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

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The embedding method [J. E. Inglesfield, J. Phys. C **14**, 3795 (1981)] for computing bound states of the Schrödinger equation is reformulated in terms of the Dirichlet-to-Neumann (DtN) and Neumann-to-Dirichlet (NtD) surface integral operators. Variational principles for energy, allowing the use of trial functions which are discontinuous in values or derivatives, are employed. A method of constructing kernels of the DtN and NtD operators from solutions to an auxiliary Steklov (Stekloff) eigenproblem is presented. Numerical results illustrating the usefulness of the DtN and NtD embedding methods are provided. After necessary modifications, the DtN-NtD formalism presented in this work may constitute the convenient framework for generalizing the embedding method to bound states of the Dirac equation.

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I. INTRODUCTION

Some years ago, Inglesfield [1] proposed a so-called *embedding method* for computing properties of bound and continuum states of a Schrödinger particle. The method is based on the observation that if a domain, in which the particle is considered, is suitably divided into two subdomains, it is possible to reduce the original mathematical problem to a problem in one of the subdomains. Inglesfield and coworkers [2] demonstrated that in many cases the reduced problem may be easier to solve than the original one [3].

Zou [4] pointed out a close mathematical relationship between the embedding method and the well-known *R*-matrix method widely used in quantum scattering theory. Zou showed that this relationship becomes evident when the *R*-matrix method is reformulated in the language of surface integral operators. An operator approach to the *R*-matrix theory was worked out in detail by one of the present authors (at that time unaware of Zou's paper) in a series of publications [5]. Inspired by Zou's observation, in the present work we use the formalism of Ref. [5] to construct two variants of the embedding method for computing energies of bound states of the Schrödinger equation in $\mathbb{R}^3$. In many aspects, results presented in this paper go beyond those contained in Refs. [1,4].

The structure of the paper is as follows. In Sec. II we divide $\mathbb{R}^3$ into a finite inner volume and an infinite remainder. Then, we present a variational principle for energy allowing the use of trial functions which are discontinuous or have discontinuous normal derivatives across the dividing interface; this variational principle will play an important role in later considerations. In Sec. III we define the Dirichlet-to-Neumann (DtN) and Neumann-to-Dirichlet (NtD) surface integral operators and show how their kernels may be constructed from solutions of some auxiliary Steklov (Stekloff) eigenvalue problem in the outer region. In Secs. IV and V the functional of Sec. II and the integral operator formalism of Sec. III are used to formulate the DtN and NtD variants of the embedding method. Problems with spherical symmetry in the outer region are considered in Sec. VI. Section VII shows how the DtN and NtD variants of the embedding method may be implemented practically, making use of the Rayleigh-Ritz linear trial functions. A numerical example illustrating the usefulness of the method is presented in Sec. VIII.

II. VARIATIONAL PRINCIPLE FOR ENERGY ALLOWING THE USE OF DISCONTINUOUS TRIAL FUNCTIONS

In this work we shall be concerned with the bound-state energy eigenvalue problem constituted by the Schrödinger equation

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

together with the asymptotic condition

$$r\Psi(\mathbf{r}) \overset{r\to\infty}{\to} 0. \tag{2.2}$$

The Hamiltonian in Eq. (2.1) has its usual Schrödinger form

$$\hat{\mathcal{H}} = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + V(\mathbf{r}), \tag{2.3}$$

with the local, real potential $V(\mathbf{r})$. We shall be assuming that the potential $V(\mathbf{r})$ is such that at least one bound-state eigensolution to the problem (2.1) and (2.2) does exist.

It is well known that the eigenproblem (2.1) and (2.2) is equivalent to the variational principle

$$\delta\mathcal{F}[\Psi] = 0, \quad E = \mathcal{F}[\Psi], \tag{2.4}$$

with the Rayleigh functional

$$\mathcal{F}[\overline{\Psi}] = \frac{\langle\overline{\Psi}|\hat{\mathcal{H}}\overline{\Psi}\rangle}{\langle\overline{\Psi}|\overline{\Psi}\rangle}. \tag{2.5}$$

The volume scalar product in Eq. (2.5) is defined as

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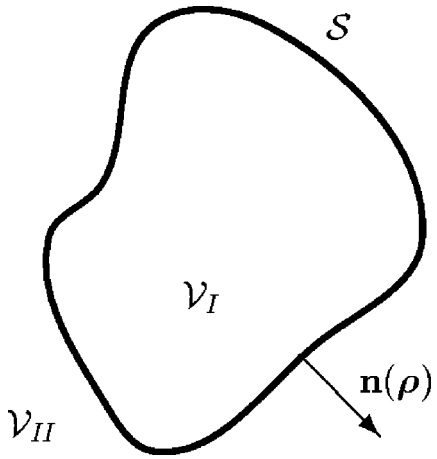

FIG. 1. Partitioning of $\mathbb{R}^3$ into the finite domain $\mathcal{V}_I$ and the infinite remainder $\mathcal{V}_{II}$, separated by the surface $\mathcal{S}$; $\mathbf{n}(\boldsymbol{\rho})$ is the unit vector normal to the surface $\mathcal{S}$ at the point $\boldsymbol{\rho}$.

$$\langle \Phi | \Phi' \rangle = \int_{\mathbb{R}^3} d^3\mathbf{r} \Phi^*(\mathbf{r}) \Phi'(\mathbf{r}). \tag{2.6}$$

It is implicit in the variational principle (2.4) and (2.5) that for any trial function $\overline{\Psi}(\mathbf{r})$ used therein both the function itself and its gradient $\boldsymbol{\nabla}\overline{\Psi}(\mathbf{r})$ are continuous throughout the whole space $\mathbb{R}^3$ and that, in analogy with Eq. (2.2), it holds that

$$r\overline{\Psi}(\mathbf{r}) \overset{r\to\infty}{\to} 0. \tag{2.7}$$

This does not mean, however, that discontinuous trial functions are not admissible in the variational approach to the eigenproblem (2.1) and (2.2). Consider the situation when the space $\mathbb{R}^3$ is artificially decomposed into a finite inner domain $\mathcal{V}_I$ and an infinite outer domain $\mathcal{V}_{II}=\mathbb{R}^3\backslash\mathcal{V}_I$, the two domains being separated by a sufficiently smooth imagined surface $\mathcal{S}$ (Fig. 1). [For convenience, throughout the paper a position vector for a point lying on the interface $\mathcal{S}$ will be denoted by $\boldsymbol{\rho}$ instead of $\mathbf{r}$. A unit vector normal to the surface $\mathcal{S}$ at the point $\boldsymbol{\rho}$, with sense from $\mathcal{V}_I$ to $\mathcal{V}_{II}$, will be denoted by $\mathbf{n}(\boldsymbol{\rho})$.] If we denote

$$\Psi_X(\mathbf{r}) = \Psi(\mathbf{r}) \quad (\mathbf{r} \in \mathcal{V}_X; X = I, II) \tag{2.8}$$

and if $\overline{\Psi}_I(\mathbf{r})$ and $\overline{\Psi}_{II}(\mathbf{r})$ are trial estimates of $\Psi_I(\mathbf{r})$ and $\Psi_{II}(\mathbf{r})$, respectively, then the variational principle (2.4) and (2.5) may be replaced by the more general one [6]

$$\delta\mathcal{F}[\Psi_I, \Psi_{II}] = 0, \quad E = \mathcal{F}[\Psi_I, \Psi_{II}], \tag{2.9}$$

with the functional

$$\begin{aligned}\mathcal{F}[\overline{\Psi}_I, \overline{\Psi}_{II}] = {} & \frac{\langle \overline{\Psi}_I | \hat{\mathcal{H}} \overline{\Psi}_I \rangle_I + \langle \overline{\Psi}_{II} | \hat{\mathcal{H}} \overline{\Psi}_{II} \rangle_{II}}{\langle \overline{\Psi}_I | \overline{\Psi}_I \rangle_I + \langle \overline{\Psi}_{II} | \overline{\Psi}_{II} \rangle_{II}} \\ & - \frac{\hbar^2}{2m} \frac{(a \nabla_\perp \overline{\Psi}_I + [1-a] \nabla_\perp \overline{\Psi}_{II} | \overline{\Psi}_I - \overline{\Psi}_{II})}{\langle \overline{\Psi}_I | \overline{\Psi}_I \rangle_I + \langle \overline{\Psi}_{II} | \overline{\Psi}_{II} \rangle_{II}} \\ & + \frac{\hbar^2}{2m} \frac{([1-a^*] \overline{\Psi}_I + a^* \overline{\Psi}_{II} | \nabla_\perp \overline{\Psi}_I - \nabla_\perp \overline{\Psi}_{II})}{\langle \overline{\Psi}_I | \overline{\Psi}_I \rangle_I + \langle \overline{\Psi}_{II} | \overline{\Psi}_{II} \rangle_{II}}\end{aligned} \tag{2.10}$$

possessing the property of being real for arbitrary trial functions:

$$\mathcal{F}[\overline{\Psi}_I, \overline{\Psi}_{II}] = \mathcal{F}^*[\overline{\Psi}_I, \overline{\Psi}_{II}]. \tag{2.11}$$

In the functional (2.10), a is an arbitrary complex constant which is *not* subjected to variation,

$$\nabla_\perp \overline{\Psi}_X(\boldsymbol{\rho}) = \mathbf{n}(\boldsymbol{\rho}) \cdot \boldsymbol{\nabla} \overline{\Psi}_X(\mathbf{r})|_{\mathbf{r}=\boldsymbol{\rho}} \tag{2.12}$$

is the normal derivative of $\overline{\Psi}_X(\mathbf{r})$ at the surface point $\boldsymbol{\rho}$,

$$\langle \Phi | \Phi' \rangle_X = \int_{\mathcal{V}_X} d^3\mathbf{r} \Phi^*(\mathbf{r}) \Phi'(\mathbf{r}) \tag{2.13}$$

is the regional volume scalar product over the domain $\mathcal{V}_X$, and

$$(\Phi | \Phi') = \oint_{\mathcal{S}} d^2\boldsymbol{\rho} \Phi^*(\boldsymbol{\rho}) \Phi'(\boldsymbol{\rho}) \tag{2.14}$$

(with $d^2\boldsymbol{\rho}$ denoting an infinitesimal *scalar* surface element around the point $\boldsymbol{\rho}$) is the surface scalar product over $\mathcal{S}$.

In the principle (2.9) and (2.10), the trial functions $\overline{\Psi}_X(\mathbf{r})$, together with their gradients, have to be continuous throughout the interiors of the relevant domains $\mathcal{V}_X$. In addition, $\overline{\Psi}_{II}(\mathbf{r})$ has to obey

$$r\overline{\Psi}_{II}(\mathbf{r}) \overset{r\to\infty}{\to} 0. \tag{2.15}$$

However, as opposed to the principle (2.4) and (2.5), the principle (2.9) and (2.10) admits the use of such trial functions $\overline{\Psi}_X(\mathbf{r})$ which do not match at the interface $\mathcal{S}$; i.e., such that

$$\overline{\Psi}_I(\boldsymbol{\rho}) \neq \overline{\Psi}_{II}(\boldsymbol{\rho}) \tag{2.16}$$

or

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

[both discontinuity relations (2.16) and (2.17) *may* hold simultaneously]. This advantage of the principle (2.9) and (2.10) will be exploited in Secs. IV and V to construct two variants of the embedding method.

III. DtN AND NtD SURFACE INTEGRAL OPERATORS

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

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

[$\hat{\mathcal{H}}$ 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)] and, in addition, obey the asymptotic condition

$$r\psi(\mathcal{E},\mathbf{r}) \overset{r\to\infty}{\to} 0. \tag{3.2}$$

We introduce two linear integral operators $\hat{\mathcal{B}}(\mathcal{E})$ and $\hat{\mathcal{R}}(\mathcal{E})$ such that for any $\psi(\mathcal{E},\mathbf{r}) \in \mathcal{D}_{II}(\mathcal{E})$ at the surface $\mathcal{S}$ it holds that

$$\nabla_\perp \psi(\mathcal{E},\boldsymbol{\rho}) = \hat{\mathcal{B}}(\mathcal{E})\psi(\mathcal{E},\boldsymbol{\rho}) \tag{3.3}$$

and

$$\hat{\mathcal{R}}(\mathcal{E})\nabla_\perp \psi(\mathcal{E},\boldsymbol{\rho}) = \psi(\mathcal{E},\boldsymbol{\rho}). \tag{3.4}$$

It follows from the above definitions that the two operators are mutually reciprocal; i.e., it holds that

$$\hat{\mathcal{B}}(\mathcal{E})\hat{\mathcal{R}}(\mathcal{E}) = \hat{\mathcal{R}}(\mathcal{E})\hat{\mathcal{B}}(\mathcal{E}) = \hat{\mathcal{I}}_{\mathcal{S}}, \tag{3.5}$$

where $\hat{\mathcal{I}}_{\mathcal{S}}$ is the unit integral operator on $\mathcal{S}$ with the kernel $\delta_{\mathcal{S}}^{(2)}(\boldsymbol{\rho}-\boldsymbol{\rho}')$. The operator $\hat{\mathcal{B}}(\mathcal{E})$, which, up to a numerical constant, coincides with the embedding potential operator defined in Eq. (10) of Ref. [1], transforms the Dirichlet datum $\psi(\mathcal{E},\boldsymbol{\rho})$ into the Neumann datum $\nabla_\perp\psi(\mathcal{E},\boldsymbol{\rho})$ and therefore it is called *the Dirichlet-to-Neumann* operator. The terms *the surface impedance* operator and *the logarithmic (log) derivative* operator are also in use. In analogy, the operator $\hat{\mathcal{R}}(\mathcal{E})$ is called the *Neumann-to-Dirichlet* operator or *the surface admittance* operator.

The operators $\hat{\mathcal{B}}(\mathcal{E})$ and $\hat{\mathcal{R}}(\mathcal{E})$ are represented by their integral kernels $\mathcal{B}(\mathcal{E},\boldsymbol{\rho},\boldsymbol{\rho}')$ and $\mathcal{R}(\mathcal{E},\boldsymbol{\rho},\boldsymbol{\rho}')$, respectively, in terms of which Eqs. (3.3)–(3.5) read

$$\nabla_\perp \psi(\mathcal{E},\boldsymbol{\rho}) = \oint_{\mathcal{S}} d^2\boldsymbol{\rho}'\, \mathcal{B}(\mathcal{E},\boldsymbol{\rho},\boldsymbol{\rho}')\psi(\mathcal{E},\boldsymbol{\rho}'), \tag{3.6}$$

$$\psi(\mathcal{E},\boldsymbol{\rho}) = \oint_{\mathcal{S}} d^2\boldsymbol{\rho}'\, \mathcal{R}(\mathcal{E},\boldsymbol{\rho},\boldsymbol{\rho}')\nabla_\perp\psi(\mathcal{E},\boldsymbol{\rho}'), \tag{3.7}$$

and

$$\begin{aligned}\oint_{\mathcal{S}} d^2\boldsymbol{\rho}''\mathcal{B}(\mathcal{E},\boldsymbol{\rho},\boldsymbol{\rho}'')\mathcal{R}(\mathcal{E},\boldsymbol{\rho}'',\boldsymbol{\rho}') &= \oint_{\mathcal{S}} d^2\boldsymbol{\rho}''\mathcal{R}(\mathcal{E},\boldsymbol{\rho},\boldsymbol{\rho}'')\mathcal{B}(\mathcal{E},\boldsymbol{\rho}'',\boldsymbol{\rho}') \\ &= \delta_{\mathcal{S}}^{(2)}(\boldsymbol{\rho}-\boldsymbol{\rho}').\end{aligned} \tag{3.8}$$

So far the operators $\hat{\mathcal{B}}(\mathcal{E})$ and $\hat{\mathcal{R}}(\mathcal{E})$ have been considered as abstract objects. To provide explicit forms of their kernels, consider the Steklov eigensystem [7]

$$\hat{\mathcal{H}}\psi_n(\mathcal{E},\mathbf{r}) = \mathcal{E}\psi_n(\mathcal{E},\mathbf{r}) \quad (\mathbf{r} \in \mathcal{V}_{II}), \tag{3.9}$$

$$r\psi_n(\mathcal{E},\mathbf{r}) \overset{r\to\infty}{\to} 0, \tag{3.10}$$

$$\nabla_\perp \psi_n(\mathcal{E},\boldsymbol{\rho}) = b_n(\mathcal{E})\psi_n(\mathcal{E},\boldsymbol{\rho}) \tag{3.11}$$

[cf. Eqs. (3.1) and (3.2)], where $\mathcal{E} \in \mathbb{R}$ is fixed and $b_n(\mathcal{E})$ is an eigenvalue. Eigenfunctions to this system, $\{\psi_n(\mathcal{E},\mathbf{r})\}$, are these particular solutions to the Schrödinger equation (3.9) in $\mathcal{V}_{II}$, obeying the asymptotic condition (3.10), which have constant normal logarithmic derivatives (Steklov eigenvalues) $\{b_n(\mathcal{E})\}$ over the surface $\mathcal{S}$. [We shall be assuming that all eigenvalues to the system (3.9)–(3.11) are finite; i.e., none of the eigenfunctions vanishes identically over the surface $\mathcal{S}$. This is not a serious restriction since in actual applications of the embedding method there is always some degree of freedom in choosing the surface $\mathcal{S}$ and this fact may be exploited to ensure that the assumption is not violated.] Applying the symmetric Green theorem to two arbitrary eigenfunctions $\psi_n(\mathcal{E},\mathbf{r})$ and $\psi_{n'}(\mathcal{E},\mathbf{r})$ yields

$$\langle\psi_n|\hat{\mathcal{H}}\psi_{n'}\rangle_{II} - \langle\hat{\mathcal{H}}\psi_n|\psi_{n'}\rangle_{II} = \frac{\hbar^2}{2m}(\psi_n|\nabla_\perp\psi_{n'}) - \frac{\hbar^2}{2m}(\nabla_\perp\psi_n|\psi_{n'}). \tag{3.12}$$

In virtue of Eq. (3.9), the left-hand side of Eq. (3.12) vanishes; hence,

$$(\psi_n|\nabla_\perp\psi_{n'}) - (\nabla_\perp\psi_n|\psi_{n'}) = 0 \tag{3.13}$$

and further, after employing Eq. (3.11),

$$[b_{n'}(\mathcal{E}) - b_n^*(\mathcal{E})](\psi_n|\psi_{n'}) = 0. \tag{3.14}$$

In the particular case when $\psi_{n'}(\mathcal{E},\mathbf{r})$ coincides with $\psi_n(\mathcal{E},\mathbf{r})$, Eq. (3.14) becomes

$$[b_n(\mathcal{E}) - b_n^*(\mathcal{E})](\psi_n|\psi_n) = 0; \tag{3.15}$$

hence, one infers that eigenvalues to the system (3.9)–(3.11) are real:

$$b_n(\mathcal{E}) = b_n^*(\mathcal{E}). \tag{3.16}$$

Combining this with Eq. (3.14) implies that eigenfunctions belonging to different eigenvalues are orthogonal with respect to the surface scalar product (2.14):

$$(\psi_n|\psi_{n'}) = 0 \quad [b_n(\mathcal{E}) \neq b_{n'}(\mathcal{E})]. \tag{3.17}$$

In what follows, we shall be assuming that all eigenfunctions to the system (3.9)–(3.11) have been normalized according to

$$(\psi_n|\psi_n) = 1 \tag{3.18}$$

and that eigenfunctions associated with degenerate eigenvalues (if there are any) have been also orthogonalized with respect to the scalar product (2.14). Then it holds that

$$(\psi_n|\psi_{n'}) = \delta_{nn'}. \tag{3.19}$$

Moreover, we shall be assuming that the surface functions $\{\psi_n(\mathcal{E},\boldsymbol{\rho})\}$ form a complete set in the space of single-valued square-integrable functions defined on $\mathcal{S}$ and therefore obey the closure relation

$$\sum_n \psi_n(\mathcal{E},\boldsymbol{\rho})\psi_n^*(\mathcal{E},\boldsymbol{\rho}') = \delta_S^{(2)}(\boldsymbol{\rho}-\boldsymbol{\rho}'). \tag{3.20}$$

It follows from the definition (3.3) of the DtN operator $\hat{\mathcal{B}}(\mathcal{E})$ and from Eq. (3.11) that it holds that

$$\hat{\mathcal{B}}(\mathcal{E})\psi_n(\mathcal{E},\boldsymbol{\rho}) = b_n(\mathcal{E})\psi_n(\mathcal{E},\boldsymbol{\rho}). \tag{3.21}$$

Equation (3.21) may be interpreted that surface parts $\{\psi_n(\mathcal{E},\boldsymbol{\rho})\}$ of the eigenfunctions $\{\psi_n(\mathcal{E},\mathbf{r})\}$ of the system (3.9)–(3.11) are eigenfunctions of the operator $\hat{\mathcal{B}}(\mathcal{E})$ with the logarithmic derivatives $\{b_n(\mathcal{E})\}$ being associated eigenvalues. Consequently, taking into account the orthonormality relation (3.19) and the closure relation (3.20), and invoking the theory of integral operators, one finds that the DtN kernel $\mathcal{B}(\mathcal{E},\boldsymbol{\rho},\boldsymbol{\rho}')$ has the spectral expansion

$$\mathcal{B}(\mathcal{E},\boldsymbol{\rho},\boldsymbol{\rho}') = \sum_n \psi_n(\mathcal{E},\boldsymbol{\rho})b_n(\mathcal{E})\psi_n^*(\mathcal{E},\boldsymbol{\rho}') \tag{3.22}$$

and that the spectral expansion of the reciprocal NtD kernel $\mathcal{R}(\mathcal{E},\boldsymbol{\rho},\boldsymbol{\rho}')$ is

$$\mathcal{R}(\mathcal{E},\boldsymbol{\rho},\boldsymbol{\rho}') = \sum_n \psi_n(\mathcal{E},\boldsymbol{\rho})b_n^{-1}(\mathcal{E})\psi_n^*(\mathcal{E},\boldsymbol{\rho}'). \tag{3.23}$$

It is evident from Eqs. (3.22) and (3.23) that the two kernels obey

$$\mathcal{B}(\mathcal{E},\boldsymbol{\rho},\boldsymbol{\rho}') = \mathcal{B}^*(\mathcal{E},\boldsymbol{\rho}',\boldsymbol{\rho}), \tag{3.24}$$

$$\mathcal{R}(\mathcal{E},\boldsymbol{\rho},\boldsymbol{\rho}') = \mathcal{R}^*(\mathcal{E},\boldsymbol{\rho}',\boldsymbol{\rho}); \tag{3.25}$$

i.e., the operators $\hat{\mathcal{B}}(\mathcal{E})$ and $\hat{\mathcal{R}}(\mathcal{E})$ are Hermitian.

IV. DtN EMBEDDING METHOD

If the trial functions $\overline{\Psi}_I(\mathbf{r})$ and $\overline{\Psi}_{II}(\mathbf{r})$ used in the functional (2.10) are constrained to match at the interface $\mathcal{S}$,

$$\overline{\Psi}_I(\boldsymbol{\rho}) = \overline{\Psi}_{II}(\boldsymbol{\rho}), \tag{4.1}$$

the functional becomes

$$\mathcal{F}^{(\mathrm{D})}[\overline{\Psi}_I,\overline{\Psi}_{II}] = \frac{\langle\overline{\Psi}_I|\hat{\mathcal{H}}\overline{\Psi}_I\rangle_I + \langle\overline{\Psi}_{II}|\hat{\mathcal{H}}\overline{\Psi}_{II}\rangle_{II} + \eta(\overline{\Psi}_I|\nabla_\perp\overline{\Psi}_I - \nabla_\perp\overline{\Psi}_{II})}{\langle\overline{\Psi}_I|\overline{\Psi}_I\rangle_I + \langle\overline{\Psi}_{II}|\overline{\Psi}_{II}\rangle_{II}} \tag{4.2}$$

[cf. Eq. (4) of Ref. [1]], where, for convenience, we have defined

$$\eta = \frac{\hbar^2}{2m}. \tag{4.3}$$

Notice that, as opposed to the unconstrained functional (2.10), the functional (4.2) does not contain the free parameter a.

Consider now the particular case when the trial function $\overline{\Psi}_{II}(\mathbf{r})$ in the functional (4.2) is

$$\overline{\Psi}_{II}(\mathbf{r}) = \psi^{(\mathrm{D})}(\mathcal{E},\mathbf{r}) \quad (\mathbf{r}\in\mathcal{V}_{II}), \tag{4.4}$$

where $\psi^{(\mathrm{D})}(\mathcal{E},\mathbf{r})$ is some function from $\mathcal{D}_{II}(\mathcal{E})$ which remains *undetermined* at this stage. In virtue of Eqs. (4.4), (3.3), and (4.1), at the interface $\mathcal{S}$ we have

$$\nabla_\perp\overline{\Psi}_{II}(\boldsymbol{\rho}) = \hat{\mathcal{B}}(\mathcal{E})\overline{\Psi}_I(\boldsymbol{\rho}). \tag{4.5}$$

Exploiting Eqs. (4.4), (3.1), and (4.5) and omitting henceforth the subscript I at the trial function in $\mathcal{V}_I$, transforms the functional (4.2) into

$$\mathcal{F}^{(\mathrm{D})}[\overline{\Psi},\psi^{(\mathrm{D})}] = \frac{\langle\overline{\Psi}|\hat{\mathcal{H}}\overline{\Psi}\rangle_I + \mathcal{E}\langle\psi^{(\mathrm{D})}|\psi^{(\mathrm{D})}\rangle_{II} + \eta(\overline{\Psi}|\nabla_\perp\overline{\Psi} - \hat{\mathcal{B}}\overline{\Psi})}{\langle\overline{\Psi}|\overline{\Psi}\rangle_I + \langle\psi^{(\mathrm{D})}|\psi^{(\mathrm{D})}\rangle_{II}}. \tag{4.6}$$

The functional (4.6) depends on the function $\psi^{(\mathrm{D})}(\mathcal{E},\mathbf{r})$ only through the volume scalar product $\langle\psi^{(\mathrm{D})}|\psi^{(\mathrm{D})}\rangle_{II}$. To eliminate this term, we differentiate Eq. (3.1) [obeyed by $\psi^{(\mathrm{D})}(\mathcal{E},\mathbf{r})$] with respect to $\mathcal{E}$, obtaining

$$\hat{\mathcal{H}}\frac{\partial \psi^{(\mathrm{D})}(\mathcal{E},\mathbf{r})}{\partial \mathcal{E}} = \psi^{(\mathrm{D})}(\mathcal{E},\mathbf{r}) + \mathcal{E}\frac{\partial \psi^{(\mathrm{D})}(\mathcal{E},\mathbf{r})}{\partial \mathcal{E}}, \tag{4.7}$$

premultiply Eq. (4.7) by $\psi^{(\mathrm{D})*}(\mathcal{E},\mathbf{r})$ and the complex conjugate of Eq. (3.1) by $\partial\psi^{(\mathrm{D})}(\mathcal{E},\mathbf{r})/\partial\mathcal{E}$, and subtract. This yields

$$-\eta\psi^{(\mathrm{D})*}(\mathcal{E},\mathbf{r})\boldsymbol{\nabla}^2\frac{\partial \psi^{(\mathrm{D})}(\mathcal{E},\mathbf{r})}{\partial \mathcal{E}} + \eta\frac{\partial \psi^{(\mathrm{D})}(\mathcal{E},\mathbf{r})}{\partial \mathcal{E}}\boldsymbol{\nabla}^2\psi^{(\mathrm{D})*}(\mathcal{E},\mathbf{r}) = \psi^{(\mathrm{D})*}(\mathcal{E},\mathbf{r})\psi^{(\mathrm{D})}(\mathcal{E},\mathbf{r}). \tag{4.8}$$

Integration of Eq. (4.8) over the volume $\mathcal{V}_{II}$, followed by application of the symmetric Green's theorem, after some rearrangement, gives

$$\langle\psi^{(\mathrm{D})}|\psi^{(\mathrm{D})}\rangle_{II} = \eta\left(\psi^{(\mathrm{D})}\middle|\nabla_\perp\frac{\partial \psi^{(\mathrm{D})}}{\partial \mathcal{E}}\right) - \eta\left(\nabla_\perp\psi^{(\mathrm{D})}\middle|\frac{\partial \psi^{(\mathrm{D})}}{\partial \mathcal{E}}\right). \tag{4.9}$$

Evidently, Eq. (4.9) may be rewritten in the form

$$\langle\psi^{(\mathrm{D})}|\psi^{(\mathrm{D})}\rangle_{II} = \eta\left(\psi^{(\mathrm{D})}\middle|\frac{\partial}{\partial \mathcal{E}}\nabla_\perp\psi^{(\mathrm{D})}\right) - \eta\left(\nabla_\perp\psi^{(\mathrm{D})}\middle|\frac{\partial \psi^{(\mathrm{D})}}{\partial \mathcal{E}}\right); \tag{4.10}$$

hence, after employing Eq. (3.3), we find

$$\langle\psi^{(\mathrm{D})}|\psi^{(\mathrm{D})}\rangle_{II} = \eta\left(\psi^{(\mathrm{D})}\middle|\frac{\partial}{\partial \mathcal{E}}\hat{\mathcal{B}}\psi^{(\mathrm{D})}\right) - \eta\left(\hat{\mathcal{B}}\psi^{(\mathrm{D})}\middle|\frac{\partial \psi^{(\mathrm{D})}}{\partial \mathcal{E}}\right) \tag{4.11}$$

or, equivalently,

$$\langle\psi^{(\mathrm{D})}|\psi^{(\mathrm{D})}\rangle_{II} = \eta\left(\psi^{(\mathrm{D})}\middle|\frac{\partial \hat{\mathcal{B}}}{\partial \mathcal{E}}\psi^{(\mathrm{D})}\right) + \eta\left(\psi^{(\mathrm{D})}\middle|\hat{\mathcal{B}}\frac{\partial \psi^{(\mathrm{D})}}{\partial \mathcal{E}}\right) - \eta\left(\hat{\mathcal{B}}\psi^{(\mathrm{D})}\middle|\frac{\partial \psi^{(\mathrm{D})}}{\partial \mathcal{E}}\right). \tag{4.12}$$

Since $\hat{\mathcal{B}}(\mathcal{E})$ is Hermitian, the second and third terms on the right-hand side of Eq. (4.12) cancel and we arrive at

$$\langle\psi^{(\mathrm{D})}|\psi^{(\mathrm{D})}\rangle_{II} = \eta\left(\psi^{(\mathrm{D})}\middle|\frac{\partial \hat{\mathcal{B}}}{\partial \mathcal{E}}\psi^{(\mathrm{D})}\right). \tag{4.13}$$

Finally, application of Eqs. (4.4) and (4.1) transforms Eq. (4.13) into

$$\langle\psi^{(\mathrm{D})}|\psi^{(\mathrm{D})}\rangle_{II} = \eta\left(\overline{\Psi}\middle|\frac{\partial \hat{\mathcal{B}}}{\partial \mathcal{E}}\overline{\Psi}\right) \tag{4.14}$$

[cf. Eq. (15) of Ref. [1]], which allows us to rewrite the functional (4.6) in the following suitable form:

$$\mathcal{F}^{(\mathrm{D})}[\overline{\Psi}] = \frac{\langle\overline{\Psi}|\hat{\mathcal{H}}\overline{\Psi}\rangle_I + \eta(\overline{\Psi}|\nabla_\perp\overline{\Psi} - \hat{\mathcal{B}}\overline{\Psi} + \mathcal{E}[\partial\hat{\mathcal{B}}/\partial\mathcal{E}]\overline{\Psi})}{\langle\overline{\Psi}|\overline{\Psi}\rangle_I + \eta(\overline{\Psi}|[\partial\hat{\mathcal{B}}/\partial\mathcal{E}]\overline{\Psi})} \tag{4.15}$$

[cf. Eq. (16) of Ref. [1]].

It may be verified that the functional (4.15) retains the property of the starting functional (2.10) to be real for any trial function $\overline{\Psi}(\mathbf{r})$:

$$\mathcal{F}^{(\mathrm{D})*}[\overline{\Psi}] = \mathcal{F}^{(\mathrm{D})}[\overline{\Psi}]. \tag{4.16}$$

We shall seek the function $\Psi^{(\mathrm{D})}(\mathbf{r})$ $(\mathbf{r}\in\mathcal{V}_I)$, which makes the functional (4.15) stationary:

$$\delta\mathcal{F}^{(\mathrm{D})}[\Psi^{(\mathrm{D})}] = 0. \tag{4.17}$$

The corresponding stationary value

$$E^{(\mathrm{D})} = \mathcal{F}^{(\mathrm{D})}[\Psi^{(\mathrm{D})}] \tag{4.18}$$

[which, by virtue of Eq. (4.16), is real] is an estimate of some eigenenergy of the original spectral problem (2.1) and (2.2). [It is to be noticed that both $E^{(\mathrm{D})}$ and $\Psi^{(\mathrm{D})}(\mathbf{r})$ depend parametrically on $\mathcal{E}$.] To find equations determining $E^{(\mathrm{D})}$ and $\Psi^{(\mathrm{D})}(\mathbf{r})$, we rewrite Eq. (4.15) as

$$\mathcal{F}^{(\mathrm{D})}[\overline{\Psi}]\left[\langle\overline{\Psi}|\overline{\Psi}\rangle_I + \eta\left(\overline{\Psi}\middle|\frac{\partial\hat{\mathcal{B}}}{\partial\mathcal{E}}\overline{\Psi}\right)\right] = \langle\overline{\Psi}|\hat{\mathcal{H}}\overline{\Psi}\rangle_I + \eta\left(\overline{\Psi}\middle|\nabla_\perp\overline{\Psi} - \hat{\mathcal{B}}\overline{\Psi} + \mathcal{E}\frac{\partial\hat{\mathcal{B}}}{\partial\mathcal{E}}\overline{\Psi}\right) \tag{4.19}$$

and vary there $\overline{\Psi}(\mathbf{r})$ around $\Psi^{(\mathrm{D})}(\mathbf{r})$. By virtue of Eqs. (4.17) and (4.18), this results in

$$\langle\delta\Psi|[\hat{\mathcal{H}} - E^{(\mathrm{D})}]\Psi^{(\mathrm{D})}\rangle_I + \langle\Psi^{(\mathrm{D})}|[\hat{\mathcal{H}} - E^{(\mathrm{D})}]\delta\Psi\rangle_I + \eta\left(\delta\Psi\middle|\nabla_\perp\Psi^{(\mathrm{D})} - \hat{\mathcal{B}}\Psi^{(\mathrm{D})} + [\mathcal{E} - E^{(\mathrm{D})}]\frac{\partial\hat{\mathcal{B}}}{\partial\mathcal{E}}\Psi^{(\mathrm{D})}\right) + \eta\left(\Psi^{(\mathrm{D})}\middle|\nabla_\perp\delta\Psi - \hat{\mathcal{B}}\delta\Psi + [\mathcal{E} - E^{(\mathrm{D})}]\frac{\partial\hat{\mathcal{B}}}{\partial\mathcal{E}}\delta\Psi\right) = 0. \tag{4.20}$$

Applying the symmetric Green's theorem to the second term on the left-hand side of Eq. (4.20) and utilizing the fact that $\hat{\mathcal{B}}(\mathcal{E})$ and $\partial\hat{\mathcal{B}}(\mathcal{E})/\partial\mathcal{E}$ are Hermitian gives

$$\langle\delta\Psi|[\hat{\mathcal{H}} - E^{(\mathrm{D})}]\Psi^{(\mathrm{D})}\rangle_I + \langle[\hat{\mathcal{H}} - E^{(\mathrm{D})}]\Psi^{(\mathrm{D})}|\delta\Psi\rangle_I + \eta\left(\delta\Psi\middle|\nabla_\perp\Psi^{(\mathrm{D})} - \hat{\mathcal{B}}\Psi^{(\mathrm{D})} + [\mathcal{E} - E^{(\mathrm{D})}]\frac{\partial\hat{\mathcal{B}}}{\partial\mathcal{E}}\Psi^{(\mathrm{D})}\right) + \eta\left(\nabla_\perp\Psi^{(\mathrm{D})} - \hat{\mathcal{B}}\Psi^{(\mathrm{D})} + [\mathcal{E} - E^{(\mathrm{D})}]\frac{\partial\hat{\mathcal{B}}}{\partial\mathcal{E}}\Psi^{(\mathrm{D})}\middle|\delta\Psi\right) = 0; \tag{4.21}$$

hence, one infers the eigensystem

$$\hat{\mathcal{H}}\Psi^{(\mathrm{D})}(\mathbf{r}) = E^{(\mathrm{D})}\Psi^{(\mathrm{D})}(\mathbf{r}) \quad (\mathbf{r}\in\mathcal{V}_I), \tag{4.22}$$

$$\left[\nabla_\perp - \hat{\mathcal{B}}(\mathcal{E}) + \mathcal{E}\frac{\partial\hat{\mathcal{B}}(\mathcal{E})}{\partial\mathcal{E}}\right]\Psi^{(\mathrm{D})}(\boldsymbol{\rho}) = E^{(\mathrm{D})}\frac{\partial\hat{\mathcal{B}}(\mathcal{E})}{\partial\mathcal{E}}\Psi^{(\mathrm{D})}(\boldsymbol{\rho}) \quad (\boldsymbol{\rho}\in\mathcal{S}), \tag{4.23}$$

obeyed by $\Psi^{(\mathrm{D})}(\mathbf{r})$ and $E^{(\mathrm{D})}$ [cf. Eq. (17) of Ref. [1]]. It is worth emphasizing that this eigensystem is of a nonstandard character since the eigenvalue $E^{(\mathrm{D})}$ appears both in the Schrödinger equation (4.22) *and* in the boundary condition (4.23).

Once the function $\Psi^{(\mathrm{D})}(\mathbf{r})$, approximating $\Psi(\mathbf{r})$ in $\mathcal{V}_I$, has been determined, the function $\psi^{(\mathrm{D})}(\mathcal{E},\mathbf{r})$, approximating $\Psi(\mathbf{r})$ in $\mathcal{V}_{II}$, may be found. [We recall that thus far $\psi^{(\mathrm{D})}(\mathcal{E},\mathbf{r})$ has played only the auxiliary role and has remained undetermined.] To this end, we expand $\psi^{(\mathrm{D})}(\mathcal{E},\mathbf{r})$ in the Steklov basis $\{\psi_n(\mathcal{E},\mathbf{r})\}$:

$$\psi^{(\mathrm{D})}(\mathcal{E},\mathbf{r}) = \sum_n c_n^{(\mathrm{D})}\psi_n(\mathcal{E},\mathbf{r}) \quad (\mathbf{r}\in\mathcal{V}_{II}). \tag{4.24}$$

The expansion coefficients in Eq. (4.24) may be found by shifting the point $\mathbf{r}$ to the surface $\mathcal{S}$, projecting the resulting equation onto the Steklov eigenfunctions, and exploiting the orthonormality relation (3.19). This yields

$$c_n^{(\mathrm{D})} = (\psi_n|\psi^{(\mathrm{D})}), \tag{4.25}$$

which, after making use of the fact that at the surface $\mathcal{S}$ it holds that

$$\psi^{(\mathrm{D})}(\mathcal{E},\boldsymbol{\rho}) = \Psi^{(\mathrm{D})}(\boldsymbol{\rho}) \tag{4.26}$$

[cf. Eqs. (4.4) and (4.1)], leads finally to

$$c_n^{(\mathrm{D})} = (\psi_n|\Psi^{(\mathrm{D})}). \tag{4.27}$$

V. NtD EMBEDDING METHOD

It is tempting to investigate what happens when the matching condition (4.1) is replaced by the weaker constraint

$$\nabla_\perp\overline{\Psi}_I(\boldsymbol{\rho}) = \nabla_\perp\overline{\Psi}_{II}(\boldsymbol{\rho}). \tag{5.1}$$

Evidently, this results in the following simplification of the functional (2.10):

$$\mathcal{F}^{(\mathrm{N})}[\overline{\Psi}_I,\overline{\Psi}_{II}] = \frac{\langle\overline{\Psi}_I|\hat{\mathcal{H}}\overline{\Psi}_I\rangle_I + \langle\overline{\Psi}_{II}|\hat{\mathcal{H}}\overline{\Psi}_{II}\rangle_{II} - \eta(\nabla_\perp\overline{\Psi}_I|\overline{\Psi}_I - \overline{\Psi}_{II})}{\langle\overline{\Psi}_I|\overline{\Psi}_I\rangle_I + \langle\overline{\Psi}_{II}|\overline{\Psi}_{II}\rangle_{II}}. \tag{5.2}$$

Consider the trial function

$$\overline{\Psi}_{II}(\mathbf{r}) = \psi^{(\mathrm{N})}(\mathcal{E},\mathbf{r}) \quad (\mathbf{r}\in\mathcal{V}_{II}), \tag{5.3}$$

where $\psi^{(\mathrm{N})}(\mathcal{E},\mathbf{r})$, at this stage undetermined, is from $\mathcal{D}_{II}(\mathcal{E})$. By virtue of Eqs. (5.3), (3.4), and (5.1), one has

$$\overline{\Psi}_{II}(\boldsymbol{\rho}) = \hat{\mathcal{R}}(\mathcal{E})\nabla_\perp\overline{\Psi}_I(\boldsymbol{\rho}) \tag{5.4}$$

and, omitting henceforth the index I at the trial function in $\mathcal{V}_I$, the functional (5.2) becomes

$$\mathcal{F}^{(\mathrm{N})}[\overline{\Psi},\psi^{(\mathrm{N})}] = \frac{\langle\overline{\Psi}|\hat{\mathcal{H}}\overline{\Psi}\rangle_I + \mathcal{E}\langle\psi^{(\mathrm{N})}|\psi^{(\mathrm{N})}\rangle_{II} + \eta(\nabla_\perp\overline{\Psi}|\hat{\mathcal{R}}\nabla_\perp\overline{\Psi} - \overline{\Psi})}{\langle\overline{\Psi}|\overline{\Psi}\rangle_I + \langle\psi^{(\mathrm{N})}|\psi^{(\mathrm{N})}\rangle_{II}}. \tag{5.5}$$

A reasoning similar to that leading to Eq. (4.14) yields

$$\langle\psi^{(\mathrm{N})}|\psi^{(\mathrm{N})}\rangle_{II} = -\eta\left(\nabla_\perp\overline{\Psi}\left|\frac{\partial\hat{\mathcal{R}}}{\partial\mathcal{E}}\nabla_\perp\overline{\Psi}\right.\right), \tag{5.6}$$

and this allows us to transform the functional (5.5) into the functional

$$\mathcal{F}^{(\mathrm{N})}[\overline{\Psi}] = \frac{\langle\overline{\Psi}|\hat{\mathcal{H}}\,\overline{\Psi}\rangle_I + \eta(\nabla_\perp\overline{\Psi}|\hat{\mathcal{R}}\,\nabla_\perp\overline{\Psi} - \mathcal{E}[\partial\hat{\mathcal{R}}/\partial\mathcal{E}]\nabla_\perp\overline{\Psi} - \overline{\Psi})}{\langle\,\overline{\Psi}|\overline{\Psi}\rangle_I - \eta(\,\nabla_\perp\overline{\Psi}|[\partial\hat{\mathcal{R}}/\partial\mathcal{E}]\nabla_\perp\overline{\Psi})} \tag{5.7}$$

[cf. Eq. (4.15)], with the property

$$\mathcal{F}^{(\mathrm{N})*}[\overline{\Psi}] = \mathcal{F}^{(\mathrm{N})}[\overline{\Psi}]. \tag{5.8}$$

Proceeding as in Sec. IV, we find that the function $\Psi^{(\mathrm{N})}(\mathbf{r})$ $(\mathbf{r}\in\mathcal{V}_I)$, which makes the functional (5.7) stationary, i.e.,

$$\delta\mathcal{F}^{(\mathrm{N})}[\Psi^{(\mathrm{N})}] = 0, \tag{5.9}$$

and the corresponding real [cf. Eq. (5.8)] stationary value

$$E^{(\mathrm{N})} = \mathcal{F}^{(\mathrm{N})}[\Psi^{(\mathrm{N})}] \tag{5.10}$$

[approximating the eigenvalue E in Eq. (2.1)] are solutions to the nonstandard eigensystem

$$\hat{\mathcal{H}}\Psi^{(\mathrm{N})}(\mathbf{r}) = E^{(\mathrm{N})}\Psi^{(\mathrm{N})}(\mathbf{r}) \quad (\mathbf{r} \in \mathcal{V}_I), \tag{5.11}$$

$$\left[\hat{\mathcal{I}}_{\mathcal{S}} - \hat{\mathcal{R}}(\mathcal{E})\nabla_\perp + \mathcal{E}\frac{\partial\hat{\mathcal{R}}(\mathcal{E})}{\partial\mathcal{E}}\nabla_\perp\right]\Psi^{(\mathrm{N})}(\boldsymbol{\rho}) = E^{(\mathrm{N})}\frac{\partial\hat{\mathcal{R}}(\mathcal{E})}{\partial\mathcal{E}}\nabla_\perp\Psi^{(\mathrm{N})}(\boldsymbol{\rho}) \quad (\boldsymbol{\rho} \in \mathcal{S}). \tag{5.12}$$

Evidently, both $E^{(\mathrm{N})}$ and $\Psi^{(\mathrm{N})}(\mathbf{r})$ depend parametrically on $\mathcal{E}$.

To facilitate comparison of the boundary condition (5.12) with that in Eq. (4.23), we operate on the former from the left with $\hat{\mathcal{B}}(\mathcal{E})$ and make use of Eq. (3.5), obtaining

$$\left[\nabla_\perp - \hat{\mathcal{B}}(\mathcal{E}) - \mathcal{E}\hat{\mathcal{B}}(\mathcal{E})\frac{\partial\hat{\mathcal{R}}(\mathcal{E})}{\partial\mathcal{E}}\nabla_\perp\right]\Psi^{(\mathrm{N})}(\boldsymbol{\rho}) = -E^{(\mathrm{N})}\hat{\mathcal{B}}(\mathcal{E})\frac{\partial\hat{\mathcal{R}}(\mathcal{E})}{\partial\mathcal{E}}\nabla_\perp\Psi^{(\mathrm{N})}(\boldsymbol{\rho}) \quad (\boldsymbol{\rho} \in \mathcal{S}). \tag{5.13}$$

This still may be transformed since from the reciprocity relation (3.5) it follows that

$$\hat{\mathcal{B}}(\mathcal{E})\frac{\partial\hat{\mathcal{R}}(\mathcal{E})}{\partial\mathcal{E}} = -\frac{\partial\hat{\mathcal{B}}(\mathcal{E})}{\partial\mathcal{E}}\hat{\mathcal{R}}(\mathcal{E}). \tag{5.14}$$

Hence, after some rearrangement, the boundary condition (5.12) becomes

$$\left[\nabla_\perp - \hat{\mathcal{B}}(\mathcal{E}) + \mathcal{E}\frac{\partial\hat{\mathcal{B}}(\mathcal{E})}{\partial\mathcal{E}}\hat{\mathcal{R}}(\mathcal{E})\nabla_\perp\right]\Psi^{(\mathrm{N})}(\boldsymbol{\rho}) = E^{(\mathrm{N})}\frac{\partial\hat{\mathcal{B}}(\mathcal{E})}{\partial\mathcal{E}}\hat{\mathcal{R}}(\mathcal{E})\nabla_\perp\Psi^{(\mathrm{N})}(\boldsymbol{\rho}) \quad (\boldsymbol{\rho} \in \mathcal{S}). \tag{5.15}$$

Comparison of Eqs. (4.23) and (5.15) shows that they *differ* in the terms containing the derivatives $\partial\hat{\mathcal{B}}(\mathcal{E})/\partial\mathcal{E}$.

Hitherto, the function $\psi^{(\mathrm{N})}(\mathcal{E},\mathbf{r})$, approximating $\Psi(\mathbf{r})$ in $\mathcal{V}_{II}$, has remained undetermined. It may be found after movements analogous to these presented at the end of Sec. IV for $\psi^{(\mathrm{D})}(\mathcal{E},\mathbf{r})$. One arrives at the expansion

$$\psi^{(\mathrm{N})}(\mathcal{E},\mathbf{r}) = \sum_n c_n^{(\mathrm{N})}\psi_n(\mathcal{E},\mathbf{r}) \quad (\mathbf{r} \in \mathcal{V}_{II}), \tag{5.16}$$

with the coefficients

$$c_n^{(\mathrm{N})} = b_n^{-1}(\mathcal{E})(\psi_n|\nabla_\perp\Psi^{(\mathrm{N})}). \tag{5.17}$$

In general the DtN and NtD embedding methods will yield *different* estimates of eigensolutions to the system (2.1) and (2.2). Differences between these estimates will provide some information about their quality.

VI. PROBLEMS WITH SPHERICAL SYMMETRY IN THE OUTER REGION

Assume that the surface $\mathcal{S}$ is a spherical shell $\mathcal{S}_\rho$ of radius ρ. Locate the coordinate origin at the center of $\mathcal{S}_\rho$ and consider the case when in the region $\mathcal{V}_{II}$ exterior to $\mathcal{S}_\rho$ the potential $V(\mathbf{r})$ is central:

$$V(\mathbf{r}) = V(r) \quad (r > \rho). \tag{6.1}$$

Then the Schrödinger equation (3.9) in $\mathcal{V}_{II}$ is separable in spherical coordinates and possesses particular solutions, satisfying the asymptotic condition (3.10), of the form

$$\psi_{lm_l}(\mathcal{E},\mathbf{r}) = \frac{f_l(\mathcal{E},r)}{\rho f_l(\mathcal{E},\rho)}Y_{lm_l}(\mathbf{n}_r). \tag{6.2}$$

Here $Y_{lm_l}(\mathbf{n}_r)$, with $\mathbf{n}_r = \mathbf{r}/r$, $l \in \mathbb{N}$ and $m_l \in \{0, \pm 1, \pm 2, \ldots, \pm l\}$, is a normalized spherical harmonic and $f_l(\mathcal{E},r)$ is that solution to the radial Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2} + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2} + V(r) - \mathcal{E}\right]rf_l(\mathcal{E},r) = 0 \quad (r > \rho), \tag{6.3}$$

which obeys

$$rf_l(\mathcal{E},r) \overset{r\to\infty}{\to} 0. \tag{6.4}$$

It is evident that at the surface $\mathcal{S}_\rho$ it holds that

$$\psi_{lm_l}(\mathcal{E},\boldsymbol{\rho}) = \rho^{-1}Y_{lm_l}(\mathbf{n}_\rho) \tag{6.5}$$

and

$$\nabla_\perp\psi_{lm_l}(\mathcal{E},\boldsymbol{\rho}) = \frac{\partial_\rho f_l(\mathcal{E},\rho)}{\rho f_l(\mathcal{E},\rho)}Y_{lm_l}(\mathbf{n}_\rho), \tag{6.6}$$

where

$$\partial_\rho f_l(\mathcal{E},\rho) = \left.\frac{\partial f_l(\mathcal{E},r)}{\partial r}\right|_{r=\rho}; \tag{6.7}$$

hence, it follows that

$$\nabla_\perp\psi_{lm_l}(\mathcal{E},\boldsymbol{\rho}) = b_l(\mathcal{E})\psi_{lm_l}(\mathcal{E},\boldsymbol{\rho}), \tag{6.8}$$

with

$$b_l(\mathcal{E}) = \frac{\partial_\rho f_l(\mathcal{E},\rho)}{f_l(\mathcal{E},\rho)}. \tag{6.9}$$

Consequently, for the problem at hand the functions (6.2) are eigenfunctions to the system (3.9)–(3.11) and the numbers (6.9) are associated real, $(2l+1)$-fold degenerate, Steklov eigenvalues. It follows from Eq. (6.5) and from the orthonormality and completeness of the spherical harmonics on the unit sphere that the functions (6.2) form the orthonormal and complete set on the sphere $\mathcal{S}_\rho$; i.e., it holds that

$$(\psi_{lm_l}|\psi_{l'm_l'}) = \delta_{ll'}\delta_{m_lm_l'}, \tag{6.10}$$

$$\sum_{l=0}^{\infty}\sum_{m_l=-l}^{l}\psi_{lm_l}(\mathcal{E},\boldsymbol{\rho})\psi_{lm_l}^*(\mathcal{E},\boldsymbol{\rho}') = \delta_{\mathcal{S}_\rho}^{(2)}(\boldsymbol{\rho}-\boldsymbol{\rho}') \tag{6.11}$$

[cf. Eqs. (3.19) and (3.20)].

Since the functions (6.2) and the numbers (6.9) are eigensolutions to the system (3.9)–(3.11), in accordance with Eqs.

(3.22) and (3.23) one finds that in the case considered here the DtN and NtD kernels are given by

$$\mathcal{B}(\mathcal{E},\boldsymbol{\rho},\boldsymbol{\rho}') = \rho^{-2}\sum_{l=0}^{\infty}\sum_{m_l=-l}^{l} b_l(\mathcal{E})Y_{lm_l}(\mathbf{n}_\rho)Y^*_{lm_l}(\mathbf{n}'_\rho) \quad (6.12)$$

and

$$\mathcal{R}(\mathcal{E},\boldsymbol{\rho},\boldsymbol{\rho}') = \rho^{-2}\sum_{l=0}^{\infty}\sum_{m_l=-l}^{l} b_l^{-1}(\mathcal{E})Y_{lm_l}(\mathbf{n}_\rho)Y^*_{lm_l}(\mathbf{n}'_\rho), \quad (6.13)$$

respectively. On employing the well-known summation formula for the spherical harmonics, Eqs. (6.12) and (6.13) may be rewritten as

$$\mathcal{B}(\mathcal{E},\boldsymbol{\rho},\boldsymbol{\rho}') = (4\pi\rho^2)^{-1}\sum_{l=0}^{\infty}(2l+1)b_l(\mathcal{E})P_l(\mathbf{n}_\rho\cdot\mathbf{n}'_\rho), \quad (6.14)$$

$$\mathcal{R}(\mathcal{E},\boldsymbol{\rho},\boldsymbol{\rho}') = (4\pi\rho^2)^{-1}\sum_{l=0}^{\infty}(2l+1)b_l^{-1}(\mathcal{E})P_l(\mathbf{n}_\rho\cdot\mathbf{n}'_\rho), \quad (6.15)$$

with $P_l(\xi)$ denoting the Legendre polynomial.

In the particular case when in the region exterior to $\mathcal{S}_\rho$ the potential vanishes,

$$V(r) \equiv 0 \quad (r > \rho), \quad (6.16)$$

nontrivial solutions to the problem (2.1) and (2.2) may exist only for $E<0$. Therefore we choose

$$\mathcal{E} < 0 \quad (6.17)$$

and define

$$K = \sqrt{-\frac{2m\mathcal{E}}{\hbar^2}}. \quad (6.18)$$

With Eq. (6.16), a solution to the radial equation (6.3), obeying the condition (6.4), is

$$f_l(\mathcal{E},r) = k_l(Kr), \quad (6.19)$$

where

$$k_l(\zeta) = \frac{\pi}{2}(-\zeta)^l\left(\frac{1}{\zeta}\frac{d}{d\zeta}\right)^l\frac{\exp(-\zeta)}{\zeta} \quad (6.20)$$

is the spherical Macdonald function (modified spherical Bessel function of the third kind) [8]. On employing the relation

$$\frac{dk_l(\zeta)}{d\zeta} = \frac{l}{\zeta}k_l(\zeta) - k_{l+1}(\zeta), \quad (6.21)$$

one finds that in the particular case (6.16) the Steklov eigenvalues (6.9) are

$$b_l(\mathcal{E}) = \frac{l}{\rho} - K\frac{k_{l+1}(K\rho)}{k_l(K\rho)}. \quad (6.22)$$

VII. APPLICATION OF RAYLEIGH-RITZ TRIAL FUNCTIONS

In practical applications of the DtN and NtD embedding methods it may be extremely difficult, or even impossible, to solve the differential eigensystems (4.22),(4.23) and (5.11),(5.12) exactly. However, the variational principle (4.17), (4.18), and (4.15) and the variational principle (5.9), (5.10), and (5.7) offer the possibility to solve these eigensystems approximately.

Let $\{\phi_\mu(\mathbf{r})\}$, $(\mu=1,\ldots,M)$, be a set of functions defined in $\mathcal{V}_I$. Consider the Rayleigh-Ritz trial function

$$\overline{\Psi}(\mathbf{r}) \equiv \overline{\Phi}(\mathbf{r}) = \sum_{\mu=1}^{M}\overline{a}_\mu\phi_\mu(\mathbf{r}) \quad (\mathbf{r}\in\mathcal{V}_I), \quad (7.1)$$

approximating some eigenfunction of the eigensystem (4.22) and (4.23), with the coefficients $\{\overline{a}_\mu\}$ to be optimized. Substitution of this trial function into the functional (4.15) yields the Rayleigh quotient

$$F^{(\mathrm{D})}[\overline{\mathrm{a}}^\dagger,\overline{\mathrm{a}}] = \frac{\overline{\mathrm{a}}^\dagger\Lambda^{(\mathrm{D})}\overline{\mathrm{a}}}{\overline{\mathrm{a}}^\dagger\Delta^{(\mathrm{D})}\overline{\mathrm{a}}}, \quad (7.2)$$

in which $\overline{\mathrm{a}}$ is an M-component column vector with elements $\{\overline{a}_\mu\}$ and $\overline{\mathrm{a}}^\dagger$ is its Hermitian adjoint, while $\Lambda^{(\mathrm{D})}$ and $\Delta^{(\mathrm{D})}$ are $M\times M$ Hermitian matrices with elements

$$\Lambda^{(\mathrm{D})}_{\mu\nu} = \langle\phi_\mu|\hat{\mathcal{H}}\phi_\nu\rangle_I + \frac{\hbar^2}{2m}(\phi_\mu|\nabla_\perp\phi_\nu - \hat{\mathcal{B}}\phi_\nu + \mathcal{E}[\partial\hat{\mathcal{B}}/\partial\mathcal{E}]\phi_\nu) \quad (7.3)$$

and

$$\Delta^{(\mathrm{D})}_{\mu\nu} = \langle\phi_\mu|\phi_\nu\rangle_I + \frac{\hbar^2}{2m}(\phi_\mu|[\partial\hat{\mathcal{B}}/\partial\mathcal{E}]\phi_\nu), \quad (7.4)$$

respectively. We shall denote by $\tilde{\mathrm{a}}^{(\mathrm{D})}$ and $\tilde{\mathrm{a}}^{(\mathrm{D})\dagger}$ these particular vectors $\overline{\mathrm{a}}$ and $\overline{\mathrm{a}}^\dagger$, for which the functional (7.2) is stationary with respect to variations in their components:

$$\delta F^{(\mathrm{D})}[\tilde{\mathrm{a}}^{(\mathrm{D})\dagger},\tilde{\mathrm{a}}^{(\mathrm{D})}] = 0. \quad (7.5)$$

Defining

$$\widetilde{E}^{(\mathrm{D})} = F^{(\mathrm{D})}[\tilde{\mathrm{a}}^{(\mathrm{D})\dagger},\tilde{\mathrm{a}}^{(\mathrm{D})}], \quad (7.6)$$

from Eqs. (7.5) and (7.2) one obtains the generalized [weighted] algebraic eigensystem

$$\Lambda^{(\mathrm{D})}\tilde{\mathrm{a}}^{(\mathrm{D})} = \widetilde{E}^{(\mathrm{D})}\Delta^{(\mathrm{D})}\tilde{\mathrm{a}}^{(\mathrm{D})} \quad (7.7)$$

and its Hermitian conjugate. In general, the eigensystem (7.7) has $M^{(\mathrm{D})}\leqslant M$ pairs of eigensolutions. The eigenvalues $\{\widetilde{E}^{(\mathrm{D})}_\gamma\}$ are second-order variational estimates of eigenvalues of the differential eigensystem (4.22) and (4.23), while components of the associated eigenvectors $\{\tilde{\mathrm{a}}^{(\mathrm{D})}_\gamma\}$ may be used in Eq. (7.1) to construct the Rayleigh-Ritz functions

$$\widetilde{\Phi}^{(\mathrm{D})}_\gamma(\mathbf{r}) = \sum_{\mu=1}^{M}\tilde{a}^{(\mathrm{D})}_{\mu\gamma}\phi_\mu(\mathbf{r}) \quad (\mathbf{r}\in\mathcal{V}_I), \quad (7.8)$$

which are first-order variational estimates of eigenfunctions of the system (4.22) and (4.23).

Proceeding in the analogous manner and using the trial function (7.1) in the functional (5.7) leads one to the generalized matrix eigensystem

$$\Lambda^{(\mathrm{N})}\tilde{\mathrm{a}}^{(\mathrm{N})} = \widetilde{E}^{(\mathrm{N})}\Delta^{(\mathrm{N})}\tilde{\mathrm{a}}^{(\mathrm{N})} \tag{7.9}$$

(and its Hermitian matrix conjugate), where $\Lambda^{(\mathrm{N})}$ and $\Delta^{(\mathrm{N})}$ are $M\times M$ Hermitian matrices with elements

$$\Lambda^{(\mathrm{N})}_{\mu\nu} = \langle\phi_\mu|\hat{\mathcal{H}}\phi_\nu\rangle_I + \frac{\hbar^2}{2m}(\nabla_\perp\phi_\mu|\hat{\mathcal{R}}\nabla_\perp\phi_\nu - \mathcal{E}[\partial\hat{\mathcal{R}}/\partial\mathcal{E}]\nabla_\perp\phi_\nu - \phi_\nu) \tag{7.10}$$

and

$$\Delta^{(\mathrm{N})}_{\mu\nu} = \langle\phi_\mu|\phi_\nu\rangle_I - \frac{\hbar^2}{2m}(\nabla_\perp\phi_\mu|[\partial\hat{\mathcal{R}}/\partial\mathcal{E}]\nabla_\perp\phi_\nu), \tag{7.11}$$

respectively. Its eigenvalues $\{\widetilde{E}^{(\mathrm{N})}_\gamma\}$ are second-order variational estimates of eigenvalues of the differential eigensystem (5.11) and (5.12), while use of components of the eigenvectors $\{\tilde{\mathrm{a}}^{(\mathrm{N})}_\gamma\}$ in Eq. (7.1) yields the functions

$$\widetilde{\Phi}^{(\mathrm{N})}_\gamma(\mathbf{r}) = \sum_{\mu=1}^{M}\tilde{a}^{(\mathrm{N})}_{\mu\gamma}\phi_\mu(\mathbf{r}) \quad (\mathbf{r}\in\mathcal{V}_I), \tag{7.12}$$

which are first-order variational estimates of eigenfunctions of the system (5.11) and (5.12).

In general, the estimates $\{\widetilde{E}^{(\mathrm{D})}_\gamma\}$ and $\{\widetilde{\Phi}^{(\mathrm{D})}_\gamma(\mathbf{r})\}$ will differ from the estimates $\{\widetilde{E}^{(\mathrm{N})}_\gamma\}$ and $\{\widetilde{\Phi}^{(\mathrm{N})}_\gamma(\mathbf{r})\}$.

VIII. NUMERICAL ILLUSTRATION

As an example illustrating the utility of the two variants of the embedding method presented above, we have considered the problem of computing variationally bound-state energies of a particle moving in the potential (Fig. 2)

$$V(\mathbf{r}) = \begin{cases} \frac{1}{2}m\omega^2(\mathbf{r}-\mathbf{r}_0)^2 - \frac{1}{2}m\omega^2(\rho+r_0)^2 & (|\mathbf{r}|<\rho), \\ 0 & (|\mathbf{r}|>\rho). \end{cases} \tag{8.1}$$

Here $\mathbf{r}_0$ is a fixed vector of length $r_0<\rho$. The regions $\mathcal{V}_I$ and $\mathcal{V}_{II}$ are the sphere of radius ρ and its exterior, respectively. Evidently, the potential (8.1) exhibits the rotational symmetry around the axis directed along the vector $\mathbf{r}_0$. Consequently, the particle's Hamiltonian does commute with the projection of the angular momentum operator onto this axis and the magnetic quantum number m_l may be used to label energy levels.

The variational bases used in our calculations have been constructed from unnormalized three-dimensional isotropic oscillator eigenfunctions

$$\phi_{nlm_l}(\mathbf{r}) = r^l\exp(-\lambda r^2/2)L_n^{(l+1/2)}(\lambda r^2)Y_{lm_l}(\mathbf{n}_r), \tag{8.2}$$

where

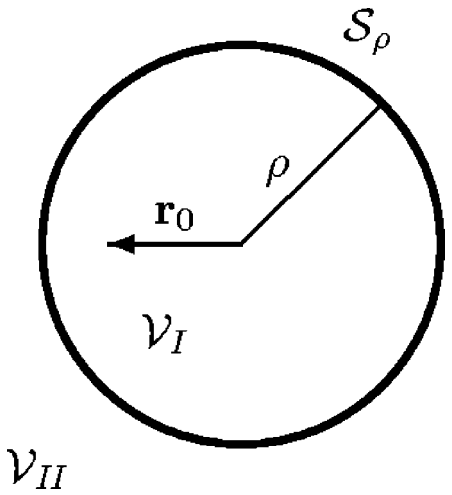

FIG. 2. Geometry of the system used in the numerical illustration. In the inner region $\mathcal{V}_I$ (the sphere of radius ρ) the potential is a superposition of that due to a three-dimensional isotropic harmonic oscillator, with its center located at the point $\mathbf{r}_0$, and that of a spherical potential well. In the outer region $\mathcal{V}_{II}$ the potential vanishes.

$$\lambda = \frac{m\omega}{\hbar} \tag{8.3}$$

and $L_n^{(\alpha)}(\xi)$ is the generalized Laguerre polynomial [9]. (The origin of the spherical coordinate system has been chosen at the center of the sphere $\mathcal{V}_I$ and the polar axis is along $\mathbf{r}_0$.) Once m_l has been chosen and fixed (cf. the preceding paragraph), a relevant variational basis is formed from the functions (8.2) with $|m_l|\leqslant l\leqslant l_{\max}$ and $0\leqslant n\leqslant n_{\max}$; the upper limits $l_{\max}$ and $n_{\max}$, constraining the basis dimension, may be varied to test convergence of variational results.

The natural units in which $m=\hbar=\omega=1$ have been used. The length parameters characterizing the potential have been chosen to be $r_0=1$, $\rho=2$. We shall report only results for the ground state with the symmetry $m_l=0$; they are representative for all cases whenever bound states in the potential (8.1) exist.

Three series of calculations have been performed.

In the first series, the truncated basis (8.2) has been used in the Rayleigh principle (2.4) and (2.5). The resulting energy estimates for four existing bound states are presented in Table I for several basis dimensions. One observes slow convergence which may be attributed to difficulty in spanning the region $r>\rho$, where exact eigenfunctions decay exponentially, with the aid of the functions (8.2) possessing Gaussian tails. The best energy estimates, computed by using the basis with $l_{\max}=40$ and $n_{\max}=40$ (which means working with 1681 basis functions), are seen to be still markedly higher than corresponding converged DtN-NtD results.

In the second and third series, the truncated basis (8.2) has been used in the variational DtN and NtD methods, respectively, in the way described in Sec. VII. To obtain the best energy estimates, calculations have been carried out iteratively. In the first step, the generalized algebraic eigensystems (7.7) and (7.9) have been solved with $\mathcal{E}$ chosen to co-

TABLE I. Variational estimates of energies of four bound states with $m_l=0$ symmetry for a particle in the potential (8.1) with $r_0=1$, $\rho=2$ (the units in which $m=\hbar=\omega=1$ are used). The results have been obtained by employing the basis functions (8.2) with $0\leqslant l\leqslant l_{\max}$ and $0\leqslant n\leqslant n_{\max}$ in the Rayleigh principle (2.4) and (2.5). For comparison, exact (chosen as the best converged DtN-NtD) energies, which should be attained in the limit $(l_{\max},n_{\max})\to(\infty,\infty)$, are provided in the last row.

$(l_{\max},n_{\max})$	$E^{(\mathrm{R})}_{1,m_l=0}$	$E^{(\mathrm{R})}_{2,m_l=0}$	$E^{(\mathrm{R})}_{3,m_l=0}$	$E^{(\mathrm{R})}_{4,m_l=0}$
(3,3)	−2.448 328 759	−1.337 158 078	−0.181 740 074	−0.108 515 116
(10,10)	−2.449 192 886	−1.339 700 783	−0.188 543 764	−0.143 283 542
(25,25)	−2.449 409 244	−1.340 437 430	−0.189 572 108	−0.146 245 353
(40,40)	−2.449 450 730	−1.340 551 206	−0.189 816 256	−0.146 496 060
DtN-NtD	−2.449 494 339	−1.340 681 212	−0.190 019 496	−0.146 705 753

incide with the (3,3) Rayleigh estimate $E^{(\mathrm{R})}_{1,m_l=0}=-2.448\,328\,759$ (cf. Table I) of the lowest energy. The resulting eigenvalues $\widetilde{E}^{(\mathrm{D\ or\ N})}_{i,m_l=0}(\mathcal{E})$, $i=1,\ldots,4$, have replaced $\mathcal{E}$ in the repeated calculations (performed henceforth separately for each i) and the procedure has been iterated (with the fixed basis dimension) until convergence in the eigenenergies has been achieved. Convergence rate of this iterative procedure for the DtN and NtD methods is illustrated, in the case of the lowest eigenenergy, by data provided in Tables II and III, respectively. Finally, converged DtN and NtD energy estimates for four existing bound states are presented in Table IV. It is seen that, at least for the problem at hand, the DtN and NtD results are of comparable quality. Moreover, comparison with entries of Table I shows that when the basis dimension increases, the DtN and NtD estimates converge to exact eigenenergies much faster than their counterparts obtained in the calculations exploiting the Rayleigh principle (2.4) and (2.5).

IX. CONCLUSIONS

There are at least three directions in which the current work may be continued. First, it would be desirable to extend present results to many-body systems. Second, it might be advantageous to reformulate in the DtN-NtD language also the embedding method for *continuum* Schrödinger states [1]. Third, our preliminary investigations show that, after necessary modifications, the DtN-NtD formalism may be the convenient framework for extending the embedding method to systems described by the Dirac equation; this thread also seems to be worth to pursue. We work on these subjects and progress will be reported in future publications.

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APPENDIX: NONVARIATIONAL APPROACH TO THE DtN AND NtD EMBEDDING METHODS

In Secs. IV and V we have derived the generalized eigensystems (4.22),(4.23) and (5.11),(5.12), respectively, by employing methods of variational calculus. A purpose of this appendix is to show that one may arrive at these two eigensystems following still another, though less elegant, procedure.

Consider at first the DtN case. The starting point is an observation that, with the aid of the DtN operator $\hat{\mathcal{B}}(E)$, one may transfer the boundary condition (2.2) from infinity to the surface $\mathcal{S}$, thus replacing the original eigensystem (2.1) and (2.2) in $\mathbb{R}^3$ by the following equivalent one in the domain $\mathcal{V}_l$:

$$\hat{\mathcal{H}}\Psi(\mathbf{r})=E\Psi(\mathbf{r})\quad(\mathbf{r}\in\mathcal{V}_l),\tag{A1}$$

$$\nabla_{\perp}\Psi(\boldsymbol{\rho})=\hat{\mathcal{B}}(E)\Psi(\boldsymbol{\rho})\quad(\boldsymbol{\rho}\in\mathcal{S}).\tag{A2}$$

The price one has to pay for shrinking the domain is that in the new eigenproblem (A1) and (A2) the energy eigenvalue E enters not only the differential equation (A1) [which is

TABLE II. Convergence rate of the DtN variational estimates of the lowest $m_l=0$ eigenenergy for a particle in the potential (8.1) with $r_0=1$, $\rho=2$ (the units in which $m=\hbar=\omega=1$ are used). The basis functions (8.2) with $0\leqslant l\leqslant l_{\max}$ and $0\leqslant n\leqslant n_{\max}$ have been employed. The input for the iteration procedure has been $\mathcal{E}=-2.448\,328\,759$, which is the (3,3) Rayleigh estimate $E^{(\mathrm{R})}_{1,m_l=0}$ of the lowest energy (cf. Table I).

Iteration	$E^{(\mathrm{D})}_{1,m_l=0}$					
	$(l_{\max},n_{\max})$					
	(3,3)	(4,4)	(5,5)	(6,6)	(7,7)	(10,10)
1	−2.449 482 118	−2.449 493 904	−2.449 494 324	−2.449 494 335	−2.449 494 335	−2.449 494 335
2	−2.449 482 122	−2.449 493 907	−2.449 494 328	−2.449 494 338	−2.449 494 339	−2.449 494 339
3	−2.449 482 122	−2.449 493 907	−2.449 494 328	−2.449 494 338	−2.449 494 339	−2.449 494 339

TABLE III. Convergence rate of the NtD variational estimates of the lowest $m_l=0$ eigenenergy for a particle in the potential (8.1) with $r_0=1$, $\rho=2$ (the units in which $m=\hbar=\omega=1$ are used). The basis functions (8.2) with $0\leqslant l\leqslant l_{\max}$ and $0\leqslant n\leqslant n_{\max}$ have been employed. The input for the iteration procedure has been $\mathcal{E}=-2.448\,328\,759$, which is the (3,3) Rayleigh estimate $E^{(\mathrm{R})}_{1,m_l=0}$ of the lowest energy (cf. Table I).

Iteration	$E^{(\mathrm{N})}_{1,m_l=0}$					
	$(l_{\max},n_{\max})$					
	(3,3)	(4,4)	(5,5)	(6,6)	(7,7)	(10,10)
1	−2.449 459 158	−2.449 493 456	−2.449 494 311	−2.449 494 329	−2.449 494 329	−2.449 494 329
2	−2.449 459 167	−2.449 493 465	−2.449 494 321	−2.449 494 338	−2.449 494 339	−2.449 494 339
3	−2.449 459 167	−2.449 493 465	−2.449 494 321	−2.449 494 338	−2.449 494 339	−2.449 494 339

seen to be identical with its counterpart (2.1) in $\mathbb{R}^3$], but also, in fact — in a very complicated way, the boundary condition (A2). Assume now that, guided by some premises or simply by intuition, we choose some real energy $\mathcal{E}$ as a zeroth-order estimate of E. Then, by Taylor's theorem, for $\hat{\mathcal{B}}(E)$ we have

$$\hat{\mathcal{B}}(E)=\sum_{n=0}^{\infty}\frac{[E-\mathcal{E}]^n}{n!}\frac{\partial^{\,n}\hat{\mathcal{B}}(\mathcal{E})}{\partial\mathcal{E}^n}, \tag{A3}$$

provided the series on the right-hand side converges. If $\mathcal{E}$ is in the vicinity of the eigenvalue E, we may approximate $\hat{\mathcal{B}}(E)$ by the first two terms in the expansion (A3):

$$\hat{\mathcal{B}}(E)\simeq\hat{\mathcal{B}}(\mathcal{E})+[E-\mathcal{E}]\frac{\partial\hat{\mathcal{B}}(\mathcal{E})}{\partial\mathcal{E}}, \tag{A4}$$

i.e., by the expression which is linear in E. This suggests that one may consider to approximate eigensolutions to the system (A1) and (A2) by solutions to the eigensystem

$$\hat{\mathcal{H}}\Psi^{(\mathrm{D})}(\mathbf{r})=E^{(\mathrm{D})}\Psi^{(\mathrm{D})}(\mathbf{r})\quad(\mathbf{r}\in\mathcal{V}_I), \tag{A5}$$

$$\left[\nabla_\perp-\hat{\mathcal{B}}(\mathcal{E})+\mathcal{E}\frac{\partial\hat{\mathcal{B}}(\mathcal{E})}{\partial\mathcal{E}}\right]\Psi^{(\mathrm{D})}(\boldsymbol{\rho})$$

$$=E^{(\mathrm{D})}\frac{\partial\hat{\mathcal{B}}(\mathcal{E})}{\partial\mathcal{E}}\Psi^{(\mathrm{D})}(\boldsymbol{\rho})\quad(\boldsymbol{\rho}\in\mathcal{S}), \tag{A6}$$

identical with that in Eqs. (4.22) and (4.23).

We turn to the NtD case. The boundary condition (A2) may be equivalently rewritten in the form

$$\Psi(\boldsymbol{\rho})=\hat{\mathcal{R}}(E)\nabla_\perp\Psi(\boldsymbol{\rho})\quad(\boldsymbol{\rho}\in\mathcal{S}). \tag{A7}$$

Truncating the Taylor's expansion

$$\hat{\mathcal{R}}(E)=\sum_{n=0}^{\infty}\frac{[E-\mathcal{E}]^n}{n!}\frac{\partial^{\,n}\hat{\mathcal{R}}(\mathcal{E})}{\partial\mathcal{E}^n} \tag{A8}$$

after the term linear in E leads to the approximation

TABLE IV. Converged DtN and NtD variational estimates of energies of four bound states with $m_l=0$ symmetry for a particle in the potential (8.1) with $r_0=1$, $\rho=2$ (the units in which $m=\hbar=\omega=1$ are used). The basis functions (8.2) with $0\leqslant l\leqslant l_{max}$ and $0\leqslant n\leqslant n_{\max}$ have been employed. The input for the iteration procedure has been $\mathcal{E}=-2.448\,328\,759$, which is the (3,3) Rayleigh estimate $E^{(\mathrm{R})}_{1,m_l=0}$ of the lowest energy (cf. Table I).

$(l_{\max},n_{\max})$	$E^{(\mathrm{D})}_{1,m_l=0}$ $E^{(\mathrm{N})}_{1,m_l=0}$	$E^{(\mathrm{D})}_{2,m_l=0}$ $E^{(\mathrm{N})}_{2,m_l=0}$	$E^{(\mathrm{D})}_{3,m_l=0}$ $E^{(\mathrm{N})}_{3,m_l=0}$	$E^{(\mathrm{D})}_{4,m_l=0}$ $E^{(\mathrm{N})}_{4,m_l=0}$
(3,3)	−2.449 482 122	−1.340 675 393	−0.190 018 190	−0.146 679 158
	−2.449 459 167	−1.340 667 882	−0.190 016 882	−0.146 638 303
(4,4)	−2.449 493 907	−1.340 681 069	−0.190 019 474	−0.146 705 173
	−2.449 493 465	−1.340 680 953	−0.190 019 458	−0.146 704 638
(5,5)	−2.449 494 328	−1.340 681 209	−0.190 019 496	−0.146 705 743
	−2.449 494 321	−1.340 681 208	−0.190 019 496	−0.146 705 737
(6,6)	−2.449 494 338	−1.340 681 212	−0.190 019 496	−0.146 705 753
	−2.449 494 338	−1.340 681 212	−0.190 019 496	−0.146 705 753
(7,7)	−2.449 494 339	−1.340 681 212	−0.190 019 496	−0.146 705 753
	−2.449 494 339	−1.340 681 212	−0.190 019 496	−0.146 705 753
(10,10)	−2.449 494 339	−1.340 681 212	−0.190 019 496	−0.146 705 753
	−2.449 494 339	−1.340 681 212	−0.190 019 496	−0.146 705 753

$$\hat{\mathcal{R}}(E) \simeq \hat{\mathcal{R}}(\mathcal{E}) + [E - \mathcal{E}]\frac{\partial \hat{\mathcal{R}}(\mathcal{E})}{\partial \mathcal{E}}. \tag{A9}$$

Replacing the operator $\hat{\mathcal{R}}(E)$ in the boundary condition (A7) by the expression on the right-hand side of Eq. (A9) and leaving the differential equation (A1) unchanged results in the eigensystem

$$\hat{\mathcal{H}}\Psi^{(\mathrm{N})}(\mathbf{r}) = E^{(\mathrm{N})}\Psi^{(\mathrm{N})}(\mathbf{r}) \quad (\mathbf{r} \in \mathcal{V}_I), \tag{A10}$$

$$\left[\hat{\mathcal{I}}_{\mathcal{S}} - \hat{\mathcal{R}}(\mathcal{E})\nabla_{\perp} + \mathcal{E}\frac{\partial \hat{\mathcal{R}}(\mathcal{E})}{\partial \mathcal{E}}\nabla_{\perp}\right]\Psi^{(\mathrm{N})}(\boldsymbol{\rho}) = E^{(\mathrm{N})}\frac{\partial \hat{\mathcal{R}}(\mathcal{E})}{\partial \mathcal{E}}\nabla_{\perp}\Psi^{(\mathrm{N})}(\boldsymbol{\rho}) \quad (\boldsymbol{\rho} \in \mathcal{S}), \tag{A11}$$

identical with that in Eqs. (5.11) and (5.12).

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