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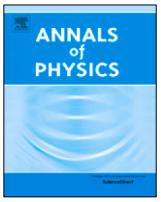

Zero-range potentials for Dirac particles: Bound-state problems

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ABSTRACT

A model in which a massive Dirac particle in $\mathbb{R}^3$ is bound by $N \geqslant 1$ spatially distributed zero-range potentials is presented. Interactions between the particle and the potentials are modeled by subjecting a particle's bispinor wave function to certain limiting conditions at the potential centers. Each of these conditions is parametrized by a 2×2 Hermitian matrix (or, equivalently, a real scalar and a real vector) and mixes the upper and the lower components of the wave function. The problem of determining particle's bound-state eigenenergies is reduced to the problem of finding real zeros of a determinant of a certain $2N \times 2N$ matrix. As the lower component of the particle's wave function is inverse-square singular at each of the potential centers, the wave function itself is not square-integrable. Nevertheless, one can define a scalar pseudo-product with the property that wave functions belonging to different eigenenergies are orthogonal with respect to it. The wave functions may then be normalized so that their self-pseudo-products are plus one, minus one or zero. An auxiliary set of Sturmian functions is constructed and used to derive an explicit representation of particle's matrix Green's function. For illustration purposes, two particular systems are studied in detail: (1) a particle bound in a field of a single zero-range potential, (2) a particle bound in a field of two identical zero-range potentials.

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1. Introduction

Useful information about some quantum mechanical systems may be obtained by analyzing models in which interactions between their constituents are of contact nature, i.e., occur only when distances between the constituents are zero. In the literature, such idealized models are often referred to as contact-, point- or delta-interaction approximations. Their variants differ among themselves in how the point interactions are mathematically built into them. One procedure, employed mainly in analysis of one-dimensional systems, is to use the Dirac delta function (and, occasionally, its first spatial derivative) in the potential energy term in the Hamiltonian of the system. Another possibility, used predominantly in studies concerning two- and three-dimensional systems, is to impose certain conditions on a wave function at those points in the configuration space that correspond to the situation when two or more components of the system are at the same location in the physical space. It is the latter approach that underlies the so-called "zero-range potential method" (or "zero-range potential approximation"), which has been popularized by Demkov and Ostrovskii [1] and by Drukarev [2], and which is sometimes used in theoretical atomic, molecular, and solid state physics.

The research conducted so far on the construction and use of point-interaction models has focused mainly on nonrelativistic systems. Only a relatively small number of works have dealt with corresponding models for particles described by relativistic wave equations; representative of that group are the publications listed in Refs. [3–12]. In particular, in Refs. [7,9] the present author outlined a formalism that generalizes the nonrelativistic one from Refs. [1,2] and enables one to study stationary scattering of Dirac particles off an arbitrary system of spatially distributed point obstacles. The purpose of the present work is to complement Refs. [7,9] by developing a model that allows one to consider massive Dirac particles bound by a system of zero-range potentials in $\mathbb{R}^3$.

The paper is structured as follows. In Section 2, we present basic principles of our model. The problem of orthogonality and normalization of particle's bound-state eigenfunctions is discussed in Section 3. An auxiliary set of Sturmian functions is introduced in Section 4. These functions are then used in Section 5 to construct an explicit representation of the Dirac–Green's function associated with the problem. Two illustrative examples – a particle interacting with a single zero-range potential center and a particle in a field of two identical zero-range potentials – are worked out in Section 6. A brief discussion of possible further developments of the model is provided in Section 7.

2. The model

We consider a Dirac particle of rest mass m, bound by a system of $N \geqslant 1$ zero-range potentials, located at the points $\boldsymbol{r}_n$, $n = 1, \ldots, N$. Everywhere in $\mathbb{R}^3$, except at the potential centers, the time-independent bispinor wave function $\Psi_a(\boldsymbol{r})$ describing the particle obeys the Dirac equation

$$[-\mathrm{i}c\hbar\boldsymbol{\alpha}\cdot\boldsymbol{\nabla} + mc^2\beta - E_a\mathcal{I}]\Psi_a(\boldsymbol{r}) = 0 \qquad (\boldsymbol{r} \neq \boldsymbol{r}_n;\, n = 1, \ldots, N), \tag{2.1}$$

where $\mathcal{I}$ is the unit 4×4 matrix, $\boldsymbol{\alpha}$ and β are the standard 4×4 Dirac matrices [13], while E_a (assumed to be real and such that $-mc^2 < E_a \leqslant mc^2$) is particle's eigenenergy which is to be determined. In the model that we propose in this work, the wave function $\Psi_a(\boldsymbol{r})$ is taken in the form

$$\Psi_a(\boldsymbol{r}) = \sum_{n=1}^{N} \begin{pmatrix} f(k_a|\boldsymbol{r}-\boldsymbol{r}_n|)\chi_{an} \\ -\mathrm{i}\varepsilon_a k_a^{-1}\boldsymbol{\sigma}\cdot\boldsymbol{\nabla} f(k_a|\boldsymbol{r}-\boldsymbol{r}_n|)\chi_{an} \end{pmatrix} \tag{2.2a}$$

or equivalently

$$\Psi_a(\boldsymbol{r}) = \sum_{n=1}^{N} \begin{pmatrix} f(k_a|\boldsymbol{r}-\boldsymbol{r}_n|)\chi_{an} \\ \mathrm{i}\varepsilon_a g(k_a|\boldsymbol{r}-\boldsymbol{r}_n|)\boldsymbol{\mu}_n(\boldsymbol{r})\cdot\boldsymbol{\sigma}\chi_{an} \end{pmatrix}. \tag{2.2b}$$

In Eqs. (2.2a) and (2.2b), and hereafter, the functions $f(z)$ and $g(z)$ are defined to be[1]

$$f(z) = \frac{\mathrm{e}^{-z}}{z} \tag{2.3a}$$

and

$$g(z) = -\frac{\mathrm{d}f(z)}{\mathrm{d}z} = \frac{\mathrm{e}^{-z}}{z} + \frac{\mathrm{e}^{-z}}{z^2}, \tag{2.3b}$$

respectively, k_a and ε_a are eigenenergy-dependent parameters defined as

$$k_a = \frac{\sqrt{(mc^2)^2 - E_a^2}}{c\hbar}, \tag{2.4a}$$

$$\varepsilon_a = \sqrt{\frac{mc^2 - E_a}{mc^2 + E_a}}, \tag{2.4b}$$

respectively, $\boldsymbol{\sigma}$ is the vector composed of the Pauli matrices and

$$\boldsymbol{\mu}_n(\boldsymbol{r}) = \frac{\boldsymbol{r} - \boldsymbol{r}_n}{|\boldsymbol{r} - \boldsymbol{r}_n|} \tag{2.5}$$

is the unit vector pointing from the center $\boldsymbol{r}_n$ to the observation point $\boldsymbol{r}$. The parameters k_a and ε_a defined in Eqs. (2.4) are easily seen to be related through

$$k_a = \frac{2mc}{\hbar}\frac{\varepsilon_a}{1 + \varepsilon_a^2}, \tag{2.6a}$$

or conversely

$$\varepsilon_a = \frac{1 \mp \sqrt{1 - (\hbar k_a/mc)^2}}{\hbar k_a/mc} = \frac{\hbar k_a/mc}{1 \pm \sqrt{1 - (\hbar k_a/mc)^2}}, \tag{2.6b}$$

with the upper (respectively, lower) signs chosen for $0 \leqslant E_a \leqslant mc^2$ (respectively, $-mc^2 < E_a \leqslant 0$). The two-component spinors χ_{an}, which are also to be determined, may be interpreted as generalized superposition coefficients in the linear combination (2.2).

The selection of $f(z)$ in the form (2.3a) guarantees that for $\boldsymbol{r} \neq \boldsymbol{r}_n$ the nth term in the sum (2.2a) does solve the Dirac equation (2.1) separately, regardless of the particular choice of the spinor χ_{an} it involves. At $\boldsymbol{r} = \boldsymbol{r}_n$, the upper and lower components of that term exhibit the first- and the second-order singularities, respectively. The reader may wish to observe that the form of the upper component of $\Psi_a(\boldsymbol{r})$ in either of Eqs. (2.2) mimics that of a wave function used in the nonrelativistic variant of the method [1,2], except that in the present case the superposition coefficients are the Pauli spinors rather than complex numbers.

To complete our model, we represent the interaction between the Dirac particle and the set of zero-range potentials by subjecting the particle's wave function to the following limiting conditions:

$$\lim_{\boldsymbol{r}\to\boldsymbol{r}_n}\left[\mathrm{i}(\boldsymbol{r} - \boldsymbol{r}_n)\cdot\boldsymbol{\alpha}^{(+)} + \frac{\hbar}{2mc}|\boldsymbol{r} - \boldsymbol{r}_n|\mathcal{K}_n^{(+)} + \varepsilon_a k_a^{-1}\beta^{(+)}\right]\Psi_a(\boldsymbol{r}) = 0 \qquad (n = 1, \ldots, N) \tag{2.7}$$

at the points where the potentials are placed (see Fig. 1). Here, the 4×4 matrices $\boldsymbol{\alpha}^{(+)}$ and $\beta^{(+)}$, and their counterparts $\boldsymbol{\alpha}^{(-)}$ and $\beta^{(-)}$ to be used later, are defined to be

$$\boldsymbol{\alpha}^{(\pm)} = \beta^{(\pm)}\boldsymbol{\alpha} = \boldsymbol{\alpha}\beta^{(\mp)}, \tag{2.8a}$$

$$\beta^{(\pm)} = \frac{1}{2}(\mathcal{I} \pm \beta), \tag{2.8b}$$

[1] In a two-dimensional model, in which both the potential centers and the Dirac particle itself are confined to the plane, the analogues of the elementary functions $f(z)$ and $g(z)$ of Eqs. (2.3a) and (2.3b) will be the cylindrical Macdonald functions $K_0(z)$ and $K_1(z)$, respectively.

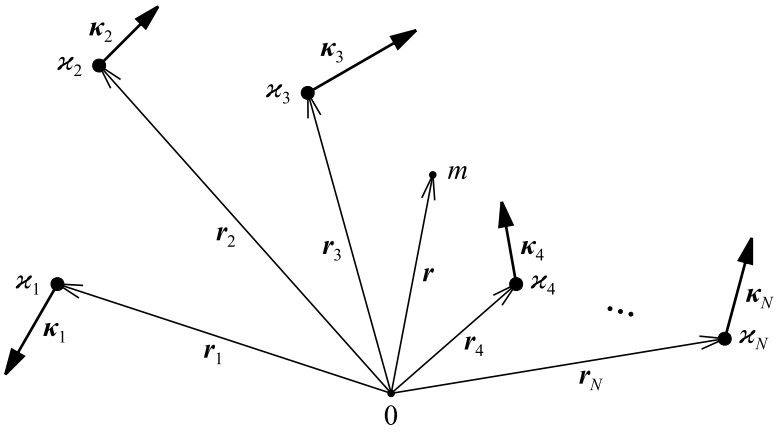

Fig. 1. The Dirac particle of mass m and the position vector $\boldsymbol{r}$ in the field of N zero-range potentials. Each potential center is characterized by its position vector $\boldsymbol{r}_n$, the real scalar $\varkappa_n$ and the real vector $\boldsymbol{\kappa}_n$. The relationship between the two latter parameters and the 2×2 interaction matrix K_n associated with the nth potential center is given in Eq. (2.10).

respectively, while $\mathcal{K}_n^{(+)}$ are 4×4 energy-independent matrices that may be expressed in terms of the 2×2 Hermitian matrices K_n as

$$\mathcal{K}_n^{(+)} = \begin{pmatrix} K_n & 0 \\ 0 & 0 \end{pmatrix}, \tag{2.9}$$

with zeros denoting the 2×2 null matrices. In later considerations we shall be exploiting the well-known fact that in the Pauli basis, consisting of the unit 2×2 matrix I and the Pauli matrix vector $\boldsymbol{\sigma}$, the matrices K_n have the representations

$$K_n = \varkappa_n I + \boldsymbol{\kappa}_n \cdot \boldsymbol{\sigma}, \tag{2.10}$$

where

$$\varkappa_n = \frac{1}{2}\mathrm{Tr}\, K_n, \tag{2.11a}$$

and

$$\boldsymbol{\kappa}_n = \frac{1}{2}\mathrm{Tr}\,(\boldsymbol{\sigma} K_n). \tag{2.11b}$$

Since the matrices K_n are presupposed to be Hermitian, the scalars $\varkappa_n$ and the vectors $\boldsymbol{\kappa}_n$ are real.

The limiting conditions (2.7) guarantee (cf. Appendix) that none of the points $\boldsymbol{r}_n$ is a source or a sink, i.e., that the flux across a spherical surface $\mathcal{S}_n$, centered at the point $\boldsymbol{r}_n$ and of radius $\rho \to 0$, does vanish:

$$\lim_{\rho \to 0} \oint_{\mathcal{S}_n} \mathrm{d}^2\boldsymbol{\rho}_n\, \boldsymbol{\mu}_n(\boldsymbol{r}_n + \boldsymbol{\rho}_n) \cdot \boldsymbol{j}_a(\boldsymbol{r}_n + \boldsymbol{\rho}_n) = 0 \qquad (n = 1, \ldots, N), \tag{2.12}$$

where $\boldsymbol{\rho}_n$ (with $|\boldsymbol{\rho}_n| = \rho$) is the radius vector (respective to the center $\boldsymbol{r}_n$) for a point on $\mathcal{S}_n$, $\boldsymbol{\mu}_n(\boldsymbol{r}_n + \boldsymbol{\rho}_n) = \boldsymbol{\rho}_n/\rho$ [cf. Eq. (2.5)] is the unit outward vector normal to $\mathcal{S}_n$ and

$$\boldsymbol{j}_a(\boldsymbol{r}) = c\Psi_a^\dagger(\boldsymbol{r})\boldsymbol{\alpha}\Psi_a(\boldsymbol{r}) \tag{2.13}$$

(here and hereafter, the dagger denotes the Hermitian adjoint matrix) is the Dirac current density vector.

Substitution of the wave function $\Psi_a(\boldsymbol{r})$ in the form (2.2b) into the limiting conditions (2.7) yields the following homogeneous algebraic system for the spinor superposition coefficients χ_{an}:

$$\left(\frac{\hbar}{2mc\varepsilon_a}K_n - I\right)\chi_{an} + \sum_{\substack{n'=1\\(n'\neq n)}}^{N} f(k_a|\boldsymbol{r}_n - \boldsymbol{r}_{n'}|)\chi_{an'} = 0 \qquad (n = 1, \ldots, N). \tag{2.14}$$

With both current and future applications in mind, we introduce a $2N \times 2N$ matrix $\mathsf{L}(E)$ built of 2×2 blocks

$$L_{nn'}(E) = \delta_{nn'}\left(\frac{\hbar}{2mc\varepsilon}K_n - I\right) + (1 - \delta_{nn'})f(k|\boldsymbol{r}_n - \boldsymbol{r}_{n'}|)I \qquad (n, n' = 1, \ldots, N), \tag{2.15}$$

where k and ε are defined in terms of an energy parameter $-mc^2 < E \leqslant mc^2$ (which may or may not be equal to one of particle's eigenenergies E_a) as [cf. Eqs. (2.4)]

$$k = \frac{\sqrt{(mc^2)^2 - E^2}}{c\hbar} \tag{2.16a}$$

and

$$\varepsilon = \sqrt{\frac{mc^2 - E}{mc^2 + E}}, \tag{2.16b}$$

respectively. Defining also a $2N$-element column vector

$$\mathsf{x}_a = \begin{pmatrix}\chi_{a1}^{\mathrm{T}} & \cdots & \chi_{aN}^{\mathrm{T}}\end{pmatrix}^{\mathrm{T}} \tag{2.17}$$

(here and hereafter, T denotes the transpose matrix), we may rewrite the system (2.14) in the compact form

$$\mathsf{L}(E_a)\mathsf{x}_a = 0. \tag{2.18}$$

The system (2.18) has nontrivial solutions x_a only if the determinant of its matrix $\mathsf{L}(E_a)$ vanishes:

$$\det \mathsf{L}(E_a) = 0. \tag{2.19}$$

This is an algebraic equation for E_a and its roots obeying the constraint $-mc^2 < E_a \leqslant mc^2$ play the role of particle's bound-state eigenenergies in our model.

From Eqs. (2.14) and (2.15), one may deduce several useful sesquilinear identities involving the spinor coefficients χ_{an}. We list four of them here. The first one is

$$\frac{\hbar^2}{2m}\sum_{n=1}^{N}\chi_{an}^{\dagger}K_n\chi_{an} + E_a k_a^{-1}\sum_{n,n'=1}^{N}\mathrm{e}^{-k_a|\boldsymbol{r}_n - \boldsymbol{r}_{n'}|}\chi_{an}^{\dagger}\chi_{an'} = c^2\hbar^2 k_a\sum_{n,n'=1}^{N}\chi_{an}^{\dagger}\left[\frac{\partial L_{nn'}(E)}{\partial E}\right]_{E=E_a}\chi_{an'}. \tag{2.20}$$

It will find an application in Section 3, in the context of normalization of the eigenfunctions (2.2). The second one,

$$\frac{E_b - E_a}{2mc^2}\sum_{n=1}^{N}\chi_{bn}^{\dagger}K_n\chi_{an} - (k_b - k_a)\sum_{n=1}^{N}\chi_{bn}^{\dagger}\chi_{an} + \sum_{\substack{n,n'=1\\(n\neq n')}}^{N}\chi_{bn}^{\dagger}\chi_{an'}\left[k_b f(k_b|\boldsymbol{r}_n - \boldsymbol{r}_{n'}|) - k_a f(k_a|\boldsymbol{r}_n - \boldsymbol{r}_{n'}|)\right] = 0 \qquad (E_b \neq E_a), \tag{2.21}$$

may be shown to be closely linked to the orthogonality relation (3.14). The last two identities,

$$(\varepsilon_b-\varepsilon_a)\sum_{n=1}^{N}\chi_{bn}^{\dagger}\chi_{an}-\sum_{\substack{n,n'=1\\(n\neq n')}}^{N}\chi_{bn}^{\dagger}\chi_{an'}\big[\varepsilon_b f(k_b|\boldsymbol{r}_n-\boldsymbol{r}_{n'}|)-\varepsilon_a f(k_a|\boldsymbol{r}_n-\boldsymbol{r}_{n'}|)\big]=0\qquad(E_b\neq E_a)\tag{2.22a}$$

and

$$\frac{\hbar}{2mc}\big(\varepsilon_b^{-1}-\varepsilon_a^{-1}\big)\sum_{n=1}^{N}\chi_{bn}^{\dagger}K_n\chi_{an}+\sum_{\substack{n,n'=1\\(n\neq n')}}^{N}\chi_{bn}^{\dagger}\chi_{an'}\big[f(k_b|\boldsymbol{r}_n-\boldsymbol{r}_{n'}|)-f(k_a|\boldsymbol{r}_n-\boldsymbol{r}_{n'}|)\big]=0$$

$$(E_b\neq E_a),\tag{2.22b}$$

are presented here because of their structural simplicity.

3. Orthogonality and normalization of eigenfunctions

Consider two bound-state eigenfunctions $\Psi_a(\boldsymbol{r})$ and $\Psi_b(\boldsymbol{r})$, belonging to the energy eigenvalues E_a and E_b, respectively. If we premultiply the Dirac equation obeyed by $\Psi_a(\boldsymbol{r})$ with $\Psi_b^{\dagger}(\boldsymbol{r})$ and integrate the result with respect to $\boldsymbol{r}$ over the domain

$$\mathbb{R}^3_{\rho}=\mathbb{R}^3\setminus\bigcup_{n=1}^{N}\mathcal{V}_n,\tag{3.1}$$

where $\mathcal{V}_n$, $n=1,\ldots,N$, is a sphere of radius

$$0<\rho<\min_{1\leqslant n'\neq n''\leqslant N}|\boldsymbol{r}_{n'}-\boldsymbol{r}_{n''}|\tag{3.2}$$

centered at $\boldsymbol{r}_n$ (for simplicity, we choose radii of all spheres $\mathcal{V}_n$ to be identical), this gives

$$\int_{\mathbb{R}^3_{\rho}}\mathrm{d}^3\boldsymbol{r}\;\Psi_b^{\dagger}(\boldsymbol{r})[\mathcal{H}-E_a\mathcal{I}]\Psi_a(\boldsymbol{r})=0,\tag{3.3}$$

where we have denoted

$$\mathcal{H}=-\mathrm{i}c\hbar\boldsymbol{\alpha}\cdot\boldsymbol{\nabla}+mc^2\beta.\tag{3.4}$$

Integrating in Eq. (3.3) by parts and exploiting the Gauss divergence theorem yields

$$\int_{\mathbb{R}^3_{\rho}}\mathrm{d}^3\boldsymbol{r}\;\{[\mathcal{H}-E_a\mathcal{I}]\Psi_b(\boldsymbol{r})\}^{\dagger}\,\Psi_a(\boldsymbol{r})-c\hbar\oint_{\mathcal{S}_{\infty}}\mathrm{d}^2\boldsymbol{\rho}_{\infty}\;\Psi_b^{\dagger}(\boldsymbol{\rho}_{\infty})\mathrm{i}\boldsymbol{n}_{\infty}\cdot\boldsymbol{\alpha}\Psi_a(\boldsymbol{\rho}_{\infty})$$
$$+\frac{c\hbar}{\rho}\sum_{n=1}^{N}\oint_{\mathcal{S}_n}\mathrm{d}^2\boldsymbol{\rho}_n\;\Psi_b^{\dagger}(\boldsymbol{r}_n+\boldsymbol{\rho}_n)\mathrm{i}\boldsymbol{\rho}_n\cdot\boldsymbol{\alpha}\Psi_a(\boldsymbol{r}_n+\boldsymbol{\rho}_n)=0,\tag{3.5}$$

where $\boldsymbol{n}_{\infty}$ is the outward unit vector on the spherical surface at infinity ($\mathcal{S}_{\infty}$) at the point characterized by the (infinite) radius vector $\boldsymbol{\rho}_{\infty}$, while $\boldsymbol{\rho}_n$ (with $|\boldsymbol{\rho}_n|=\rho$) is the radius vector (respective to the center $\boldsymbol{r}_n$) for a point on the spherical surface $\mathcal{S}_n$ bounding $\mathcal{V}_n$ [cf. the comments following Eq. (2.12)]. We observe that because both eigenfunctions $\Psi_a(\boldsymbol{r})$ and $\Psi_b(\boldsymbol{r})$ decay exponentially for $r\to\infty$, the surface integral over $\mathcal{S}_{\infty}$ vanishes. As regards the surface integrals over $\mathcal{S}_n$, with the use of the identity

$$\boldsymbol{\alpha}=\boldsymbol{\alpha}^{(+)}+\boldsymbol{\alpha}^{(-)}\tag{3.6}$$

we split each of them into two integrals and then modify the one containing the matrix $\boldsymbol{\alpha}^{(-)}$ using

$$\boldsymbol{\alpha}^{(-)}=\boldsymbol{\alpha}^{(+)\dagger}.\tag{3.7}$$

This converts Eq. (3.5) into

$$(E_b - E_a)\int_{\mathbb{R}^3_\rho} \mathrm{d}^3\boldsymbol{r}\; \Psi_b^\dagger(\boldsymbol{r})\Psi_a(\boldsymbol{r}) + \frac{c\hbar}{\rho}\sum_{n=1}^{N}\oint_{\mathcal{S}_n} \mathrm{d}^2\boldsymbol{\rho}_n\; \Psi_b^\dagger(\boldsymbol{r}_n+\boldsymbol{\rho}_n)\mathrm{i}\boldsymbol{\rho}_n\cdot\boldsymbol{\alpha}^{(+)}\Psi_a(\boldsymbol{r}_n+\boldsymbol{\rho}_n)$$
$$-\frac{c\hbar}{\rho}\sum_{n=1}^{N}\oint_{\mathcal{S}_n} \mathrm{d}^2\boldsymbol{\rho}_n\,[\mathrm{i}\boldsymbol{\rho}_n\cdot\boldsymbol{\alpha}^{(+)}\Psi_b(\boldsymbol{r}_n+\boldsymbol{\rho}_n)]^\dagger\Psi_a(\boldsymbol{r}_n+\boldsymbol{\rho}_n) = 0. \tag{3.8}$$

So far, the radius ρ has been arbitrary except for being subjected to the constraint (3.2). At this stage, we let it tend to zero. Transforming the surface integrals over $\mathcal{S}_n$ with the aid of the limiting conditions (2.7) and making use of the fact that

$$\varepsilon_b k_b^{-1} - \varepsilon_a k_a^{-1} = -\frac{E_b - E_a}{c\hbar}(\varepsilon_b k_b^{-1})(\varepsilon_a k_a^{-1}) \tag{3.9}$$

casts Eq. (3.8) into the form

$$(E_b - E_a)\lim_{\rho\to 0}\left\{\int_{\mathbb{R}^3_\rho} \mathrm{d}^3\boldsymbol{r}\; \Psi_b^\dagger(\boldsymbol{r})\Psi_a(\boldsymbol{r})\right.$$
$$\left. -\frac{(\varepsilon_b k_b^{-1})(\varepsilon_a k_a^{-1})}{\rho}\sum_{n=1}^{N}\oint_{\mathcal{S}_n} \mathrm{d}^2\boldsymbol{\rho}_n\; \Psi_b^\dagger(\boldsymbol{r}_n+\boldsymbol{\rho}_n)\beta^{(+)}\Psi_a(\boldsymbol{r}_n+\boldsymbol{\rho}_n)\right\} = 0. \tag{3.10}$$

From Eq. (3.10), we see that if E_a and E_b are distinct, then the eigenfunctions $\Psi_a(\boldsymbol{r})$ and $\Psi_b(\boldsymbol{r})$ are orthogonal in the sense of

$$\lim_{\rho\to 0}\left\{\int_{\mathbb{R}^3_\rho} \mathrm{d}^3\boldsymbol{r}\; \Psi_b^\dagger(\boldsymbol{r})\Psi_a(\boldsymbol{r}) - \frac{(\varepsilon_b k_b^{-1})(\varepsilon_a k_a^{-1})}{\rho}\sum_{n=1}^{N}\oint_{\mathcal{S}_n} \mathrm{d}^2\boldsymbol{\rho}_n\; \Psi_b^\dagger(\boldsymbol{r}_n+\boldsymbol{\rho}_n)\beta^{(+)}\Psi_a(\boldsymbol{r}_n+\boldsymbol{\rho}_n)\right\} = 0$$
$$(E_a \neq E_b). \tag{3.11}$$

If for any two sufficiently regular four-component functions $\Phi(\boldsymbol{r})$ and $\Phi'(\boldsymbol{r})$ we define their volume

$$\big\langle\Phi\big|\Phi'\big\rangle_{\mathbb{R}^3_\rho} \equiv \int_{\mathbb{R}^3_\rho} \mathrm{d}^3\boldsymbol{r}\; \Phi^\dagger(\boldsymbol{r})\Phi'(\boldsymbol{r}) \tag{3.12}$$

and surface

$$\big(\Phi\big|\Phi'\big)_{\mathcal{S}_n} = \oint_{\mathcal{S}_n} \mathrm{d}^2\boldsymbol{\rho}_n\; \Phi^\dagger(\boldsymbol{r}_n+\boldsymbol{\rho}_n)\Phi'(\boldsymbol{r}_n+\boldsymbol{\rho}_n) \tag{3.13}$$

scalar products, then the orthogonality relation (3.11) may be compactly rewritten as

$$\lim_{\rho\to 0}\left\{\big\langle\Psi_b\big|\Psi_a\big\rangle_{\mathbb{R}^3_\rho} - \frac{(\varepsilon_b k_b^{-1})(\varepsilon_a k_a^{-1})}{\rho}\sum_{n=1}^{N}\big(\Psi_b\big|\beta^{(+)}\Psi_a\big)_{\mathcal{S}_n}\right\} = 0 \qquad (E_a \neq E_b). \tag{3.14}$$

In what follows, we shall be assuming that eigenfunctions belonging to degenerate energy eigenvalues (if there are any) have been linearly transformed among themselves so that the orthogonality relation

$$\lim_{\rho\to 0}\left\{\big\langle\Psi_b\big|\Psi_a\big\rangle_{\mathbb{R}^3_\rho} - \frac{(\varepsilon_b k_b^{-1})(\varepsilon_a k_a^{-1})}{\rho}\sum_{n=1}^{N}\big(\Psi_b\big|\beta^{(+)}\Psi_a\big)_{\mathcal{S}_n}\right\} = 0 \qquad (a \neq b) \tag{3.15}$$

holds as long as $\Psi_a(\boldsymbol{r})$ and $\Psi_b(\boldsymbol{r})$ are linearly independent, even if $E_a = E_b$ (i.e., if $\varepsilon_a = \varepsilon_b$ and $k_a = k_b$).

One may look on the sesquilinear form

$$\langle\!\langle\Psi_b\big|\Psi_a\rangle\!\rangle \stackrel{\text{def}}{=} \lim_{\rho\to 0}\left\{\big\langle\Psi_b\big|\Psi_a\big\rangle_{\mathbb{R}^3_\rho} - \frac{(\varepsilon_b k_b^{-1})(\varepsilon_a k_a^{-1})}{\rho}\sum_{n=1}^{N}\big(\Psi_b\big|\beta^{(+)}\Psi_a\big)_{\mathcal{S}_n}\right\} \tag{3.16}$$

as a scalar pseudo-product of two eigenfunctions $\Psi_b(\boldsymbol{r})$ and $\Psi_a(\boldsymbol{r})$. It is not sign-definite since in the product of $\Psi_a(\boldsymbol{r})$ with itself, i.e., in the form

$$\langle\!\langle\Psi_a\big|\Psi_a\rangle\!\rangle = \lim_{\rho\to 0}\left\{\big\langle\Psi_a\big|\Psi_a\big\rangle_{\mathbb{R}^3_\rho} - \frac{\varepsilon_a^2 k_a^{-2}}{\rho}\sum_{n=1}^{N}\big(\Psi_a\big|\beta^{(+)}\Psi_a\big)_{\mathcal{S}_n}\right\}, \tag{3.17}$$

the expression between the curly brackets is a difference of two nonnegative terms and nothing can be said a priori about the sign of its limit. We define the pseudo-norm $\|\Psi_a\|$ of the eigenfunction $\Psi_a(\boldsymbol{r})$ as

$$\|\Psi_a\| = \sqrt{|\langle\!\langle\Psi_a\big|\Psi_a\rangle\!\rangle|} \geqslant 0. \tag{3.18}$$

The eigenfunctions with vanishing pseudo-norm, i.e., those for which it holds that

$$\langle\!\langle\Psi_a\big|\Psi_a\rangle\!\rangle = 0, \tag{3.19}$$

will be called null-eigenfunctions. In addition, we define the signature $\Delta_a \in \{0, \pm 1\}$ of the eigenfunction $\Psi_a(\boldsymbol{r})$ as

$$\Delta_a = \operatorname{sgn}\langle\!\langle\Psi_a\big|\Psi_a\rangle\!\rangle \tag{3.20}$$

(please observe that null-eigenfunctions have signature zero).

In standard quantum mechanics, it is frequently convenient to work with bound-state eigenfunctions normalized to the unity with respect to the natural norm induced by a scalar product under which eigenfunctions belonging to different eigenvalues are orthogonal. Provided that $\Delta_a = \pm 1$, in our case the analogous normalizing role is played by the constraint

$$\langle\!\langle\Psi_a\big|\Psi_a\rangle\!\rangle = \Delta_a, \tag{3.21}$$

which, at least formally, determines $\Psi_a(\boldsymbol{r})$ up to a multiplicative phase factor. On combining Eq. (3.21) with the orthogonality constraint (3.15), we then obtain the generalized orthonormality relation

$$\langle\!\langle\Psi_b\big|\Psi_a\rangle\!\rangle = \delta_{ba}\Delta_a \tag{3.22}$$

obeyed by the eigenfunctions to the problem we study here.

Equations (3.21) and (3.17) are important from the theoretical point of view. However, it turns out that except for the simplest case of a particle bound in the field of a single zero-range potential (cf. Section 6.1), this pair cannot be used to practically perform the eigenfunction normalization process. The reason for this is that if more than one potential center is involved, the volume integral $\big\langle\Psi_a\big|\Psi_a\big\rangle_{\mathbb{R}^3_\rho}$ appearing in Eq. (3.17) is not amenable to direct analytical evaluation. To overcome the difficulty, we shall transform the formal definition (3.16) of the pseudo-product $\langle\!\langle\Psi_b\big|\Psi_a\rangle\!\rangle$ to an operational form. To this end, consider the easily provable operator identity

$$\mathcal{H}\beta^{(-)} - \beta^{(+)}\mathcal{H} + mc^2\mathcal{I} = 0, \tag{3.23}$$

which is obeyed by the Dirac Hamiltonian (3.4). Premultiplying Eq. (3.23) with $\Psi_b^\dagger(\boldsymbol{r})$, postmultiplying with $\Psi_a(\boldsymbol{r})$ and integrating over the domain $\mathbb{R}^3_\rho$ yields

$$\big\langle\Psi_b\big|\mathcal{H}\beta^{(-)}\Psi_a\big\rangle_{\mathbb{R}^3_\rho} - \big\langle\Psi_b\big|\beta^{(+)}\mathcal{H}\Psi_a\big\rangle_{\mathbb{R}^3_\rho} + mc^2\big\langle\Psi_b\big|\Psi_a\big\rangle_{\mathbb{R}^3_\rho} = 0. \tag{3.24}$$

If in the first term on the left-hand side the action of $\mathcal{H}$ is transferred to the left with the aid of the integration by parts, this gives

$$\big\langle\mathcal{H}\Psi_b\big|\beta^{(-)}\Psi_a\big\rangle_{\mathbb{R}^3_\rho} + \frac{c\hbar}{\rho}\sum_{n=1}^{N}\big(\Psi_b\big|\mathrm{i}\boldsymbol{\rho}_n\cdot\boldsymbol{\alpha}\beta^{(-)}\Psi_a\big)_{\mathcal{S}_n} - \big\langle\Psi_b\big|\beta^{(+)}\mathcal{H}\Psi_a\big\rangle_{\mathbb{R}^3_\rho} + mc^2\big\langle\Psi_b\big|\Psi_a\big\rangle_{\mathbb{R}^3_\rho} = 0, \tag{3.25}$$

where we have exploited the fact that the surface integral over the infinite sphere $\mathcal{S}_\infty$ vanishes. Since $\Psi_a(\boldsymbol{r})$ and $\Psi_b(\boldsymbol{r})$ are eigenfunctions belonging to the energy eigenvalues E_a and E_b, respectively,

and since the identity (2.8a) holds, Eq. (3.25) may be rewritten in the form

$$\left\langle\Psi_b\middle|\left[E_b\beta^{(-)}-E_a\beta^{(+)}+mc^2\mathcal{I}\right]\Psi_a\right\rangle_{\mathbb{R}^3_\rho}+\frac{c\hbar}{\rho}\sum_{n=1}^{N}\left(\Psi_b\middle|\mathrm{i}\boldsymbol{\rho}_n\cdot\boldsymbol{\alpha}^{(+)}\Psi_a\right)_{\mathcal{S}_n}=0. \tag{3.26}$$

In the limit $\rho\to 0$, with the use of the interaction conditions (2.7), Eq. (3.26) goes over into

$$\begin{aligned}&\lim_{\rho\to 0}\left\{\left\langle\Psi_b\middle|\left[E_b\beta^{(-)}-E_a\beta^{(+)}+mc^2\mathcal{I}\right]\Psi_a\right\rangle_{\mathbb{R}^3_\rho}-\frac{c\hbar\varepsilon_a k_a^{-1}}{\rho}\sum_{n=1}^{N}\left(\Psi_b\middle|\beta^{(+)}\Psi_a\right)_{\mathcal{S}_n}\right\}\\&\quad=\frac{\hbar^2}{2m}\lim_{\rho\to 0}\sum_{n=1}^{N}\left(\Psi_b\middle|\mathcal{K}_n^{(+)}\Psi_a\right)_{\mathcal{S}_n}.\end{aligned} \tag{3.27}$$

Using elementary properties of the matrices $\beta^{(\pm)}$, the above result may be further transformed into the integral identity

$$\begin{aligned}&(E_b+mc^2)\lim_{\rho\to 0}\left\{\left\langle\Psi_b\middle|\Psi_a\right\rangle_{\mathbb{R}^3_\rho}-\frac{(\varepsilon_b k_b^{-1})(\varepsilon_a k_a^{-1})}{\rho}\sum_{n=1}^{N}\left(\Psi_b\middle|\beta^{(+)}\Psi_a\right)_{\mathcal{S}_n}\right\}\\&\quad=(E_b+E_a)\left\langle\Psi_b\middle|\beta^{(+)}\Psi_a\right\rangle_{\mathbb{R}^3}+\frac{\hbar^2}{2m}\lim_{\rho\to 0}\sum_{n=1}^{N}\left(\Psi_b\middle|\mathcal{K}_n^{(+)}\Psi_a\right)_{\mathcal{S}_n},\end{aligned} \tag{3.28}$$

where we have made use of the fact that

$$\lim_{\rho\to 0}\left\langle\Psi_b\middle|\beta^{(+)}\Psi_a\right\rangle_{\mathbb{R}^3_\rho}=\left\langle\Psi_b\middle|\beta^{(+)}\Psi_a\right\rangle_{\mathbb{R}^3}. \tag{3.29}$$

On invoking Eq. (3.16), the left-hand side of Eq. (3.28) is seen to be a multiple of the pseudo-product $\langle\!\langle\Psi_b\middle|\Psi_a\rangle\!\rangle$. If the orthogonality relation (3.15) holds, which we shall assume to be the case, then irrespective of whether the eigenfunctions have been normalized in the sense of Eq. (3.21) or not, Eq. (3.28) may be cast into the symmetric form

$$\langle\!\langle\Psi_b\middle|\Psi_a\rangle\!\rangle=\frac{(E_b+E_a)\left\langle\Psi_b\middle|\beta^{(+)}\Psi_a\right\rangle_{\mathbb{R}^3}+\dfrac{\hbar^2}{2m}\lim\limits_{\rho\to 0}\sum\limits_{n=1}^{N}\left(\Psi_b\middle|\mathcal{K}_n^{(+)}\Psi_a\right)_{\mathcal{S}_n}}{\sqrt{(E_b+mc^2)(E_a+mc^2)}}. \tag{3.30}$$

This is the sought alternative representation for $\langle\!\langle\Psi_b\middle|\Psi_a\rangle\!\rangle$. In the particular case of $b=a$, it becomes

$$\langle\!\langle\Psi_a\middle|\Psi_a\rangle\!\rangle=\left(1-\varepsilon_a^2\right)\left\langle\Psi_a\middle|\beta^{(+)}\Psi_a\right\rangle_{\mathbb{R}^3}+\frac{\hbar}{2mc}\varepsilon_a k_a^{-1}\lim_{\rho\to 0}\sum_{n=1}^{N}\left(\Psi_a\middle|\mathcal{K}_n^{(+)}\Psi_a\right)_{\mathcal{S}_n}. \tag{3.31}$$

The practical advantage of the representation of $\langle\!\langle\Psi_a\middle|\Psi_a\rangle\!\rangle$ given in Eq. (3.31) over the one in Eq. (3.17) is that the surface and the volume integrals appearing in the former may be reduced analytically to closed-form algebraic expressions. Using Eqs. (2.2b) and (2.3a), with no difficulty one shows that

$$\lim_{\rho\to 0}\left(\Psi_a\middle|\mathcal{K}_n^{(+)}\Psi_a\right)_{\mathcal{S}_n}=\frac{4\pi}{k_a^2}\chi_{an}^\dagger K_n\chi_{an}. \tag{3.32}$$

Reduction of the volume integral $\left\langle\Psi_a\middle|\beta^{(+)}\Psi_a\right\rangle_{\mathbb{R}^3}$ is a bit more involved. We have

$$\left\langle\Psi_a\middle|\beta^{(+)}\Psi_a\right\rangle_{\mathbb{R}^3}=\frac{1}{k_a^2}\sum_{n,n'=1}^{N}\chi_{an}^\dagger\chi_{an'}\int_{\mathbb{R}^3}\mathrm{d}^3\boldsymbol{r}\,\frac{\mathrm{e}^{-k_a|\boldsymbol{r}-\boldsymbol{r}_n|}}{|\boldsymbol{r}-\boldsymbol{r}_n|}\frac{\mathrm{e}^{-k_a|\boldsymbol{r}-\boldsymbol{r}_{n'}|}}{|\boldsymbol{r}-\boldsymbol{r}_{n'}|}. \tag{3.33}$$

The integral in Eq. (3.33) may be evaluated in the prolate spheroidal coordinates $\xi_{nn'}$, $\eta_{nn'}$, $\varphi_{nn'}$. The former two are defined as

$$\xi_{nn'} = \frac{|\boldsymbol{r}-\boldsymbol{r}_n| + |\boldsymbol{r}-\boldsymbol{r}_{n'}|}{|\boldsymbol{r}_n - \boldsymbol{r}_{n'}|} \tag{3.34a}$$

and

$$\eta_{nn'} = \frac{|\boldsymbol{r}-\boldsymbol{r}_n| - |\boldsymbol{r}-\boldsymbol{r}_{n'}|}{|\boldsymbol{r}_n - \boldsymbol{r}_{n'}|}, \tag{3.34b}$$

respectively, whereas the latter is a rotational angle in a plane perpendicular to the vector $\boldsymbol{r}_n - \boldsymbol{r}_{n'}$. The ranges in which these coordinates vary are

$$1 \leqslant \xi_{nn'} < \infty, \qquad -1 \leqslant \eta_{nn'} \leqslant 1, \qquad 0 \leqslant \varphi_{nn'} < 2\pi. \tag{3.35}$$

Since from Eqs. (3.34a) and (3.34b) one has

$$|\boldsymbol{r}-\boldsymbol{r}_n| = \frac{1}{2}|\boldsymbol{r}_n - \boldsymbol{r}_{n'}|(\xi_{nn'} + \eta_{nn'}), \tag{3.36a}$$

$$|\boldsymbol{r}-\boldsymbol{r}_{n'}| = \frac{1}{2}|\boldsymbol{r}_n - \boldsymbol{r}_{n'}|(\xi_{nn'} - \eta_{nn'}), \tag{3.36b}$$

and since in the prolate spheroidal coordinates the infinitesimal volume element $\mathrm{d}^3\boldsymbol{r}$ is

$$\mathrm{d}^3\boldsymbol{r} = \frac{|\boldsymbol{r}_n - \boldsymbol{r}_{n'}|^3}{8}\left(\xi_{nn'}^2 - \eta_{nn'}^2\right)\mathrm{d}\xi_{nn'}\mathrm{d}\eta_{nn'}\mathrm{d}\varphi_{nn'}, \tag{3.37}$$

elementary integrations over the three variables yield the result

$$\int_{\mathbb{R}^3} \mathrm{d}^3\boldsymbol{r}\, \frac{\mathrm{e}^{-k_a|\boldsymbol{r}-\boldsymbol{r}_n|}}{|\boldsymbol{r}-\boldsymbol{r}_n|}\frac{\mathrm{e}^{-k_a|\boldsymbol{r}-\boldsymbol{r}_{n'}|}}{|\boldsymbol{r}-\boldsymbol{r}_{n'}|} = \frac{2\pi}{k_a}\mathrm{e}^{-k_a|\boldsymbol{r}_n-\boldsymbol{r}_{n'}|}. \tag{3.38}$$

It then follows that

$$\left\langle \Psi_a \middle| \beta^{(+)}\Psi_a \right\rangle_{\mathbb{R}^3} = \frac{2\pi}{k_a^3}\sum_{n,n'=1}^{N} \chi_{an}^\dagger \chi_{an'}\mathrm{e}^{-k_a|\boldsymbol{r}_n-\boldsymbol{r}_{n'}|}. \tag{3.39}$$

On combining Eqs. (3.31), (3.32) and (3.39), we infer the following algebraic representation of the pseudo-product $\langle\!\langle \Psi_a | \Psi_a \rangle\!\rangle$:

$$\langle\!\langle \Psi_a \middle| \Psi_a \rangle\!\rangle = \frac{2\pi}{k_a^3}\left[\left(1-\varepsilon_a^2\right)\sum_{n,n'=1}^{N} \chi_{an}^\dagger \chi_{an'}\mathrm{e}^{-k_a|\boldsymbol{r}_n-\boldsymbol{r}_{n'}|} + \frac{\hbar\varepsilon_a}{mc}\sum_{n=1}^{N}\chi_{an}^\dagger K_n \chi_{an}\right]. \tag{3.40}$$

Hence, the relation (3.21) may be rewritten in the following form:

$$\frac{2\pi}{k_a^3}\left[\left(1-\varepsilon_a^2\right)\sum_{n,n'=1}^{N} \chi_{an}^\dagger \chi_{an'}\mathrm{e}^{-k_a|\boldsymbol{r}_n-\boldsymbol{r}_{n'}|} + \frac{\hbar\varepsilon_a}{mc}\sum_{n=1}^{N}\chi_{an}^\dagger K_n \chi_{an}\right] = \Delta_a. \tag{3.41}$$

If $\Delta_a \neq 0$, Eq. (3.41) fixes the absolute value of a common multiplicative factor in the spinors χ_{an}, and thus actually normalizes $\Psi_a(\boldsymbol{r})$.

It is profitable to juggle a bit with the form of Eq. (3.40). If we transform its right-hand side with the aid of Eq. (2.4b), this gives

$$\langle\!\langle \Psi_a \middle| \Psi_a \rangle\!\rangle = \frac{4\pi\varepsilon_a}{c\hbar k_a^3}\left[E_a k_a^{-1}\sum_{n,n'=1}^{N} \chi_{an}^\dagger \chi_{an'}\mathrm{e}^{-k_a|\boldsymbol{r}_n-\boldsymbol{r}_{n'}|} + \frac{\hbar^2}{2m}\sum_{n=1}^{N}\chi_{an}^\dagger K_n \chi_{an}\right]. \tag{3.42}$$

It is immediately seen that the expression in the square bracket coincides with the left-hand side of Eq. (2.20). Hence, we get the remarkable relationship

$$\langle\!\langle \Psi_a \middle| \Psi_a \rangle\!\rangle = 4\pi c\hbar\varepsilon_a k_a^{-2}\mathsf{x}_a^\dagger\left[\frac{\partial \mathsf{L}(E)}{\partial E}\right]_{E=E_a}\mathsf{x}_a. \tag{3.43}$$

If it is combined with the normalization relation (3.21), the latter takes the form

$$4\pi c\hbar\varepsilon_a k_a^{-2}\mathsf{x}_a^\dagger\left[\frac{\partial\mathsf{L}(E)}{\partial E}\right]_{E=E_a}\mathsf{x}_a=\Delta_a. \tag{3.44}$$

Equation (3.44) will find an application at the end of the next section, where we shall exploit it to derive a useful relationship between a normalized eigenfunction $\Psi_a(\boldsymbol{r})$ and a related Sturmian function $\Sigma_a(E,\boldsymbol{r})$.

4. The Sturmian functions

The Sturmian functions for our model are defined as these solutions to the Dirac equation

$$[-\mathrm{i}c\hbar\boldsymbol{\alpha}\cdot\boldsymbol{\nabla}+mc^2\beta-E\mathcal{I}]\Sigma_a(E,\boldsymbol{r})=0\qquad(\boldsymbol{r}\neq\boldsymbol{r}_n;\,n=1,\ldots,N), \tag{4.1}$$

which are of the form

$$\Sigma_a(E,\boldsymbol{r})=\sum_{n=1}^{N}\begin{pmatrix}f(k|\boldsymbol{r}-\boldsymbol{r}_n|)\eta_{an}(E)\\ \mathrm{i}\varepsilon g(k|\boldsymbol{r}-\boldsymbol{r}_n|)\boldsymbol{\mu}_n(\boldsymbol{r})\cdot\boldsymbol{\sigma}\eta_{an}(E)\end{pmatrix}, \tag{4.2}$$

with $f(z)$, $g(z)$, $\mu_n(\boldsymbol{r})$, k and ε defined in Eqs. (2.3), (2.5) and (2.16), respectively, and which are forced to obey the constraining conditions

$$\lim_{\boldsymbol{r}\to\boldsymbol{r}_n}\left\{\mathrm{i}(\boldsymbol{r}-\boldsymbol{r}_n)\cdot\boldsymbol{\alpha}^{(+)}+\frac{\hbar}{2mc}|\boldsymbol{r}-\boldsymbol{r}_n|\mathcal{K}_n^{(+)}-\lambda_a(E)\varepsilon|\boldsymbol{r}-\boldsymbol{r}_n|\beta^{(+)}+\varepsilon k^{-1}\beta^{(+)}\right\}\Sigma_a(E,\boldsymbol{r})=0$$
$$(n=1,\ldots,N) \tag{4.3}$$

[cf. Eq. (2.7)], with $\mathcal{K}_n^{(+)}$ defined as in Eqs. (2.9)–(2.11). In Eqs. (4.1)–(4.3), E is presumed to have a *fixed* value from the range $-mc^2<E\leqslant mc^2$ [in general, E need not coincide with any of the eigenenergies to the eigenproblem constituted by Eqs. (2.1), (2.2) and (2.7)], whereas the role of an eigenparameter is now taken over by the parameter $\lambda_a(E)$ entering the limiting conditions (4.3). The two-component spinors $\eta_{an}(E)$ [not to be confused with the spheroidal coordinate $\eta_{nn'}$ defined in Eq. (3.34b)] entering Eq. (4.2) play the role of generalized linear combination coefficients and may be determined by solving the algebraic eigensystem

$$\left\{\frac{\hbar}{2mc\varepsilon}K_n-[\lambda_a(E)+1]I\right\}\eta_{an}(E)+\sum_{\substack{n'=1\\(n'\neq n)}}^{N}f(k|\boldsymbol{r}_n-\boldsymbol{r}_{n'}|)\eta_{an'}(E)=0\qquad(n=1,\ldots,N) \tag{4.4}$$

emerging after Eq. (4.2) is inserted into Eq. (4.3). If the spinors $\eta_{an}(E)$ are collected in a $2N$-component vector

$$\mathsf{y}_a(E)=\begin{pmatrix}\eta_{a1}^{\mathrm{T}}(E) & \cdots & \eta_{aN}^{\mathrm{T}}(E)\end{pmatrix}^{\mathrm{T}}, \tag{4.5}$$

the eigensystem (4.4) may be rewritten compactly as

$$\mathsf{L}(E)\mathsf{y}_a(E)=\lambda_a(E)\mathsf{y}_a(E), \tag{4.6}$$

where $\mathsf{L}(E)$ is the $2N\times 2N$ matrix with its 2×2 block-elements defined in Eq. (2.15). We see that $\lambda_a(E)$ and $\mathsf{y}_a(E)$ are an eigenvalue and an associated eigenvector of the matrix $\mathsf{L}(E)$, respectively. Since k and ε are real, $\mathsf{L}(E)$ is Hermitian and therefore we know in advance that all its eigenvalues $\lambda_a(E)$ are real, and also that eigenvectors belonging to different eigenvalues are orthogonal in the sense of

$$\mathsf{y}_b^\dagger(E)\mathsf{y}_a(E)=0\qquad[\lambda_b(E)\neq\lambda_a(E)]. \tag{4.7}$$

In what follows, we shall be assuming that eigenvectors associated with degenerate eigenvalues (if there are any) have been orthogonalized in the same manner, and consequently it holds that

$$\mathsf{y}_b^\dagger(E)\mathsf{y}_a(E)=0\qquad(b\neq a). \tag{4.8}$$

Temporarily, we leave aside the issue of normalization of the eigenvectors $\mathsf{y}_a(E)$ and turn to the problem of orthogonality and normalization of the Sturmian functions.

To this end, consider the volume integral $\big\langle \Sigma_b(E)\big|[\mathcal{H}-E\mathcal{I}]\Sigma_a(E)\big\rangle_{\mathbb{R}^3_\rho}$ over the domain $\mathbb{R}^3_\rho$ defined in Eq. (3.1). If the action of the operator $\mathcal{H}-E\mathcal{I}$ is transferred to the left with the use of the Gauss integral formula, this leads to the identity

$$\big\langle \Sigma_b(E)\big|[\mathcal{H}-E\mathcal{I}]\Sigma_a(E)\big\rangle_{\mathbb{R}^3_\rho} = \big\langle [\mathcal{H}-E\mathcal{I}]\Sigma_b(E)\big|\,\Sigma_a(E)\big\rangle_{\mathbb{R}^3_\rho} + \frac{c\hbar}{\rho}\sum_{n=1}^{N}\big(\Sigma_b(E)\big|\mathrm{i}\boldsymbol{\rho}_n\cdot\boldsymbol{\alpha}\Sigma_a(E)\big)_{\mathcal{S}_n}, \quad (4.9)$$

where the integral over the surface of an infinitely distant sphere $\mathcal{S}_\infty$ has been omitted, being zero in view of the exponential decay of both $\Sigma_a(E,\boldsymbol{r})$ and $\Sigma_b(E,\boldsymbol{r})$. Since the operator $\mathcal{H}-E\mathcal{I}$ annihilates both Sturmians $\Sigma_a(E,\boldsymbol{r})$ and $\Sigma_b(E,\boldsymbol{r})$ [cf. Eq. (4.1)], the two volume integrals in Eq. (4.9) vanish, yielding

$$\frac{1}{\rho}\sum_{n=1}^{N}\big(\Sigma_b(E)\big|\mathrm{i}\boldsymbol{\rho}_n\cdot\boldsymbol{\alpha}\Sigma_a(E)\big)_{\mathcal{S}_n} = 0 \quad (4.10)$$

and then, with the aid of Eqs. (3.6) and (3.7),

$$\frac{1}{\rho}\sum_{n=1}^{N}\big(\Sigma_b(E)\big|\mathrm{i}\boldsymbol{\rho}_n\cdot\boldsymbol{\alpha}^{(+)}\Sigma_a(E)\big)_{\mathcal{S}_n} - \frac{1}{\rho}\sum_{n=1}^{N}\big(\mathrm{i}\boldsymbol{\rho}_n\cdot\boldsymbol{\alpha}^{(+)}\Sigma_b(E)\big|\,\Sigma_a(E)\big)_{\mathcal{S}_n} = 0. \quad (4.11)$$

If we let the common radius ρ of the spheres $\mathcal{S}_n$ tend to zero, after exploiting the constraints (4.3) we obtain

$$[\lambda_a(E)-\lambda_b(E)]\lim_{\rho\to 0}\sum_{n=1}^{N}\big(\Sigma_b(E)\big|\beta^{(+)}\Sigma_a(E)\big)_{\mathcal{S}_n} = 0, \quad (4.12)$$

where we have also made use of the fact that the Sturmian eigenvalues are real [cf. the remark preceding Eq. (4.7)]. Equation (4.12) implies that the Sturmian functions obey the orthogonality relation

$$\lim_{\rho\to 0}\sum_{n=1}^{N}\big(\Sigma_b(E)\big|\beta^{(+)}\Sigma_a(E)\big)_{\mathcal{S}_n} = 0 \qquad [\lambda_b(E)\neq\lambda_a(E)]. \quad (4.13)$$

Actually, Eq. (4.13) does not offer anything more than Eq. (4.7) does. Indeed, using Eq. (4.2) it is straightforward to show that

$$\lim_{\rho\to 0}\big(\Sigma_b(E)\big|\beta^{(+)}\Sigma_a(E)\big)_{\mathcal{S}_n} = \frac{4\pi}{k^2}\eta^{\dagger}_{bn}(E)\eta_{an}(E), \quad (4.14)$$

hence, it follows that

$$\lim_{\rho\to 0}\sum_{n=1}^{N}\big(\Sigma_b(E)\big|\beta^{(+)}\Sigma_a(E)\big)_{\mathcal{S}_n} = \frac{4\pi}{k^2}\mathsf{y}^{\dagger}_b(E)\mathsf{y}_a(E), \quad (4.15)$$

which implies the equivalence of Eqs. (4.7) and (4.13). But if Eq. (4.15) is combined with Eq. (4.8), one obtains a still more general orthogonality relation, namely

$$\lim_{\rho\to 0}\sum_{n=1}^{N}\big(\Sigma_b(E)\big|\beta^{(+)}\Sigma_a(E)\big)_{\mathcal{S}_n} = 0 \qquad (b\neq a). \quad (4.16)$$

If we normalize the Sturmian functions in accordance with

$$\lim_{\rho\to 0}\sum_{n=1}^{N}\big(\Sigma_a(E)\big|\beta^{(+)}\Sigma_a(E)\big)_{\mathcal{S}_n} = 1, \quad (4.17)$$

we have the integral orthonormality relation

$$\lim_{\rho\to 0}\sum_{n=1}^{N}\bigl(\Sigma_b(E)\bigl|\beta^{(+)}\Sigma_a(E)\bigr)_{\mathcal{S}_n}=\delta_{ba}. \tag{4.18}$$

Concluding this thread, we observe that imposing the constraint (4.17) we have automatically normalized the eigenvectors $\mathsf{y}_a(E)$, so that Eq. (4.8) may be replaced with the more general algebraic orthonormality relation

$$\frac{4\pi}{k^2}\mathsf{y}_b^\dagger(E)\mathsf{y}_a(E)=\delta_{ba}. \tag{4.19}$$

Until this moment, the index used to distinguish between different Sturmian eigenpairs $\lambda_a(E)$ and $\Sigma_a(E,\boldsymbol{r})$ has not been related in any way to the index labeling particle's eigenenergies E_a and their associated eigenfunctions $\Psi_a(\boldsymbol{r})$. However, it is convenient to correlate these indices to have

$$\lambda_a(E_a)=0 \quad\text{and}\quad \mathsf{y}_a(E_a)=A_a\mathsf{x}_a, \tag{4.20}$$

where A_a is a proportionality factor which is to be determined. Then it holds that

$$\Sigma_a(E_a,\boldsymbol{r})=A_a\Psi_a(\boldsymbol{r}). \tag{4.21}$$

To determine the coefficient A_a, we invoke the Hellmann–Feynman theorem for the matrix $\mathsf{L}(E)$, which is

$$\mathsf{y}_a^\dagger(E)\frac{\partial\mathsf{L}(E)}{\partial E}\mathsf{y}_a(E)=\frac{\partial\lambda_a(E)}{\partial E}\mathsf{y}_a^\dagger(E)\mathsf{y}_a(E). \tag{4.22}$$

After the limit $E\to E_a$ is taken and then, on the left-hand side only, the use is made of the second of Eqs. (4.20), Eq. (4.22) becomes

$$|A_a|^2\mathsf{x}_a^\dagger\left[\frac{\partial\mathsf{L}(E)}{\partial E}\right]_{E=E_a}\mathsf{x}_a=\left[\frac{\partial\lambda_a(E)}{\partial E}\right]_{E=E_a}\mathsf{y}_a^\dagger(E_a)\mathsf{y}_a(E_a). \tag{4.23}$$

A simplification occurs after the left-hand side of Eq. (4.23) is transformed with the aid of Eq. (3.44) and the right-hand side with the aid of Eq. (4.19), the latter being taken in the case of $b=a$ and $E=E_a$. This gives

$$|A_a|^2\Delta_a=c\hbar\varepsilon_a\left[\frac{\partial\lambda_a(E)}{\partial E}\right]_{E=E_a}. \tag{4.24}$$

From this one finds that

$$A_a=\sqrt{c\hbar\varepsilon_a|\partial\lambda_a(E)/\partial E|_{E=E_a}}\qquad(\Delta_a\neq 0), \tag{4.25}$$

an adjustable phase factor in A_a being chosen to have A_a real and positive, and also that

$$\Delta_a=\operatorname{sgn}\left[\frac{\partial\lambda_a(E)}{\partial E}\right]_{E=E_a}. \tag{4.26}$$

In summary, we see that once the Sturmian eigenpairs $\lambda_a(E)$ and $\Sigma_a(E,\boldsymbol{r})$ have been found, with $\Sigma_a(E,\boldsymbol{r})$ normalized in the sense of Eq. (4.17), one may determine the particle's eigenenergies E_a from the first of Eqs. (4.20), whereas the associated eigenfunctions $\Psi_a(\boldsymbol{r})$, normalized in the sense of Eq. (3.21), are given by

$$\Psi_a(\boldsymbol{r})=\frac{\Sigma_a(E_a,\boldsymbol{r})}{\sqrt{c\hbar\varepsilon_a|\partial\lambda_a(E)/\partial E|_{E=E_a}}}\qquad(\Delta_a\neq 0). \tag{4.27}$$

It should be observed that if E_a is degenerate, the associated eigenfunctions resulting from Eq. (4.27) may need to be orthogonalized to obey the orthonormality relation (3.22).

5. The matrix Green's function and its Sturmian representation

In our model, the matrix Green's function $\mathcal{G}(E,\boldsymbol{r},\boldsymbol{r}')$ due to a source located at the point $\boldsymbol{r}'\neq\boldsymbol{r}_n$, $n=1,\ldots,N$, satisfies the inhomogeneous differential equation

$$[-\mathrm{i}c\hbar\boldsymbol{\alpha}\cdot\boldsymbol{\nabla}+mc^2\beta-E\mathcal{I}]\mathcal{G}(E,\boldsymbol{r},\boldsymbol{r}')=\delta^{(3)}(\boldsymbol{r}-\boldsymbol{r}')\mathcal{I}\qquad(\boldsymbol{r},\boldsymbol{r}'\neq\boldsymbol{r}_n;\,n=1,\ldots,N),\tag{5.1}$$

the asymptotic condition

$$\mathcal{G}(E,\boldsymbol{r},\boldsymbol{r}')\overset{r\to\infty}{\longrightarrow}\mathcal{A}(E,\boldsymbol{r}')\frac{\mathrm{e}^{-kr}}{r},\tag{5.2}$$

where $\mathcal{A}(E,\boldsymbol{r}')$ is a certain 4×4 amplitude matrix, and also the limiting constraints

$$\lim_{\boldsymbol{r}\to\boldsymbol{r}_n}\left[\mathrm{i}(\boldsymbol{r}-\boldsymbol{r}_n)\cdot\boldsymbol{\alpha}^{(+)}+\frac{\hbar}{2mc}|\boldsymbol{r}-\boldsymbol{r}_n|\mathcal{K}_n^{(+)}+\varepsilon k^{-1}\beta^{(+)}\right]\mathcal{G}(E,\boldsymbol{r},\boldsymbol{r}')=0\qquad(n=1,\ldots,N)\tag{5.3}$$

at locations of the potential centers [cf. Eq. (2.7)]. The energy parameter E is constrained to the interval $-mc^2<E\leqslant mc^2$. We shall seek $\mathcal{G}(E,\boldsymbol{r},\boldsymbol{r}')$ in the form

$$\mathcal{G}(E,\boldsymbol{r},\boldsymbol{r}')=\mathcal{G}_0(E,\boldsymbol{r},\boldsymbol{r}')+\sum_{a=1}^{2N}\Sigma_a(E,\boldsymbol{r})C_a^\dagger(E,\boldsymbol{r}'),\tag{5.4}$$

where

$$\begin{aligned}\mathcal{G}_0(E,\boldsymbol{r},\boldsymbol{r}')&=\frac{1}{4\pi c^2\hbar^2}[-\mathrm{i}c\hbar\boldsymbol{\alpha}\cdot\boldsymbol{\nabla}+mc^2\beta+E\mathcal{I}]\frac{\mathrm{e}^{-k|\boldsymbol{r}-\boldsymbol{r}'|}}{|\boldsymbol{r}-\boldsymbol{r}'|}\\&=\frac{k}{4\pi c^2\hbar^2}\begin{pmatrix}(E+mc^2)f(k|\boldsymbol{r}-\boldsymbol{r}'|)I & \mathrm{i}c\hbar kg(k|\boldsymbol{r}-\boldsymbol{r}'|)\boldsymbol{\mu}(\boldsymbol{r},\boldsymbol{r}')\cdot\boldsymbol{\sigma}\\ \mathrm{i}c\hbar kg(k|\boldsymbol{r}-\boldsymbol{r}'|)\boldsymbol{\mu}(\boldsymbol{r},\boldsymbol{r}')\cdot\boldsymbol{\sigma} & (E-mc^2)f(k|\boldsymbol{r}-\boldsymbol{r}'|)I\end{pmatrix},\end{aligned}\tag{5.5}$$

with

$$\boldsymbol{\mu}(\boldsymbol{r},\boldsymbol{r}')=\frac{\boldsymbol{r}-\boldsymbol{r}'}{|\boldsymbol{r}-\boldsymbol{r}'|},\tag{5.6}$$

is the free-particle Dirac–Green's function, $\Sigma_a(E,\boldsymbol{r})$ are the Sturmian functions of Section 4, while $C_a^\dagger(E,\boldsymbol{r})$ are spinor expansion coefficients which remain to be determined. From the fact that $\mathcal{G}_0(E,\boldsymbol{r},\boldsymbol{r}')$ is known to obey the inhomogeneous equation

$$[-\mathrm{i}c\hbar\boldsymbol{\alpha}\cdot\boldsymbol{\nabla}+mc^2\beta-E\mathcal{I}]\mathcal{G}_0(E,\boldsymbol{r},\boldsymbol{r}')=\delta^{(3)}(\boldsymbol{r}-\boldsymbol{r}')\mathcal{I},\tag{5.7}$$

whereas the Sturmian functions solve the homogeneous equation (4.1), we see that the function $\mathcal{G}(E,\boldsymbol{r},\boldsymbol{r}')$ defined above does indeed satisfy the inhomogeneous equation (5.1). In turn, it follows from Eqs. (5.5), (4.2) and (2.3) that the asymptotic condition (5.2) is also fulfilled. Hence, it remains to adjust the coefficients $C_a^\dagger(E,\boldsymbol{r}')$ so that the constraints (5.3) are complied with.

To achieve the above goal, at first we observe that if the source point $\boldsymbol{r}'$ is located in the domain $\mathbb{R}^3_\rho$ defined in Eq. (3.1), from Eqs. (5.1) one has

$$\big\langle\Sigma_a(E)\big|[\mathcal{H}-E\mathcal{I}]\mathcal{G}(E,\boldsymbol{r}')\big\rangle_{\mathbb{R}^3_\rho}=\Sigma_a^\dagger(E,\boldsymbol{r}'),\tag{5.8}$$

where $\mathcal{H}$ stands for the Dirac Hamiltonian (3.4). Then it trivially follows that

$$\lim_{\rho\to0}\big\langle\Sigma_a(E)\big|[\mathcal{H}-E\mathcal{I}]\mathcal{G}(E,\boldsymbol{r}')\big\rangle_{\mathbb{R}^3_\rho}=\Sigma_a^\dagger(E,\boldsymbol{r}').\tag{5.9}$$

On the other hand, if in the integral $\big\langle\Sigma_a(E)\big|[\mathcal{H}-E\mathcal{I}]\mathcal{G}(E,\boldsymbol{r}')\big\rangle_{\mathbb{R}^3_\rho}$ action of the operator $\mathcal{H}-E\mathcal{I}$ is transferred to the left, with the aid of the Gauss divergence formula one obtains

$$\big\langle\Sigma_a(E)\big|[\mathcal{H}-E\mathcal{I}]\mathcal{G}(E,\boldsymbol{r}')\big\rangle_{\mathbb{R}^3_\rho}=\big\langle[\mathcal{H}-E\mathcal{I}]\Sigma_a(E)\big|\mathcal{G}(E,\boldsymbol{r}')\big\rangle_{\mathbb{R}^3_\rho}+\frac{c\hbar}{\rho}\sum_{n=1}^{N}\big(\Sigma_a(E)\big|\mathrm{i}\boldsymbol{\rho}_n\cdot\boldsymbol{\alpha}\mathcal{G}(E,\boldsymbol{r}')\big)_{\mathcal{S}_n},\tag{5.10}$$

the omitted integral over the infinite sphere $\mathcal{S}_\infty$ being zero. Now, the volume integral on the right-hand side vanishes by virtue of Eq. (4.1), while use of Eqs. (3.6) and (3.7) splits each of the surface integrals into two ones. This leads to

$$\begin{aligned}&\big\langle\Sigma_a(E)\big|[\mathcal{H}-E\mathcal{I}]\mathcal{G}(E,\boldsymbol{r}')\big\rangle_{\mathbb{R}^3_\rho}\\&\quad=\frac{c\hbar}{\rho}\sum_{n=1}^{N}\big(\Sigma_a(E)\big|\mathrm{i}\boldsymbol{\rho}_n\cdot\boldsymbol{\alpha}^{(+)}\mathcal{G}(E,\boldsymbol{r}')\big)_{\mathcal{S}_n}-\frac{c\hbar}{\rho}\sum_{n=1}^{N}\big(\mathrm{i}\boldsymbol{\rho}_n\cdot\boldsymbol{\alpha}^{(+)}\Sigma_a(E)\big|\mathcal{G}(E,\boldsymbol{r}')\big)_{\mathcal{S}_n}.\end{aligned}\tag{5.11}$$

Applying the limit $\rho\to 0$ to both sides of Eq. (5.11) and transforming the right-hand side with the aid of the limiting relations (4.3) and (5.3) gives

$$\lim_{\rho\to0}\big\langle\Sigma_a(E)\big|[\mathcal{H}-E\mathcal{I}]\mathcal{G}(E,\boldsymbol{r}')\big\rangle_{\mathbb{R}^3_\rho}=-c\hbar\varepsilon\lambda_a(E)\lim_{\rho\to0}\sum_{n=1}^{N}\big(\Sigma_a(E)\big|\beta^{(+)}\mathcal{G}(E,\boldsymbol{r}')\big)_{\mathcal{S}_n}.\tag{5.12}$$

Now, from Eq. (5.4) one has

$$\begin{aligned}&\lim_{\rho\to0}\sum_{n=1}^{N}\big(\Sigma_a(E)\big|\beta^{(+)}\mathcal{G}(E,\boldsymbol{r}')\big)_{\mathcal{S}_n}\\&\quad=\lim_{\rho\to0}\sum_{n=1}^{N}\big(\Sigma_a(E)\big|\beta^{(+)}\mathcal{G}_0(E,\boldsymbol{r}')\big)_{\mathcal{S}_n}+\sum_{b=1}^{2N}\left[\lim_{\rho\to0}\sum_{n=1}^{N}\big(\Sigma_a(E)\big|\beta^{(+)}\Sigma_b(E)\big)_{\mathcal{S}_n}\right]C_b^\dagger(E,\boldsymbol{r}').\end{aligned}\tag{5.13}$$

The first term on the right-hand side of Eq. (5.13) is zero, whereas the second one simplifies after the orthonormality relation (4.18) is applied, yielding

$$\lim_{\rho\to0}\sum_{n=1}^{N}\big(\Sigma_a(E)\big|\beta^{(+)}\mathcal{G}(E,\boldsymbol{r}')\big)_{\mathcal{S}_n}=C_a^\dagger(E,\boldsymbol{r}').\tag{5.14}$$

Hence, one has

$$\lim_{\rho\to0}\big\langle\Sigma_a(E)\big|[\mathcal{H}-E\mathcal{I}]\mathcal{G}(E,\boldsymbol{r}')\big\rangle_{\mathbb{R}^3_\rho}=-c\hbar\varepsilon\lambda_a(E)C_a^\dagger(E,\boldsymbol{r}')\tag{5.15}$$

and further, after Eq. (5.15) is combined with Eq. (5.9),

$$C_a^\dagger(E,\boldsymbol{r}')=-\frac{1}{c\hbar\varepsilon}\lambda_a^{-1}(E)\Sigma_a^\dagger(E,\boldsymbol{r}').\tag{5.16}$$

Consequently, the sought form of the Sturmian representation (5.4) of $\mathcal{G}(E,\boldsymbol{r},\boldsymbol{r}')$ is

$$\mathcal{G}(E,\boldsymbol{r},\boldsymbol{r}')=\mathcal{G}_0(E,\boldsymbol{r},\boldsymbol{r}')-\frac{1}{c\hbar\varepsilon}\sum_{a=1}^{2N}\lambda_a^{-1}(E)\Sigma_a(E,\boldsymbol{r})\Sigma_a^\dagger(E,\boldsymbol{r}').\tag{5.17}$$

From Eqs. (5.17) and (5.5) the Green's function is seen to be symmetric in the sense of

$$\mathcal{G}(E,\boldsymbol{r},\boldsymbol{r}')=\mathcal{G}^\dagger(E,\boldsymbol{r}',\boldsymbol{r}).\tag{5.18}$$

6. Illustrative applications

6.1. Particle bound in a field of a single zero-range potential

6.1.1. Bound-state eigenenergies and associated eigenfunctions

Consider a particle moving in a field of a single zero-range potential located at the point $\boldsymbol{r}_1=\boldsymbol{0}$. The 2×2 interaction matrix K (for brevity, we omit the subscript 1) is

$$K=\varkappa I+\boldsymbol{\kappa}\cdot\boldsymbol{\sigma}.\tag{6.1}$$

The matrix $\mathsf{L}(E_a)$ is simply

$$\mathsf{L}(E_a) = \frac{\hbar}{2mc\varepsilon_a} K - I \tag{6.2}$$

and its determinant is

$$\det \mathsf{L}(E_a) = \left(\frac{\hbar\varkappa}{2mc\varepsilon_a} - 1\right)^2 - \left(\frac{\hbar\kappa}{2mc\varepsilon_a}\right)^2, \tag{6.3}$$

where $\kappa = |\boldsymbol{\kappa}|$. Equating the right-hand side to zero [cf. Eq. (2.19)] and solving the resulting equation for ε_a yields

$$\varepsilon_\pm = \frac{\hbar(\varkappa \pm \kappa)}{2mc}, \tag{6.4}$$

where we have put $a = \pm$ with reference to the two signs which appear on the right-hand side. Since, by virtue of the definition (2.4b), $\varepsilon_\pm$ cannot be negative, we have the following three possibilities:

$$\begin{cases} \varkappa < -\kappa & \Rightarrow \text{ there are no bound states} \\ -\kappa \leqslant \varkappa < \kappa & \Rightarrow \text{ there is one bound state of energy } E_+ \\ \varkappa \geqslant \kappa & \Rightarrow \text{ there are two bound states of energies } E_\pm, \end{cases} \tag{6.5}$$

where

$$E_\pm = mc^2 \frac{1 - \left[\dfrac{\hbar(\varkappa \pm \kappa)}{2mc}\right]^2}{1 + \left[\dfrac{\hbar(\varkappa \pm \kappa)}{2mc}\right]^2}. \tag{6.6}$$

In accordance with the definition (2.4a) or with the relation in Eq. (2.6a), wave numbers associated with the eigenenergies (6.6) are

$$k_\pm = \frac{\varkappa \pm \kappa}{1 + \left[\dfrac{\hbar(\varkappa \pm \kappa)}{2mc}\right]^2}. \tag{6.7}$$

It follows from what has been said above that in the limiting case when $\boldsymbol{\kappa} = \mathbf{0}$ and $\varkappa \neq 0$ (which is the case of a 'purely scalar' interaction), there are no bound states if $\varkappa < 0$, whereas if $\varkappa > 0$, then there are two degenerate bound states of energy

$$E = mc^2 \frac{1 - \left(\dfrac{\hbar\varkappa}{2mc}\right)^2}{1 + \left(\dfrac{\hbar\varkappa}{2mc}\right)^2}, \tag{6.8}$$

the redundant subscript at E being omitted. In the second limiting case, i.e., for $\varkappa = 0$ and $\boldsymbol{\kappa} \neq \mathbf{0}$ (which is the case of a 'purely vector' interaction), there will always be only one bound state of energy

$$E_+ = mc^2 \frac{1 - \left(\dfrac{\hbar\kappa}{2mc}\right)^2}{1 + \left(\dfrac{\hbar\kappa}{2mc}\right)^2}. \tag{6.9}$$

In the nonrelativistic approximation, Eqs. (6.6) and (6.7) go over into

$$E_\pm \simeq mc^2 - \frac{\hbar^2(\varkappa \pm \kappa)^2}{2m} \tag{6.10}$$

and

$$k_\pm = \varkappa \pm \kappa, \tag{6.11}$$

respectively. Approximations analogous to that in Eq. (6.10) obviously hold for Eqs. (6.8) and (6.9).

Next, we turn to the eigenfunctions. Adapting Eq. (2.2b) to the present case, we see that the eigenfunctions which belong to the eigenenergies $E_\pm$ are

$$\Psi_\pm(\boldsymbol{r}) = \begin{pmatrix} f(k_\pm r)\chi_\pm \\ \mathrm{i}\varepsilon_\pm g(k_\pm r)\boldsymbol{n}_r\cdot\boldsymbol{\sigma}\chi_\pm \end{pmatrix}, \tag{6.12}$$

where $\boldsymbol{n}_r = \boldsymbol{r}/r$ is the unit vector in the direction of the position vector $\boldsymbol{r}$ and where the spinor coefficients $\chi_\pm$ solve [cf. Eq. (2.14)]

$$\left(\frac{\hbar}{2mc\varepsilon_\pm}K - I\right)\chi_\pm = 0. \tag{6.13}$$

Invoking Eq. (6.1), it is easy to see that the spinors $\chi_\pm$ may be written as

$$\chi_\pm = c_\pm\xi_\pm, \tag{6.14}$$

where $c_\pm$ are normalization coefficients to be determined later, whereas $\xi_\pm$ are normalized (in the sense of $\xi_\pm^\dagger\xi_\pm = 1$) eigenvectors of the matrix $\boldsymbol{\kappa}\cdot\boldsymbol{\sigma}$ and obey

$$\boldsymbol{\kappa}\cdot\boldsymbol{\sigma}\xi_\pm = \pm\kappa\xi_\pm. \tag{6.15}$$

The explicit forms of the spinors $\xi_\pm$ are

$$\xi_+ = \begin{pmatrix} \cos(\theta_\kappa/2) \\ \sin(\theta_\kappa/2)\mathrm{e}^{\mathrm{i}\phi_\kappa} \end{pmatrix}, \qquad \xi_- = \begin{pmatrix} \sin(\theta_\kappa/2) \\ -\cos(\theta_\kappa/2)\mathrm{e}^{\mathrm{i}\phi_\kappa} \end{pmatrix}, \tag{6.16}$$

where $0 \leqslant \theta_\kappa \leqslant \pi$ and $0 \leqslant \phi_\kappa < 2\pi$ are the spherical angles of the vector $\boldsymbol{\kappa}$.

In Section 3, we have mentioned that the single-center system considered here is the one for which the eigenfunctions may be effectively normalized using any of the two available representations of the self-pseudo-product. To show that this is indeed the case, consider at first the pseudo-product $\langle\!\langle\Psi_\pm|\Psi_\pm\rangle\!\rangle$ in the form (3.17), i.e.,

$$\langle\!\langle\Psi_\pm|\Psi_\pm\rangle\!\rangle = \lim_{\rho\to 0}\left\{\langle\Psi_\pm|\Psi_\pm\rangle_{\mathbb{R}^3_\rho} - \frac{\varepsilon_\pm^2 k_\pm^{-2}}{\rho}\big(\Psi_\pm\big|\beta^{(+)}\Psi_\pm\big)_{\mathcal{S}}\right\} \tag{6.17}$$

(the redundant subscript at $\mathcal{S}$ has been omitted intentionally). With no difficulty one finds that

$$\langle\Psi_\pm|\Psi_\pm\rangle_{\mathbb{R}^3_\rho} = \frac{2\pi}{k_\pm^3}\left[1 + \varepsilon_\pm^2\left(1 + \frac{2}{k_\pm\rho}\right)\right]\mathrm{e}^{-2k_\pm\rho}\chi_\pm^\dagger\chi_\pm \tag{6.18a}$$

and

$$\big(\Psi_\pm\big|\beta^{(+)}\Psi_\pm\big)_{\mathcal{S}} = \frac{4\pi}{k_\pm^2}\mathrm{e}^{-2k_\pm\rho}\chi_\pm^\dagger\chi_\pm, \tag{6.18b}$$

and consequently one has

$$\lim_{\rho\to 0}\left\{\langle\Psi_\pm|\Psi_\pm\rangle_{\mathbb{R}^3_\rho} - \frac{\varepsilon_\pm^2 k_\pm^{-2}}{\rho}\big(\Psi_\pm\big|\beta^{(+)}\Psi_\pm\big)_{\mathcal{S}}\right\} = \frac{2\pi}{k_\pm^3}\big(1+\varepsilon_\pm^2\big)\chi_\pm^\dagger\chi_\pm. \tag{6.19}$$

Alternatively, we may take the pseudo-product $\langle\!\langle\Psi_\pm|\Psi_\pm\rangle\!\rangle$ in the form

$$\langle\!\langle\Psi_\pm|\Psi_\pm\rangle\!\rangle = \big(1-\varepsilon_\pm^2\big)\langle\Psi_\pm|\beta^{(+)}\Psi_\pm\rangle_{\mathbb{R}^3} + \frac{\hbar}{2mc}\varepsilon_\pm k_\pm^{-1}\lim_{\rho\to 0}\big(\Psi_\pm\big|\mathcal{K}^{(+)}\Psi_\pm\big)_{\mathcal{S}}, \tag{6.20}$$

which follows from Eq. (3.31). For the two integrals involved one easily obtains

$$\langle\Psi_\pm|\beta^{(+)}\Psi_\pm\rangle_{\mathbb{R}^3} = \frac{2\pi}{k_\pm^3}\chi_\pm^\dagger\chi_\pm \tag{6.21a}$$

and

$$\big(\Psi_\pm\big|\mathcal{K}^{(+)}\Psi_\pm\big)_{\mathcal{S}} = \frac{4\pi(\varkappa\pm\kappa)}{k_\pm^2}\mathrm{e}^{-2k_\pm\rho}\chi_\pm^\dagger\chi_\pm, \tag{6.21b}$$

respectively. This brings the right-hand side of Eq. (6.20) to the form

$$\big(1-\varepsilon_\pm^2\big)\big\langle\Psi_\pm\big|\beta^{(+)}\Psi_\pm\big\rangle_{\mathbb{R}^3} + \frac{\hbar}{2mc}\varepsilon_\pm k_\pm^{-1}\lim_{\rho\to0}\big(\Psi_\pm\big|\mathcal{K}^{(+)}\Psi_\pm\big)_{\mathcal{S}} = \frac{2\pi}{k_\pm^3}\big(1+\varepsilon_\pm^2\big)\chi_\pm^\dagger\chi_\pm. \tag{6.22}$$

We thus see that no matter which of the two available representations of $\langle\!\langle\Psi_\pm\big|\Psi_\pm\rangle\!\rangle$ is used, one gets

$$\langle\!\langle\Psi_\pm\big|\Psi_\pm\rangle\!\rangle = \frac{2\pi}{k_\pm^3}\big(1+\varepsilon_\pm^2\big)\chi_\pm^\dagger\chi_\pm. \tag{6.23}$$

The right-hand side of Eq. (6.23) is positive and this implies that the signatures of the eigenfunctions $\Psi_\pm(\boldsymbol{r})$ are

$$\Delta_\pm = +1. \tag{6.24}$$

Hence, the explicit form of the normalization condition (3.21) is

$$\frac{2\pi}{k_\pm^3}\big(1+\varepsilon_\pm^2\big)\chi_\pm^\dagger\chi_\pm = 1. \tag{6.25}$$

On combining Eq. (6.25) with the relation

$$\chi_\pm^\dagger\chi_\pm = |c_\pm|^2, \tag{6.26}$$

which follows from Eq. (6.14) and from the unitary normalization of $\xi_\pm$, one arrives at the result

$$c_\pm = \sqrt{\frac{k_\pm^3}{2\pi\big(1+\varepsilon_\pm^2\big)}}. \tag{6.27}$$

For convenience, an indeterminable phase factor has been chosen to make $c_\pm$ real and positive. Hence, the normalized eigenfunctions are

$$\Psi_\pm(\boldsymbol{r}) = \sqrt{\frac{k_\pm^3}{2\pi\big(1+\varepsilon_\pm^2\big)}}\begin{pmatrix} f(k_\pm r)\xi_\pm \\ \mathrm{i}\varepsilon_\pm g(k_\pm r)\boldsymbol{n}_r\cdot\boldsymbol{\sigma}\xi_\pm\end{pmatrix}, \tag{6.28}$$

with the caveat that if the only energy eigenvalue is E_+, then only $\Psi_+(\boldsymbol{r})$ is a physically meaningful eigenfunction.

6.1.2. The Sturmian functions

To construct the Sturmian functions (4.2) for the system under consideration, we have to solve the eigenvalue problem

$$\mathsf{L}(E)\eta_a(E) = \lambda_a(E)\eta_a(E) \tag{6.29}$$

with the matrix $\mathsf{L}(E)$ given by

$$\mathsf{L}(E) = \frac{\hbar}{2mc\varepsilon}K - I. \tag{6.30}$$

The Sturmian eigenvalues, i.e., the roots of the characteristic equation

$$\det[\mathsf{L}(E) - \lambda_a(E)I] = 0, \tag{6.31}$$

are

$$\lambda_\pm(E) = \frac{\hbar(\varkappa\pm\kappa)}{2mc\varepsilon} - 1 = \frac{\varepsilon_\pm}{\varepsilon} - 1, \tag{6.32}$$

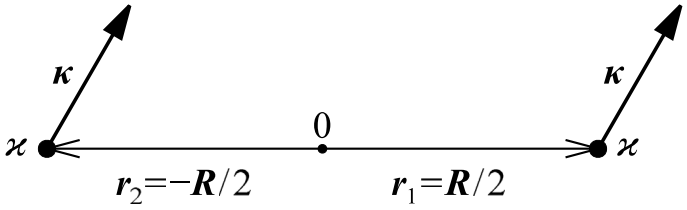

Fig. 2. Two identical zero-range potentials located at the points $\boldsymbol{r}_1 = \boldsymbol{R}/2$ and $\boldsymbol{r}_2 = -\boldsymbol{R}/2$, respectively. Each potential is characterized by the real scalar $\varkappa$ and the real vector $\boldsymbol{\kappa}$, which together define the 2×2 interaction matrix K in accordance with Eq. (6.1).

with $\varepsilon_\pm$ defined in Eq. (6.4). Associated spinor coefficients $\eta_\pm(E)$, normalized in accordance with

$$\eta_\pm^\dagger(E)\eta_\pm(E) = \frac{k^2}{4\pi} \tag{6.33}$$

and suitably phased, are then found to be

$$\eta_\pm(E) = \frac{k}{\sqrt{4\pi}}\xi_\pm. \tag{6.34}$$

This yields the sought Sturmian functions in the form

$$\Sigma_\pm(E,\boldsymbol{r}) = \frac{k}{\sqrt{4\pi}}\begin{pmatrix} f(kr)\xi_\pm \\ \mathrm{i}\varepsilon g(kr)\boldsymbol{n}_r\cdot\boldsymbol{\sigma}\xi_\pm \end{pmatrix}. \tag{6.35}$$

Since it holds that

$$\left[\frac{\partial\lambda_\pm(E)}{\partial E}\right]_{E=E_\pm} = \frac{m}{\hbar^2 k_\pm^2}, \tag{6.36}$$

with $E_\pm$ and $k_\pm$ defined in Eqs. (6.6) and (6.7), respectively, upon exploiting Eq. (4.27) we arrive at the relationship

$$\Psi_\pm(\boldsymbol{r}) = \sqrt{\frac{2k_\pm}{1+\varepsilon_\pm^2}}\,\Sigma_\pm(E_\pm,\boldsymbol{r}), \tag{6.37}$$

which, by virtue of Eq. (6.35), is seen to be in agreement with the result in Eq. (6.28).

6.2. *Particle bound in a field of two identical zero-range potentials*

As the second example, let us consider a particle bound in the field of two identical zero-range potentials which are located at the points

$$\boldsymbol{r}_1 = \frac{1}{2}\boldsymbol{R}, \qquad \boldsymbol{r}_2 = -\frac{1}{2}\boldsymbol{R}, \tag{6.38}$$

respectively (cf. Fig. 2), and are characterized by the 2×2 interaction matrices

$$K_1 = K_2 = K, \tag{6.39}$$

with K defined as in Eq. (6.1). This time we shall consider the relevant Sturmian problem first and then proceed to the analysis of the energy eigenproblem.

6.2.1. The Sturmian functions

The matrix $\mathsf{L}(E)$ for the system under study is

$$\mathsf{L}(E) = \begin{pmatrix} \dfrac{\hbar}{2mc\varepsilon}(\varkappa I + \boldsymbol{\kappa}\cdot\boldsymbol{\sigma}) - I & \dfrac{\mathrm{e}^{-kR}}{kR} I \\ \dfrac{\mathrm{e}^{-kR}}{kR} I & \dfrac{\hbar}{2mc\varepsilon}(\varkappa I + \boldsymbol{\kappa}\cdot\boldsymbol{\sigma}) - I \end{pmatrix}. \tag{6.40}$$

It is not difficult to show that its four eigenvalues are

$$\lambda_{\pm g}(E) = \frac{\hbar(\varkappa \pm \kappa)}{2mc\varepsilon} - 1 + \frac{\mathrm{e}^{-kR}}{kR}, \tag{6.41a}$$

$$\lambda_{\pm u}(E) = \frac{\hbar(\varkappa \pm \kappa)}{2mc\varepsilon} - 1 - \frac{\mathrm{e}^{-kR}}{kR}, \tag{6.41b}$$

and that the associated eigenvectors normalized in accordance with Eq. (4.19) are

$$\mathsf{y}_{\pm g}(E) = \frac{k}{\sqrt{8\pi}} \begin{pmatrix} \xi_\pm^{\mathrm{T}} & \xi_\pm^{\mathrm{T}} \end{pmatrix}^{\mathrm{T}}, \tag{6.42a}$$

$$\mathsf{y}_{\pm u}(E) = \frac{k}{\sqrt{8\pi}} \begin{pmatrix} \xi_\pm^{\mathrm{T}} & -\xi_\pm^{\mathrm{T}} \end{pmatrix}^{\mathrm{T}}, \tag{6.42b}$$

where $\xi_\pm$ are the eigenvectors of the matrix $\boldsymbol{\kappa}\cdot\boldsymbol{\sigma}$ displayed in Eq. (6.16). Hence, the Sturmian functions for the current problem are given by

$$\Sigma_{\pm g}(E,\boldsymbol{r}) = \frac{k}{\sqrt{8\pi}} \begin{pmatrix} \big[f(k|\boldsymbol{r}-\boldsymbol{R}/2|) + f(k|\boldsymbol{r}+\boldsymbol{R}/2|)\big]\xi_\pm \\ \mathrm{i}\varepsilon\big[g(k|\boldsymbol{r}-\boldsymbol{R}/2|)\boldsymbol{\mu}(\boldsymbol{r},\boldsymbol{R}/2) + g(k|\boldsymbol{r}+\boldsymbol{R}/2|)\boldsymbol{\mu}(\boldsymbol{r},-\boldsymbol{R}/2)\big]\cdot\boldsymbol{\sigma}\xi_\pm \end{pmatrix}, \tag{6.43a}$$

$$\Sigma_{\pm u}(E,\boldsymbol{r}) = \frac{k}{\sqrt{8\pi}} \begin{pmatrix} \big[f(k|\boldsymbol{r}-\boldsymbol{R}/2|) - f(k|\boldsymbol{r}+\boldsymbol{R}/2|)\big]\xi_\pm \\ \mathrm{i}\varepsilon\big[g(k|\boldsymbol{r}-\boldsymbol{R}/2|)\boldsymbol{\mu}(\boldsymbol{r},\boldsymbol{R}/2) - g(k|\boldsymbol{r}+\boldsymbol{R}/2|)\boldsymbol{\mu}(\boldsymbol{r},-\boldsymbol{R}/2)\big]\cdot\boldsymbol{\sigma}\xi_\pm \end{pmatrix}, \tag{6.43b}$$

[for the definition of the unit vectors $\boldsymbol{\mu}(\boldsymbol{r},\pm\boldsymbol{R}/2)$ see Eq. (5.6)]. It is evident that the Sturmian functions with the subscript g (respectively, u) are eigenfunctions of the Dirac parity operator Π [defined through its action on an arbitrary bispinor function $\Phi(\boldsymbol{r})$ in the following way: $\Pi\Phi(\boldsymbol{r}) \equiv \beta\Phi(-\boldsymbol{r})$, where β is the Dirac beta matrix] associated with the eigenvalue $+1$ (respectively, -1).

6.2.2. Bound-state eigenenergies

Algebraic equations leading to particle's energy eigenvalues are obtained by equating each of the Sturmian eigenvalues (6.41) to zero:

$$\lambda_{\pm g}(E_{\pm g}) \equiv \frac{\hbar(\varkappa \pm \kappa)}{2mc}\sqrt{\frac{mc^2 + E_{\pm g}}{mc^2 - E_{\pm g}}} - 1 + \frac{c\hbar}{R}\frac{\mathrm{e}^{-\sqrt{(mc^2)^2 - E_{\pm g}^2}(R/c\hbar)}}{\sqrt{(mc^2)^2 - E_{\pm g}^2}} = 0, \tag{6.44a}$$

$$\lambda_{\pm u}(E_{\pm u}) \equiv \frac{\hbar(\varkappa \pm \kappa)}{2mc}\sqrt{\frac{mc^2 + E_{\pm u}}{mc^2 - E_{\pm u}}} - 1 - \frac{c\hbar}{R}\frac{\mathrm{e}^{-\sqrt{(mc^2)^2 - E_{\pm u}^2}(R/c\hbar)}}{\sqrt{(mc^2)^2 - E_{\pm u}^2}} = 0. \tag{6.44b}$$

It is not difficult to see that roots to Eqs. (6.44) may be expressed in the following manner:

$$E_{\pm g} = mc^2\epsilon_g\left(\frac{\hbar}{mcR}, (\varkappa \pm \kappa)R\right), \tag{6.45a}$$

$$E_{\pm u} = mc^2\epsilon_u\left(\frac{\hbar}{mcR}, (\varkappa \pm \kappa)R\right) \tag{6.45b}$$

in terms of two universal functions $\epsilon_g(x,y):\mathbb{R}_+\times\mathbb{R}\to(-1,+1]$ and $\epsilon_u(x,y):\mathbb{R}_+\times\mathbb{R}\to(-1,+1]$, which are solutions to the transcendental algebraic equations

$$\frac{1}{2}xy\sqrt{\frac{1+\epsilon_g(x,y)}{1-\epsilon_g(x,y)}}-1+\frac{x\exp\left(-\frac{1}{x}\sqrt{1-\epsilon_g^2(x,y)}\right)}{\sqrt{1-\epsilon_g^2(x,y)}}=0 \tag{6.46a}$$

and

$$\frac{1}{2}xy\sqrt{\frac{1+\epsilon_u(x,y)}{1-\epsilon_u(x,y)}}-1-\frac{x\exp\left(-\frac{1}{x}\sqrt{1-\epsilon_u^2(x,y)}\right)}{\sqrt{1-\epsilon_u^2(x,y)}}=0, \tag{6.46b}$$

respectively. Equations (6.46) define $\epsilon_g(x,y)$ and $\epsilon_u(x,y)$ in an implicit manner. Explicit algebraic representations of the two functions remain unknown and to make graphs of $\epsilon_g(x,y)$ and $\epsilon_u(x,y)$, one has to solve Eqs. (6.46) numerically. We have done this with Mathematica 12.3. Representative plots, obtained for two fixed values of x and for varying y, are depicted in Fig. 3. It is seen that behaviors of the two functions are completely different. The function $\epsilon_u(x,y)$ exists for $y\geqslant 1$. It is single-valued and decreases monotonically from $\epsilon_u(x,1)=1$ to $\lim_{y\to\infty}\epsilon_u(x,y)=-1$. To the contrary, $\epsilon_g(x,y)$ is a two-branched function. The branch $\epsilon_g^{(+)}(x,y)$, which exists for $-1\leqslant y\leqslant y_c(x)$, decreases monotonically from $\epsilon_g^{(+)}(x,-1)=1$ to $\epsilon_g^{(+)}\big(x,y_c(x)\big)=\epsilon_{gc}(x)$, with $[\partial\epsilon_g^{(+)}(x,y)/\partial y]_{y=y_c(x)}=-\infty$. The branch $\epsilon_g^{(-)}(x,y)$, which exists for $-\infty<y\leqslant y_c(x)$, increases monotonically from $\lim_{y\to-\infty}\epsilon_g^{(-)}(x,y)=-1$ to $\epsilon_g^{(-)}\big(x,y_c(x)\big)=\epsilon_{gc}(x)$, with $[\partial\epsilon_g^{(-)}(x,y)/\partial y]_{y=y_c(x)}=\infty$. The two branches match smoothly at the point $\{y_c(x),\epsilon_{gc}(x)\}$. Hence, the function $\epsilon_g(x,y)$ is single-valued in the interval $-\infty<y<-1$ and at the point $y=y_c(x)$, being double-valued in the interval $-1\leqslant y<y_c(x)$. The coordinates of the matching point $\{y_c(x),\epsilon_{gc}(x)\}$ may be found by solving the algebraic system

$$\begin{cases}\dfrac{1}{2}xy_c(x)\sqrt{\dfrac{1+\epsilon_{gc}(x)}{1-\epsilon_{gc}(x)}}-1+\dfrac{x\exp\left(-\frac{1}{x}\sqrt{1-\epsilon_{gc}^2(x)}\right)}{\sqrt{1-\epsilon_{gc}^2(x)}}=0,\\[2ex] \dfrac{1}{2}xy_c(x)\sqrt{\dfrac{1+\epsilon_{gc}(x)}{1-\epsilon_{gc}(x)}}+\epsilon_{gc}(x)\left(1+\dfrac{x}{\sqrt{1-\epsilon_{gc}^2(x)}}\right)\exp\left(-\dfrac{1}{x}\sqrt{1-\epsilon_{gc}^2(x)}\right)=0.\end{cases} \tag{6.47}$$

The first equation in this system follows from the fact that the pair $\{y_c(x),\epsilon_{gc}(x)\}$ has to obey Eq. (6.46a). The second one is the consequence of the fact that at the matching point the slope of $\epsilon_g(x,y)$ versus y is infinite [cf. the text preceding Eq. (6.47)]. Its explicit form results after Eq. (6.46a) is differentiated with respect to y, the resulting identity is divided by $\partial\epsilon_g(x,y)/\partial y$ and then the constraint $\partial\epsilon_g(x,y)/\partial y=\pm\infty$ is imposed for $y=y_c(x)$ and $\epsilon_g\big(x,y_c(x)\big)=\epsilon_{gc}(x)$.

Although exact analytical representations of $\epsilon_g^{(\pm)}(x,y)$ and $\epsilon_u(x,y)$ are not available, employing iteration methods we have been able to derive the following truncated-series approximations to these functions:

$$\epsilon_g^{(+)}(x,y)\overset{x\to0+0}{\sim}1-\frac{x^2}{2}\left[y+W_0\big(\mathrm{e}^{-y}\big)\right]^2+\frac{x^4}{8}\frac{\left[y+W_0\big(\mathrm{e}^{-y}\big)\right]^3}{1+W_0\big(\mathrm{e}^{-y}\big)}\Big\{y-(y+1)W_0\big(\mathrm{e}^{-y}\big)-\left[W_0\big(\mathrm{e}^{-y}\big)\right]^2\Big\}+O\big(x^6\big), \tag{6.48}$$

$$\epsilon_g^{(+)}(x,y)\overset{y\to-1+0}{\sim}1-\frac{1}{8}x^2(y+1)^2-\frac{1}{64}x^2(x^2+2)(y+1)^3+O\big((y+1)^4\big), \tag{6.49}$$

$$\epsilon_g^{(-)}(x,y)\overset{y\to-\infty}{\sim}-1+\frac{2}{|y|}-\frac{8}{x|y|^{3/2}}+\frac{20}{x^2|y|^2}+\frac{4(3x^2-32)}{3x^3|y|^{5/2}}-\frac{4(27x^2-71)}{3x^4|y|^3}+O\big(|y|^{-7/2}\big), \tag{6.50}$$

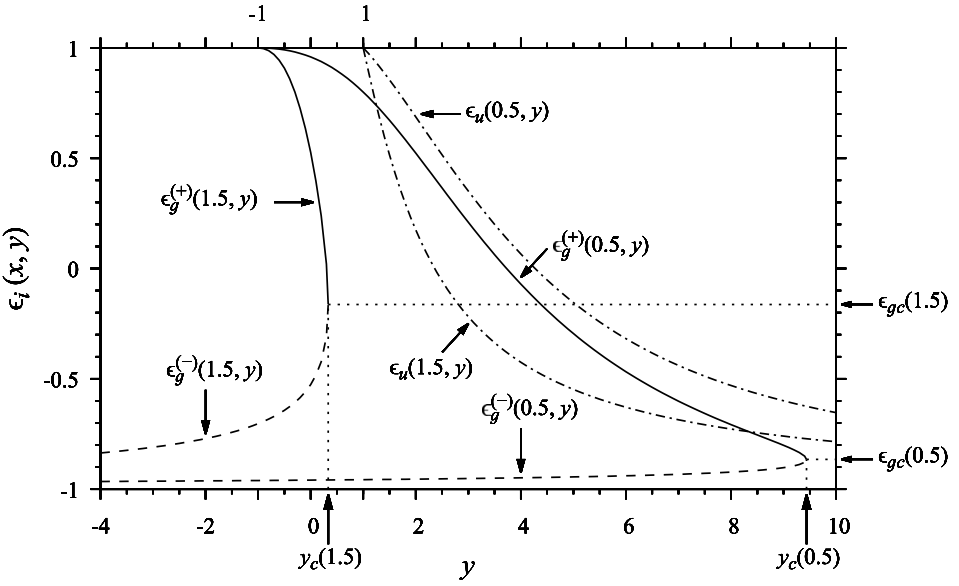

Fig. 3. Plots of the functions $\epsilon_g(x,y)$ and $\epsilon_u(x,y)$ [being real solutions to Eqs. (6.46a) and (6.46b), respectively] versus y for $x = 0.5$ and for $x = 1.5$. The function $\epsilon_u(x,y)$ is single-valued. The function $\epsilon_g(x,y)$ has two branches, denoted as $\epsilon_g^{(+)}(x,y)$ and $\epsilon_g^{(-)}(x,y)$, which match smoothly, with an infinite slope, at the point $\{y_c(x), \epsilon_{gc}(x)\}$. One has $\{y_c(0.5) = 9.437..., \epsilon_{gc}(0.5) = -0.865...\}$ and $\{y_c(1.5) = 0.334..., \epsilon_{gc}(1.5) = -0.163...\}$ (for more precise values of the y_c's and ϵ_{gc}'s, see Table 2).

$$\epsilon_u(x,y) \overset{x\to 0+0}{\sim} 1 - \frac{x^2}{2}\left[y + W_0\left(-\mathrm{e}^{-y}\right)\right]^2 + \frac{x^4}{8}\frac{\left[y + W_0\left(-\mathrm{e}^{-y}\right)\right]^3}{1 + W_0\left(-\mathrm{e}^{-y}\right)}\left\{y - (y+1)W_0\left(-\mathrm{e}^{-y}\right) - \left[W_0\left(-\mathrm{e}^{-y}\right)\right]^2\right\} + O\left(x^6\right), \tag{6.51}$$

$$\epsilon_u(x,y) \overset{y\to 1+0}{\sim} 1 - 2\frac{x^2}{x^2+2}(y-1) - \frac{8}{3}\frac{x^2}{(x^2+2)^{5/2}}(y-1)^{3/2} + \frac{2}{3}\frac{x^2(3x^6+6x^4+2x^2-4)}{(x^2+2)^4}(y-1)^2 + O\left((y-1)^{5/2}\right), \tag{6.52}$$

$$\epsilon_u(x,y) \overset{y\to\infty}{\sim} -1 + \frac{2}{y} + \frac{4}{x^2y^2} - \frac{8}{3x^3y^{5/2}} - \frac{4(3x^2-7)}{3x^4y^3} + O\left(y^{-7/2}\right). \tag{6.53}$$

In Eqs. (6.48) and (6.51), $W_0(z)$ denotes the principal branch of the Lambert function (the product logarithm) [14,15].

Using Table 1, one may establish which bound-state energy eigenvalues exist for a given set of physical parameters characterizing the particle (m) and the potentials (R, $\varkappa$, κ). There are two extremes. The first one occurs if m and R are such that

$$\frac{\hbar}{mcR} > x_c \tag{6.54a}$$

Table 1
The table marks existence ($\surd$) or non-existence (–) of the solutions $\epsilon_g^{(-)}(x,y)$ and $\epsilon_g^{(+)}(x,y)$ to Eq. (6.46a) and the solution $\epsilon_u(x,y)$ to Eq. (6.46b) for various combinations of subdomains that x and y may belong to. For $y = y_c(x)$, the equality sign placed between the second and third columns reminds that $\epsilon_g^{(-)}(x,y_c(x)) = \epsilon_g^{(+)}\big(x,y_c(x)\big) = \epsilon_{gc}(x)$. For the critical value of $x = x_c = 1.198\,076\ldots$, one has $y = y_c(x_c) = 1$ and $\epsilon_g^{(-)}(x_c,1) = \epsilon_g^{(+)}(x_c,1) = \epsilon_{gc}(x_c) = -0.379162\ldots$.

Range of y	$\epsilon_g^{(-)}(x,y)$		$\epsilon_g^{(+)}(x,y)$	$\epsilon_u(x,y)$
$0 < x < x_c$				
$-\infty < y < -1$	$\surd$		–	–
$-1 \leqslant y < 1$	$\surd$		$\surd$	–
$1 \leqslant y < y_c(x)$	$\surd$		$\surd$	$\surd$
$y = y_c(x)$	$\surd$	=	$\surd$	$\surd$
$y_c(x) < y < \infty$	–		–	$\surd$
$x = x_c = 1.198\,076\ldots$				
$-\infty < y < -1$	$\surd$		–	–
$-1 \leqslant y < y_c(x_c) = 1$	$\surd$		$\surd$	–
$y = y_c(x_c) = 1$	$\surd$	=	$\surd$	$\surd$
$1 = y_c(x_c) < y < \infty$	–		–	$\surd$
$x_c < x < \infty$				
$-\infty < y < -1$	$\surd$		–	–
$-1 \leqslant y < y_c(x)$	$\surd$		$\surd$	–
$y = y_c(x)$	$\surd$	=	$\surd$	–
$y_c(x) < y < 1$	–		–	–
$1 \leqslant y < \infty$	–		–	$\surd$

[here and then in Eqs. (6.55a) and (6.57a), $x_c = 1.198\,076\ldots$ is the root to the equation $y_c(x_c) = 1$] and if simultaneously R, $\varkappa$ and κ are such that

$$y_c\left(\frac{\hbar}{mcR}\right) < (\varkappa - \kappa)R \leqslant (\varkappa + \kappa)R < 1. \tag{6.54b}$$

Then the discrete part of the particle's energy spectrum is seen to be empty. The other extreme occurs if m and R are such that

$$\frac{\hbar}{mcR} < x_c \tag{6.55a}$$

and if simultaneously R, $\varkappa$ and κ are such that

$$1 \leqslant (\varkappa - \kappa)R \leqslant (\varkappa + \kappa)R < y_c\left(\frac{\hbar}{mcR}\right). \tag{6.55b}$$

Then the bound-state part of the particle's energy spectrum consists of six eigenenergies

$$E_{\pm g}^{(+)} = mc^2\epsilon_g^{(+)}\left(\frac{\hbar}{mcR}, (\varkappa \pm \kappa)R\right), \tag{6.56a}$$

$$E_{\pm g}^{(-)} = mc^2\epsilon_g^{(-)}\left(\frac{\hbar}{mcR}, (\varkappa \pm \kappa)R\right) \tag{6.56b}$$

and

$$E_{\pm u} = mc^2\epsilon_u\left(\frac{\hbar}{mcR}, (\varkappa \pm \kappa)R\right) \tag{6.56c}$$

(for $\kappa = 0$ the degeneracies $E_{+g}^{(+)} = E_{-g}^{(+)}$, $E_{+g}^{(-)} = E_{-g}^{(-)}$ and $E_{+u} = E_{-u}$ are seen to occur). For the remaining possible combinations of $\hbar/mcR$ and $(\varkappa - \kappa)R \leqslant (\varkappa + \kappa)R$ a variety of intermediate cases arises. For instance, if

$$\frac{\hbar}{mcR} > x_c \tag{6.57a}$$

Table 2
Numerical values of the solutions $\epsilon_g^{(-)}(x,y)$ and $\epsilon_g^{(+)}(x,y)$ to Eq. (6.46a) and of the solution $\epsilon_u(x,y)$ to Eq. (6.46b) for selected values of x and y. For $y = y_c(x)$, corresponding entries in the second and the third columns are identical and equal to $\epsilon_{gc}(x)$. For each value of x considered, the corresponding value of $y_c(x)$ is displayed with the accuracy necessary to reproduce the common entry in the second and third columns with the given precision.

y	$\epsilon_g^{(-)}(x,y)$	$\epsilon_g^{(+)}(x,y)$	$\epsilon_u(x,y)$
$x = 0.01$			
$y \to -\infty$	$-1 + 2/\lvert y\rvert$	–	–
-100	$-1 + 1.6054 \times 10^{-5}$	–	–
-10	$-1 + 1.6080 \times 10^{-5}$	–	–
-1	$-1 + 1.6082 \times 10^{-5}$	1 (exact)	–
1	$-1 + 1.6083 \times 10^{-5}$	$1 - 8.1723 \times 10^{-5}$	1 (exact)
10	$-1 + 1.6086 \times 10^{-5}$	$1 - 4.9876 \times 10^{-3}$	$1 - 4.9875 \times 10^{-3}$
100	$-1 + 1.6112 \times 10^{-5}$	6.0000×10^{-1}	6.0000×10^{-1}
1 000	$-1 + 1.6381 \times 10^{-5}$	$-1 + 7.6923 \times 10^{-2}$	$-1 + 7.6923 \times 10^{-2}$
10 000	$-1 + 1.9939 \times 10^{-5}$	$-1 + 7.9219 \times 10^{-4}$	$-1 + 8.0687 \times 10^{-4}$
$y_c(0.01) = 25\,401.358\,108\,598\ldots$	$-1 + 5.6189 \times 10^{-5}$	$-1 + 5.6189 \times 10^{-5}$	$-1 + 1.5048 \times 10^{-4}$
100 000	–	–	$-1 + 2.3836 \times 10^{-5}$
$y \to \infty$	–	–	$-1 + 2/y$
$x = 0.5$			
$y \to -\infty$	$-1 + 2/\lvert y\rvert$	–	–
-100	$-1 + 9.6266 \times 10^{-3}$	–	–
-10	$-1 + 2.8822 \times 10^{-2}$	–	–
-1	$-1 + 3.9225 \times 10^{-2}$	1 (exact)	–
1	$-1 + 4.3115 \times 10^{-2}$	7.9970×10^{-1}	1 (exact)
$y_c(0.5) = 9.436\,540\,350\,268\ldots$	-8.6525×10^{-1}	-8.6525×10^{-1}	-6.2449×10^{-1}
10	–	–	-6.5311×10^{-1}
100	–	–	$-1 + 2.1489 \times 10^{-2}$
$y \to \infty$	–	–	$-1 + 2/y$
$x = 1.5$			
$y \to -\infty$	$-1 + 2/\lvert y\rvert$	–	–
-100	$-1 + 1.5460 \times 10^{-2}$	–	–
-10	$-1 + 9.4260 \times 10^{-2}$	–	
-1	-7.0313×10^{-1}	1 (exact)	–
$y_c(1.5) = 0.333\,896\,179\,26\ldots$	-1.6277×10^{-1}	-1.6277×10^{-1}	–
$y_c(1.5) < y < 1$	–	–	–
1	–	–	1 (exact)
10	–	–	-7.8507×10^{-1}
100	–	–	$-1 + 2.0170 \times 10^{-2}$
$y \to \infty$	–	–	$-1 + 2/y$

and

$$y_c\left(\frac{\hbar}{mcR}\right) < (\varkappa - \kappa)R < 1 \leqslant (\varkappa + \kappa)R, \tag{6.57b}$$

then there is only one bound-state with eigenenergy

$$E_{+u} = mc^2\epsilon_u\left(\frac{\hbar}{mcR}, (\varkappa + \kappa)R\right). \tag{6.58}$$

Next, we shall consider the question of determining the signatures Δ_a of the individual eigenstates. It appears that Δ_a may be correlated with the sign of the derivative $[\partial\epsilon_a(\hbar/mcR, y)/\partial y]_{y=(\varkappa\pm\kappa)R}$, i.e., with the sign of the slope of the corresponding curve $\epsilon_a(x,y)$ in Fig. 3. Indeed, it follows from Eqs. (6.41) that

$$\lambda_a(E) \equiv \lambda_a\big(E, (\varkappa \pm \kappa)R\big) = \frac{\hbar}{2mcR}[(\varkappa \pm \kappa)R]\sqrt{\frac{mc^2 + E}{mc^2 - E}} - 1 + \sigma_a\frac{c\hbar}{R}\frac{\mathrm{e}^{-\sqrt{(mc^2)^2 - E^2}(R/c\hbar)}}{\sqrt{(mc^2)^2 - E^2}}, \tag{6.59}$$

with $\sigma_a = +1$ for the g states and $\sigma_a = -1$ for the u states. Now, it is an exercise in elementary calculus to prove that if $x = x_0(b)$ is a root to the algebraic equation $F(x, b) = 0$, in which x is a variable and b is a parameter, then it holds that

$$\left[\frac{\partial F(x,b)}{\partial x}\right]_{x=x_0(b)} = -\left[\frac{\partial F(x,b)}{\partial b}\right]_{x=x_0(b)}\left[\frac{\mathrm{d}x_0(b)}{\mathrm{d}b}\right]^{-1} \tag{6.60}$$

(notice the minus sign in front of the right-hand side). On employing the lemma (6.60) and Eqs. (6.45), from Eq. (6.59) we deduce that

$$\left[\frac{\partial\lambda_a\big(E,(\varkappa\pm\kappa)R\big)}{\partial E}\right]_{E=E_a} = -\frac{\hbar}{2m^2c^3R}\sqrt{\frac{mc^2+E_a}{mc^2-E_a}}\left[\frac{\partial\epsilon_a(\hbar/mcR,y)}{\partial y}\right]^{-1}_{y=(\varkappa\pm\kappa)R}, \tag{6.61}$$

from which, by virtue of Eq. (4.26), it follows that

$$\Delta_a = -\mathrm{sgn}\left[\frac{\partial\epsilon_a(\hbar/mcR,y)}{\partial y}\right]^{-1}_{y=(\varkappa\pm\kappa)R}. \tag{6.62}$$

In conclusion, one has

$$\Delta_a = \begin{cases} +1 & \text{for states with } \epsilon_a = \epsilon_g^{(+)} \text{ or } \epsilon_a = \epsilon_u \\ 0 & \text{for states with } \epsilon_a = \epsilon_{gc} \\ -1 & \text{for states with } \epsilon_a = \epsilon_g^{(-)}. \end{cases} \tag{6.63}$$

It remains to comment on the eigenfunctions $\Psi_a(\boldsymbol{r})$. If $\Delta_a = 0$ (i.e., if $\epsilon_a = \epsilon_{gc}$), the corresponding eigenfunction $\Psi_{gc}(\boldsymbol{r})$ is an arbitrary nonzero multiple of the Sturmian function displayed in Eq. (6.43a), with $k = k_{gc}$ and $\varepsilon = \varepsilon_{gc}$. If $\Delta_a = \pm 1$, the normalized [in the sense of Eq. (3.21)] eigenfunctions arise after one combines Eqs. (4.21) and (4.25) with Eqs. (6.43) and with the relation

$$\left[\frac{\partial\lambda_a(E)}{\partial E}\right]_{E=E_a} = \frac{1}{2c\hbar\varepsilon_a k_a}\left[\left(1+\sigma_a\mathrm{e}^{-k_aR}\right)+\varepsilon_a^2\left(1-\sigma_a\mathrm{e}^{-k_aR}-\sigma_a\frac{2\mathrm{e}^{-k_aR}}{k_aR}\right)\right], \tag{6.64}$$

which follows once Eq. (6.59) is differentiated with respect to E and then the result is simplified with the aid of Eqs. (6.44) and (2.4).

Our considerations would be incomplete without saying a few words about the nonrelativistic limits of the energy eigenvalues. Mathematically, the nonrelativistic regime is approached by imposing the constraint

$$\frac{\hbar}{mcR} \ll 1. \tag{6.65}$$

Hence, upon retaining two leading terms in each of the truncated series displayed in Eqs. (6.48) and (6.51), one finds the following approximate expressions for these energy levels which are located in the vicinity of the rest-energy threshold mc^2:

$$E_{\pm g}^{(+)} \simeq mc^2 - \frac{\hbar^2}{2mR^2}\left[(\varkappa\pm\kappa)R + W_0\big(\mathrm{e}^{-(\varkappa\pm\kappa)R}\big)\right]^2 \qquad [(\varkappa\pm\kappa)R \geqslant -1], \tag{6.66a}$$

$$E_{\pm u} \simeq mc^2 - \frac{\hbar^2}{2mR^2}\left[(\varkappa\pm\kappa)R + W_0\big(-\mathrm{e}^{-(\varkappa\pm\kappa)R}\big)\right]^2 \qquad [(\varkappa\pm\kappa)R \geqslant 1], \tag{6.66b}$$

where, we recall, $W_0(z)$ is the principal branch of the Lambert function. We have verified that the above formulas agree with those we would get if our considerations were nonrelativistic from the beginning.

7. Conclusions

In the previous pages, we have presented the basics of the mathematical model for a Dirac particle bound by a set of spatially distributed zero-range potentials. Although the applications

presented in Section 6 have been limited to only the simplest one- and two-center systems, the developed formalism may find applications in modeling Dirac fermions interacting with multicenter systems such as large biomolecules, chains, lattices, and crystals, either perfect or with structural defects.

There are several directions in which the model might be further developed. To study systems subjected to external static electric or magnetic fields, a suitable variant of the Rayleigh–Schrödinger perturbation theory should be constructed. Another challenge would be to extend the formalism to systems involving potential centers with internal degrees of freedom. It would be also desirable to make it applicable to description of time-dependent processes; for that purpose, a prior Lorentz-invariant reformulation of the method would be necessary.

Declaration of competing interest

The author declares that he has no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix. A proof of the zero-flux relation (2.12)

On employing Eq. (2.13), the integral that stands on the left-hand side of Eq. (2.12) takes the form

$$\oint_{\mathcal{S}_n} \mathrm{d}^2\boldsymbol{\rho}_n\, \boldsymbol{\mu}_n \cdot c\Psi_a^\dagger(\boldsymbol{r}_n+\boldsymbol{\rho}_n)\boldsymbol{\alpha}\Psi_a(\boldsymbol{r}_n+\boldsymbol{\rho}_n). \tag{A.1}$$

The meaning of all symbols appearing in Eq. (A.1) is the same as in Eqs. (2.12) and (2.13), except that for convenience we have abbreviated $\boldsymbol{\mu}_n(\boldsymbol{r}_n+\boldsymbol{\rho}_n)=\boldsymbol{\rho}_n/\rho$ to $\boldsymbol{\mu}_n$. Since the infinitesimal element $\mathrm{d}^2\boldsymbol{\rho}_n$ of the spherical surface $\mathcal{S}_n$ is

$$\mathrm{d}^2\boldsymbol{\rho}_n = \rho^2\mathrm{d}^2\boldsymbol{\mu}_n, \tag{A.2}$$

where $\mathrm{d}^2\boldsymbol{\mu}_n$ is the infinitesimal solid angle around the direction of the unit vector $\boldsymbol{\mu}_n$ and with its apex at $\boldsymbol{r}_n$, and since $\rho\boldsymbol{\mu}_n=\boldsymbol{\rho}_n$, the integral (A.1) may be rewritten as

$$\oint_{4\pi} \mathrm{d}^2\boldsymbol{\mu}_n \underbrace{c\rho\Psi_a^\dagger(\boldsymbol{r}_n+\boldsymbol{\rho}_n)\boldsymbol{\rho}_n\cdot\boldsymbol{\alpha}\Psi_a(\boldsymbol{r}_n+\boldsymbol{\rho}_n)}_{F_a(\boldsymbol{\rho}_n)}. \tag{A.3}$$

By virtue of Eqs. (3.6) and (3.7), the integrand in Eq. (A.3) may be cast into the form

$$F_a(\boldsymbol{\rho}_n) = 2c\mathrm{Im}\big[\rho\Psi_a^\dagger(\boldsymbol{r}_n+\boldsymbol{\rho}_n)\mathrm{i}\boldsymbol{\rho}_n\cdot\boldsymbol{\alpha}^{(+)}\Psi_a(\boldsymbol{r}_n+\boldsymbol{\rho}_n)\big]. \tag{A.4}$$

Now, the matrix $\frac{\hbar}{2mc}\rho\mathcal{K}_n^{(+)}+\varepsilon_a k_a^{-1}\beta^{(+)}$ is Hermitian (we remind that ε_a and k_a are real), and consequently it holds that

$$2c\mathrm{Im}\left\{\rho\Psi_a^\dagger(\boldsymbol{r}_n+\boldsymbol{\rho}_n)\left[\frac{\hbar}{2mc}\rho\mathcal{K}_n^{(+)}+\varepsilon_a k_a^{-1}\beta^{(+)}\right]\Psi_a(\boldsymbol{r}_n+\boldsymbol{\rho}_n)\right\}=0. \tag{A.5}$$

This implies that Eq. (A.4) may be equivalently written as

$$F_a(\boldsymbol{\rho}_n) = 2c\mathrm{Im}\left\{\rho\Psi_a^\dagger(\boldsymbol{r}_n+\boldsymbol{\rho}_n)\left[\mathrm{i}\boldsymbol{\rho}_n\cdot\boldsymbol{\alpha}^{(+)}+\frac{\hbar}{2mc}\rho\mathcal{K}_n^{(+)}+\varepsilon_a k_a^{-1}\beta^{(+)}\right]\Psi_a(\boldsymbol{r}_n+\boldsymbol{\rho}_n)\right\}. \tag{A.6}$$

Since the matrix that stands between the square brackets obeys $[\ldots] = \beta^{(+)}[\ldots]$ and since $\beta^{(+)}$ is Hermitian, it is possible to transform Eq. (A.6) into

$$F_a(\boldsymbol{\rho}_n) = 2c\mathrm{Im}\left\{\left[\rho\beta^{(+)}\Psi_a(\boldsymbol{r}_n+\boldsymbol{\rho}_n)\right]^\dagger\left[\mathrm{i}\boldsymbol{\rho}_n\cdot\boldsymbol{\alpha}^{(+)}+\frac{\hbar}{2mc}\rho\mathcal{K}_n^{(+)}+\varepsilon_a k_a^{-1}\beta^{(+)}\right]\Psi_a(\boldsymbol{r}_n+\boldsymbol{\rho}_n)\right\}. \tag{A.7}$$

It follows from Eqs. (2.2) and (2.3a) that the limit of $\rho\beta^{(+)}\Psi_a(\boldsymbol{r}_n+\boldsymbol{\rho}_n)$ as $\rho\to 0$ is finite. On the other hand, by virtue of the constraints (2.7), one has

$$\lim_{\rho\to 0}\left[\mathrm{i}\boldsymbol{\rho}_n\cdot\boldsymbol{\alpha}^{(+)}+\frac{\hbar}{2mc}\rho\mathcal{K}_n^{(+)}+\varepsilon_a k_a^{-1}\beta^{(+)}\right]\Psi_a(\boldsymbol{r}_n+\boldsymbol{\rho}_n)=0. \tag{A.8}$$

This implies that in the limit $\rho\to 0$ the integrand in Eq. (A.3) vanishes. Remembering the equivalence of the integrals in Eqs. (A.3) and (A.1), we thus obtain

$$\lim_{\rho\to 0}\oint_{\mathcal{S}_n}\mathrm{d}^2\boldsymbol{\rho}_n\,\boldsymbol{\mu}_n(\boldsymbol{r}_n+\boldsymbol{\rho}_n)\cdot c\Psi_a^\dagger(\boldsymbol{r}_n+\boldsymbol{\rho}_n)\boldsymbol{\alpha}\Psi_a(\boldsymbol{r}_n+\boldsymbol{\rho}_n)=0, \tag{A.9}$$

which, after being combined with Eq. (2.13), is seen to coincide with Eq. (2.12).

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