal{B}}(\mathcal{E})$ appearing in a formulation of the non-relativistic embedding method; similarly, the operators $\hat{\mathcal{R}}^{(\pm)}(\mathcal{E})$ are formal analogues of the non-relativistic Neumann-to-Dirichlet operator $\hat{\mathcal{R}}(\mathcal{E})$; for this reason, we shall call $\hat{\mathcal{B}}^{(\pm)}(\mathcal{E})$ and $\hat{\mathcal{R}}^{(\pm)}(\mathcal{E})$ the Dirac DtN and NtD operators, respectively. Concluding this thread, we observe that although in the relativistic regime, as opposed to the non-relativistic one [26], we have introduced *four* (i.e., *two* DtN and *two* NtD) operators, in view of the constraining relationships (3.37) we should not expect to be able to formulate more than *two* independent variants of the embedding method for bound states of the Dirac equation.

4. Embedding method with the DtN operators $\hat{\mathcal{B}}^{(\pm)}(\mathcal{E})$

Let us assume that the trial functions $\overline{\Psi}_I(\boldsymbol{r})$ and $\overline{\Psi}_{II}(\boldsymbol{r})$ used in the variational principle (2.7) and (2.8) are such that at the interface $\mathcal{S}$ they match *either* in their upper *or* in their lower spinor components:

$$\beta^{(\pm)}\overline{\Psi}_I(\boldsymbol{\rho}) = \beta^{(\pm)}\overline{\Psi}_{II}(\boldsymbol{\rho}). \tag{4.1}$$

Evidently, with the aid of the identity (A.11), equation (4.1) may be equivalently rewritten as

$$\alpha_\perp^{(\mp)}(\boldsymbol{\rho})\overline{\Psi}_I(\boldsymbol{\rho}) = \alpha_\perp^{(\mp)}(\boldsymbol{\rho})\overline{\Psi}_{II}(\boldsymbol{\rho}). \tag{4.2}$$

Now, substitution of the constraints (4.2) into equation (2.8), followed by some straightforward manipulations exploiting the relationships (A.10) and (A.4), as well as equation (4.1), yields two essentially different functionals:

$$\mathcal{F}^{(\pm)}[\overline{\Psi}_I, \overline{\Psi}_{II}] = \frac{\langle\overline{\Psi}_I|\hat{\mathcal{H}}\overline{\Psi}_I\rangle_I + \langle\overline{\Psi}_{II}|\hat{\mathcal{H}}\overline{\Psi}_{II}\rangle_{II} + c\hbar\left(\overline{\Psi}_I\middle|\mathrm{i}\alpha_\perp^{(\pm)}\overline{\Psi}_I - \mathrm{i}\alpha_\perp^{(\pm)}\overline{\Psi}_{II}\right)}{\langle\overline{\Psi}_I|\overline{\Psi}_I\rangle_I + \langle\overline{\Psi}_{II}|\overline{\Psi}_{II}\rangle_{II}} \tag{4.3}$$

(note that, in the course of considerations leading to equation (4.3), the parameter a has dropped out in a natural way).

In the next step, we require that the outer-region trial function $\overline{\Psi}_{II}(\boldsymbol{r})$, appearing in the functionals (4.3), is chosen to be some, at this stage remaining unknown, function from $\mathcal{D}_{II}(\mathcal{E})$:

$$\overline{\Psi}_{II}(\boldsymbol{r}) = \psi(\mathcal{E}, \boldsymbol{r}) \qquad (\boldsymbol{r} \in \mathcal{V}_{II}) \tag{4.4}$$

where $\mathcal{E} \in \mathbb{R}$ is some estimate of a particular sought eigenenergy E to the eigensystem (2.1) and (2.2). Then, combining equation (4.4) with equations (3.4), (3.3) and (4.1), one obtains

$$\mathrm{i}\alpha_\perp^{(\pm)}(\boldsymbol{\rho})\overline{\Psi}_{II}(\boldsymbol{\rho}) = \gamma^{(\pm)}\hat{\mathcal{B}}^{(\pm)}(\mathcal{E})\overline{\Psi}_I(\boldsymbol{\rho}). \tag{4.5}$$

Insertion of equations (4.4) and (4.5) into equation (4.3) furnishes

$$\mathcal{F}^{(\pm)}[\mathcal{E}; \overline{\Psi}_I, \psi] = \frac{\langle\overline{\Psi}_I|\hat{\mathcal{H}}\overline{\Psi}_I\rangle_I + \mathcal{E}\langle\psi|\psi\rangle_{II} + c\hbar\left(\overline{\Psi}_I\middle|\mathrm{i}\alpha_\perp^{(\pm)}\overline{\Psi}_I - \gamma^{(\pm)}\hat{\mathcal{B}}^{(\pm)}\overline{\Psi}_I\right)}{\langle\overline{\Psi}_I|\overline{\Psi}_I\rangle_I + \langle\psi|\psi\rangle_{II}}. \tag{4.6}$$

The functionals in equation (4.6) depend on $\psi(\mathcal{E}, \boldsymbol{r})$ only through the volume scalar product $\langle\psi|\psi\rangle_{II}$. This dependence may be eliminated in the following way. We differentiate the Dirac equation (3.1) with respect to $\mathcal{E}$, obtaining

$$\hat{\mathcal{H}}\frac{\partial\psi(\mathcal{E}, \boldsymbol{r})}{\partial\mathcal{E}} = \psi(\mathcal{E}, \boldsymbol{r}) + \mathcal{E}\frac{\partial\psi(\mathcal{E}, \boldsymbol{r})}{\partial\mathcal{E}} \qquad (\boldsymbol{r} \in \mathcal{V}_{II}). \tag{4.7}$$

Premultiplying this equation with $\psi^\dagger(\mathcal{E}, \boldsymbol{r})$, postmultiplying the matrix Hermitian conjugate of equation (3.1) with $\partial\psi(\mathcal{E}, \boldsymbol{r})/\partial\mathcal{E}$, and subtracting, after some rearrangements, gives

$$\psi^\dagger(\mathcal{E}, \boldsymbol{r})\psi(\mathcal{E}, \boldsymbol{r}) = -\mathrm{i}c\hbar\boldsymbol{\nabla}\cdot\left[\psi^\dagger(\mathcal{E}, \boldsymbol{r})\boldsymbol{\alpha}\frac{\partial\psi(\mathcal{E}, \boldsymbol{r})}{\partial\mathcal{E}}\right] \qquad (\boldsymbol{r} \in \mathcal{V}_{II}). \tag{4.8}$$

Integrating this throughout the domain $\mathcal{V}_{II}$ and employing the Gauss divergence theorem, one finds

$$\langle\psi|\psi\rangle_{II} = c\hbar\left(\psi\middle|\mathrm{i}\alpha_\perp\frac{\partial\psi}{\partial\mathcal{E}}\right). \tag{4.9}$$

(The absence of the minus sign on the right-hand side of equation (4.9) is a consequence of our convention concerning orientation of the normal unit vector $\boldsymbol{n}(\boldsymbol{\rho})$ at $\mathcal{S}$.) Equation (4.9) may be further transformed, with the aid of the identities (A.1) and (A.3), to yield

$$\langle\psi|\psi\rangle_{II} = c\hbar\left(\psi\middle|\mathrm{i}\alpha_\perp^{(\pm)}\frac{\partial\psi}{\partial\mathcal{E}}\right) - c\hbar\left(\mathrm{i}\alpha_\perp^{(\pm)}\psi\middle|\frac{\partial\psi}{\partial\mathcal{E}}\right) \tag{4.10}$$

or, equivalently,

$$\langle\psi|\psi\rangle_{II} = c\hbar\left(\psi\middle|\frac{\partial}{\partial\mathcal{E}}\mathrm{i}\alpha_\perp^{(\pm)}\psi\right) - c\hbar\left(\mathrm{i}\alpha_\perp^{(\pm)}\psi\middle|\frac{\partial\psi}{\partial\mathcal{E}}\right). \tag{4.11}$$

After employing equation (3.4), the last equation may be rewritten as

$$\langle\psi|\psi\rangle_{II} = c\hbar\gamma^{(\pm)}\left(\psi\middle|\frac{\partial}{\partial\mathcal{E}}\hat{\mathcal{B}}^{(\pm)}\psi\right) - c\hbar\gamma^{(\pm)}\left(\hat{\mathcal{B}}^{(\pm)}\psi\middle|\frac{\partial\psi}{\partial\mathcal{E}}\right). \tag{4.12}$$

Hence, one finds

$$\langle\psi|\psi\rangle_{II} = c\hbar\gamma^{(\pm)}\left(\psi\left|\frac{\partial\hat{\mathcal{B}}^{(\pm)}}{\partial\mathcal{E}}\psi\right.\right) + c\hbar\gamma^{(\pm)}\left(\psi\left|\hat{\mathcal{B}}^{(\pm)}\frac{\partial\psi}{\partial\mathcal{E}}\right.\right) - c\hbar\gamma^{(\pm)}\left(\hat{\mathcal{B}}^{(\pm)}\psi\left|\frac{\partial\psi}{\partial\mathcal{E}}\right.\right). \tag{4.13}$$

Because of the Hermiticity properties of their kernels, expressed by equation (3.34), the DtN operators $\hat{\mathcal{B}}^{(\pm)}(\mathcal{E})$ are Hermitian with respect to the surface scalar product (2.13). Consequently, the second and the third terms on the right-hand side of equation (4.13) cancel out and one gets

$$\langle\psi|\psi\rangle_{II} = c\hbar\gamma^{(\pm)}\left(\psi\left|\frac{\partial\hat{\mathcal{B}}^{(\pm)}}{\partial\mathcal{E}}\psi\right.\right). \tag{4.14}$$

In the final step, the right-hand side of the above equation is transformed with the aid of equations (3.3), (A.4), (4.4) and (4.1), which results in the sought relationship:

$$\langle\psi|\psi\rangle_{II} = c\hbar\gamma^{(\pm)}\left(\overline{\Psi}_I\left|\frac{\partial\hat{\mathcal{B}}^{(\pm)}}{\partial\mathcal{E}}\overline{\Psi}_I\right.\right). \tag{4.15}$$

Inserting equation (4.15) into equation (4.6) furnishes two functionals

$$\mathcal{F}^{(\pm)}[\mathcal{E};\overline{\Psi}_I] = \frac{\langle\overline{\Psi}_I|\hat{\mathcal{H}}\overline{\Psi}_I\rangle_I + c\hbar\left(\overline{\Psi}_I\left|\mathrm{i}\alpha_\perp^{(\pm)}\overline{\Psi}_I - \gamma^{(\pm)}\hat{\mathcal{B}}^{(\pm)}\overline{\Psi}_I + \gamma^{(\pm)}\mathcal{E}[\partial\hat{\mathcal{B}}^{(\pm)}/\partial\mathcal{E}]\overline{\Psi}_I\right.\right)}{\langle\overline{\Psi}_I|\overline{\Psi}_I\rangle_I + c\hbar\gamma^{(\pm)}(\overline{\Psi}_I|[\partial\hat{\mathcal{B}}^{(\pm)}/\partial\mathcal{E}]\overline{\Psi}_I)} \tag{4.16}$$

which depend solely on the trial function $\overline{\Psi}_I(\boldsymbol{r})$ defined in the interior of the volume $\mathcal{V}_I$ and on the surface $\mathcal{S}$. It may be readily verified that both functionals in equation (4.16) assume real values for an arbitrary $\overline{\Psi}_I(\boldsymbol{r})$.

Given the functionals (4.16), we shall seek the functions $\widetilde{\Psi}_I^{(\pm)}(\mathcal{E},\boldsymbol{r})$, $(\boldsymbol{r}\in\mathcal{V}_I)$, which make these functionals stationary:

$$\delta\mathcal{F}^{(\pm)}\big[\mathcal{E};\widetilde{\Psi}_I^{(\pm)}\big] = 0. \tag{4.17}$$

(The superscripts at $\widetilde{\Psi}_I^{(\pm)}(\mathcal{E},\boldsymbol{r})$ indicate that, in general, extremals of $\mathcal{F}^{(+)}$ and $\mathcal{F}^{(-)}$ will differ.) If these functions are considered as approximations (in the interior domain $\mathcal{V}_I$) to some particular eigenfunction $\Psi(E,\boldsymbol{r})$ of the spectral problem (2.1) and (2.2), the corresponding stationary values

$$\widetilde{E}^{(\pm)}(\mathcal{E}) = \mathcal{F}^{(\pm)}\big[\mathcal{E};\widetilde{\Psi}_I^{(\pm)}\big] \tag{4.18}$$

are estimates to the associated eigenenergy E. To find eigensystems determining $\widetilde{E}^{(\pm)}(\mathcal{E})$ and $\widetilde{\Psi}_I^{(\pm)}(\mathcal{E},\boldsymbol{r})$, it is first convenient to rewrite equation (4.16) as

$$\begin{aligned}\mathcal{F}^{(\pm)}[\mathcal{E};\overline{\Psi}_I]&\left[\langle\overline{\Psi}_I|\overline{\Psi}_I\rangle_I + c\hbar\gamma^{(\pm)}\left(\overline{\Psi}_I\left|\frac{\partial\hat{\mathcal{B}}^{(\pm)}}{\partial\mathcal{E}}\overline{\Psi}_I\right.\right)\right]\\ &= \langle\overline{\Psi}_I|\hat{\mathcal{H}}\overline{\Psi}_I\rangle_I + c\hbar\left(\overline{\Psi}_I\left|\mathrm{i}\alpha_\perp^{(\pm)}\overline{\Psi}_I - \gamma^{(\pm)}\hat{\mathcal{B}}^{(\pm)}\overline{\Psi}_I + \gamma^{(\pm)}\mathcal{E}\frac{\partial\hat{\mathcal{B}}^{(\pm)}}{\partial\mathcal{E}}\overline{\Psi}_I\right.\right)\end{aligned} \tag{4.19}$$

and then vary there $\overline{\Psi}_I(\boldsymbol{r})$ around $\widetilde{\Psi}_I^{(\pm)}(\mathcal{E},\boldsymbol{r})$. After exploiting equations (4.17) and (4.18), this yields

$$\begin{aligned}&\big\langle\delta\overline{\Psi}_I\big|[\hat{\mathcal{H}}-\widetilde{E}^{(\pm)}]\widetilde{\Psi}_I^{(\pm)}\big\rangle_I + \big\langle\widetilde{\Psi}_I^{(\pm)}\big|[\hat{\mathcal{H}}-\widetilde{E}^{(\pm)}]\delta\overline{\Psi}_I\big\rangle_I\\ &\quad + c\hbar\left(\delta\overline{\Psi}_I\left|\mathrm{i}\alpha_\perp^{(\pm)}\widetilde{\Psi}_I^{(\pm)} - \gamma^{(\pm)}\hat{\mathcal{B}}^{(\pm)}\widetilde{\Psi}_I^{(\pm)} + \gamma^{(\pm)}[\mathcal{E}-\widetilde{E}^{(\pm)}]\frac{\partial\hat{\mathcal{B}}^{(\pm)}}{\partial\mathcal{E}}\widetilde{\Psi}_I^{(\pm)}\right.\right)\\ &\quad + c\hbar\left(\widetilde{\Psi}_I^{(\pm)}\left|\mathrm{i}\alpha_\perp^{(\pm)}\delta\overline{\Psi}_I - \gamma^{(\pm)}\hat{\mathcal{B}}^{(\pm)}\delta\overline{\Psi}_I + \gamma^{(\pm)}[\mathcal{E}-\widetilde{E}^{(\pm)}]\frac{\partial\hat{\mathcal{B}}^{(\pm)}}{\partial\mathcal{E}}\delta\overline{\Psi}_I\right.\right) = 0.\end{aligned} \tag{4.20}$$

Applying the Gauss divergence formula to the second term on the left-hand side of equation (4.20), and utilizing the fact that $\hat{\mathcal{B}}^{(\pm)}(\mathcal{E})$, hence also $\partial\hat{\mathcal{B}}^{(\pm)}(\mathcal{E})/\partial\mathcal{E}$, are Hermitian with respect to the surface scalar product (2.13), gives

$$\begin{aligned}\big\langle\delta\overline{\Psi}_I\big|[\hat{\mathcal{H}}-\widetilde{E}^{(\pm)}]\widetilde{\Psi}_I^{(\pm)}\big\rangle_I+\big\langle[\hat{\mathcal{H}}-\widetilde{E}^{(\pm)}]\widetilde{\Psi}_I^{(\pm)}\big|\delta\overline{\Psi}_I\big\rangle_I\\ +c\hbar\left(\delta\overline{\Psi}_I\left|\mathrm{i}\alpha_\perp^{(\pm)}\widetilde{\Psi}_I^{(\pm)}-\gamma^{(\pm)}\hat{\mathcal{B}}^{(\pm)}\widetilde{\Psi}_I^{(\pm)}+\gamma^{(\pm)}[\mathcal{E}-\widetilde{E}^{(\pm)}]\frac{\partial\hat{\mathcal{B}}^{(\pm)}}{\partial\mathcal{E}}\widetilde{\Psi}_I^{(\pm)}\right.\right)\\ +c\hbar\left(\mathrm{i}\alpha_\perp^{(\pm)}\widetilde{\Psi}_I^{(\pm)}-\gamma^{(\pm)}\hat{\mathcal{B}}^{(\pm)}\widetilde{\Psi}_I^{(\pm)}+\gamma^{(\pm)}[\mathcal{E}-\widetilde{E}^{(\pm)}]\frac{\partial\hat{\mathcal{B}}^{(\pm)}}{\partial\mathcal{E}}\widetilde{\Psi}_I^{(\pm)}\left|\delta\overline{\Psi}_I\right.\right).\end{aligned}\tag{4.21}$$

Hence, in virtue of arbitrariness of the variations $\delta\overline{\Psi}_I(\boldsymbol{r})$ and $\delta\overline{\Psi}_I(\boldsymbol{\rho})$, one deduces the sought integro-differential eigensystems

$$\hat{\mathcal{H}}\widetilde{\Psi}_I^{(\pm)}(\mathcal{E},\boldsymbol{r})=\widetilde{E}^{(\pm)}(\mathcal{E})\widetilde{\Psi}_I^{(\pm)}(\mathcal{E},\boldsymbol{r})\qquad(\boldsymbol{r}\in\mathcal{V}_I)\tag{4.22}$$

$$\begin{aligned}&\left[\mathrm{i}\alpha_\perp^{(\pm)}(\boldsymbol{\rho})\hat{\mathcal{I}}_{\mathcal{S}}-\gamma^{(\pm)}\hat{\mathcal{B}}^{(\pm)}(\mathcal{E})+\gamma^{(\pm)}\mathcal{E}\frac{\partial\hat{\mathcal{B}}^{(\pm)}(\mathcal{E})}{\partial\mathcal{E}}\right]\widetilde{\Psi}_I^{(\pm)}(\mathcal{E},\boldsymbol{\rho})\\ &\qquad=\gamma^{(\pm)}\widetilde{E}^{(\pm)}(\mathcal{E})\frac{\partial\hat{\mathcal{B}}^{(\pm)}(\mathcal{E})}{\partial\mathcal{E}}\widetilde{\Psi}_I^{(\pm)}(\mathcal{E},\boldsymbol{\rho})\qquad(\boldsymbol{\rho}\in\mathcal{S})\end{aligned}\tag{4.23}$$

obeyed by $\widetilde{\Psi}_I^{(\pm)}(\mathcal{E},\boldsymbol{r})$ and $\widetilde{E}^{(\pm)}(\mathcal{E})$. Since the eigenvalues $\widetilde{E}^{(\pm)}(\mathcal{E})$ appear both in the Dirac equations (4.22) and in the boundary conditions (4.23), the eigensystems constituted by these equations are of a non-standard (albeit this time also non-Steklov) character. We recall that, in general, the eigensolutions $\{\widetilde{E}^{(+)}(\mathcal{E}),\widetilde{\Psi}_I^{(+)}(\mathcal{E},\boldsymbol{r})\}$ will *differ* from the eigensolutions $\{\widetilde{E}^{(-)}(\mathcal{E}),\widetilde{\Psi}_I^{(-)}(\mathcal{E},\boldsymbol{r})\}$.

At this stage, we already know equations from which the functions $\widetilde{\Psi}_I^{(\pm)}(\mathcal{E},\boldsymbol{r})$, approximating the eigenfunction $\Psi(E,\boldsymbol{r})$ in $\mathcal{V}_I$, may be determined. However, thus far the function $\psi(\mathcal{E},\boldsymbol{r})\in\mathcal{D}_{II}(\mathcal{E})$, approximating the eigenfunction $\Psi(E,\boldsymbol{r})$ in $\mathcal{V}_{II}$, has played an entirely auxiliary role in our considerations and we have paid no attention to the problem of its determination. Since we need to approximate $\Psi(E,\boldsymbol{r})$ throughout the whole space $\mathbb{R}^3$, we have to face this problem now.

We begin with the observation that each of the two interior estimates $\widetilde{\Psi}_I^{(\pm)}(\mathcal{E},\boldsymbol{r})$ should give rise to its corresponding exterior estimate

$$\widetilde{\Psi}_{II}^{(\pm)}(\mathcal{E},\boldsymbol{r})\equiv\psi^{(\pm)}(\mathcal{E},\boldsymbol{r})\qquad(\boldsymbol{r}\in\mathcal{V}_{II})\tag{4.24}$$

such that (cf equation (4.1))

$$\beta^{(\pm)}\widetilde{\Psi}_I^{(\pm)}(\mathcal{E},\boldsymbol{\rho})=\beta^{(\pm)}\widetilde{\Psi}_{II}^{(\pm)}(\mathcal{E},\boldsymbol{\rho}).\tag{4.25}$$

To find the functions $\widetilde{\Psi}_{II}^{(\pm)}(\mathcal{E},\boldsymbol{r})$, we expand them in the Steklov basis $\{\psi_n(\mathcal{E},\boldsymbol{r})\}$:

$$\widetilde{\Psi}_{II}^{(\pm)}(\mathcal{E},\boldsymbol{r})=\sum_n c_n^{(\pm)}(\mathcal{E})\psi_n(\mathcal{E},\boldsymbol{r})\qquad(\boldsymbol{r}\in\mathcal{V}_{II})\tag{4.26}$$

with the coefficients $\{c_n^{(\pm)}(\mathcal{E})\}$ to be determined. Letting the point $\boldsymbol{r}$ tend in equation (4.26) to the surface $\mathcal{S}$, operating on the result with $\beta^{(\pm)}$ and employing equation (4.25) gives

$$\beta^{(\pm)}\widetilde{\Psi}_I^{(\pm)}(\mathcal{E},\boldsymbol{\rho})=\sum_n c_n^{(\pm)}(\mathcal{E})\beta^{(\pm)}\psi_n(\mathcal{E},\boldsymbol{\rho}).\tag{4.27}$$

Then, projecting equation (4.27) onto the surface parts of the Steklov eigenfunctions $\{\psi_n(\mathcal{E},\boldsymbol{r})\}$ and exploiting subsequently the orthogonality relations (3.23) and (3.26), yields

$$c_n^{(+)}(\mathcal{E}) = \left(\psi_n \middle| \beta^{(+)}\widetilde{\Psi}_I^{(+)}\right) \tag{4.28a}$$

$$c_n^{(-)}(\mathcal{E}) = (\gamma^{(-)})^2 b_n^{-2}(\mathcal{E})\left(\psi_n \middle| \beta^{(-)}\widetilde{\Psi}_I^{(-)}\right). \tag{4.28b}$$

Insertion of equations (4.28*a*) and (4.28*b*) into equation (4.26) completes the problem of finding the estimates $\widetilde{\Psi}_{II}^{(\pm)}(\mathcal{E}, \boldsymbol{r})$ of the eigenfunction $\Psi(E, \boldsymbol{r})$ in the exterior domain $\mathcal{V}_{II}$.

5. Embedding method with the NtD operators $\hat{\mathcal{R}}^{(\pm)}(\mathcal{E})$

In considerations of section 4, extensive use has been made of the DtN operators $\hat{\mathcal{B}}^{(\pm)}(\mathcal{E})$. However, nothing prevents one to formulate the method in terms of the NtD operators $\hat{\mathcal{R}}^{(\pm)}(\mathcal{E})$. Most easily, this goal may be achieved rewriting the main results of section 4 with the aid of the relationships (3.37) and some of the identities listed in the appendix. In this way, for the volume integral $\langle\psi|\psi\rangle_{II}$ one obtains

$$\langle\psi|\psi\rangle_{II} = c\hbar\gamma^{(\pm)}\left(\mathrm{i}\alpha_\perp^{(\mp)}\overline{\Psi}_I \middle| \frac{\partial\hat{\mathcal{R}}^{(\mp)}}{\partial\mathcal{E}}\mathrm{i}\alpha_\perp^{(\mp)}\overline{\Psi}_I\right) \tag{5.1}$$

the functionals (4.16) transform into

$$\begin{aligned}\mathcal{F}^{(\pm)}[\mathcal{E}; \overline{\Psi}_I] = {} & \frac{\langle\overline{\Psi}_I|\hat{\mathcal{H}}\overline{\Psi}_I\rangle_I}{\langle\overline{\Psi}_I|\overline{\Psi}_I\rangle_I + c\hbar\gamma^{(\pm)}\left(\mathrm{i}\alpha_\perp^{(\mp)}\overline{\Psi}_I\middle|[\partial\hat{\mathcal{R}}^{(\mp)}/\partial\mathcal{E}]\mathrm{i}\alpha_\perp^{(\mp)}\overline{\Psi}_I\right)} \\ & + \frac{c\hbar\left(\mathrm{i}\alpha_\perp^{(\mp)}\overline{\Psi}_I\middle|\gamma^{(\pm)}\mathcal{E}[\partial\hat{\mathcal{R}}^{(\mp)}/\partial\mathcal{E}]\mathrm{i}\alpha_\perp^{(\mp)}\overline{\Psi}_I - \gamma^{(\pm)}\hat{\mathcal{R}}^{(\mp)}\mathrm{i}\alpha_\perp^{(\mp)}\overline{\Psi}_I - \beta^{(\mp)}\overline{\Psi}_I\right)}{\langle\overline{\Psi}_I|\overline{\Psi}_I\rangle_I + c\hbar\gamma^{(\pm)}\left(\mathrm{i}\alpha_\perp^{(\mp)}\overline{\Psi}_I\middle|[\partial\hat{\mathcal{R}}^{(\mp)}/\partial\mathcal{E}]\mathrm{i}\alpha_\perp^{(\mp)}\overline{\Psi}_I\right)}\end{aligned} \tag{5.2}$$

while the boundary conditions (4.23) obeyed by the extremals $\widetilde{\Psi}_I^{(\pm)}(\mathcal{E}, \boldsymbol{r})$ (defined by equation (4.17)) of the above functionals become

$$\begin{aligned}&\left[\beta^{(\mp)}\hat{\mathcal{I}}_{\mathcal{S}} + \gamma^{(\pm)}\hat{\mathcal{R}}^{(\mp)}(\mathcal{E})\mathrm{i}\alpha_\perp^{(\mp)}(\boldsymbol{\rho}) - \gamma^{(\pm)}\mathcal{E}\frac{\partial\hat{\mathcal{R}}^{(\mp)}(\mathcal{E})}{\partial\mathcal{E}}\mathrm{i}\alpha_\perp^{(\mp)}(\boldsymbol{\rho})\right]\widetilde{\Psi}_I^{(\pm)}(\mathcal{E}, \boldsymbol{\rho}) \\ &\qquad = -\gamma^{(\pm)}\widetilde{E}^{(\pm)}(\mathcal{E})\frac{\partial\hat{\mathcal{R}}^{(\mp)}(\mathcal{E})}{\partial\mathcal{E}}\mathrm{i}\alpha_\perp^{(\mp)}(\boldsymbol{\rho})\widetilde{\Psi}_I^{(\pm)}(\mathcal{E}, \boldsymbol{\rho}) \qquad (\boldsymbol{\rho}\in\mathcal{S})\end{aligned} \tag{5.3}$$

(throughout the domain $\mathcal{V}_I$, the extremals $\widetilde{\Psi}_I^{(\pm)}(\mathcal{E}, \boldsymbol{r})$ still satisfy the Dirac equation (4.22)).

It has to be emphasized that the two NtD embedding approaches based on the use of the operators $\hat{\mathcal{R}}^{(\pm)}(\mathcal{E})$ are completely equivalent to the two DtN embedding methods exploiting the operators $\hat{\mathcal{B}}^{(\mp)}(\mathcal{E})$ (notice, however, the arrangements of the superscripts).

The reader is suggested to compare results of sections 4 and 5 of the present paper with those from sections IV and V of [26].

6. Algebraization of the variational principle (4.16)–(4.18)

Let $\{\phi_\mu(\boldsymbol{r})\}$, $(\mu = 1, \ldots, M)$, be a set of suitably chosen four-component spinor functions defined in $\overline{\mathcal{V}}_I$. Consider the following approximation:

$$\overline{\Psi}_I(\boldsymbol{r}) \equiv \overline{\Phi}(\boldsymbol{r}) = \sum_{\mu=1}^{M}\overline{a}_\mu\phi_\mu(\boldsymbol{r}) \qquad (\boldsymbol{r}\in\mathcal{V}_I) \tag{6.1}$$

to some particular eigenfunctions $\widetilde{\Psi}_I^{(\pm)}(\mathcal{E},\boldsymbol{r})$ of the integro-differential system (4.22) and (4.23); at this stage, the coefficients $\{\overline{a}_\mu\}$ remain undetermined. Insertion of this function into the functionals defined in equations (4.16) yields the Rayleigh quotients

$$F^{(\pm)}[\mathcal{E},\overline{\mathsf{a}}^\dagger,\overline{\mathsf{a}}]=\frac{\overline{\mathsf{a}}^\dagger\Lambda^{(\pm)}(\mathcal{E})\overline{\mathsf{a}}}{\overline{\mathsf{a}}^\dagger\Delta^{(\pm)}(\mathcal{E})\overline{\mathsf{a}}} \tag{6.2}$$

in which $\overline{\mathsf{a}}$ is an M-component column vector with elements $\{\overline{a}_\mu\}$, while $\Lambda^{(\pm)}(\mathcal{E})$ and $\Delta^{(\pm)}(\mathcal{E})$ are $M\times M$ Hermitian matrices with elements

$$\Lambda_{\mu\nu}^{(\pm)}(\mathcal{E})=\langle\phi_\mu|\hat{\mathcal{H}}\phi_\nu\rangle_I+c\hbar\big(\phi_\mu\big|\mathrm{i}\alpha_\perp^{(\pm)}\phi_\nu-\gamma^{(\pm)}\hat{\mathcal{B}}^{(\pm)}\phi_\nu+\gamma^{(\pm)}\mathcal{E}[\partial\hat{\mathcal{B}}^{(\pm)}/\partial\mathcal{E}]\phi_\nu\big) \tag{6.3}$$

and

$$\Delta_{\mu\nu}^{(\pm)}(\mathcal{E})=\langle\phi_\mu|\phi_\nu\rangle_I+c\hbar\gamma^{(\pm)}\big(\phi_\mu\big|[\partial\hat{\mathcal{B}}^{(\pm)}/\partial\mathcal{E}]\phi_\nu\big) \tag{6.4}$$

respectively. Varying independently the vectors $\overline{\mathsf{a}}$ and $\overline{\mathsf{a}}^\dagger$, denoting by $\widetilde{\mathsf{a}}^{(\pm)}(\mathcal{E})$ and $\widetilde{\mathsf{a}}^{(\pm)\dagger}(\mathcal{E})$ these particular $\overline{\mathsf{a}}$ and $\overline{\mathsf{a}}^\dagger$, for which the functionals in equation (6.2) are stationary:

$$\delta F^{(\pm)}[\mathcal{E},\widetilde{\mathsf{a}}^{(\pm)\dagger}(\mathcal{E}),\widetilde{\mathsf{a}}^{(\pm)}(\mathcal{E})]=0 \tag{6.5}$$

and defining

$$\widetilde{\mathscr{E}}^{(\pm)}(\mathcal{E})=F^{(\pm)}[\mathcal{E},\widetilde{\mathsf{a}}^{(\pm)\dagger}(\mathcal{E}),\widetilde{\mathsf{a}}^{(\pm)}(\mathcal{E})] \tag{6.6}$$

leads to the weighted algebraic eigensystems

$$\Lambda^{(\pm)}(\mathcal{E})\widetilde{\mathsf{a}}^{(\pm)}(\mathcal{E})=\widetilde{\mathscr{E}}^{(\pm)}(\mathcal{E})\Delta^{(\pm)}(\mathcal{E})\widetilde{\mathsf{a}}^{(\pm)}(\mathcal{E}) \tag{6.7}$$

and their Hermitian conjugates. In general, the eigensystems (6.7) have $M^{(\pm)}\leqslant M$ eigenvalues $\big\{\widetilde{\mathscr{E}}_\gamma^{(\pm)}(\mathcal{E})\big\}$ and associated eigenvectors $\big\{\widetilde{\mathsf{a}}_\gamma^{(\pm)}(\mathcal{E})\big\}$. These eigenvalues are second-order variational estimates of some from among eigenvalues of the system (4.22) and (4.23). Moreover, use of the components $\big\{\widetilde{a}_{\mu\gamma}^{(\pm)}(\mathcal{E})\big\}$ of the eigenvectors $\big\{\widetilde{\mathsf{a}}_\gamma^{(\pm)}(\mathcal{E})\big\}$ in equation (6.1) results in $M^{(\pm)}$ functions

$$\widetilde{\Phi}_\gamma^{(\pm)}(\mathcal{E},\boldsymbol{r})=\sum_{\mu=1}^{M}\widetilde{a}_{\mu\gamma}^{(\pm)}(\mathcal{E})\phi_\mu(\boldsymbol{r})\qquad(\boldsymbol{r}\in\mathcal{V}_I) \tag{6.8}$$

which are first-order variational estimates of the eigenfunctions $\widetilde{\Psi}_I^{(\pm)}(\mathcal{E},\boldsymbol{r})$ associated with some from among the eigenvalues $\widetilde{E}^{(\pm)}(\mathcal{E})$.

7. Problems with spherical symmetry in the outer region

7.1. Generalities

Thus far, in our considerations neither we have been imposing any restrictions on the shape of the interface $\mathcal{S}$ separating the domains $\mathcal{V}_I$ and $\mathcal{V}_{II}$ (except for assuming that $\mathcal{S}$ is sufficiently smooth), nor we have been constraining a functional form of the potential $V(\boldsymbol{r})$. In this section, we shall confine ourselves to the particular case when this interface, denoted hereafter $\mathcal{S}_\rho$, is a spherical shell of radius ρ. Moreover, locating an origin of a coordinate system used in the centre of the sphere $\mathcal{V}_I$, we shall be assuming that in the outer region $\mathcal{V}_{II}$ the potential $V(\boldsymbol{r})$ is central:

$$V(\boldsymbol{r})=V(r)\qquad(r\geqslant\rho). \tag{7.1}$$

With the above assumptions, the Dirac equation (3.12) is separable in $\mathcal{V}_{II}$ in spherical coordinates and possesses elementary solutions of the form

$$\psi_{\varkappa\mu}(\mathcal{E},\boldsymbol{r})=\frac{1}{rf_\varkappa(\mathcal{E},\rho)}\begin{pmatrix}f_\varkappa(\mathcal{E},r)\Omega_{\varkappa\mu}(\boldsymbol{n}_r)\\ \mathrm{i}g_\varkappa(\mathcal{E},r)\Omega_{-\varkappa\mu}(\boldsymbol{n}_r)\end{pmatrix}\qquad(r\geqslant\rho) \tag{7.2}$$

(here $\Omega_{\varkappa\mu}(\boldsymbol{n}_r)$, with $\boldsymbol{n}_r = \boldsymbol{r}/r$, $\varkappa = \pm1, \pm2, \ldots$, and $\mu = \pm\frac{1}{2}, \ldots, \pm\left(|\varkappa| - \frac{1}{2}\right)$, is a spherical spinor), provided the radial functions $f_\varkappa(\mathcal{E}, r)$ and $g_\varkappa(\mathcal{E}, r)$ obey the radial Dirac system

$$\begin{pmatrix} mc^2 - \mathcal{E} + V(r) & c\hbar(-\partial/\partial r + \varkappa/r) \\ c\hbar(\partial/\partial r + \varkappa/r) & -mc^2 - \mathcal{E} + V(r) \end{pmatrix} \begin{pmatrix} f_\varkappa(\mathcal{E}, r) \\ g_\varkappa(\mathcal{E}, r) \end{pmatrix} = 0 \qquad (r \geqslant \rho). \tag{7.3}$$

To enforce the functions (7.2) to obey the asymptotic condition (3.13), we subject the solutions of equation (7.3) to the constraints

$$\lim_{r\to\infty} r^{1/2} f_\varkappa(\mathcal{E}, r) = 0 \qquad \lim_{r\to\infty} r^{1/2} g_\varkappa(\mathcal{E}, r) = 0. \tag{7.4}$$

Since the matrix differential operator in equation (7.3) is real, imposing the limiting conditions (7.4) implies that the functions $f_\varkappa(\mathcal{E}, r)$ and $g_\varkappa(\mathcal{E}, r)$ are real up to a common multiplicative factor. Finally, exploiting the well-known property of the spherical spinors:

$$\boldsymbol{n}\cdot\boldsymbol{\sigma}\Omega_{\varkappa\mu}(\boldsymbol{n}) = -\Omega_{-\varkappa\mu}(\boldsymbol{n}) \tag{7.5}$$

($\boldsymbol{\sigma}$ is the Pauli matrix vector) and observing that in the present context it holds that $\boldsymbol{n}(\boldsymbol{\rho}) = \boldsymbol{n}_\rho$, we find that on the surface $\mathcal{S}_\rho$ the functions (7.2) obey the boundary condition (3.14) (or, equivalently, (3.25)) with

$$b_\varkappa(\mathcal{E}) = -\gamma^{(-)}\frac{g_\varkappa(\mathcal{E}, \rho)}{f_\varkappa(\mathcal{E}, \rho)}. \tag{7.6}$$

Hence, it follows that the functions (7.2) are the Steklov eigenfunctions for the problem at hand, while the real numbers (7.6) are the associated, μ-independent (hence, $2|\varkappa|$-fold degenerate), Steklov eigenvalues.

The multiplier $1/f_\varkappa(\mathcal{E}, \rho)$ in the definition of the Steklov eigenfunctions (7.2), together with the orthonormality relation for the spherical spinors:

$$\oint_{4\pi} \mathrm{d}^2\boldsymbol{n}\, \Omega^\dagger_{\varkappa\mu}(\boldsymbol{n})\Omega_{\varkappa'\mu'}(\boldsymbol{n}) = \delta_{\varkappa\varkappa'}\delta_{\mu\mu'} \tag{7.7}$$

guarantee that the Steklov eigenfunctions (7.2) satisfy the orthonormality relation (3.23), which in the present case reads

$$(\psi_{\varkappa\mu}|\beta^{(+)}\psi_{\varkappa'\mu'}) = \delta_{\varkappa\varkappa'}\delta_{\mu\mu'}. \tag{7.8}$$

In addition, exploiting the known completeness relation for the spherical spinors:

$$\sum_{\substack{\varkappa=-\infty \\ (\varkappa\neq0)}}^{\infty} \sum_{\mu=-|\varkappa|+1/2}^{|\varkappa|-1/2} \Omega_{\varkappa\mu}(\boldsymbol{n}_\rho)\Omega^\dagger_{\varkappa\mu}(\boldsymbol{n}'_\rho) = \pi^{-1}\delta(1 - \boldsymbol{n}_\rho\cdot\boldsymbol{n}'_\rho)I \equiv \rho^2\delta^{(2)}_{\mathcal{S}_\rho}(\boldsymbol{\rho} - \boldsymbol{\rho}')I \tag{7.9}$$

(I is the 2×2 unit matrix), with no difficulty one obtains that

$$\sum_{\substack{\varkappa=-\infty \\ (\varkappa\neq0)}}^{\infty} \sum_{\mu=-|\varkappa|+1/2}^{|\varkappa|-1/2} \beta^{(+)}\psi_{\varkappa\mu}(\mathcal{E}, \boldsymbol{\rho})\psi^\dagger_{\varkappa\mu}(\mathcal{E}, \boldsymbol{\rho}')\beta^{(+)} = \delta^{(2)}_{\mathcal{S}_\rho}(\boldsymbol{\rho} - \boldsymbol{\rho}')\beta^{(+)} \tag{7.10}$$

i.e., the relation (3.24) particularized to the present case. (Observe that while in section 3 the validity of the closure relation (3.24) for an arbitrarily shaped interface $\mathcal{S}$ has been *postulated* by us, above we have shown that the validity of its particular form (7.10) for the spherically shaped $\mathcal{S}(=\mathcal{S}_\rho)$ may be *proved*.) Finally, inserting equations (7.2) and (7.6) into the right-hand sides of equations (3.30)–(3.33), after utilizing the following summation formula for the spherical spinors [52, 53]:

$$\sum_{\mu=-|\varkappa|+1/2}^{|\varkappa|-1/2} \Omega_{\varkappa\mu}(\boldsymbol{n})\Omega^\dagger_{\varkappa\mu}(\boldsymbol{n}') \equiv \Pi_\varkappa(\boldsymbol{n}, \boldsymbol{n}') = \frac{|\varkappa|}{4\pi}P_l(\boldsymbol{n}\cdot\boldsymbol{n}')I + \mathrm{i}\frac{\mathrm{sgn}(\varkappa)}{4\pi}P'_l(\boldsymbol{n}\cdot\boldsymbol{n}')(\boldsymbol{n}\times\boldsymbol{n}')\cdot\boldsymbol{\sigma} \tag{7.11}$$

where

$$l = \left|\varkappa + \tfrac{1}{2}\right| - \tfrac{1}{2} \tag{7.12}$$

$P_l(x)$ is the Legendre polynomial [54, section 5.4], and $P_l'(x)$ is its first derivative with respect to the variable x, one finds that for problems exhibiting the spherical symmetry in the outer domain, the spectral expansions of the DtN and NtD kernels can be cast into the following forms:

$$\mathcal{B}^{(+)}(\mathcal{E}, \boldsymbol{\rho}, \boldsymbol{\rho}') = \rho^{-2} \sum_{\substack{\varkappa=-\infty \\ (\varkappa\neq 0)}}^{\infty} b_\varkappa(\mathcal{E}) \begin{pmatrix} \Pi_\varkappa(\boldsymbol{n}_\rho, \boldsymbol{n}_\rho') & 0 \\ 0 & 0 \end{pmatrix} \tag{7.13a}$$

$$\mathcal{B}^{(-)}(\mathcal{E}, \boldsymbol{\rho}, \boldsymbol{\rho}') = \rho^{-2} \sum_{\substack{\varkappa=-\infty \\ (\varkappa\neq 0)}}^{\infty} b_\varkappa^{-1}(\mathcal{E}) \begin{pmatrix} 0 & 0 \\ 0 & \Pi_{-\varkappa}(\boldsymbol{n}_\rho, \boldsymbol{n}_\rho') \end{pmatrix} \tag{7.13b}$$

$$\mathcal{R}^{(+)}(\mathcal{E}, \boldsymbol{\rho}, \boldsymbol{\rho}') = \rho^{-2} \sum_{\substack{\varkappa=-\infty \\ (\varkappa\neq 0)}}^{\infty} b_\varkappa^{-1}(\mathcal{E}) \begin{pmatrix} \Pi_\varkappa(\boldsymbol{n}_\rho, \boldsymbol{n}_\rho') & 0 \\ 0 & 0 \end{pmatrix} \tag{7.14a}$$

$$\mathcal{R}^{(-)}(\mathcal{E}, \boldsymbol{\rho}, \boldsymbol{\rho}') = \rho^{-2} \sum_{\substack{\varkappa=-\infty \\ (\varkappa\neq 0)}}^{\infty} b_\varkappa(\mathcal{E}) \begin{pmatrix} 0 & 0 \\ 0 & \Pi_{-\varkappa}(\boldsymbol{n}_\rho, \boldsymbol{n}_\rho') \end{pmatrix} \tag{7.14b}$$

with zeros denoting 2×2 null matrices. From the above, it is seen that, in the case considered here, the DtN and NtD kernels depend on $\mathcal{E}$ solely through the dependence of the Steklov eigenvalues $\{b_\varkappa(\mathcal{E})\}$ on this parameter.

It appears that, in principle, it is possible to compute the Steklov eigenvalue $b_\varkappa(\mathcal{E})$ by solving a nonlinear Riccati-type differential equation. To show this, we define the radial function

$$b_\varkappa(\mathcal{E}, r) = -\gamma^{(-)} \frac{g_\varkappa(\mathcal{E}, r)}{f_\varkappa(\mathcal{E}, r)} \qquad (r \geqslant \rho). \tag{7.15}$$

Combining this definition with the definition (7.6), one has

$$b_\varkappa(\mathcal{E}) = b_\varkappa(\mathcal{E}, \rho). \tag{7.16}$$

Further, differentiating equation (7.15) with respect to r and transforming subsequently the right-hand side of the resulting equation with the aid of the definition (7.15) and the system (7.3), yields the sought nonlinear equation [55–59]

$$\begin{aligned} \frac{\partial b_\varkappa(\mathcal{E}, r)}{\partial r} = &-\frac{\gamma^{(+)}}{c\hbar}[\mathcal{E} + mc^2 - V(r)]b_\varkappa^2(\mathcal{E}, r) + 2\frac{\varkappa}{r}b_\varkappa(\mathcal{E}, r) \\ &+ \frac{\gamma^{(-)}}{c\hbar}[\mathcal{E} - mc^2 - V(r)] \qquad (r \geqslant \rho) \end{aligned} \tag{7.17}$$

which should be integrated *inwards*, from $r = \infty$ down to $r = \rho$, subject to the initial condition

$$b_\varkappa(\mathcal{E}, \infty) = -\gamma^{(-)} \lim_{r\to\infty} \frac{g_\varkappa(\mathcal{E}, r)}{f_\varkappa(\mathcal{E}, r)}. \tag{7.18}$$

The limit on the right-hand side of the above equation may be found by analysing asymptotic forms of solutions to the radial system (7.3).

Unfortunately, equation (7.17) appears to be unsuitable for computational purposes because of singularities occurring in the function $b_\varkappa(\mathcal{E}, r)$ at some intermediate values of the variable r. The remedy is to introduce a new function, $\varphi_\varkappa(\mathcal{E}, r)$, related to $b_\varkappa(\mathcal{E}, r)$ through

$$b_\varkappa(\mathcal{E}, r) = -\gamma^{(-)} \tan \varphi_\varkappa(\mathcal{E}, r) \qquad (r \geqslant \rho). \tag{7.19}$$

This function appears to be free of afflicting singularities and satisfies the following, easily derivable from equations (7.19) and (7.17), nonlinear differential equation

$$\frac{\partial \varphi_\varkappa(\mathcal{E}, r)}{\partial r} = -\frac{1}{2}\gamma^{(-)} \cos[2\varphi_\varkappa(\mathcal{E}, r)] + \frac{\varkappa}{r} \sin[2\varphi_\varkappa(\mathcal{E}, r)] - \frac{1}{c\hbar}[\mathcal{E} - V(r)] \qquad (r \geqslant \rho) \tag{7.20}$$

subject to the initial condition

$$\varphi_\varkappa(\mathcal{E}, \infty) = \arctan[\gamma^{(+)} b_\varkappa(\mathcal{E}, \infty)]. \tag{7.21}$$

Once the above initial-value problem is integrated down to $r = \rho$, the Steklov eigenvalue $b_\varkappa(\mathcal{E})$ is found to be

$$b_\varkappa(\mathcal{E}) = -\gamma^{(-)} \tan \varphi_\varkappa(\mathcal{E}, \rho). \tag{7.22}$$

In the general considerations presented in sections 4 and 5, we have encountered not only the DtN and NtD operators but also their derivatives with respect to the scalar parameter $\mathcal{E}$. In view of the aforementioned dependence of the DtN and NtD kernels on $\mathcal{E}$ only through $\{b_\varkappa(\mathcal{E})\}$, to evaluate kernels of these derivative operators one needs to know the derivatives $\{\partial b_\varkappa(\mathcal{E})/\partial \mathcal{E}\}$. However, differentiating equation (7.22) with respect to $\mathcal{E}$, one has

$$\frac{\partial b_\varkappa(\mathcal{E})}{\partial \mathcal{E}} = -\frac{\gamma^{(-)}}{\cos^2 \varphi_\varkappa(\mathcal{E}, \rho)} \frac{\partial \varphi_\varkappa(\mathcal{E}, \rho)}{\partial \mathcal{E}}. \tag{7.23}$$

This shows that, once the system (7.20) and (7.21) has been solved for $\varphi_\varkappa(\mathcal{E}, r)$, and thus $\varphi_\varkappa(\mathcal{E}, \rho)$ is known, the problem of finding $\partial b_\varkappa(\mathcal{E})/\partial \mathcal{E}$ may be replaced by that of determining the derivative $\partial \varphi_\varkappa(\mathcal{E}, \rho)/\partial \mathcal{E}$. The latter quantity may be found using an approach similar to that we proposed for seeking $\varphi_\varkappa(\mathcal{E}, \rho)$. Indeed, differentiation of equations (7.20) and (7.21) with respect to $\mathcal{E}$ leads to the inhomogeneous linear differential equation

$$\frac{\partial}{\partial r}\left(\frac{\partial \varphi_\varkappa(\mathcal{E}, r)}{\partial \mathcal{E}}\right) = \left\{\gamma^{(-)} \sin[2\varphi_\varkappa(\mathcal{E}, r)] + 2\frac{\varkappa}{r} \cos[2\varphi_\varkappa(\mathcal{E}, r)]\right\} \frac{\partial \varphi_\varkappa(\mathcal{E}, r)}{\partial \mathcal{E}} - \frac{1}{c\hbar} \qquad (r \geqslant \rho) \tag{7.24}$$

together with the relationship

$$\frac{\partial \varphi_\varkappa(\mathcal{E}, \infty)}{\partial \mathcal{E}} = -\frac{\gamma^{(-)}}{(\gamma^{(-)})^2 + b_\varkappa^2(\mathcal{E}, \infty)} \frac{\partial b_\varkappa(\mathcal{E}, \infty)}{\partial \mathcal{E}}. \tag{7.25}$$

Integrating equation (7.24) inwards from $r = \infty$ down to $r = \rho$, with the relation (7.25) taken as an initial condition, yields $\partial \varphi_\varkappa(\mathcal{E}, \rho)/\partial \mathcal{E}$.

7.2. Example: potential vanishing in the external domain

As the first application of the deliberations from section 7.1, consider the case when in the outer region the potential $V(r)$ vanishes identically:

$$V(r) \equiv 0 \qquad (r > \rho). \tag{7.26}$$

Then, assuming that

$$-mc^2 < \mathcal{E} < mc^2 \tag{7.27}$$

and defining

$$\mathcal{K} = \frac{\sqrt{(mc^2)^2 - \mathcal{E}^2}}{c\hbar} \qquad \varepsilon = \sqrt{\frac{mc^2 - \mathcal{E}}{mc^2 + \mathcal{E}}} \tag{7.28}$$

asymptotically vanishing particular solutions to the Dirac system (7.3), i.e., the (unnormalized) radial components of the pertinent Steklov eigenfunctions, are found to be

$$f_\varkappa(\mathcal{E}, r) = r k_l(\mathcal{K}r) \tag{7.29a}$$

$$g_\varkappa(\mathcal{E}, r) = -\varepsilon r k_{l'}(\mathcal{K}r) \tag{7.29b}$$

where l is defined by equation (7.12),

$$l' = \left|-\varkappa + \tfrac{1}{2}\right| - \tfrac{1}{2} = l - \operatorname{sgn}(\varkappa) \tag{7.30}$$

and

$$k_l(x) = \frac{\pi}{2}(-x)^l \left(\frac{1}{x}\frac{\mathrm{d}}{\mathrm{d}x}\right)^l \frac{\mathrm{e}^{-x}}{x} \tag{7.31}$$

is the spherical Macdonald function (the modified spherical Bessel function of the third kind) [60]. Hence, in this example the analytical evaluation of the Steklov eigenvalues presents no difficulty and from equations (7.6), (7.29*a*) and (7.29*b*) one deduces that

$$b_\varkappa(\mathcal{E}) = \varepsilon\gamma^{(-)}\frac{k_{l'}(\mathcal{K}\rho)}{k_l(\mathcal{K}\rho)}. \tag{7.32}$$

Differentiating this expression with respect to $\mathcal{E}$, after making use of recurrence relations obeyed by the spherical Macdonald functions [60], the derivative $\partial b_\varkappa(\mathcal{E})/\partial\mathcal{E}$ is found to be

$$\frac{\partial b_\varkappa(\mathcal{E})}{\partial\mathcal{E}} = \frac{\rho\gamma^{(+)}(\varepsilon^{-2} - 1)}{2c\hbar} b_\varkappa^2(\mathcal{E}) + \frac{(2\varkappa - 1)\varepsilon^2 - (2\varkappa + 1)}{2c\hbar\varepsilon\mathcal{K}} b_\varkappa(\mathcal{E}) + \frac{\rho\gamma^{(-)}(1 - \varepsilon^2)}{2c\hbar}. \tag{7.33}$$

7.3. Example: potential with a pure Coulomb tail in the external domain

The second example we wish to consider here is the one in which in the outer domain the potential $V(r)$ is purely Coulombic:

$$V(r) = -\frac{Ze^2}{r} \qquad (0 < Z < \alpha^{-1}; r > \rho) \tag{7.34}$$

($\alpha = e^2/c\hbar$ is the Sommerfeld fine structure constant). Assuming that the constraint (7.27) holds, with some effort it may be shown that solutions to the radial Dirac system (7.3), satisfying the asymptotic conditions (7.4), are

$$f_\varkappa(\mathcal{E}, r) = r^{-1/2}[(\varkappa + \xi) W_{\eta-1/2,\gamma}(2\mathcal{K}r) + W_{\eta+1/2,\gamma}(2\mathcal{K}r)] \tag{7.35a}$$

$$g_\varkappa(\mathcal{E}, r) = \varepsilon r^{-1/2}[(\varkappa + \xi) W_{\eta-1/2,\gamma}(2\mathcal{K}r) - W_{\eta+1/2,\gamma}(2\mathcal{K}r)] \tag{7.35b}$$

where $W_{\kappa\mu}(z)$ is the Whittaker function of the second kind [54, chapter 7], $\mathcal{K}$ and ε have been defined in equation (7.28),

$$\eta = \tfrac{1}{2}\zeta(\varepsilon^{-1} - \varepsilon) \qquad \xi = \tfrac{1}{2}\zeta(\varepsilon^{-1} + \varepsilon) \tag{7.36}$$

and

$$\gamma = \sqrt{\varkappa^2 - \zeta^2} \tag{7.37}$$

with

$$\zeta = \alpha Z. \tag{7.38}$$

Hence, after invoking equation (7.6), one finds

$$b_\varkappa(\mathcal{E}) = -\varepsilon\gamma^{(-)}\frac{(\varkappa+\xi)W_{\eta-1/2,\gamma}(2\mathcal{K}\rho) - W_{\eta+1/2,\gamma}(2\mathcal{K}\rho)}{(\varkappa+\xi)W_{\eta-1/2,\gamma}(2\mathcal{K}\rho) + W_{\eta+1/2,\gamma}(2\mathcal{K}\rho)}. \tag{7.39}$$

In principle, the derivative $\partial b_\varkappa(\mathcal{E})/\partial\mathcal{E}$ may be found from equation (7.39) by differentiating the latter with respect to $\mathcal{E}$. In practice, however, carrying out this differentiation would be a formidable task since not only the arguments of both the Whittaker functions in equation (7.39), but also their first indices, i.e., $\eta \pm 1/2$ (as well as ε and ξ) depend on $\mathcal{E}$. Therefore, in actual calculations it will be much more convenient to find both $b_\varkappa(\mathcal{E})$ and $\partial b_\varkappa(\mathcal{E})/\partial\mathcal{E}$ by integrating numerically equations (7.20) and (7.24) and then utilizing equations (7.22) and (7.23). Of necessity, these numerical integrations must not start at $r = \infty$ but rather at some large value of r, say r_s. Pertinent initial conditions, found from equations (7.15), (7.35*a*), (7.35*b*) and (7.19), and from the known asymptotic representation of the Whittaker function [54, chapter 7]:

$$W_{\kappa\mu}(z) \overset{|z|\to\infty}{\sim} z^\kappa \mathrm{e}^{-z/2}{}_2F_0\left(\tfrac{1}{2}-\kappa+\mu, \tfrac{1}{2}-\kappa-\mu; ; -z^{-1}\right) \qquad (|\arg(z)| < 3\pi/2) \tag{7.40}$$

are

$$\varphi_\varkappa(\mathcal{E}, r_s) \simeq -\arctan\varepsilon + \gamma^{(+)}\frac{\varkappa+\xi}{r_s} \qquad (\mathcal{K}r_s \gg 1) \tag{7.41}$$

and

$$\frac{\partial\varphi_\varkappa(\mathcal{E}, r_s)}{\partial\mathcal{E}} \simeq \frac{1}{2c\hbar\mathcal{K}}\left(1+\frac{\eta}{\mathcal{K}r_s}\right) \qquad (\mathcal{K}r_s \gg 1) \tag{7.42}$$

respectively.

8. An illustrative numerical application

Consider a Dirac particle bound in the potential

$$V(r) = \begin{cases} -\dfrac{Ze^2}{\rho} & \text{for} \quad r \leqslant \rho \\ -\dfrac{Ze^2}{r} & \text{for} \quad r > \rho \end{cases} \qquad (0 < Z < \alpha^{-1}). \tag{8.1}$$

Discrete energy levels E for this system, for each value of $\varkappa \neq 0$, are roots of the transcendental equation

$$\mathrm{sgn}(\varkappa)\epsilon_0\frac{j_{l'}(K_0\rho)}{j_l(K_0\rho)} = \epsilon\frac{(\varkappa+\xi)W_{\eta-1/2,\gamma}(2K\rho) - W_{\eta+1/2,\gamma}(2K\rho)}{(\varkappa+\xi)W_{\eta-1/2,\gamma}(2K\rho) + W_{\eta+1/2,\gamma}(2K\rho)} \tag{8.2}$$

where l and l' are defined as in equations (7.12) and (7.30), respectively,

$$K = \frac{\sqrt{(mc^2)^2 - E^2}}{c\hbar} \qquad \epsilon = \sqrt{\frac{mc^2 - E}{mc^2 + E}} \tag{8.3}$$

$$K_0 = \frac{\sqrt{(E+V_0)^2 - (mc^2)^2}}{c\hbar} \qquad \epsilon_0 = \sqrt{\frac{E+V_0-mc^2}{E+V_0+mc^2}} \tag{8.4}$$

with

$$V_0 = \frac{Ze^2}{\rho} \tag{8.5}$$

η and ξ are defined as in equation (7.36), but this time with ε replaced by ϵ defined in equation (8.3), while $j_l(z)$ is the spherical Bessel function [60]. Equation (8.2) may be solved numerically, for instance by the method of bisection, and throughout the remainder of this section energy levels computed in this way will be designated as 'exact.'

We aim at determining variationally the discrete energy levels in the potential (8.1). As the variational basis, we choose the set of eigenfunctions of the three-dimensional Dirac oscillator [61, 62]:

$$\phi_{n\varkappa\mu}(\lambda; \boldsymbol{r}) = \frac{1}{r}\begin{pmatrix} P_{n\varkappa}(\lambda; r)\Omega_{\varkappa\mu}(\boldsymbol{n}_r) \\ \mathrm{i}Q_{n\varkappa}(\lambda; r)\Omega_{-\varkappa\mu}(\boldsymbol{n}_r) \end{pmatrix} \tag{8.6}$$

with the radial parts

$$P_{n\varkappa}(\lambda; r) = \sqrt{\frac{\lambda|n|!(E_{n\varkappa} + mc^2)}{\Gamma\left(|n| + l + \frac{3}{2}\right) E_{n\varkappa}}}(\lambda r)^{l+1}\mathrm{e}^{-\lambda^2 r^2/2} L_{|n|}^{(l+1/2)}(\lambda^2 r^2) \tag{8.7a}$$

and

$$Q_{n\varkappa}(\lambda; r) = \pm\mathrm{sgn}(\varkappa)\sqrt{\frac{\lambda|n'|!(E_{n\varkappa} - mc^2)}{\Gamma\left(|n'| + l' + \frac{3}{2}\right) E_{n\varkappa}}}(\lambda r)^{l'+1}\mathrm{e}^{-\lambda^2 r^2/2} L_{|n'|}^{(l'+1/2)}(\lambda^2 r^2). \tag{8.7b}$$

(In equation (8.7*b*) we adopt the convention that if $\varkappa < 0$, then the upper sign is to be chosen for $n \geqslant 0$ and the lower one for $n < 0$, while if $\varkappa > 0$, then the upper sign is to be chosen for $n = +0, +1, +2, \ldots$ and the lower one for $n = -0, -1, -2, \ldots$ (for $\varkappa > 0$ it is absolutely necessary to distinguish between the cases $n = +0$ and $n = -0$).) In equations (8.7*a*) and (8.7*b*), l and l' have the same meanings as in equations (7.12) and (7.30), respectively, while $L_n^{(\alpha)}(x)$ is the generalized Laguerre polynomial [54, section 5.5]; moreover,

$$|n'| = \begin{cases} |n| - 1 & \text{for} \quad \varkappa < 0 \\ |n| & \text{for} \quad \varkappa > 0 \end{cases} \tag{8.8}$$

$$E_{n\varkappa} = \pm mc^2\sqrt{1 + 4|n|\left(\frac{\hbar\lambda}{mc}\right)^2} \qquad (\varkappa < 0; n = 0, \pm1, \pm2, \ldots) \tag{8.9a}$$

$$E_{n\varkappa} = \pm mc^2\sqrt{1 + 4\left(|n| + l + \tfrac{1}{2}\right)\left(\frac{\hbar\lambda}{mc}\right)^2} \qquad (\varkappa > 0; n = \pm0, \pm1, \pm2, \ldots) \tag{8.9b}$$

(the same sign convention as in equation (8.7*b*) applies in equations (8.9*a*) and (8.9*b*)), while λ is a real, positive, adjustable parameter, related to the oscillator's frequency ω through

$$\lambda = \sqrt{\frac{m\omega}{\hbar}}. \tag{8.10}$$

Numerical calculations have been carried out for the system for which $Z = 80$ and $\rho = 1a_0$ ($a_0 = \hbar^2/me^2$ is the Bohr radius); the scaling parameter λ characterizing the oscillator basis (8.6) has been fixed at $\lambda = 1a_0^{-1}$. Working of necessity with truncated basis sets, for each $\varkappa < 0$ we have used an odd number $2N + 1$ of the eigenfunctions (8.6) with the radial quantum numbers $n \in \{0, \pm1, \pm2, \ldots, \pm N\}$, while for each $\varkappa > 0$ we have used an even number $2N + 2$ of such eigenfunctions with the radial quantum numbers $n \in \{\pm0, \pm1, \pm2, \ldots, \pm N\}$; in both cases N has been admitted to vary.

Table 1. Convergence rate of the Rayleigh–Ritz variational calculations of *the lowest discrete* energy levels in the potential (8.1) for the angular symmetries $\varkappa = \mp 1$. The parameters of the potential are $Z = 80$ and $\rho = 1a_0$. The variational basis employed has been the Dirac oscillator basis (8.6) with $\lambda = 1a_0^{-1}$. A total number of $2N^{(\mathrm{R})} + 1$ basis functions with $n \in \{0, \pm 1, \pm 2, \ldots, \pm N^{(\mathrm{R})}\}$ have been used for $\varkappa = -1$ and of $2N^{(\mathrm{R})} + 2$ basis functions with $n \in \{\pm 0, \pm 1, \pm 2, \ldots, \pm N^{(\mathrm{R})}\}$ for $\varkappa = +1$. Exact values, obtained by solving numerically the transcendental equation (8.2), are presented in the last row.

$N^{(\mathrm{R})}$	$\widetilde{E}^{(\mathrm{R})}_{\varkappa=-1} - mc^2$ (au)	$\widetilde{E}^{(\mathrm{R})}_{\varkappa=+1} - mc^2$ (au)
5	−76.857 0551	−73.412 4410
10	−76.914 7255	−73.722 2469
20	−76.942 6595	−73.809 0758
40	−76.950 2447	−73.825 1431
80	−76.951 3219	−73.828 3316
Exact	−76.951 6007	−73.828 9214

Table 2. Convergence rate of the DtN/NtD variational estimates of *the lowest discrete* eigenenergy with $\varkappa = -1$ for a Dirac particle in the potential (8.1) with $Z = 80$ and $\rho = 1a_0$. The variational basis employed has been the Dirac oscillator basis (8.6) with $\lambda = 1a_0^{-1}$. A total number of $2N + 1$ basis functions with $n \in \{0, \pm 1, \pm 2, \ldots, \pm N\}$ have been used. The energy input for the iteration procedures in both versions of the method has been $\mathcal{E}_{\varkappa=-1} - mc^2 = -76.942\,6595$ au. Row (a) presents results obtained with the operator $\hat{\mathcal{B}}^{(+)}$ (or equivalently $\hat{\mathcal{R}}^{(-)}$), row (b) results obtained with the operator $\hat{\mathcal{B}}^{(-)}$ (or equivalently $\hat{\mathcal{R}}^{(+)}$). The exact value, obtained by solving numerically the transcendental equation (8.2), is presented in the last row.

		$\widetilde{\mathscr{E}}^{(\pm)}_{\varkappa=-1} - mc^2$ (au)			
Iteration		$N = 3$	$N = 4$	$N = 5$	$N = 6$
1	(a)	−76.951 6006	−76.951 6006	−76.951 6006	−76.951 6006
	(b)	−76.951 6001	−76.951 6003	−76.951 6003	−76.951 6003
2	(a)	−76.951 6007	−76.951 6007	−76.951 6007	−76.951 6007
	(b)	−76.951 6005	−76.951 6007	−76.951 6007	−76.951 6007
3	(a)	−76.951 6007	−76.951 6007	−76.951 6007	−76.951 6007
	(b)	−76.951 6005	−76.951 6007	−76.951 6007	−76.951 6007
Exact		−76.951 6007			

Three series of calculations have been performed. We shall report only results for *the lowest discrete* eigenstates belonging to the angular symmetries $\varkappa = \mp 1$, since they have been found to be sufficiently representative for the problem considered.

First, we have used the basis (8.6) in the standard Rayleigh–Ritz principle based on the functional (2.15). The results are presented in table 1, from which it is seen that for both angular symmetries the convergence rate to the exact results, with the latter obtained by solving numerically the transcendental equation (8.2), is moderately rapid; no symptoms of the variational collapse have been observed.

In the remaining two series of calculations, the DtN embedding methods based on the use of the operators $\hat{\mathcal{B}}^{(\pm)}(\mathcal{E})$ (equivalent to the NtD embedding methods exploiting the operators $\hat{\mathcal{R}}^{(\mp)}(\mathcal{E})$) have been applied. For each dimension of the variational basis characterized by N (cf above), the calculations have been carried out iteratively. In the first step, the algebraic eigensystems (6.7) have been solved with the matrices $\Lambda^{(\pm)}$ and $\Delta^{(\pm)}$ constructed with $\mathcal{E}_{\varkappa=-1} - mc^2 = -76.942\,6595$ au or $\mathcal{E}_{\varkappa=+1} - mc^2 = -73.809\,0758$ au, with the latter

Table 3. Convergence rate of the DtN/NtD variational estimates of *the lowest discrete* eigenenergy with $\varkappa = +1$ for a Dirac particle in the potential (8.1) with $Z = 80$ and $\rho = 1a_0$. The variational basis employed has been the Dirac oscillator basis (8.6) with $\lambda = 1a_0^{-1}$. A total number of $2N + 2$ basis functions with $n \in \{\pm 0, \pm 1, \pm 2, \ldots, \pm N\}$ have been used. The input for the iteration procedures in both versions of the method has been $\mathcal{E}_{\varkappa=+1} - mc^2 = -73.809\,0758$ au. Row (a) presents results obtained with the operator $\hat{\mathcal{B}}^{(+)}$ (or equivalently $\hat{\mathcal{R}}^{(-)}$), row (b) results obtained with the operator $\hat{\mathcal{B}}^{(-)}$ (or equivalently $\hat{\mathcal{R}}^{(+)}$). The exact value, obtained by solving numerically the transcendental equation (8.2), is presented in the last row.

		$\widetilde{\mathcal{E}}^{(\pm)}_{\varkappa=+1} - mc^2$ (au)			
Iteration		$N = 3$	$N = 4$	$N = 5$	$N = 6$
1	(a)	−73.828 9201	−73.828 9201	−73.828 9201	−73.828 9201
	(b)	−73.828 9104	−73.828 9107	−73.828 9107	−73.828 9107
2	(a)	−73.828 9214	−73.828 9214	−73.828 9214	−73.828 9214
	(b)	−73.828 9210	−73.828 9214	−73.828 9214	−73.828 9214
3	(a)	−73.828 9214	−73.828 9214	−73.828 9214	−73.828 9214
	(b)	−73.828 9210	−73.828 9214	−73.828 9214	−73.828 9214
Exact		−73.828 9214			

two being the Rayleigh–Ritz estimates of $E_{\varkappa=\mp 1} - mc^2$ obtained with $N^{(\mathrm{R})} = 20$ (cf table 1). Then, the procedure has been iterated with $\mathcal{E}_{\varkappa=\mp 1}$ replaced successively by the eigenvalues $\widetilde{\mathcal{E}}^{(\pm)}_{\varkappa=\mp 1}$ obtained in the preceding iteration step. The results are presented in tables 2 and 3. It is seen that for the lowest discrete eigenvalues considered here, convergence of this iteration process has been very rapid and exact results have been obtained with much smaller bases than in the case of the Rayleigh–Ritz calculations. (For some excited states convergence could not be achieved for very small bases; however, in all the cases we have investigated the choice $N = 10$ has been sufficient to obtain the results converged to the exact value.)

9. Conclusions

In this paper, we have extended the embedding method of Inglesfield [1] to bound states of Dirac particles. Although our approach has many points of contact with that adopted in a recent paper by Crampin [25] on the same subject, there are also some marked differences between the two papers. In particular, while Crampin, following closely the reasoning from [1], based his considerations on the Green functions technique, in the present work we have made an extensive use of the suitably adapted formalism of Dirac analogues of the Dirichlet-to-Neumann and Neumann-to-Dirichlet surface integral operators [29, 30, 32, 34, 35]. This has allowed us to develop *two* variants of the method. We have carried out some numerical studies, results of which seem to confirm the supposition of Crampin [25] that, at least for bound state problems, the Dirac embedding method may be a useful practical tool for computing characteristics of relativistic systems. In a later publication we plan to present an application of the formalism of the DtN and NtD operators to computations of properties of continuum states of Dirac particles.

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Appendix. Some useful identities obeyed by the matrices $\alpha_\perp^{(\pm)}(\rho)$ and $\beta^{(\pm)}$

The matrices $\alpha_\perp^{(\pm)}(\boldsymbol{\rho})$ and $\beta^{(\pm)}$ have been defined by equations (2.9)–(2.11). Directly from these definitions and from the well-known properties of the Dirac matrices $\boldsymbol{\alpha}$ and β, one may derive the following set of identities, which we have relied on heavily throughout sections 3–5:

$$\alpha_\perp^{(+)}(\boldsymbol{\rho}) + \alpha_\perp^{(-)}(\boldsymbol{\rho}) = \alpha_\perp(\boldsymbol{\rho}) \tag{A.1}$$

$$\beta^{(+)} + \beta^{(-)} = \mathcal{I} \tag{A.2}$$

$$\alpha_\perp^{(\pm)\dagger}(\boldsymbol{\rho}) = \alpha_\perp^{(\mp)}(\boldsymbol{\rho}) \tag{A.3}$$

$$\beta^{(\pm)\dagger} = \beta^{(\pm)} \tag{A.4}$$

$$\alpha_\perp^{(\pm)}(\boldsymbol{\rho})\alpha_\perp^{(\pm)}(\boldsymbol{\rho}) = 0 \tag{A.5}$$

$$\alpha_\perp^{(\pm)}(\boldsymbol{\rho})\alpha_\perp^{(\mp)}(\boldsymbol{\rho}) = \beta^{(\pm)} \tag{A.6}$$

$$\beta^{(\pm)}\beta^{(\pm)} = \beta^{(\pm)} \tag{A.7}$$

$$\beta^{(\pm)}\beta^{(\mp)} = 0 \tag{A.8}$$

$$\alpha_\perp^{(\pm)}(\boldsymbol{\rho})\beta^{(\pm)} = 0 \tag{A.9}$$

$$\beta^{(\pm)}\alpha_\perp^{(\pm)}(\boldsymbol{\rho}) = \alpha_\perp^{(\pm)}(\boldsymbol{\rho}) \tag{A.10}$$

$$\alpha_\perp^{(\pm)}(\boldsymbol{\rho})\beta^{(\mp)} = \alpha_\perp^{(\pm)}(\boldsymbol{\rho}) \tag{A.11}$$

$$\beta^{(\pm)}\alpha_\perp^{(\mp)}(\boldsymbol{\rho}) = 0. \tag{A.12}$$

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