Unified construction of variational *R*-matrix methods for the Dirac equation

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A systematic construction, based on a unified approach described by Gerjuoy, Rau, and Spruch [Rev. Mod. Phys. **55**, 725 (1983)], of unrestricted variational principles related to the *R*-matrix theory for the Dirac equation is presented. Variational principles for eigenvalues and matrix elements of the operators $\hat{\mathcal{R}}^{(\pm)}(E)$ and $\hat{\mathcal{B}}^{(\pm)}(E)$, relating values of upper and lower components of spinor wave functions on a surface $\mathcal{S}$ of a closed volume $\mathcal{V}$ inside which the functions satisfy the Dirac equation at energy E, are derived. A variational principle for eigenvalues of the operators $\hat{\mathcal{R}}^{(-)}(E)$ and $\hat{\mathcal{B}}^{(+)}(E)$ has been already found before by Hamacher and Hinze [Phys. Rev. A **44**, 1705 (1991)] but other variational principles are constructed in this paper.
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I. INTRODUCTION

Among a variety of theoretical methods used for a description of such atomic processes as electron-atom scattering, atomic photoionization, and spectra of Rydberg atoms, finite volume treatments, usually referred to as *R*-matrix methods, play a very prominent role [1–3]. It is a common feature of such methods that the configuration space of the total system, target plus electron, is divided into separate domains, at least one of which has a finite volume. The dynamics of the system is considered independently in each domain. The total wave function Ψ, describing behavior of the system in the whole configuration space, is obtained by matching solutions of the wave equation at interfaces between adjacent domains. It may be shown that complete information required for the matching procedure at a surface $\mathcal{S}$ enclosing a particular domain $\mathcal{V}$ is embodied in a square matrix R (or, equivalently, in its inverse $\mathsf{B}=\mathsf{R}^{-1}$, frequently denoted also as Y). To explain the meaning of the matrix R, assume that a complete discrete set of orthonormal functions spanning the surface $\mathcal{S}$ is known. Then an arbitrary sufficiently regular function, including the function Ψ, may be expanded in this set on the surface $\mathcal{S}$. If the particle is described by a Schrödinger equation, the matrix R transforms a vector of expansion coefficients of the normal gradient $\nabla_n\Psi$ into a vector of expansion coefficients of the function Ψ. Obviously, the matrices R and B are not unique since the expansion basis at the surface $\mathcal{S}$ may be chosen in an infinite number of ways. In this connection, Nesbet [4–6] and Szmytkowski [7] pointed out that it is more natural and fundamental to build the nonrelativistic theory on *integral operators* $\hat{\mathcal{R}}(E)$ and $\hat{\mathcal{B}}(E)$, of which $\mathsf{R}(E)$ and $\mathsf{B}(E)$ are *matrix representations*. The operator $\hat{\mathcal{R}}(E)$ is defined so that when it acts at $\mathcal{S}$ on normal derivatives of functions that in $\mathcal{V}$ are solutions of the Schrödinger equation at energy E, values of these functions on $\mathcal{S}$ are produced. The operator $\hat{\mathcal{B}}(E)$ is the inverse of $\hat{\mathcal{R}}(E)$. The primary goal of the theory is to find the operators $\hat{\mathcal{R}}(E)$ and $\hat{\mathcal{B}}(E)$ by constructing their kernels or, equivalently, to find the matrices $\mathsf{R}(E)$ and $\mathsf{B}(E)$ by determining their matrix elements. Among several approaches enabling one to achieve this goal [1–3,8–11], there are methods employing the calculus of variations. A variety of variational principles related to the nonrelativistic *R*-matrix theory has been invented during the last fifty years [12–42] and some of them have been successfully applied in atomic physics calculations [3,34]. Recently, Szmytkowski [7], following a remark made by Raşeev [30], has shown that, on combining a general method for construction of variational principles described by Gerjuoy, Rau, and Spruch [43] (cf. also Refs. [44, 45]) with the operator formulation of the *R*-matrix theory [4–7], all the finite-volume variational principles that have already been known, and also some new, may be derived in a systematic way [46].

Recent years have seen a rapid growth of interest in analysis of relativistic effects in atomic processes [47,48]. In view of the conspicuous success of the nonrelativistic variational *R*-matrix methods in describing atomic phenomena [3,34], it is natural to expect that their relativistic counterparts should be equally helpful when the relativity has to be taken into account. The need for the relativistic versions of variational *R*-matrix methods has been recently articulated by Aymar, Greene, and Luc-Koenig [3]. In response to this request, in the present paper we attempt to generalize the results of Ref. [7] to the case when the wave equation governing dynamics of a system is a Dirac equation. For the sake of brevity and aiming to keep the presentation as simple as possible, we restrict our considerations to the case of potential scattering. In Sec. II, the relativistic *R*-matrix theory is formulated in terms of integral operators $\hat{\mathcal{R}}^{(\pm)}(E)$ and $\hat{\mathcal{B}}^{(\pm)}(E)$, which on the surface $\mathcal{S}$ link upper and lower components of those wave spinors Ψ which in the volume $\mathcal{V}$ enclosed by $\mathcal{S}$ satisfy a Dirac equation at energy E. The operators $\hat{\mathcal{R}}^{(+)}(E)$ and $\hat{\mathcal{B}}^{(+)}(E)$ are, in some sense, the analogs of the operators $\hat{\mathcal{R}}(E)$ and $\hat{\mathcal{B}}(E)$, respectively, encountered in the nonrelativistic theory. The specific feature of the relativistic case is that two other operators $\hat{\mathcal{R}}^{(-)}(E)$ and $\hat{\mathcal{B}}^{(-)}(E)$ appear in the course of development of the theory and these operators must be treated on an equal foot with the operators $\hat{\mathcal{R}}^{(+)}(E)$ and $\hat{\mathcal{B}}^{(+)}(E)$. After analysis of properties of the operators $\hat{\mathcal{R}}^{(\pm)}(E)$ and $\hat{\mathcal{B}}^{(\pm)}(E)$ and their integral kernels, in Sec. III we apply the general powerful approach of Gerjuoy, Rau, and Spruch [43] and derive variational principles for eigenvalues and matrix elements of the operators $\hat{\mathcal{R}}^{(\pm)}(E)$ and $\hat{\mathcal{B}}^{(\pm)}(E)$. In particular, we rederive a variational principle for (common) eigenvalues of $\hat{\mathcal{R}}^{(-)}(E)$ and $\hat{\mathcal{B}}^{(+)}(E)$ found, in an alternative way, several years ago by Hamacher and Hinze [49]. The variational principles derived in Sec. III are unrestricted, which means that no particular constraints need to be imposed on trial wave functions used. In some cases it may be desirable, however, to use trial functions that are subjected to some subsidiary conditions. Therefore, in Sec. IV we present constrained forms of the variational principles found in Sec. III. The principles derived in Secs. III and IV are linear, bilinear, or fractional bilinear in trial functions and therefore are ideally suited for the use with linear trial functions of the Rayleigh-Ritz form. Examples of applications of such functions to variational principles constructed in Sec. III are presented in Sec. V. The paper concludes with a brief discussion of the results presented in Sec. VI.

II. THE OPERATORS $\hat{\mathcal{B}}^{(\pm)}(E)$ AND $\hat{\mathcal{R}}^{(\pm)}(E)$

We shall be concerned with a Dirac particle of a given real energy E moving in a real, local, in general noncentral potential $V(\boldsymbol{r})$. The wave equation governing the dynamics of the particle is

$$[\hat{H}-E]\Psi(E,\boldsymbol{r})=0, \tag{1}$$

where $\hat{H}$ is the Dirac Hamiltonian

$$\hat{H}=-ic\hbar\boldsymbol{\alpha}\cdot\boldsymbol{\nabla}+\beta mc^2+V(\boldsymbol{r}) \tag{2}$$

with the Hermitian 4×4 matrices $\boldsymbol{\alpha}$ and β defined as usual [50].

As in all R-matrix treatments, we restrict our considerations to a finite volume $\mathcal{V}$ enclosed by a surface $\mathcal{S}$. We wish to find a homogeneous boundary condition satisfied on $\mathcal{S}$ by solutions of Eq. (1). In what follows, $\boldsymbol{r}$ is a position vector of a point in the volume $\mathcal{V}$. If the point $\boldsymbol{r}$ lies on the surface $\mathcal{S}$, we denote this using the symbol $\boldsymbol{\rho}$ instead of $\boldsymbol{r}$. To denote volume and surface integrals containing products of two spinor functions, we shall use the following notation:

$$\langle\Phi|\Phi'\rangle\equiv\int_{\mathcal{V}}d^3\boldsymbol{r}\,\Phi^{\dagger}(\boldsymbol{r})\Phi'(\boldsymbol{r}),$$

$$(\Phi|\Phi')\equiv\int_{\mathcal{S}}d^2\boldsymbol{\rho}\,\Phi^{\dagger}(\boldsymbol{\rho})\Phi'(\boldsymbol{\rho}), \tag{3}$$

where the dagger denotes the matrix Hermitian conjugation. Here $d^3\boldsymbol{r}$ is an infinitesimal volume element around the point $\boldsymbol{r}$ and $d^2\boldsymbol{\rho}$ is an infinitesimal *scalar* surface element around the point $\boldsymbol{\rho}$. We define also a surface delta function $\delta^{(2)}(\boldsymbol{\rho}-\boldsymbol{\rho}')$ such that for any reasonable four-component spinor function $\Phi(\boldsymbol{\rho})$ defined on the surface $\mathcal{S}$ one has

$$\int_{\mathcal{S}}d^2\boldsymbol{\rho}'\,\delta^{(2)}(\boldsymbol{\rho}-\boldsymbol{\rho}')\Phi(\boldsymbol{\rho}')=\Phi(\boldsymbol{\rho}),$$

$$\int_{\mathcal{S}}d^2\boldsymbol{\rho}'\,\delta^{(2)}(\boldsymbol{\rho}-\boldsymbol{\rho}')\Phi^{\dagger}(\boldsymbol{\rho}')=\Phi^{\dagger}(\boldsymbol{\rho}). \tag{4}$$

Let $\Psi(E,\boldsymbol{r})$ and $\Psi'(E,\boldsymbol{r})$ be two particular solutions to the Dirac equation (1) corresponding to the same real energy E. Applying the Gauss divergence theorem we obtain

$$\langle\hat{H}\Psi'|\Psi\rangle-\langle\Psi'|\hat{H}\Psi\rangle=(\Psi'|ic\hbar\alpha_n\Psi). \tag{5}$$

Here $\alpha_n(\boldsymbol{\rho})$ is the 4×4 Hermitian matrix defined as

$$\alpha_n(\boldsymbol{\rho})=\boldsymbol{n}(\boldsymbol{\rho})\cdot\boldsymbol{\alpha}, \tag{6}$$

where $\boldsymbol{n}(\boldsymbol{\rho})$ is an outward unit vector normal to the surface $\mathcal{S}$ at the point $\boldsymbol{\rho}$. In virtue of the reality of E the left-hand side of Eq. (5) vanishes yielding

$$(\Psi'|i\alpha_n\Psi)=0 \tag{7}$$

(for reasons that should become clear shortly, we have retained in Eq. (7) the imaginary unit i). To proceed further we define matrices

$$\beta^{(\pm)}=\frac{I\pm\beta}{2},\quad \alpha_n^{(\pm)}(\boldsymbol{\rho})=\beta^{(\pm)}\alpha_n(\boldsymbol{\rho}), \tag{8}$$

where I is the unit 4×4 matrix. Obviously, one has

$$\beta^{(+)}+\beta^{(-)}=I,\quad \alpha_n^{(+)}(\boldsymbol{\rho})+\alpha_n^{(-)}(\boldsymbol{\rho})=\alpha_n(\boldsymbol{\rho}). \tag{9}$$

The matrices $\beta^{(\pm)}$ are Hermitian while

$$\alpha_n^{(\pm)\dagger}(\boldsymbol{\rho})=\alpha_n^{(\mp)}(\boldsymbol{\rho}). \tag{10}$$

For the sake of later applications we notice the following properties of the matrices $\beta^{(\pm)}$ and $\alpha_n^{(\pm)}(\boldsymbol{\rho})$:

$$\beta^{(\pm)}\beta^{(\pm)}=\beta^{(\pm)},\quad \beta^{(\pm)}\beta^{(\mp)}=0,\quad \alpha_n^{(\pm)}(\boldsymbol{\rho})\alpha_n^{(\pm)}(\boldsymbol{\rho})=0,$$

$$\alpha_n^{(\pm)}(\boldsymbol{\rho})\alpha_n^{(\mp)}(\boldsymbol{\rho})=\beta^{(\pm)}, \tag{11}$$

$$\alpha_n^{(\pm)}(\boldsymbol{\rho})\beta^{(\pm)}=0,\quad \beta^{(\pm)}\alpha_n^{(\pm)}(\boldsymbol{\rho})=\alpha_n^{(\pm)}(\boldsymbol{\rho}),$$

$$\beta^{(\pm)}\alpha_n^{(\mp)}(\boldsymbol{\rho})=0,\quad \alpha_n^{(\pm)}(\boldsymbol{\rho})\beta^{(\mp)}=\alpha_n^{(\pm)}(\boldsymbol{\rho}), \tag{12}$$

which may be easily derived from the definitions (8) and the anticommutation relations satisfied by the matrices $\boldsymbol{\alpha}$ and β [50]. With the matrices $\alpha_n^{(\pm)}(\boldsymbol{\rho})$ the relation (7) may be rewritten in two equivalent forms:

$$(i\alpha_n^{(+)}\Psi'|\Psi)=(\Psi'|i\alpha_n^{(+)}\Psi),$$

$$(i\alpha_n^{(-)}\Psi'|\Psi)=(\Psi'|i\alpha_n^{(-)}\Psi), \tag{13}$$

where it may be interpreted that the matrices $i\alpha_n^{(+)}(\boldsymbol{\rho})$ and $i\alpha_n^{(-)}(\boldsymbol{\rho})$, considered as operators acting on solutions of the

Dirac equation (1) at fixed energy E, are Hermitian with respect to the surface scalar product $(|)$.

With the matrices $i\alpha_n^{(\pm)}(\boldsymbol{\rho})$ one may associate linear Hermitian integral operators $\hat{\mathcal{B}}^{(\pm)}(E)$ such that

$$i\alpha_n^{(\pm)}(\boldsymbol{\rho})\Psi(E,\boldsymbol{\rho})=\pm\hat{\mathcal{B}}^{(\pm)}(E)\Psi(E,\boldsymbol{\rho}) \tag{14}$$

for any solution of Eq. (1) at energy E. The operators $\hat{\mathcal{B}}^{(\pm)}(E)$ are represented by their integral kernels $\mathcal{B}^{(\pm)}(E,\boldsymbol{\rho},\boldsymbol{\rho}')$ and Eq. (14) may be equivalently rewritten in the form

$$i\alpha_n^{(\pm)}(\boldsymbol{\rho})\Psi(E,\boldsymbol{\rho})=\pm\int_{\mathcal{S}}d^2\boldsymbol{\rho}'\,\mathcal{B}^{(\pm)}(E,\boldsymbol{\rho},\boldsymbol{\rho}')\Psi(E,\boldsymbol{\rho}') \tag{15}$$

[notice that the kernels $\mathcal{B}^{(\pm)}(E,\boldsymbol{\rho},\boldsymbol{\rho}')$ are the 4×4 matrices]. Since the left-hand side of this equation remains invariant after premultiplication with $\beta^{(\pm)}$, this restricts a class of admissible kernels $\mathcal{B}^{(\pm)}(E,\boldsymbol{\rho},\boldsymbol{\rho}')$ to such that

$$\mathcal{B}^{(\pm)}(E,\boldsymbol{\rho},\boldsymbol{\rho}')=\beta^{(\pm)}\mathcal{B}^{(\pm)}(E,\boldsymbol{\rho},\boldsymbol{\rho}'). \tag{16}$$

Further constraints follow from the fact that, to represent the Hermitian operators $\hat{\mathcal{B}}^{(\pm)}(E)$, the kernels $\mathcal{B}^{(\pm)}(E,\boldsymbol{\rho},\boldsymbol{\rho}')$ must be Hermitian themselves, i.e.,

$$\mathcal{B}^{(\pm)}(E,\boldsymbol{\rho},\boldsymbol{\rho}')=\mathcal{B}^{(\pm)\dagger}(E,\boldsymbol{\rho}',\boldsymbol{\rho}). \tag{17}$$

Equations (16) and (17) imply

$$\mathcal{B}^{(\pm)}(E,\boldsymbol{\rho},\boldsymbol{\rho}')=\beta^{(\pm)}\mathcal{B}^{(\pm)}(E,\boldsymbol{\rho},\boldsymbol{\rho}')\beta^{(\pm)}. \tag{18}$$

It must be emphasized that the operators $i\alpha_n^{(\pm)}(\boldsymbol{\rho})$ and $\pm\hat{\mathcal{B}}^{(\pm)}(E)$ are *not* identical and for an arbitrary four-component spinor function $\Phi(\boldsymbol{r})$ in general one has

$$i\alpha_n^{(\pm)}(\boldsymbol{\rho})\Phi(\boldsymbol{\rho})\neq\pm\hat{\mathcal{B}}^{(\pm)}(E)\Phi(\boldsymbol{\rho}) \tag{19}$$

unless $\Phi(\boldsymbol{r})$ obeys in $\mathcal{V}$ the Dirac equation (1) at energy E.

In applications it will be convenient to use the Hermitian integral operators $\hat{\mathcal{R}}^{(\pm)}(E)$ defined by

$$\beta^{(\pm)}\Psi(E,\boldsymbol{\rho})=\pm\hat{\mathcal{R}}^{(\pm)}(E)i\alpha_n^{(\pm)}(\boldsymbol{\rho})\Psi(E,\boldsymbol{\rho}) \tag{20}$$

for any solution to Eq. (1) at energy E. In terms of the associated 4×4 matrix kernels $\mathcal{R}^{(\pm)}(E,\boldsymbol{\rho},\boldsymbol{\rho}')$ Eq. (20) may be rewritten as

$$\beta^{(\pm)}\Psi(E,\boldsymbol{\rho})=\pm\int_{\mathcal{S}}d^2\boldsymbol{\rho}'\,\mathcal{R}^{(\pm)}(E,\boldsymbol{\rho},\boldsymbol{\rho}')i\alpha_n^{(\pm)}(\boldsymbol{\rho}')\Psi(E,\boldsymbol{\rho}'). \tag{21}$$

The operators $\hat{\mathcal{R}}^{(\pm)}(E)$ and $\hat{\mathcal{B}}^{(\pm)}(E)$ are reciprocal in the sense of

$$\hat{\mathcal{R}}^{(\pm)}(E)\hat{\mathcal{B}}^{(\pm)}(E)=\hat{\mathcal{B}}^{(\pm)}(E)\hat{\mathcal{R}}^{(\pm)}(E)=\beta^{(\pm)}. \tag{22}$$

The corresponding reciprocity relation for the kernels $\mathcal{R}^{(\pm)}(E,\boldsymbol{\rho},\boldsymbol{\rho}')$ and $\mathcal{B}^{(\pm)}(E,\boldsymbol{\rho},\boldsymbol{\rho}')$ is

$$\begin{aligned}\int_{\mathcal{S}}d^2\boldsymbol{\rho}''\mathcal{R}^{(\pm)}(E,\boldsymbol{\rho},\boldsymbol{\rho}'')\mathcal{B}^{(\pm)}(E,\boldsymbol{\rho}'',\boldsymbol{\rho}')\\ =\int_{\mathcal{S}}d^2\boldsymbol{\rho}''\mathcal{B}^{(\pm)}(E,\boldsymbol{\rho},\boldsymbol{\rho}'')\mathcal{R}^{(\pm)}(E,\boldsymbol{\rho}'',\boldsymbol{\rho}')\\ =\delta^{(2)}(\boldsymbol{\rho}-\boldsymbol{\rho}')\beta^{(\pm)}.\end{aligned} \tag{23}$$

The kernels $\mathcal{R}^{(\pm)}(E,\boldsymbol{\rho},\boldsymbol{\rho}')$ are Hermitian,

$$\mathcal{R}^{(\pm)}(E,\boldsymbol{\rho},\boldsymbol{\rho}')=\mathcal{R}^{(\pm)\dagger}(E,\boldsymbol{\rho}',\boldsymbol{\rho}), \tag{24}$$

and possess the property [cf. Eq. (18)]

$$\mathcal{R}^{(\pm)}(E,\boldsymbol{\rho},\boldsymbol{\rho}')=\beta^{(\pm)}\mathcal{R}^{(\pm)}(E,\boldsymbol{\rho},\boldsymbol{\rho}')\beta^{(\pm)}. \tag{25}$$

Consider now those particular solutions $\{\Psi_i(E,\boldsymbol{r})\}$ to the Dirac equation (1) that on the surface $\mathcal{S}$ satisfy the relation

$$i\alpha_n^{(+)}(\boldsymbol{\rho})\Psi_i(E,\boldsymbol{\rho})=b_i(E)\beta^{(+)}\Psi_i(E,\boldsymbol{\rho}). \tag{26}$$

By utilizing Eq. (14) we may rewrite this relation in the form

$$\hat{\mathcal{B}}^{(+)}(E)\Psi_i(E,\boldsymbol{\rho})=b_i(E)\beta^{(+)}\Psi_i(E,\boldsymbol{\rho}). \tag{27}$$

It follows that the surface functions $\{\Psi_i(E,\boldsymbol{\rho})\}$ may be interpreted as eigenfunctions of the operator $\hat{\mathcal{B}}^{(+)}(E)$ with the singular weight $\beta^{(+)}$. The constants $\{b_i(E)\}$ are corresponding eigenvalues. Since the operators $\hat{\mathcal{B}}^{(+)}(E)$ and $\beta^{(+)}$ are Hermitian, the eigenvalues $\{b_i(E)\}$ are real and eigenfunctions associated with different eigenvalues are orthogonal with respect to the weight $\beta^{(+)}$ over the surface $\mathcal{S}$

$$(\Psi_i|\beta^{(+)}\Psi_j)=0,\quad b_i(E)\neq b_j(E). \tag{28}$$

Without loss of generality we shall assume that eigenfunctions associated with degenerate eigenvalues (if there are any) are also mutually orthogonal over the surface $\mathcal{S}$ and that all eigenfunctions are normalized to unity in the sense of

$$(\Psi_i|\beta^{(+)}\Psi_i)=1. \tag{29}$$

Then for two arbitrary eigenfunctions of the operator $\hat{\mathcal{B}}^{(+)}(E)$ one has

$$(\Psi_i|\beta^{(+)}\Psi_j)=\delta_{ij}. \tag{30}$$

The functions $\{\beta^{(+)}\Psi_i(E,\boldsymbol{\rho})\}$ form a complete set on the surface $\mathcal{S}$ in the subspace of *upper* components (this is a consequence of singularity of the weight $\beta^{(+)}$) and the corresponding closure relation is

$$\sum_{\text{all }i}\beta^{(+)}\Psi_i(E,\boldsymbol{\rho})\Psi_i^\dagger(E,\boldsymbol{\rho}')\beta^{(+)}=\delta^{(2)}(\boldsymbol{\rho}-\boldsymbol{\rho}')\beta^{(+)}. \tag{31}$$

We have defined the functions $\{\Psi_i(E,\boldsymbol{r})\}$ as those solutions to the Dirac equation (1) that on the surface $\mathcal{S}$ are eigenfunctions of the operator $\hat{\mathcal{B}}^{(+)}(E)$ with the weight $\beta^{(+)}$ [cf. Eq. (27)]. It appears that the surface functions $\{\Psi_i(E,\boldsymbol{\rho})\}$ are simultaneously eigenfunctions of the operator

$\hat{\mathcal{B}}^{(-)}(E)$ with the weight $\beta^{(-)}$. Indeed, upon premultiplying both sides of Eq. (26) with the matrix $\alpha_n^{(-)}(\boldsymbol{\rho})$ one has

$$i\alpha_n^{(-)}(\boldsymbol{\rho})\Psi_i(E,\boldsymbol{\rho}) = -b_i^{-1}(E)\beta^{(-)}\Psi_i(E,\boldsymbol{\rho}), \qquad (32)$$

which, after utilizing Eq. (14), may be rewritten as

$$\hat{\mathcal{B}}^{(-)}(E)\Psi_i(E,\boldsymbol{\rho}) = b_i^{-1}(E)\beta^{(-)}\Psi_i(E,\boldsymbol{\rho}). \qquad (33)$$

This proves the conjecture and shows also that eigenvalues of the operator $\hat{\mathcal{B}}^{(-)}(E)$ are $\{b_i^{-1}(E)\}$. With the normalization (29) adopted above one finds the orthogonality relation

$$(\Psi_i|\beta^{(-)}\Psi_j) = b_i^2(E)\delta_{ij} \qquad (34)$$

and the corresponding closure relation in the subspace of *lower* components

$$\sum_{\text{all } i} \beta^{(-)}\Psi_i(E,\boldsymbol{\rho})b_i^{-2}(E)\Psi_i^\dagger(E,\boldsymbol{\rho}')\beta^{(-)} = \delta^{(2)}(\boldsymbol{\rho}-\boldsymbol{\rho}')\beta^{(-)}. \qquad (35)$$

For the sake of completeness of our discussion, we present eigenvalue equations for the operators $\hat{\mathcal{R}}^{(\pm)}(E)$:

$$\hat{\mathcal{R}}^{(+)}(E)\Psi_i(E,\boldsymbol{\rho}) = b_i^{-1}(E)\beta^{(+)}\Psi_i(E,\boldsymbol{\rho}), \qquad (36)$$

$$\hat{\mathcal{R}}^{(-)}(E)\Psi_i(E,\boldsymbol{\rho}) = b_i(E)\beta^{(-)}\Psi_i(E,\boldsymbol{\rho}). \qquad (37)$$

It is to be noticed that the operators $\hat{\mathcal{B}}^{(+)}(E)$ and $\hat{\mathcal{R}}^{(-)}(E)$ have a common set of eigenvalues as do the operators $\hat{\mathcal{B}}^{(-)}(E)$ and $\hat{\mathcal{R}}^{(+)}(E)$.

Given the eigenfunctions $\{\Psi_i(E,\boldsymbol{\rho})\}$ and the eigenvalues $\{b_i(E)\}$, one may reconstruct the kernels $\mathcal{B}^{(\pm)}(E,\boldsymbol{\rho},\boldsymbol{\rho}')$ and $\mathcal{R}^{(\pm)}(E,\boldsymbol{\rho},\boldsymbol{\rho}')$. By combining Eqs. (15), (26), and (32) one obtains integral eigenvalue equations for the surface functions $\{\Psi_i(E,\boldsymbol{\rho})\}$:

$$\int_{\mathcal{S}} d^2\boldsymbol{\rho}'\,\mathcal{B}^{(+)}(E,\boldsymbol{\rho},\boldsymbol{\rho}')\Psi_i(E,\boldsymbol{\rho}') = b_i(E)\beta^{(+)}\Psi_i(E,\boldsymbol{\rho}), \qquad (38)$$

$$\int_{\mathcal{S}} d^2\boldsymbol{\rho}'\,\mathcal{B}^{(-)}(E,\boldsymbol{\rho},\boldsymbol{\rho}')\Psi_i(E,\boldsymbol{\rho}') = b_i^{-1}(E)\beta^{(-)}\Psi_i(E,\boldsymbol{\rho}). \qquad (39)$$

By virtue of the relations (30), (31), (34), and (35) these eigenvalue equations imply spectral representations of the kernels $\mathcal{B}^{(\pm)}(E,\boldsymbol{\rho},\boldsymbol{\rho}')$:

$$\mathcal{B}^{(+)}(E,\boldsymbol{\rho},\boldsymbol{\rho}') = \sum_{\text{all } i} \beta^{(+)}\Psi_i(E,\boldsymbol{\rho})b_i(E)\Psi_i^\dagger(E,\boldsymbol{\rho}')\beta^{(+)}, \qquad (40)$$

$$\mathcal{B}^{(-)}(E,\boldsymbol{\rho},\boldsymbol{\rho}') = \sum_{\text{all } i} \beta^{(-)}\Psi_i(E,\boldsymbol{\rho})b_i^{-3}(E)\Psi_i^\dagger(E,\boldsymbol{\rho}')\beta^{(-)}. \qquad (41)$$

Similarly, the integral eigenvalue equations

$$\int_{\mathcal{S}} d^2\boldsymbol{\rho}'\,\mathcal{R}^{(+)}(E,\boldsymbol{\rho},\boldsymbol{\rho}')\Psi_i(E,\boldsymbol{\rho}') = b_i^{-1}(E)\beta^{(+)}\Psi_i(E,\boldsymbol{\rho}), \qquad (42)$$

$$\int_{\mathcal{S}} d^2\boldsymbol{\rho}'\,\mathcal{R}^{(-)}(E,\boldsymbol{\rho},\boldsymbol{\rho}')\Psi_i(E,\boldsymbol{\rho}') = b_i(E)\beta^{(-)}\Psi_i(E,\boldsymbol{\rho}), \qquad (43)$$

stemming from Eqs. (36) and (37), imply the spectral representations of the kernels $\mathcal{R}^{(\pm)}(E,\boldsymbol{\rho},\boldsymbol{\rho}')$:

$$\mathcal{R}^{(+)}(E,\boldsymbol{\rho},\boldsymbol{\rho}') = \sum_{\text{all } i} \beta^{(+)}\Psi_i(E,\boldsymbol{\rho})b_i^{-1}(E)\Psi_i^\dagger(E,\boldsymbol{\rho}')\beta^{(+)}, \qquad (44)$$

$$\mathcal{R}^{(-)}(E,\boldsymbol{\rho},\boldsymbol{\rho}') = \sum_{\text{all } i} \beta^{(-)}\Psi_i(E,\boldsymbol{\rho})b_i^{-1}(E)\Psi_i^\dagger(E,\boldsymbol{\rho}')\beta^{(-)}. \qquad (45)$$

Notice the asymmetry between the representations (40)–(41) and (44)–(45).

We have seen that the operators $\hat{\mathcal{B}}^{(+)}(E)$ and $\hat{\mathcal{R}}^{(-)}(E)$ have a common set of eigenvalues $\{b_i(E)\}$. Similarly, a common set of eigenvalues of the operators $\hat{\mathcal{B}}^{(-)}(E)$ and $\hat{\mathcal{R}}^{(+)}(E)$ is $\{b_i^{-1}(E)\}$. Moreover, the four operators have a common set of eigenfunctions $\{\Psi_i(E,\boldsymbol{\rho})\}$. This suggests that the kernels $\mathcal{B}^{(+)}(E,\boldsymbol{\rho},\boldsymbol{\rho}')$ and $\mathcal{R}^{(-)}(E,\boldsymbol{\rho},\boldsymbol{\rho}')$ should be related as should be the kernels $\mathcal{B}^{(-)}(E,\boldsymbol{\rho},\boldsymbol{\rho}')$ and $\mathcal{R}^{(+)}(E,\boldsymbol{\rho},\boldsymbol{\rho}')$. To obtain the desired relations we operate on Eqs. (40) and (41) from the left with $\alpha_n^{(-)}(\boldsymbol{\rho})$ and $\alpha_n^{(+)}(\boldsymbol{\rho})$, respectively, and then on the resulting equations from the right with $\alpha_n^{(+)}(\boldsymbol{\rho}')$ and $\alpha_n^{(-)}(\boldsymbol{\rho}')$, respectively. Upon utilizing the properties of the matrices $\alpha_n^{(\pm)}(\boldsymbol{\rho})$ and $\beta^{(\pm)}$, making use of the eigenvalue equations (26) and (32) and comparing the results with the spectral representations (44) and (45) one finds

$$\mathcal{R}^{(\pm)}(E,\boldsymbol{\rho},\boldsymbol{\rho}') = \alpha_n^{(\pm)}(\boldsymbol{\rho})\mathcal{B}^{(\mp)}(E,\boldsymbol{\rho},\boldsymbol{\rho}')\alpha_n^{(\mp)}(\boldsymbol{\rho}'). \qquad (46)$$

III. CONSTRUCTION OF VARIATIONAL PRINCIPLES

A. Variational principles for eigenvalues of $\hat{\mathcal{B}}^{(\pm)}(E)$ and $\hat{\mathcal{R}}^{(\pm)}(E)$

In this subsection we shall derive variational principles for eigenvalues of the operators $\hat{\mathcal{B}}^{(\pm)}(E)$ and $\hat{\mathcal{R}}^{(\pm)}(E)$. [We recall that the operators $\hat{\mathcal{B}}^{(+)}(E)$ and $\hat{\mathcal{R}}^{(-)}(E)$ and the operators $\hat{\mathcal{B}}^{(-)}(E)$ and $\hat{\mathcal{R}}^{(+)}(E)$ have common sets of eigenvalues, respectively. Also, eigenvalues of the operators $\hat{\mathcal{B}}^{(-)}(E)$ and $\hat{\mathcal{R}}^{(+)}(E)$ are reciprocals of eigenvalues of the operators $\hat{\mathcal{B}}^{(+)}(E)$ and $\hat{\mathcal{R}}^{(-)}(E)$.] For the sake of brevity, throughout this subsection we shall omit all indices labeling eigenvalues and corresponding eigenfunctions.

Following the ideas of Gerjuoy, Rau, and Spruch [43] (cf. also Refs. [44,45]), we treat the defining Eqs. (1), (26), and (32) as constraints and consider the functionals

$$F^{(\pm)}[\overline{b^{\pm1}},\overline{\lambda^{(\pm)}},\overline{\Lambda^{(\pm)}},\overline{\Psi}]$$
$$=\overline{b^{\pm1}}+(\overline{\lambda^{(\pm)}}|i\alpha_n^{(\pm)}\overline{\Psi}\mp\overline{b^{\pm1}}\beta^{(\pm)}\overline{\Psi})$$
$$+\langle\overline{\Lambda^{(\pm)}}|[\hat{H}-E]\overline{\Psi}\rangle. \tag{47}$$

Here $\overline{b^{+1}}\equiv\overline{b}$ and $\overline{b^{-1}}$ are numbers (possibly complex), $\overline{\lambda^{(\pm)}}(\boldsymbol{\rho})$ are regular functions defined on the surface $\mathcal{S}$, while $\overline{\Lambda^{(\pm)}}(\boldsymbol{r})$ and $\overline{\Psi}(\boldsymbol{r})$ are regular functions defined in the volume $\mathcal{V}$. The functions $\overline{\lambda^{(\pm)}}(\boldsymbol{\rho})$ and $\overline{\Lambda^{(\pm)}}(\boldsymbol{r})$ are the Lagrange functions for the problem discussed and are responsible for incorporation of the constraints (26) and (1) (if the upper superscripts are chosen) or the constraints (32) and (1) (if the lower superscripts are chosen), respectively.

The functionals (47) possess an important property. If the number $\overline{b}$ equals some eigenvalue, say $b(E)$, of the operators $\hat{\mathcal{B}}^{(+)}(E)$ and $\hat{\mathcal{R}}^{(-)}(E)$ and if simultaneously $\overline{\Psi}(\boldsymbol{r})$ coincides with a corresponding eigenfunction $\Psi(E,\boldsymbol{r})$, the value of the functional $F^{(+)}$ is $b(E)$ irrespective of particular forms of the Lagrange functions $\overline{\lambda^{(+)}}(\boldsymbol{\rho})$ and $\overline{\Lambda^{(+)}}(\boldsymbol{r})$. Similarly, if $\overline{b^{-1}}=b^{-1}(E)$ and $\overline{\Psi}(\boldsymbol{r})=\Psi(E,\boldsymbol{r})$, then the value of the functional $F^{(-)}$ is $b^{-1}(E)$ regardless of forms of the functions $\overline{\lambda^{(-)}}(\boldsymbol{\rho})$ and $\overline{\Lambda^{(-)}}(\boldsymbol{r})$. According to Gerjuoy, Rau, and Spruch [43], this property may be exploited and it is possible to find such optimal forms of the Lagrange functions, we shall denote them by $\lambda^{(\pm)}(\boldsymbol{\rho})$ and $\Lambda^{(\pm)}(\boldsymbol{r})$, that the functionals (47) will be stationary subject to small and otherwise arbitrary variations of $\overline{b^{\pm1}}$, $\overline{\lambda^{(\pm)}}(\boldsymbol{\rho})$, $\overline{\Lambda^{(\pm)}}(\boldsymbol{r})$, and $\overline{\Psi}(\boldsymbol{r})$ around $b^{\pm1}(E)$, $\lambda^{(\pm)}(\boldsymbol{\rho})$, $\Lambda^{(\pm)}(\boldsymbol{r})$, and $\Psi(E,\boldsymbol{r})$, respectively. To find the functions $\lambda^{(\pm)}(\boldsymbol{\rho})$ and $\Lambda^{(\pm)}(\boldsymbol{r})$, we vary Eq. (47) obtaining

$$\delta F^{(\pm)}[b^{\pm1},\lambda^{(\pm)},\Lambda^{(\pm)},\Psi]$$
$$=\delta b^{\pm1}+(\delta\lambda^{(\pm)}|i\alpha_n^{(\pm)}\Psi\mp b^{\pm1}\beta^{(\pm)}\Psi)$$
$$\mp\delta b^{\pm1}(\lambda^{(\pm)}|\beta^{(\pm)}\Psi)+(\lambda^{(\pm)}|i\alpha_n^{(\pm)}\delta\Psi$$
$$\mp b^{\pm1}\beta^{(\pm)}\delta\Psi)+\langle\delta\Lambda^{(\pm)}|[\hat{H}-E]\Psi\rangle$$
$$+\langle\Lambda^{(\pm)}|[\hat{H}-E]\delta\Psi\rangle \tag{48}$$

[here $\delta b^{\pm1}$ means $\delta(b^{\pm1})$ and *not* $(\delta b)^{\pm1}$]. Because of Eqs. (1), (26), and (32), the terms containing the variations $\delta\lambda^{(\pm)}(\boldsymbol{\rho})$ and $\delta\Lambda^{(\pm)}(\boldsymbol{r})$ vanish and Eq. (48) takes the form

$$\delta F^{(\pm)}[b^{\pm1},\lambda^{(\pm)},\Lambda^{(\pm)},\Psi]$$
$$=\delta b^{\pm1}[1\mp(\lambda^{(\pm)}|\beta^{(\pm)}\Psi)]+(\lambda^{(\pm)}|i\alpha_n^{(\pm)}\delta\Psi$$
$$\mp b^{\pm1}\beta^{(\pm)}\delta\Psi)+\langle\Lambda^{(\pm)}|[\hat{H}-E]\delta\Psi\rangle. \tag{49}$$

The right-hand side of Eq. (49) may be conveniently transformed by utilizing the Gauss divergence theorem, which, applied to the volume integral in Eq. (49), states that

$$\langle\Lambda^{(\pm)}|[\hat{H}-E]\delta\Psi\rangle=\langle[\hat{H}-E]\Lambda^{(\pm)}|\delta\Psi\rangle$$
$$-(\Lambda^{(\pm)}|ic\hbar\alpha_n\delta\Psi). \tag{50}$$

This gives

$$\delta F^{(\pm)}[b^{\pm1},\lambda^{(\pm)},\Lambda^{(\pm)},\Psi]$$
$$=\delta b^{\pm1}[1\mp(\lambda^{(\pm)}|\beta^{(\pm)}\Psi)]+(ic\hbar\alpha_n\Lambda^{(\pm)}-i\alpha_n^{(\mp)}\lambda^{(\pm)}$$
$$\mp b^{\pm1}\beta^{(\pm)}\lambda^{(\pm)}|\delta\Psi)+\langle[\hat{H}-E]\Lambda^{(\pm)}|\delta\Psi\rangle. \tag{51}$$

We see that to make the functionals (47) stationary, which is equivalent to

$$\delta F^{(\pm)}[b^{\pm1},\lambda^{(\pm)},\Lambda^{(\pm)},\Psi]=0, \tag{52}$$

it is necessary to impose the conditions

$$1\mp(\lambda^{(\pm)}|\beta^{(\pm)}\Psi)=0, \tag{53}$$

$$[\hat{H}-E]\Lambda^{(\pm)}(\boldsymbol{r})=0 \quad \text{in } \mathcal{V} \tag{54}$$

and

$$ic\hbar\alpha_n(\boldsymbol{\rho})\Lambda^{(\pm)}(\boldsymbol{\rho})-i\alpha_n^{(\mp)}(\boldsymbol{\rho})\lambda^{(\pm)}(\boldsymbol{\rho})\mp b^{\pm1}(E)\beta^{(\pm)}\lambda^{(\pm)}(\boldsymbol{\rho})$$
$$=0 \quad \text{on } \mathcal{S}. \tag{55}$$

We may conveniently split Eq. (55) premultiplying it by suitably chosen matrices. Operating from the left with $\beta^{(\pm)}$ we obtain

$$ic\hbar\alpha_n^{(\pm)}(\boldsymbol{\rho})\Lambda^{(\pm)}(\boldsymbol{\rho})\mp b^{\pm1}(E)\beta^{(\pm)}\lambda^{(\pm)}(\boldsymbol{\rho})=0 \tag{56}$$

while operating with $\alpha_n^{(\pm)}(\boldsymbol{\rho})$ we get

$$ic\hbar\beta^{(\pm)}\Lambda^{(\pm)}(\boldsymbol{\rho})-i\beta^{(\pm)}\lambda^{(\pm)}(\boldsymbol{\rho})=0. \tag{57}$$

Hence the boundary conditions satisfied by the functions $\Lambda^{(\pm)}(\boldsymbol{r})$ on the surface $\mathcal{S}$ follow

$$i\alpha_n^{(\pm)}(\boldsymbol{\rho})\Lambda^{(\pm)}(\boldsymbol{\rho})\mp b^{\pm1}(E)\beta^{(\pm)}\Lambda^{(\pm)}(\boldsymbol{\rho})=0. \tag{58}$$

Comparison of this result with Eqs. (26) and (32) shows that the Lagrange functions $\Lambda^{(\pm)}(\boldsymbol{r})$ satisfy on the surface $\mathcal{S}$ the same homogeneous boundary condition as the eigenfunction $\Psi(E,\boldsymbol{r})$. Moreover, in virtue of Eqs. (1) and (54) the functions $\Psi(E,\boldsymbol{r})$ and $\Lambda^{(\pm)}(\boldsymbol{r})$ are solutions of the same differential equations. This implies that the functions $\Lambda^{(\pm)}(\boldsymbol{r})$ may be chosen [43] as

$$\Lambda^{(\pm)}(\boldsymbol{r})=\gamma^{(\pm)}\Psi(E,\boldsymbol{r}), \tag{59}$$

where the proportionality factors $\gamma^{(\pm)}$ are to be determined. This is done with the aid of Eq. (57) and the condition (53). One obtains

$$\gamma^{(\pm)}=\pm\frac{1}{c\hbar}\frac{1}{(\Psi|\beta^{(\pm)}\Psi)} \tag{60}$$

and consequently

$$\Lambda^{(\pm)}(\boldsymbol{r})=\pm\frac{1}{c\hbar}\frac{1}{(\Psi|\beta^{(\pm)}\Psi)}\Psi(E,\boldsymbol{r}). \tag{61}$$

Furthermore, Eqs. (57) and (61) give

$$\beta^{(\pm)}\lambda^{(\pm)}(\boldsymbol{\rho})=\pm\frac{1}{(\Psi|\beta^{(\pm)}\Psi)}\beta^{(\pm)}\Psi(E,\boldsymbol{\rho}). \tag{62}$$

It may seem distressing that the construction presented above does not provide the lower component of the spinor $\lambda^{(+)}(\boldsymbol{\rho})$ and the upper component of the spinor $\lambda^{(-)}(\boldsymbol{\rho})$ but we shall see in a moment that this does not cause any problems.

The relations (61) and (62) between the functions $\Lambda^{(\pm)}(\boldsymbol{r})$ and $\lambda^{(\pm)}(\boldsymbol{\rho})$ and the eigenfunction $\Psi(E,\boldsymbol{r})$ suggest that in variational calculations it should be convenient to choose the trial Lagrange functions as

$$\overline{\Lambda^{(\pm)}}(\boldsymbol{r})=\pm\frac{1}{c\hbar}\frac{1}{(\overline{\Psi}|\beta^{(\pm)}\overline{\Psi})}\overline{\Psi}(\boldsymbol{r}), \tag{63}$$

$$\beta^{(\pm)}\overline{\lambda^{(\pm)}}(\boldsymbol{\rho})=\pm\frac{1}{(\overline{\Psi}|\beta^{(\pm)}\overline{\Psi})}\beta^{(\pm)}\overline{\Psi}(\boldsymbol{\rho}). \tag{64}$$

On substituting these particular forms of $\overline{\Lambda^{(\pm)}}(\boldsymbol{r})$ and $\beta^{(\pm)}\overline{\lambda^{(\pm)}}(\boldsymbol{\rho})$ to the functionals (47) and utilizing the relation

$$(\overline{\lambda^{(\pm)}}|\alpha_n^{(\pm)}\overline{\Psi})=(\beta^{(\pm)}\overline{\lambda^{(\pm)}}|\alpha_n^{(\pm)}\overline{\Psi}), \tag{65}$$

following from the properties of the matrices $\alpha_n^{(\pm)}(\boldsymbol{\rho})$ and $\beta^{(\pm)}$ [the relation (65) shows that we do not need to know anything about the lower component of the spinor $\overline{\lambda^{(+)}}(\boldsymbol{\rho})$ and the upper component of the spinor $\overline{\lambda^{(-)}}(\boldsymbol{\rho})$, which may be arbitrary], we find the functionals

$$F^{(\pm)}[\overline{\Psi}]=\pm\frac{(\overline{\Psi}|i\alpha_n^{(\pm)}\overline{\Psi})}{(\overline{\Psi}|\beta^{(\pm)}\overline{\Psi})}\pm\frac{1}{c\hbar}\frac{\langle\overline{\Psi}|[\hat{H}-E]\overline{\Psi}\rangle}{(\overline{\Psi}|\beta^{(\pm)}\overline{\Psi})} \tag{66}$$

with the desirable property

$$F^{(\pm)}[\overline{\Psi}]=F^{(\pm)*}[\overline{\Psi}] \tag{67}$$

(the asterisk denotes the complex conjugation). The sought variational principles, the analogs of the nonrelativistic variational principles (52) and (76) of Ref. [7], are

$$b(E)=\mathrm{stat}\left\{\frac{(\overline{\Psi}|i\alpha_n^{(+)}\overline{\Psi})}{(\overline{\Psi}|\beta^{(+)}\overline{\Psi})}+\frac{1}{c\hbar}\frac{\langle\overline{\Psi}|[\hat{H}-E]\overline{\Psi}\rangle}{(\overline{\Psi}|\beta^{(+)}\overline{\Psi})}\right\}, \tag{68}$$

$$b^{-1}(E)=\mathrm{stat}\left\{-\frac{(\overline{\Psi}|i\alpha_n^{(-)}\overline{\Psi})}{(\overline{\Psi}|\beta^{(-)}\overline{\Psi})}-\frac{1}{c\hbar}\frac{\langle\overline{\Psi}|[\hat{H}-E]\overline{\Psi}\rangle}{(\overline{\Psi}|\beta^{(-)}\overline{\Psi})}\right\}. \tag{69}$$

The principle (68), the relativistic counterpart of the celebrated Kohn variational principle [12], has been found earlier in a different way by Hamacher and Hinze [49].

B. Variational principles for matrix elements of $\hat{\mathcal{R}}^{(\pm)}(E)$ and their reciprocals

In this subsection we shall derive variational principles for matrix elements $(\Phi|\hat{\mathcal{R}}^{(\pm)}\Phi')$ and their reciprocals, $(\Phi|\hat{\mathcal{R}}^{(\pm)}\Phi')^{-1}$, where $\hat{\mathcal{R}}^{(\pm)}(E)$ are the integral operators defined in Sec. II while $\Phi(\boldsymbol{\rho})$ and $\Phi'(\boldsymbol{\rho})$ are sufficiently regular spinor functions defined on the surface $\mathcal{S}$. For this purpose, we shall need auxiliary spinor functions $\Psi^{(\pm)}(E,\boldsymbol{r})$ and $\Psi'^{(\pm)}(E,\boldsymbol{r})$ defined as those particular solutions of the relativistic wave equation (1), which on the enclosing surface $\mathcal{S}$ satisfy inhomogeneous boundary conditions

$$i\alpha_n^{(\pm)}(\boldsymbol{\rho})\Psi^{(\pm)}(E,\boldsymbol{\rho})=\pm\beta^{(\pm)}\Phi(\boldsymbol{\rho}),$$
$$i\alpha_n^{(\pm)}(\boldsymbol{\rho})\Psi'^{(\pm)}(E,\boldsymbol{\rho})=\pm\beta^{(\pm)}\Phi'(\boldsymbol{\rho}). \tag{70}$$

The conditions (70) are the analogs of the inhomogeneous Neumann boundary conditions used in the nonrelativistic theory [7]. Since the functions $\Psi^{(\pm)}(E,\boldsymbol{r})$ and $\Psi'^{(\pm)}(E,\boldsymbol{r})$ satisfy the Dirac equation (1), we may utilize Eq. (20) and rewrite the conditions (70) in the form containing the operators $\hat{\mathcal{R}}^{(\pm)}(E)$:

$$\beta^{(\pm)}\Psi^{(\pm)}(E,\boldsymbol{\rho})=\hat{\mathcal{R}}^{(\pm)}(E)\Phi(\boldsymbol{\rho}),$$
$$\beta^{(\pm)}\Psi'^{(\pm)}(E,\boldsymbol{\rho})=\hat{\mathcal{R}}^{(\pm)}(E)\Phi'(\boldsymbol{\rho}). \tag{71}$$

At first we shall construct functionals whose stationary values are $(\Phi|\hat{\mathcal{R}}^{(\pm)}\Phi')$. To this end, we treat Eqs. (1), (70), and (71) as constraints and consider the functionals

$$\begin{aligned}F^{(\pm)}&[\Phi,\Phi';\hat{\overline{\mathcal{R}}}^{(\pm)},\overline{\chi^{(\pm)}},\overline{\lambda^{(\pm)}},\overline{\Lambda^{(\pm)}},\overline{\Psi'^{(\pm)}}]\\&=(\Phi|\hat{\overline{\mathcal{R}}}^{(\pm)}\Phi')+(\overline{\chi^{(\pm)}}|\beta^{(\pm)}\overline{\Psi'^{(\pm)}}-\hat{\overline{\mathcal{R}}}^{(\pm)}\Phi')\\&\quad+(\overline{\lambda^{(\pm)}}|i\alpha_n^{(\pm)}\overline{\Psi'^{(\pm)}}\mp\beta^{(\pm)}\Phi')\\&\quad+\langle\overline{\Lambda^{(\pm)}}|[\hat{H}-E]\overline{\Psi'^{(\pm)}}\rangle.\end{aligned} \tag{72}$$

Here $\hat{\overline{\mathcal{R}}}^{(\pm)}$ are some (possibly non-Hermitian) linear integral operators acting on functions defined on the surface $\mathcal{S}$, $\overline{\chi^{(\pm)}}(\boldsymbol{\rho})$ and $\overline{\lambda^{(\pm)}}(\boldsymbol{\rho})$ are sufficiently regular functions defined on $\mathcal{S}$, while $\overline{\Lambda^{(\pm)}}(\boldsymbol{r})$ and $\overline{\Psi'^{(\pm)}}(\boldsymbol{r})$ are sufficiently regular functions defined in the volume $\mathcal{V}$. The functions $\overline{\chi^{(\pm)}}(\boldsymbol{\rho})$, $\overline{\lambda^{(\pm)}}(\boldsymbol{\rho})$, and $\overline{\Lambda^{(\pm)}}(\boldsymbol{r})$ are the Lagrange functions incorporating the constraints (71), (70), and (1), respectively. We seek such functions $\chi^{(\pm)}(\boldsymbol{\rho})$, $\lambda^{(\pm)}(\boldsymbol{\rho})$, and $\Lambda^{(\pm)}(\boldsymbol{r})$ that the first variations of the functionals (72) due to small variations of $\hat{\overline{\mathcal{R}}}^{(\pm)}$, $\overline{\chi^{(\pm)}}(\boldsymbol{\rho})$, $\overline{\lambda^{(\pm)}}(\boldsymbol{\rho})$, $\overline{\Lambda^{(\pm)}}(\boldsymbol{r})$, and $\overline{\Psi'^{(\pm)}}(\boldsymbol{r})$ around $\hat{\mathcal{R}}^{(\pm)}(E)$, $\chi^{(\pm)}(\boldsymbol{\rho})$, $\lambda^{(\pm)}(\boldsymbol{\rho})$, $\Lambda^{(\pm)}(\boldsymbol{r})$, and $\Psi'^{(\pm)}(E,\boldsymbol{r})$, respectively, vanish. We have

$$\begin{aligned}\delta F^{(\pm)}&[\Phi,\Phi';\hat{\mathcal{R}}^{(\pm)},\chi^{(\pm)},\lambda^{(\pm)},\Lambda^{(\pm)},\Psi'^{(\pm)}]\\&=(\Phi|\delta\hat{\mathcal{R}}^{(\pm)}\Phi')+(\chi^{(\pm)}|\beta^{(\pm)}\delta\Psi'^{(\pm)}-\delta\hat{\mathcal{R}}^{(\pm)}\Phi')\\&\quad+(\lambda^{(\pm)}|i\alpha_n^{(\pm)}\delta\Psi'^{(\pm)})+\langle\Lambda^{(\pm)}|[\hat{H}-E]\delta\Psi'^{(\pm)}\rangle,\end{aligned} \tag{73}$$

where we have utilized the fact that terms containing the variations $\delta\chi^{(\pm)}(\boldsymbol{\rho})$, $\delta\lambda^{(\pm)}(\boldsymbol{\rho})$, and $\delta\Lambda^{(\pm)}(\boldsymbol{r})$ vanish due to the constraints (71), (70), and (1). Application of the Gauss theorem to the volume integral transforms Eq. (73) to the form

$$\delta F^{(\pm)}[\Phi,\Phi';\hat{\mathcal{R}}^{(\pm)},\chi^{(\pm)},\lambda^{(\pm)},\Lambda^{(\pm)},\Psi'^{(\pm)}] = (\Phi-\chi^{(\pm)}|\delta\hat{\mathcal{R}}^{(\pm)}\Phi') + (\beta^{(\pm)}\chi^{(\pm)} - i\alpha_n^{(\mp)}\lambda^{(\pm)} + ic\hbar\alpha_n\Lambda^{(\pm)}|\delta\Psi'^{(\pm)}) + \langle[\hat{H}-E]\Lambda^{(\pm)}|\delta\Psi'^{(\pm)}\rangle. \tag{74}$$

On stipulating

$$\delta F^{(\pm)}[\Phi,\Phi';\hat{\mathcal{R}}^{(\pm)},\chi^{(\pm)},\lambda^{(\pm)},\Lambda^{(\pm)},\Psi'^{(\pm)}]=0 \tag{75}$$

we find

$$[\hat{H}-E]\Lambda^{(\pm)}(\boldsymbol{r})=0 \quad \text{in } \mathcal{V}, \tag{76}$$

$$\Phi(\boldsymbol{\rho})-\chi^{(\pm)}(\boldsymbol{\rho})=0 \quad \text{on } \mathcal{S}, \tag{77}$$

and

$$\beta^{(\pm)}\chi^{(\pm)}(\boldsymbol{\rho}) - i\alpha_n^{(\mp)}(\boldsymbol{\rho})\lambda^{(\pm)}(\boldsymbol{\rho}) + ic\hbar\alpha_n(\boldsymbol{\rho})\Lambda^{(\pm)}(\boldsymbol{\rho})=0 \quad \text{on } \mathcal{S}. \tag{78}$$

Premultiplying Eq. (78) by $\beta^{(\pm)}$ and utilizing the relations (11) and (12) we have

$$\beta^{(\pm)}\chi^{(\pm)}(\boldsymbol{\rho}) + ic\hbar\alpha_n^{(\pm)}(\boldsymbol{\rho})\Lambda^{(\pm)}(\boldsymbol{\rho})=0 \tag{79}$$

while premultiplying by $\alpha_n^{(\pm)}(\boldsymbol{\rho})$ we obtain

$$-i\beta^{(\pm)}\lambda^{(\pm)}(\boldsymbol{\rho}) + ic\hbar\beta^{(\pm)}\Lambda^{(\pm)}(\boldsymbol{\rho})=0. \tag{80}$$

From Eq. (77) it follows that

$$\chi^{(\pm)}(\boldsymbol{\rho})=\Phi(\boldsymbol{\rho}) \tag{81}$$

while Eqs. (79) and (81) imply

$$i\alpha_n^{(\pm)}(\boldsymbol{\rho})\Lambda^{(\pm)}(\boldsymbol{\rho}) = -\frac{1}{c\hbar}\beta^{(\pm)}\Phi(\boldsymbol{\rho}). \tag{82}$$

Comparison of Eqs. (76) and (82) with Eqs. (1) and (70) shows that the Lagrange functions $\Lambda^{(\pm)}(\boldsymbol{r})$ satisfy the same differential equation in $\mathcal{V}$ as the functions $\Psi^{(\pm)}(E,\boldsymbol{r})$ do and obey on $\mathcal{S}$ the inhomogeneous boundary conditions that differ from those satisfied by $\Psi^{(\pm)}(E,\boldsymbol{r})$ only by the multiplicative factors $\mp 1/c\hbar$ in inhomogeneous terms. This implies that we may choose

$$\Lambda^{(\pm)}(\boldsymbol{r}) = \mp\frac{1}{c\hbar}\Psi^{(\pm)}(E,\boldsymbol{r}) \tag{83}$$

and consequently [cf. Eq. (80)]

$$\beta^{(\pm)}\lambda^{(\pm)}(\boldsymbol{\rho}) = \mp\beta^{(\pm)}\Psi^{(\pm)}(E,\boldsymbol{\rho}). \tag{84}$$

The relations (81), (83), and (84) between the functions $\chi^{(\pm)}(\boldsymbol{\rho})$, $\lambda^{(\pm)}(\boldsymbol{\rho})$, and $\Lambda^{(\pm)}(\boldsymbol{r})$ and the functions $\Phi(\boldsymbol{\rho})$ and $\Psi^{(\pm)}(E,\boldsymbol{r})$ suggest that we may restrict our considerations to the following trial forms of the Lagrange functions:

$$\overline{\chi^{(\pm)}}(\boldsymbol{\rho})=\Phi(\boldsymbol{\rho}), \tag{85}$$

$$\beta^{(\pm)}\overline{\lambda^{(\pm)}}(\boldsymbol{\rho}) = \mp\beta^{(\pm)}\overline{\Psi}^{(\pm)}(\boldsymbol{\rho}) \tag{86}$$

and

$$\overline{\Lambda^{(\pm)}}(\boldsymbol{r}) = \mp\frac{1}{c\hbar}\,\overline{\Psi}^{(\pm)}(\boldsymbol{r}). \tag{87}$$

Substitution of these particular forms of $\overline{\chi^{(\pm)}}(\boldsymbol{\rho})$, $\overline{\lambda^{(\pm)}}(\boldsymbol{\rho})$, and $\overline{\Lambda^{(\pm)}}(\boldsymbol{r})$ to the definition (72) gives the variational functionals

$$F^{(\pm)}[\Phi,\Phi';\overline{\Psi}^{(\pm)},\overline{\Psi}'^{(\pm)}] = (\Phi|\beta^{(\pm)}\overline{\Psi}'^{(\pm)}) + (\beta^{(\pm)}\overline{\Psi}^{(\pm)}|\Phi') \mp (\overline{\Psi}^{(\pm)}|i\alpha_n^{(\pm)}\overline{\Psi}'^{(\pm)}) \mp \frac{1}{c\hbar}\langle\overline{\Psi}^{(\pm)}|[\hat{H}-E]\overline{\Psi}'^{(\pm)}\rangle. \tag{88}$$

By applying the Gauss divergence theorem to the volume integral appearing on the right-hand side of this equation, it may be easily shown that the functionals (88) possess a symmetry property

$$F^{(\pm)}[\Phi,\Phi';\overline{\Psi}^{(\pm)},\overline{\Psi}'^{(\pm)}] = F^{(\pm)*}[\Phi',\Phi;\overline{\Psi}'^{(\pm)},\overline{\Psi}^{(\pm)}]. \tag{89}$$

The functionals (88) are stationary for small, smooth, and otherwise arbitrary variations of $\overline{\Psi}^{(\pm)}(\boldsymbol{r})$ and $\overline{\Psi}'^{(\pm)}(\boldsymbol{r})$ around $\Psi^{(\pm)}(E,\boldsymbol{r})$ and $\Psi'^{(\pm)}(E,\boldsymbol{r})$, respectively, and their stationary values are $(\Phi|\hat{\mathcal{R}}^{(\pm)}\Phi')$. We have thus the variational principles

$$(\Phi|\hat{\mathcal{R}}^{(\pm)}\Phi') = \mathrm{stat}\left\{(\Phi|\beta^{(\pm)}\overline{\Psi}'^{(\pm)}) + (\beta^{(\pm)}\overline{\Psi}^{(\pm)}|\Phi') \mp (\overline{\Psi}^{(\pm)}|i\alpha_n^{(\pm)}\overline{\Psi}'^{(\pm)}) \mp \frac{1}{c\hbar}\langle\overline{\Psi}^{(\pm)}|[\hat{H}-E]\overline{\Psi}'^{(\pm)}\rangle\right\}, \tag{90}$$

which are the counterparts of the nonrelativistic variational principle (96) of Ref. [7].

Next we shall derive variational principles for reciprocals of the matrix elements of the operators $\hat{\mathcal{R}}^{(\pm)}(E)$, i.e., for $(\Phi|\hat{\mathcal{R}}^{(\pm)}\Phi')^{-1}$. To this end we construct the functionals

$$F^{(\pm)}[\Phi,\Phi';\hat{\bar{\mathcal{R}}}^{(\pm)},\overline{\chi}^{(\pm)},\overline{\lambda}^{(\pm)},\overline{\Lambda}^{(\pm)},\overline{\Psi}'^{(\pm)}]$$
$$=\frac{1}{(\Phi|\hat{\bar{\mathcal{R}}}^{(\pm)}\Phi')}+(\overline{\chi}^{(\pm)}|\beta^{(\pm)}\overline{\Psi}'^{(\pm)}-\hat{\bar{\mathcal{R}}}^{(\pm)}\Phi')$$
$$+(\overline{\lambda}^{(\pm)}|i\alpha_n^{(\pm)}\overline{\Psi}'^{(\pm)}\mp\beta^{(\pm)}\Phi')$$
$$+\langle\overline{\Lambda}^{(\pm)}|[\hat{H}-E]\overline{\Psi}'^{(\pm)}\rangle. \tag{91}$$

We seek such forms $\chi^{(\pm)}(\boldsymbol{\rho})$, $\lambda^{(\pm)}(\boldsymbol{\rho})$, and $\Lambda^{(\pm)}(\boldsymbol{r})$ of the Lagrange functions $\overline{\chi}^{(\pm)}(\boldsymbol{\rho})$, $\overline{\lambda}^{(\pm)}(\boldsymbol{\rho})$, and $\overline{\Lambda}^{(\pm)}(\boldsymbol{r})$ [incorporating the subsidiary conditions (71), (70), and (1), respectively] that the functionals (91) are stationary for small variations of $\hat{\bar{\mathcal{R}}}^{(\pm)}$, $\overline{\chi}^{(\pm)}(\boldsymbol{\rho})$, $\overline{\lambda}^{(\pm)}(\boldsymbol{\rho})$, $\overline{\Lambda}^{(\pm)}(\boldsymbol{r})$, and $\overline{\Psi}'^{(\pm)}(\boldsymbol{r})$ around $\hat{\mathcal{R}}^{(\pm)}(E)$, $\chi^{(\pm)}(\boldsymbol{\rho})$, $\lambda^{(\pm)}(\boldsymbol{\rho})$, $\Lambda^{(\pm)}(\boldsymbol{r})$, and $\Psi'^{(\pm)}(E,\boldsymbol{r})$. Varying Eq. (91) we obtain

$$\delta F^{(\pm)}[\Phi,\Phi';\hat{\mathcal{R}}^{(\pm)},\chi^{(\pm)},\lambda^{(\pm)},\Lambda^{(\pm)},\Psi'^{(\pm)}]$$
$$=-\frac{(\Phi|\delta\hat{\mathcal{R}}^{(\pm)}\Phi')}{(\Phi|\hat{\mathcal{R}}^{(\pm)}\Phi')^2}+(\chi^{(\pm)}|\beta^{(\pm)}\delta\Psi'^{(\pm)}-\delta\hat{\mathcal{R}}^{(\pm)}\Phi')$$
$$+(\lambda^{(\pm)}|i\alpha_n^{(\pm)}\delta\Psi'^{(\pm)})+\langle\Lambda^{(\pm)}|[\hat{H}-E]\delta\Psi'^{(\pm)}\rangle. \tag{92}$$

To simplify this equation, we use the Gauss theorem and transfer the operation $[\hat{H}-E]$ on $\delta\Psi'^{(\pm)}(\boldsymbol{r})$ to $\Lambda^{(\pm)}(\boldsymbol{r})$. This yields

$$\delta F^{(\pm)}[\Phi,\Phi';\hat{\mathcal{R}}^{(\pm)},\chi^{(\pm)},\lambda^{(\pm)},\Lambda^{(\pm)},\Psi'^{(\pm)}]$$
$$=-\left[\frac{(\Phi|\delta\hat{\mathcal{R}}^{(\pm)}\Phi')}{(\Phi|\hat{\mathcal{R}}^{(\pm)}\Phi')^2}+(\chi^{(\pm)}|\delta\hat{\mathcal{R}}^{(\pm)}\Phi')\right]$$
$$+(\beta^{(\pm)}\chi^{(\pm)}-i\alpha_n^{(\mp)}\lambda^{(\pm)}+ic\hbar\,\alpha_n\Lambda^{(\pm)}|\delta\Psi'^{(\pm)})$$
$$+\langle[\hat{H}-E]\Lambda^{(\pm)}|\delta\Psi'^{(\pm)}\rangle. \tag{93}$$

To ensure that

$$\delta F^{(\pm)}[\Phi,\Phi';\hat{\mathcal{R}}^{(\pm)},\chi^{(\pm)},\lambda^{(\pm)},\Lambda^{(\pm)},\Psi'^{(\pm)}]=0 \tag{94}$$

holds for essentially arbitrary $\delta\hat{\mathcal{R}}^{(\pm)}$ and $\delta\Psi'^{(\pm)}(\boldsymbol{r})$, we must require

$$[\hat{H}-E]\Lambda^{(\pm)}(\boldsymbol{r})=0 \quad \text{in } \mathcal{V}, \tag{95}$$

$$\frac{1}{(\hat{\mathcal{R}}^{(\pm)}\Phi'|\Phi)^2}\Phi(\boldsymbol{\rho})+\chi^{(\pm)}(\boldsymbol{\rho})=0 \quad \text{on } \mathcal{S} \tag{96}$$

and

$$\beta^{(\pm)}\chi^{(\pm)}(\boldsymbol{\rho})-i\alpha_n^{(\mp)}(\boldsymbol{\rho})\lambda^{(\pm)}(\boldsymbol{\rho})+ic\hbar\,\alpha_n(\boldsymbol{\rho})\Lambda^{(\pm)}(\boldsymbol{\rho})=0 \quad \text{on } \mathcal{S}. \tag{97}$$

Operating on Eq. (97) from the left with $\beta^{(\pm)}$ gives

$$\beta^{(\pm)}\chi^{(\pm)}(\boldsymbol{\rho})+ic\hbar\,\alpha_n^{(\pm)}(\boldsymbol{\rho})\Lambda^{(\pm)}(\boldsymbol{\rho})=0 \tag{98}$$

and with $\alpha_n^{(\pm)}(\boldsymbol{\rho})$ gives

$$-i\beta^{(\pm)}\lambda^{(\pm)}(\boldsymbol{\rho})+ic\hbar\,\beta^{(\pm)}\Lambda^{(\pm)}(\boldsymbol{\rho})=0. \tag{99}$$

We deduce from Eq. (96) that

$$\chi^{(\pm)}(\boldsymbol{\rho})=-\frac{1}{(\hat{\mathcal{R}}^{(\pm)}\Phi'|\Phi)^2}\Phi(\boldsymbol{\rho}) \tag{100}$$

and from Eqs. (98) and (100) that

$$i\alpha_n^{(\pm)}(\boldsymbol{\rho})\Lambda^{(\pm)}(\boldsymbol{\rho})=\frac{1}{c\hbar}\frac{1}{(\hat{\mathcal{R}}^{(\pm)}\Phi'|\Phi)^2}\beta^{(\pm)}\Phi(\boldsymbol{\rho}). \tag{101}$$

Utilizing the boundary conditions (71) and the Hermicity property of the operators $\hat{\mathcal{R}}^{(\pm)}(E)$, it is convenient to rewrite Eqs. (100) and (101) in the forms

$$\chi^{(\pm)}(\boldsymbol{\rho})=-\frac{1}{(\beta^{(\pm)}\Psi'^{(\pm)}|\Phi)(\hat{\mathcal{R}}^{(\pm)}\Phi'|\Phi)}\Phi(\boldsymbol{\rho}), \tag{102}$$

$$i\alpha_n^{(\pm)}(\boldsymbol{\rho})\Lambda^{(\pm)}(\boldsymbol{\rho})=\frac{1}{c\hbar}\frac{1}{(\Phi'|\beta^{(\pm)}\Psi^{(\pm)})(\beta^{(\pm)}\Psi'^{(\pm)}|\Phi)}\times\beta^{(\pm)}\Phi(\boldsymbol{\rho}). \tag{103}$$

Comparison of Eqs. (95), (103), (1), and (70) shows that we may choose

$$\Lambda^{(\pm)}(\boldsymbol{r})=\pm\frac{1}{c\hbar}\frac{1}{(\Phi'|\beta^{(\pm)}\Psi^{(\pm)})(\beta^{(\pm)}\Psi'^{(\pm)}|\Phi)}\Psi^{(\pm)}(E,\boldsymbol{r}) \tag{104}$$

and consequently [cf. Eq. (99)]

$$\beta^{(\pm)}\lambda^{(\pm)}(\boldsymbol{\rho})=\pm\frac{1}{(\Phi'|\beta^{(\pm)}\Psi^{(\pm)})(\beta^{(\pm)}\Psi'^{(\pm)}|\Phi)}\times\beta^{(\pm)}\Psi^{(\pm)}(E,\boldsymbol{\rho}). \tag{105}$$

It is then natural to choose trial estimates of $\chi^{(\pm)}(\boldsymbol{\rho})$, $\lambda^{(\pm)}(\boldsymbol{\rho})$, and $\Lambda^{(\pm)}(\boldsymbol{r})$ as

$$\overline{\chi}^{(\pm)}(\boldsymbol{\rho})=-\frac{1}{(\beta^{(\pm)}\overline{\Psi}'^{(\pm)}|\Phi)(\hat{\bar{\mathcal{R}}}^{(\pm)}\Phi'|\Phi)}\Phi(\boldsymbol{\rho}), \tag{106}$$

$$\beta^{(\pm)}\overline{\lambda}^{(\pm)}(\boldsymbol{\rho})=\pm\frac{1}{(\Phi'|\beta^{(\pm)}\overline{\Psi}^{(\pm)})(\beta^{(\pm)}\overline{\Psi}'^{(\pm)}|\Phi)},\times\beta^{(\pm)}\overline{\Psi}^{(\pm)}(\boldsymbol{\rho}), \tag{107}$$

and

$$\overline{\Lambda}^{(\pm)}(\boldsymbol{r})=\pm\frac{1}{c\hbar}\frac{1}{(\Phi'|\beta^{(\pm)}\overline{\Psi}^{(\pm)})(\beta^{(\pm)}\overline{\Psi}'^{(\pm)}|\Phi)}\overline{\Psi}^{(\pm)}(\boldsymbol{r}), \tag{108}$$

which leads us to the symmetric [in the sense of Eq. (89)] functionals

$$F^{(\pm)}[\Phi,\Phi';\overline{\Psi}^{(\pm)},\overline{\Psi}'^{(\pm)}]=\pm\frac{(\overline{\Psi}^{(\pm)}|i\alpha_n^{(\pm)}\overline{\Psi}'^{(\pm)})}{(\Phi|\beta^{(\pm)}\overline{\Psi}'^{(\pm)})(\beta^{(\pm)}\overline{\Psi}^{(\pm)}|\Phi')}\pm\frac{1}{c\hbar}\frac{\langle\overline{\Psi}^{(\pm)}|[\hat{H}-E]\overline{\Psi}'^{(\pm)}\rangle}{(\Phi|\beta^{(\pm)}\overline{\Psi}'^{(\pm)})(\beta^{(\pm)}\overline{\Psi}^{(\pm)}|\Phi')}. \qquad (109)$$

The resulting variational principles

$$(\Phi|\hat{\mathcal{R}}^{(\pm)}\Phi')^{-1}=\mathrm{stat}\left\{\pm\frac{(\overline{\Psi}^{(\pm)}|i\alpha_n^{(\pm)}\overline{\Psi}'^{(\pm)})}{(\Phi|\beta^{(\pm)}\overline{\Psi}'^{(\pm)})(\beta^{(\pm)}\overline{\Psi}^{(\pm)}|\Phi')}\pm\frac{1}{c\hbar}\frac{\langle\overline{\Psi}^{(\pm)}|[\hat{H}-E]\overline{\Psi}'^{(\pm)}\rangle}{(\Phi|\beta^{(\pm)}\overline{\Psi}'^{(\pm)})(\beta^{(\pm)}\overline{\Psi}^{(\pm)}|\Phi')}\right\} \qquad (110)$$

are the analogs of the nonrelativistic variational principle (115) of Ref. [7].

C. Variational principles for matrix elements of $\hat{\mathcal{B}}^{(\pm)}(E)$ and their reciprocals

In this subsection we shall derive variational principles for matrix elements $(\Phi|\hat{\mathcal{B}}^{(\pm)}\Phi')$ and their reciprocals $(\Phi|\hat{\mathcal{B}}^{(\pm)}\Phi')^{-1}$, where $\hat{\mathcal{B}}^{(\pm)}(E)$ are the integral operators defined in Sec. II while $\Phi(\boldsymbol{\rho})$ and $\Phi'(\boldsymbol{\rho})$ are any reasonable spinor functions defined on the surface $\mathcal{S}$. As in the preceding subsection, we introduce auxiliary spinor functions $\Psi^{(\pm)}(E,\boldsymbol{r})$ and $\Psi'^{(\pm)}(E,\boldsymbol{r})$ satisfying in $\mathcal{V}$ the wave equation (1). This time, however, the functions $\Psi^{(\pm)}(E,\boldsymbol{r})$ and $\Psi'^{(\pm)}(E,\boldsymbol{r})$ are enforced to satisfy on the surface $\mathcal{S}$ the inhomogeneous boundary conditions

$$\beta^{(\pm)}\Psi^{(\pm)}(E,\boldsymbol{\rho})=\pm\beta^{(\pm)}\Phi(\boldsymbol{\rho}),$$

$$\beta^{(\pm)}\Psi'^{(\pm)}(E,\boldsymbol{\rho})=\pm\beta^{(\pm)}\Phi'(\boldsymbol{\rho}), \qquad (111)$$

which may be viewed as the analogs of the inhomogeneous Dirichlet boundary conditions used in the nonrelativistic theory [7]. By virtue of Eq. (14), the conditions (111) may be rewritten in the form

$$i\alpha_n^{(\pm)}(\boldsymbol{\rho})\Psi^{(\pm)}(E,\boldsymbol{\rho})=\hat{\mathcal{B}}^{(\pm)}(E)\Phi(\boldsymbol{\rho}),$$

$$i\alpha_n^{(\pm)}(\boldsymbol{\rho})\Psi'^{(\pm)}(E,\boldsymbol{\rho})=\hat{\mathcal{B}}^{(\pm)}(E)\Phi'(\boldsymbol{\rho}). \qquad (112)$$

To derive variational principles for the matrix elements $(\Phi|\hat{\mathcal{B}}^{(\pm)}\Phi')$, we start with the functionals

$$\begin{aligned}F^{(\pm)}[\Phi,\Phi';\overline{\hat{\mathcal{B}}}^{(\pm)},\overline{\chi}^{(\pm)},\overline{\lambda}^{(\pm)},\overline{\Lambda}^{(\pm)},\overline{\Psi}'^{(\pm)}]&=(\Phi|\overline{\hat{\mathcal{B}}}^{(\pm)}\Phi')+(\overline{\chi}^{(\pm)}|i\alpha_n^{(\pm)}\overline{\Psi}'^{(\pm)}-\overline{\hat{\mathcal{B}}}^{(\pm)}\Phi')\\&\quad+(\overline{\lambda}^{(\pm)}|\beta^{(\pm)}\overline{\Psi}'^{(\pm)}\mp\beta^{(\pm)}\Phi')\\&\quad+\langle\overline{\Lambda}^{(\pm)}|[\hat{H}-E]\overline{\Psi}'^{(\pm)}\rangle. \qquad (113)\end{aligned}$$

The notation used in Eq. (113) is similar to that used in Sec. III B and should be self-explanatory. The first variation of Eq. (113) is

$$\begin{aligned}\delta F^{(\pm)}[\Phi,\Phi';\hat{\mathcal{B}}^{(\pm)},\chi^{(\pm)},\lambda^{(\pm)},\Lambda^{(\pm)},\Psi'^{(\pm)}]&=(\Phi|\delta\hat{\mathcal{B}}^{(\pm)}\Phi')+(\chi^{(\pm)}|i\alpha_n^{(\pm)}\delta\Psi'^{(\pm)}-\delta\hat{\mathcal{B}}^{(\pm)}\Phi')\\&\quad+(\lambda^{(\pm)}|\beta^{(\pm)}\delta\Psi'^{(\pm)})+\langle\Lambda^{(\pm)}|[\hat{H}-E]\delta\Psi'^{(\pm)}\rangle \qquad (114)\end{aligned}$$

and, making use of the Gauss theorem, may be transformed to the form

$$\begin{aligned}\delta F^{(\pm)}[\Phi,\Phi';\hat{\mathcal{B}}^{(\pm)},\chi^{(\pm)},\lambda^{(\pm)},\Lambda^{(\pm)},\Psi'^{(\pm)}]&=(\Phi-\chi^{(\pm)}|\delta\hat{\mathcal{B}}^{(\pm)}\Phi')+(-i\alpha_n^{(\mp)}\chi^{(\pm)}+\beta^{(\pm)}\lambda^{(\pm)}\\&\quad+ic\hbar\alpha_n\Lambda^{(\pm)}|\delta\Psi'^{(\pm)})+\langle[\hat{H}-E]\Lambda^{(\pm)}|\delta\Psi'^{(\pm)}\rangle. \qquad (115)\end{aligned}$$

To make the right-hand side of Eq. (115) vanish for arbitrary $\delta\hat{\mathcal{B}}^{(\pm)}$ and $\delta\Psi'^{(\pm)}(\boldsymbol{r})$,

$$\delta F^{(\pm)}[\Phi,\Phi';\hat{\mathcal{B}}^{(\pm)},\chi^{(\pm)},\lambda^{(\pm)},\Lambda^{(\pm)},\Psi'^{(\pm)}]=0, \qquad (116)$$

it is necessary to require

$$[\hat{H}-E]\Lambda^{(\pm)}(\boldsymbol{r})=0 \quad \text{in } \mathcal{V}, \qquad (117)$$

$$\Phi(\boldsymbol{\rho})-\chi^{(\pm)}(\boldsymbol{\rho})=0 \quad \text{on } \mathcal{S}, \qquad (118)$$

and

$$-i\alpha_n^{(\mp)}(\boldsymbol{\rho})\chi^{(\pm)}(\boldsymbol{\rho})+\beta^{(\pm)}\lambda^{(\pm)}(\boldsymbol{\rho})+ic\hbar\alpha_n(\boldsymbol{\rho})\Lambda^{(\pm)}(\boldsymbol{\rho})=0 \quad \text{on } \mathcal{S}. \qquad (119)$$

Equation (119) implies

$$\beta^{(\pm)}\lambda^{(\pm)}(\boldsymbol{\rho})+ic\hbar\alpha_n^{(\pm)}(\boldsymbol{\rho})\Lambda^{(\pm)}(\boldsymbol{\rho})=0 \quad \text{on } \mathcal{S}, \qquad (120)$$

$$-i\beta^{(\pm)}\chi^{(\pm)}(\boldsymbol{\rho})+ic\hbar\beta^{(\pm)}\Lambda^{(\pm)}(\boldsymbol{\rho})=0 \quad \text{on } \mathcal{S} \tag{121}$$

and from Eqs. (118) and (121) we find

$$\chi^{(\pm)}(\boldsymbol{\rho})=\Phi(\boldsymbol{\rho}), \tag{122}$$

$$\beta^{(\pm)}\Lambda^{(\pm)}(\boldsymbol{\rho})=\frac{1}{c\hbar}\beta^{(\pm)}\Phi(\boldsymbol{\rho}). \tag{123}$$

Eqs. (117), (123), (1), and (111) give

$$\Lambda^{(\pm)}(\boldsymbol{r})=\pm\frac{1}{c\hbar}\Psi^{(\pm)}(E,\boldsymbol{r}) \tag{124}$$

and consequently [cf. Eq. (120)]

$$\beta^{(\pm)}\lambda^{(\pm)}(\boldsymbol{\rho})=\mp i\alpha_n^{(\pm)}(\boldsymbol{\rho})\Psi^{(\pm)}(E,\boldsymbol{\rho}). \tag{125}$$

Choosing trial forms of the Lagrange functions as

$$\overline{\chi}^{(\pm)}(\boldsymbol{\rho})=\Phi(\boldsymbol{\rho}), \tag{126}$$

$$\beta^{(\pm)}\overline{\lambda}^{(\pm)}(\boldsymbol{\rho})=\mp i\alpha_n^{(\pm)}(\boldsymbol{\rho})\overline{\Psi}^{(\pm)}(\boldsymbol{\rho}), \tag{127}$$

$$\overline{\Lambda}^{(\pm)}(\boldsymbol{r})=\pm\frac{1}{c\hbar}\,\overline{\Psi}^{(\pm)}(\boldsymbol{r}) \tag{128}$$

and substituting these estimates to Eq. (113) yields the functionals

$$\begin{aligned}F^{(\pm)}[\Phi,\Phi';\overline{\Psi}^{(\pm)},\overline{\Psi}'^{(\pm)}]=&(\Phi|i\alpha_n^{(\pm)}\overline{\Psi}'^{(\pm)})\\&+(i\alpha_n^{(\pm)}\overline{\Psi}^{(\pm)}|\Phi')\\&\mp(i\alpha_n^{(\pm)}\overline{\Psi}^{(\pm)}|\overline{\Psi}'^{(\pm)})\\&\pm\frac{1}{c\hbar}\langle\overline{\Psi}^{(\pm)}|[\hat{H}-E]\overline{\Psi}'^{(\pm)}\rangle,\end{aligned} \tag{129}$$

possessing the symmetry property (89). The sought variational principles are

$$\begin{aligned}(\Phi|\hat{\mathcal{B}}^{(\pm)}\Phi')=\text{stat}\Big\{&(\Phi|i\alpha_n^{(\pm)}\overline{\Psi}'^{(\pm)})+(i\alpha_n^{(\pm)}\overline{\Psi}^{(\pm)}|\Phi')\\&\mp(i\alpha_n^{(\pm)}\overline{\Psi}^{(\pm)}|\overline{\Psi}'^{(\pm)})\\&\pm\frac{1}{c\hbar}\langle\overline{\Psi}^{(\pm)}|[\hat{H}-E]\overline{\Psi}'^{(\pm)}\rangle\Big\}\end{aligned} \tag{130}$$

and are akin to the nonrelativistic stationary principle (135) of Ref. [7].

Finally, we shall construct variational principles for the reciprocals of the matrix elements $(\Phi|\hat{\mathcal{B}}^{(\pm)}\Phi')$. The starting points are the functionals

$$\begin{aligned}&F^{(\pm)}[\Phi,\Phi';\hat{\overline{\mathcal{B}}}^{(\pm)},\overline{\chi}^{(\pm)},\overline{\lambda}^{(\pm)},\overline{\Lambda}^{(\pm)},\overline{\Psi}'^{(\pm)}]\\&=\frac{1}{(\Phi|\hat{\overline{\mathcal{B}}}^{(\pm)}\Phi')}+(\overline{\chi}^{(\pm)}|i\alpha_n^{(\pm)}\overline{\Psi}'^{(\pm)}-\hat{\overline{\mathcal{B}}}^{(\pm)}\Phi')\\&\quad+(\overline{\lambda}^{(\pm)}|\beta^{(\pm)}\overline{\Psi}'^{(\pm)}\mp\beta^{(\pm)}\Phi')\\&\quad+\langle\overline{\Lambda}^{(\pm)}|[\hat{H}-E]\overline{\Psi}'^{(\pm)}\rangle.\end{aligned} \tag{131}$$

Varying Eq. (131) we obtain

$$\begin{aligned}&\delta F^{(\pm)}[\Phi,\Phi';\hat{\mathcal{B}}^{(\pm)},\chi^{(\pm)},\lambda^{(\pm)},\Lambda^{(\pm)},\Psi'^{(\pm)}]\\&=-\frac{(\Phi|\delta\hat{\mathcal{B}}^{(\pm)}\Phi')}{(\Phi|\hat{\mathcal{B}}^{(\pm)}\Phi')^2}+(\chi^{(\pm)}|i\alpha_n^{(\pm)}\delta\Psi'^{(\pm)}-\delta\hat{\mathcal{B}}^{(\pm)}\Phi')\\&\quad+(\lambda^{(\pm)}|\beta^{(\pm)}\delta\Psi'^{(\pm)})+\langle\Lambda^{(\pm)}|[\hat{H}-E]\delta\Psi'^{(\pm)}\rangle\end{aligned} \tag{132}$$

and, after application of the Gauss theorem,

$$\begin{aligned}&\delta F^{(\pm)}[\Phi,\Phi';\hat{\mathcal{B}}^{(\pm)},\chi^{(\pm)},\lambda^{(\pm)},\Lambda^{(\pm)},\Psi'^{(\pm)}]\\&=-\left[\frac{(\Phi|\delta\hat{\mathcal{B}}^{(\pm)}\Phi')}{(\Phi|\hat{\mathcal{B}}^{(\pm)}\Phi')^2}+(\chi^{(\pm)}|\delta\hat{\mathcal{B}}^{(\pm)}\Phi')\right]\\&\quad+(-i\alpha_n^{(\mp)}\chi^{(\pm)}+\beta^{(\pm)}\lambda^{(\pm)}+ic\hbar\alpha_n\Lambda^{(\pm)}|\delta\Psi'^{(\pm)})\\&\quad+\langle[\hat{H}-E]\Lambda^{(\pm)}|\delta\Psi'^{(\pm)}\rangle.\end{aligned} \tag{133}$$

Demanding

$$\delta F^{(\pm)}[\Phi,\Phi';\hat{\mathcal{B}}^{(\pm)},\chi^{(\pm)},\lambda^{(\pm)},\Lambda^{(\pm)},\Psi'^{(\pm)}]=0 \tag{134}$$

yields

$$[\hat{H}-E]\Lambda^{(\pm)}(\boldsymbol{r})=0 \quad \text{in } \mathcal{V}, \tag{135}$$

$$\frac{1}{(\hat{\mathcal{B}}^{(\pm)}\Phi'|\Phi)^2}\Phi(\boldsymbol{\rho})+\chi^{(\pm)}(\boldsymbol{\rho})=0 \quad \text{on } \mathcal{S}, \tag{136}$$

$$-i\alpha_n^{(\mp)}(\boldsymbol{\rho})\chi^{(\pm)}(\boldsymbol{\rho})+\beta^{(\pm)}\lambda^{(\pm)}(\boldsymbol{\rho})+ic\hbar\alpha_n(\boldsymbol{\rho})\Lambda^{(\pm)}(\boldsymbol{\rho})=0 \quad \text{on } \mathcal{S}. \tag{137}$$

Premultiplying Eq. (137) by $\beta^{(\pm)}$ or $\alpha_n^{(\pm)}(\boldsymbol{\rho})$ gives, respectively,

$$\beta^{(\pm)}\lambda^{(\pm)}(\boldsymbol{\rho})+ic\hbar\alpha_n^{(\pm)}(\boldsymbol{\rho})\Lambda^{(\pm)}(\boldsymbol{\rho})=0, \tag{138}$$

$$-i\beta^{(\pm)}\chi^{(\pm)}(\boldsymbol{\rho})+ic\hbar\beta^{(\pm)}\Lambda^{(\pm)}(\boldsymbol{\rho})=0. \tag{139}$$

Hence, we find

$$\chi^{(\pm)}(\boldsymbol{\rho})=-\frac{1}{(\hat{\mathcal{B}}^{(\pm)}\Phi'|\Phi)^2}\Phi(\boldsymbol{\rho}), \tag{140}$$

$$\beta^{(\pm)}\Lambda^{(\pm)}(\boldsymbol{\rho})=-\frac{1}{c\hbar}\frac{1}{(\hat{\mathcal{B}}^{(\pm)}\Phi'|\Phi)^2}\beta^{(\pm)}\Phi(\boldsymbol{\rho}). \tag{141}$$

The Hermicity of the operators $\hat{\mathcal{B}}^{(\pm)}(E)$ and Eq. (112) allows us to rewrite these relations in the more convenient forms

$$\chi^{(\pm)}(\boldsymbol{\rho})=-\frac{1}{(i\alpha_n^{(\pm)}\Psi'^{(\pm)}|\Phi)(\hat{\mathcal{B}}^{(\pm)}\Phi'|\Phi)}\Phi(\boldsymbol{\rho}), \tag{142}$$

$$\beta^{(\pm)}\Lambda^{(\pm)}(\boldsymbol{\rho})=-\frac{1}{c\hbar}\frac{1}{(\Phi'|i\alpha_n^{(\pm)}\Psi^{(\pm)})(i\alpha_n^{(\pm)}\Psi'^{(\pm)}|\Phi)}\times\beta^{(\pm)}\Phi(\boldsymbol{\rho}). \tag{143}$$

Comparison of Eqs. (135), (143), (1), and (111) yields

$$\Lambda^{(\pm)}(\boldsymbol{r})=\mp\frac{1}{c\hbar}\frac{1}{(\Phi'|i\alpha_n^{(\pm)}\Psi^{(\pm)})(i\alpha_n^{(\pm)}\Psi'^{(\pm)}|\Phi)}\times\Psi^{(\pm)}(E,\boldsymbol{r}) \tag{144}$$

and consequently [cf. Eq. (138)]

$$\beta^{(\pm)}\lambda^{(\pm)}(\boldsymbol{\rho})=\pm\frac{1}{(\Phi'|i\alpha_n^{(\pm)}\Psi^{(\pm)})(i\alpha_n^{(\pm)}\Psi'^{(\pm)}|\Phi)}\times i\alpha_n^{(\pm)}(\boldsymbol{\rho})\Psi^{(\pm)}(E,\boldsymbol{\rho}). \tag{145}$$

Choosing

$$\overline{\chi}^{(\pm)}(\boldsymbol{\rho})=-\frac{1}{(i\alpha_n^{(\pm)}\overline{\Psi}'^{(\pm)}|\Phi)(\hat{\overline{\mathcal{B}}}^{(\pm)}\Phi'|\Phi)}\Phi(\boldsymbol{\rho}), \tag{146}$$

$$\beta^{(\pm)}\overline{\lambda}^{(\pm)}(\boldsymbol{\rho})=\pm\frac{1}{(\Phi'|i\alpha_n^{(\pm)}\overline{\Psi}^{(\pm)})(i\alpha_n^{(\pm)}\overline{\Psi}'^{(\pm)}|\Phi)}\times i\alpha_n^{(\pm)}(\boldsymbol{\rho})\overline{\Psi}^{(\pm)}(\boldsymbol{\rho}), \tag{147}$$

$$\overline{\Lambda}^{(\pm)}(\boldsymbol{r})=\mp\frac{1}{c\hbar}\frac{1}{(\Phi'|i\alpha_n^{(\pm)}\overline{\Psi}^{(\pm)})(i\alpha_n^{(\pm)}\overline{\Psi}'^{(\pm)}|\Phi)}\overline{\Psi}^{(\pm)}(\boldsymbol{r}) \tag{148}$$

we get the symmetric [in the sense of Eq. (89)] functionals

$$F^{(\pm)}[\Phi,\Phi';\overline{\Psi}^{(\pm)},\overline{\Psi}'^{(\pm)}]=\pm\frac{(i\alpha_n^{(\pm)}\overline{\Psi}^{(\pm)}|\overline{\Psi}'^{(\pm)})}{(\Phi|i\alpha_n^{(\pm)}\overline{\Psi}'^{(\pm)})(i\alpha_n^{(\pm)}\overline{\Psi}^{(\pm)}|\Phi')}\mp\frac{1}{c\hbar}\frac{\langle\overline{\Psi}^{(\pm)}|[\hat{H}-E]\overline{\Psi}'^{(\pm)}\rangle}{(\Phi|i\alpha_n^{(\pm)}\overline{\Psi}'^{(\pm)})(i\alpha_n^{(\pm)}\overline{\Psi}^{(\pm)}|\Phi')} \tag{149}$$

and arrive at the variational principles

$$(\Phi|\hat{\mathcal{B}}^{(\pm)}\Phi')^{-1}=\mathrm{stat}\left\{\pm\frac{(i\alpha_n^{(\pm)}\overline{\Psi}^{(\pm)}|\overline{\Psi}'^{(\pm)})}{(\Phi|i\alpha_n^{(\pm)}\overline{\Psi}'^{(\pm)})(i\alpha_n^{(\pm)}\overline{\Psi}^{(\pm)}|\Phi')}\mp\frac{1}{c\hbar}\frac{\langle\overline{\Psi}^{(\pm)}|[\hat{H}-E]\overline{\Psi}'^{(\pm)}\rangle}{(\Phi|i\alpha_n^{(\pm)}\overline{\Psi}'^{(\pm)})(i\alpha_n^{(\pm)}\overline{\Psi}^{(\pm)}|\Phi')}\right\} \tag{150}$$

analogous to the nonrelativistic principle (154) of Ref. [7].

IV. VARIATIONAL PRINCIPLES WITH CONSTRAINED TRIAL FUNCTIONS

The variational principles derived in Sec. III are *unconstrained*, which means that trial functions used are not required to satisfy any restrictive conditions apart from the reasonable requirement of continuity of their upper and lower components across any surface subdividing the volume $\mathcal{V}$. In particular, the approximating functions $\overline{\Psi}^{(\pm)}(\boldsymbol{r})$ and $\overline{\Psi}'^{(\pm)}(\boldsymbol{r})$ used in the variational principles (90) and (110) do not need to satisfy the ''Neumann'' boundary conditions (70) obeyed on the enclosing surface $\mathcal{S}$ by the exact solutions $\Psi^{(\pm)}(E,\boldsymbol{r})$ and $\Psi'^{(\pm)}(E,\boldsymbol{r})$. Similarly, it is not necessary that approximating functions used in the variational principles (130) and (150) should satisfy the ''Dirichlet'' boundary conditions (111).

In actual applications, however, it may be profitable to restrict a class of admissible trial functions to those satisfying the same boundary condition as the exact solution does. The advantages may be twofold. First, this may facilitate the optimal choice of trial functions. Second, the restriction may lead to a simpler form of a functional varied. We shall illustrate the second advantage considering the variational principles (90) and (130).

Consider at first the variational principle (90). If the trial functions $\overline{\Psi}^{(\pm)}(\boldsymbol{r})$ and $\overline{\Psi}'^{(\pm)}(\boldsymbol{r})$ are forced to satisfy on the surface $\mathcal{S}$ the ''Neumann'' boundary conditions [cf. Eq. (70)]

$$i\alpha_n^{(\pm)}(\boldsymbol{\rho})\overline{\Psi}^{(\pm)}(\boldsymbol{\rho})=\pm\beta^{(\pm)}\Phi(\boldsymbol{\rho}),$$

$$i\alpha_n^{(\pm)}(\boldsymbol{\rho})\overline{\Psi}'^{(\pm)}(\boldsymbol{\rho})=\pm\beta^{(\pm)}\Phi'(\boldsymbol{\rho}), \tag{151}$$

the second and the third terms on the right-hand side of Eq. (90) cancel yielding the analog of the nonrelativistic Jackson variational principle [cf. Eq. (160) of Ref. [7]]

$$(\Phi|\hat{\mathcal{R}}^{(\pm)}\Phi') = \mathrm{stat}\left\{ (\Phi|\beta^{(\pm)}\overline{\Psi}'^{(\pm)}) \mp \frac{1}{c\hbar}\langle \overline{\Psi}^{(\pm)}|[\hat{H}-E]\overline{\Psi}'^{(\pm)}\rangle \right\}. \quad (152)$$

Similarly, if in the variational principle (130) the approximating functions $\overline{\Psi}^{(\pm)}(\boldsymbol{r})$ and $\overline{\Psi}'^{(\pm)}(\boldsymbol{r})$ are restricted to satisfy the ''Dirichlet'' boundary conditions [cf. Eq. (111)]

$$\beta^{(\pm)}\overline{\Psi}^{(\pm)}(\boldsymbol{\rho}) = \pm\beta^{(\pm)}\Phi(\boldsymbol{\rho}),$$

$$\beta^{(\pm)}\overline{\Psi}'^{(\pm)}(\boldsymbol{\rho}) = \pm\beta^{(\pm)}\Phi'(\boldsymbol{\rho}), \quad (153)$$

this yields the constrained variational principle

$$(\Phi|\hat{\mathcal{B}}^{(\pm)}\Phi') = \mathrm{stat}\left\{ (\Phi|i\alpha_n^{(\pm)}\overline{\Psi}'^{(\pm)}) \pm \frac{1}{c\hbar}\langle \overline{\Psi}^{(\pm)}|[\hat{H}-E]\overline{\Psi}'^{(\pm)}\rangle \right\} \quad (154)$$

analogous to the nonrelativistic principle (162) of Ref. [7].

V. APPLICATION OF LINEAR TRIAL FUNCTIONS

Analysis of the variational principles derived in Secs. III and IV shows that trial functions enter them in a linear, bilinear, or fractional bilinear way. This implies that these variational principles are ideally suited for approximate computations of actual eigenvalues and matrix elements with the use of the Rayleigh-Ritz linear trial functions. While particular steps in the derivation of the variational principles in the relativistic theory presented in Sec. III differ in details from their counterparts in the nonrelativistic theory, the details of the use of the Rayleigh-Ritz trial functions are nearly identical in both cases. Therefore, we shall omit these details here (an interested reader is referred to Ref. [7] for a thorough description of all necessary movements) and present only final results with relevant definitions.

We begin with the variational principle (68) for common eigenvalues of the operators $\hat{\mathcal{B}}^{(+)}(E)$ and $\hat{\mathcal{R}}^{(-)}(E)$. Choosing a trial function in the form

$$\overline{\Psi}(\boldsymbol{r}) = \sum_{i=1}^{N} c_i^{(+)}\phi_i(\boldsymbol{r}), \quad (155)$$

where $\{\phi_i(\boldsymbol{r})\}$ are given basis spinor functions and $\{c_i^{(+)}\}$ are variational parameters and substituting Eq. (155) into the principle (68) one finds that approximations to the eigenvalues of $\hat{\mathcal{B}}^{(+)}(E)$ and $\hat{\mathcal{R}}^{(-)}(E)$, we shall denote them as $\widetilde{b}$, are eigenvalues of the generalized matrix eigenproblem

$$\mathsf{S}^{(+)}\mathsf{c}^{(+)} = \mathsf{M}^{(+)}\mathsf{c}^{(+)}\widetilde{b}. \quad (156)$$

Here $\mathsf{S}^{(+)}$ and $\mathsf{M}^{(+)}$ are square $N\times N$ matrices with elements

$$S_{ij}^{(+)} = (\phi_i|i\alpha_n^{(+)}\phi_j) + \frac{1}{c\hbar}\langle\phi_i|[\hat{H}-E]\phi_j\rangle \quad (157)$$

and

$$M_{ij}^{(+)} = (\phi_i|\beta^{(+)}\phi_j), \quad (158)$$

respectively and $\mathsf{c}^{(+)}$ is an N-dimensional column eigenvector with elements $\{c_i^{(+)}\}$ corresponding to the eigenvalue $\widetilde{b}$. Similarly, the use of the trial function

$$\overline{\Psi}(\boldsymbol{r}) = \sum_{i=1}^{N} c_i^{(-)}\phi_i(\boldsymbol{r}) \quad (159)$$

in the variational principle (69) yields estimates of the eigenvalues of $\hat{\mathcal{B}}^{(-)}(E)$ and $\hat{\mathcal{R}}^{(+)}(E)$. Any such estimate, $\widetilde{b^{-1}}$, is an eigenvalue of the generalized matrix eigenproblem

$$\mathsf{S}^{(-)}\mathsf{c}^{(-)} = \mathsf{M}^{(-)}\mathsf{c}^{(-)}\widetilde{b^{-1}}, \quad (160)$$

where $\mathsf{S}^{(-)}$ and $\mathsf{M}^{(-)}$ are square $N\times N$ matrices with elements

$$S_{ij}^{(-)} = -(\phi_i|i\alpha_n^{(-)}\phi_j) - \frac{1}{c\hbar}\langle\phi_i|[\hat{H}-E]\phi_j\rangle, \quad (161)$$

$$M_{ij}^{(-)} = (\phi_i|\beta^{(-)}\phi_j), \quad (162)$$

and $\mathsf{c}^{(-)}$ is a corresponding eigenvector.

To find variational estimates of the matrix elements $(\Phi|\hat{\mathcal{R}}^{(\pm)}\Phi')$ and $(\Phi|\hat{\mathcal{B}}^{(\pm)}\Phi')$ one may employ trial functions

$$\overline{\Psi}^{(\pm)}(\boldsymbol{r}) = \sum_{i=1}^{N} c_i^{(\pm)}\phi_i(\boldsymbol{r}), \quad \overline{\Psi}'^{(\pm)}(\boldsymbol{r}) = \sum_{i=1}^{N} c_i'^{(\pm)}\phi_i(\boldsymbol{r}). \quad (163)$$

The use of these functions in the principles (90) and (110) gives approximate values of $(\Phi|\hat{\mathcal{R}}^{(\pm)}\Phi')$:

$$(\Phi|\hat{\tilde{\mathcal{R}}}^{(\pm)}\Phi') = \mathsf{f}^{(\pm)\dagger}[\mathsf{S}^{(\pm)}]^{-1}\mathsf{f}'^{(\pm)} \equiv \sum_{i,j=1}^{N} (\Phi|\beta^{(\pm)}\phi_i)([\mathsf{S}^{(\pm)}]^{-1})_{ij}(\beta^{(\pm)}\phi_j|\Phi'). \quad (164)$$

Here $\mathsf{f}^{(\pm)\dagger}$ are N-dimensional *row* vectors with elements $\{f_i^{(\pm)*} = (\Phi|\beta^{(\pm)}\phi_i)\}$, $\mathsf{f}'^{(\pm)}$ are N-dimensional *column* vectors with elements $\{f_i'^{(\pm)} = (\beta^{(\pm)}\phi_i|\Phi')\}$, and $\mathsf{S}^{(\pm)}$ are square $N\times N$ matrices with elements defined by Eqs. (157) and (161), respectively. Analogously, the use of the trial functions (163) in the principles (130) and (150) gives variational estimates of $(\Phi|\hat{\mathcal{B}}^{(\pm)}\Phi')$:

$$(\Phi|\hat{\tilde{\mathcal{B}}}^{(\pm)}\Phi') = \mathsf{g}^{(\pm)\dagger}[\mathsf{T}^{(\pm)}]^{-1}\mathsf{g}'^{(\pm)} \equiv \sum_{i,j=1}^{N} (\Phi|i\alpha_n^{(\pm)}\phi_i)([\mathsf{T}^{(\pm)}]^{-1})_{ij}(i\alpha_n^{(\pm)}\phi_j|\Phi'), \quad (165)$$

where $\mathsf{g}^{(\pm)\dagger}$ are N-dimensional *row* vectors with elements $\{g_i^{(\pm)*}=(\Phi|i\alpha_n^{(\pm)}\phi_i)\}$, $\mathsf{g}'^{(\pm)}$ are N-dimensional *column* vectors with elements $\{g_i'^{(\pm)}=(i\alpha_n^{(\pm)}\phi_i|\Phi')\}$, and $\mathsf{T}^{(\pm)}$ are square $N\times N$ matrices with elements

$$T_{ij}^{(\pm)}=\pm(i\alpha_n^{(\pm)}\phi_i|\phi_j)\mp\frac{1}{c\hbar}\langle\phi_i|[\hat{H}-E]\phi_j\rangle. \quad (166)$$

VI. CONCLUDING REMARKS

In this paper we have achieved two goals. Firstly, we have succeeded in formulating the R-matrix theory for the Dirac equation (cf. Refs. [51,52]) in the language of integral operators rather than matrices. Such a generalization facilitates further development of the theory. This has been shown in the course of achieving the second goal of the paper: a derivation of a variety of stationary principles for eigenvalues and matrix elements of the integral operators $\hat{\mathcal{R}}^{(\pm)}(E)$ and $\hat{\mathcal{B}}^{(\pm)}(E)$ playing a central role in the theory. The principles have been constructed in *a systematic manner* (which is in marked contrast with a common procedure of *guessing* variational principles) by using the general approach described by Gerjuoy, Rau, and Spruch [43] (cf. also Refs. [44,45]). Our success illustrates the power of the Gerjuoy-Rau-Spruch's procedure, which is not sufficiently appreciated yet.

The variational principles derived in the present work may serve as a starting point for developing numerical codes suitable for the use for the relativistic description of atomic processes. Currently we are working on the application of the variational principles (68) and (69) to analysis of relativistic effects in low-energy electron–atom collisions.

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