Operator formulation of Wigner's *R*-matrix theories for the Schrödinger and Dirac equations

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The *R*-matrix theories for the Schrödinger and Dirac equations are formulated in the language of integral operators. In the nonrelativistic theory the central role is played by an integral operator $\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}(E)$ relating function values to normal derivatives on a surface $\mathscr{S}$ of a closed volume $\mathscr{V}$, inside which the function satisfies the Schrödinger equation at energy *E*. In the relativistic theory, the same role is played by two integral operators, $\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}^{(+)}(E)$ and $\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}^{(-)}(E)$, linking on the surface $\mathscr{S}$ values of upper and lower components of spinor wave functions satisfying in the volume $\mathscr{V}$ the Dirac equation at energy *E*. Systematic procedures for constructing the operators $\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}(E)$ and $\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}^{(\pm)}(E)$, generalizing the methods due to Kapur and Peierls and to Wigner, are presented.
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I. INTRODUCTION

The *R*-matrix theory originated in the late 1930s[1] within the framework of the nuclear reactions theory. At the early stages of the evolvement of the method, the most significant contributions were made by Wigner[2–6] and since then the method has been invariably associated with his name. In the field of nuclear physics the theory achieved the most spectacular successes in the 1950s and the early 1960s.[7,8] Later, the interest of the nuclear physics community in the *R*-matrix theory diminished but at nearly the same time it was recognized that the method was ideally suited for applications in atomic and molecular physics. Over the last 30 years the *R*-matrix theory has evolved into one of the most popular and accurate methods used in theoretical studies of such atomic and molecular phenomena as electron collisions with atoms, molecules and ions, atomic and molecular photoionization and spectra of Rydberg systems.[9–11]

To summarize the most important features of the *R*-matrix theory, let us consider scattering of a particle of energy *E* in a field of a real local potential $V(\mathbf{r})$. In the *R*-matrix approach one divides the physical space into two regions separated by an imagined closed surface $\mathscr{S}$. It is assumed that in the external region the potential $V(\mathbf{r})$ is so simple that a general solution of a time-independent wave equation governing the dynamics of the particle in that region is known either analytically or at least in a numerical form. To the contrary, in the internal region $\mathscr{V}$ the potential $V(\mathbf{r})$ may be much more complicated. It was pointed out by Kapur and Peierls[1] and by Wigner and co-workers[2–6] that from the point of view of the external region, the domain $\mathscr{V}$ may be treated as a ''black box'' and the collision matrix $\mathsf{U}(E)$ may still be found provided one knows a natural boundary condition obeyed on the surface $\mathscr{S}$ by all solutions of the wave equation considered. It was shown by Teichmann and Wigner[6] that if an orthonormal set of basis functions $\{\Phi_i\}$ spanning the surface $\mathscr{S}$ is given, a general matrix form of such a natural boundary condition for the Schrödinger equation is

$$\mathsf{P}(E)=\mathsf{R}_{\mathsf{b}}(E)[\mathsf{D}(E)-\mathsf{b}\mathsf{P}(E)]. \tag{1}$$

In Eq. (1) $\mathsf{P}(E)$ and $\mathsf{D}(E)$ are column matrices containing, respectively, projections of the wave function Ψ and its normal derivative $\nabla_n\Psi$ at the surface $\mathscr{S}$ onto the surface basis functions $\{\Phi_i\}$, b is an arbitrary Hermitian matrix which may be chosen at one's will. The goal of the theory is to find the energy-dependent matrix $\mathsf{R}_{\mathsf{b}}(E)$. Once this goal is achieved, the collision matrix $\mathsf{U}(E)$ may be expressed in terms of the *R*-matrix $\mathsf{R}_{\mathsf{b}}(E)$.[6–8]

Some years ago Nesbet[12,13] pointed out that since the Schrödinger equation is not a matrix equation but a partial differential equation, it is more fundamental to formulate the theory in terms of integral operators rather than in terms of matrices. According to Nesbet, in the nonrelativistic theory the central role is played not by the matrix $\mathsf{R}_{\mathfrak{b}}(E)$ itself but by an integral operator $\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}(E)$ such that

$$\Psi(E,\boldsymbol{\rho})=\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}(E)[\nabla_n\Psi(E,\boldsymbol{\rho})-\hat{\mathfrak{b}}\Psi(E,\boldsymbol{\rho})]. \tag{2}$$

Here $\boldsymbol{\rho}$ is an arbitrary point on the surface $\mathscr{S}$ and $\hat{\mathfrak{b}}$ is a Hermitian integral operator acting on functions defined on the surface $\mathscr{S}$ which may be chosen at our will. The operator $\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}(E)$ is independent of the choice of a particular basis set spanning the surface $\mathscr{S}$. However, once such a basis set is chosen, matrix elements of the operator $\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}(E)$ between basis functions form the matrix $\mathsf{R}_{\mathfrak{b}}(E)$ in that particular representation.

In this work we present the thorough discussion of the operator formulation of the version of the *R*-matrix theory due to Kapur and Peierls[1,14] and to Wigner.[2,3,4,6] We consider both the nonrelativistic case when the wave equation of the particle is the Schrödinger equation as well as the relativistic case of a particle whose dynamics are governed by the Dirac equation. There are two main motivations for undertaking this work. First, the operator formulation of the *R*-matrix theory is more general and elegant than the matrix approach. It is more transparent and therefore better suited for examining mathematical aspects of the method. Such a formulation is also in accord with the permanent trend in theoretical physics to make a mathematical formalism underlying any theoretical method as general and (to a reasonable extent) as rigorous as possible. Even if providing a general mathematical formulation of a particular method does not result in an immediate breakthrough in practical applications, usually it leads to better understanding of the essence of the method and may stimulate its further development. The second motivation is of a more practical nature. It appears that the operator formulation of the *R*-matrix theory relatively simply yields results which are valid for an arbitrarily shaped volume $\mathscr{V}$. This is of particular significance in the case of the *R*-matrix theory for the Dirac equation since previous attempts to develop such a theory based on a matrix approach[15–18] led to difficulties: the resulting theories either contained an error (this was shown by Szmytkowski and Hinze[17,18]) or were restricted solely to a spherically symmetric volume $\mathscr{V}$.[17,18]

The plan of the paper is as follows. In Sec. II the notation used subsequently is introduced. Section III deals with the nonrelativistic *R*-matrix theory. In Sec. III A it is shown how the operator $\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}(E)$ arises in the theory. A method of constructing the integral kernel of the operator $\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}(E)$ is discussed in Sec. III B. The operator formulation of the *R*-matrix theory for the Dirac equation is the subject of Sec. IV. In Sec. IV A two operators $\hat{\mathscr{R}}^{(+)}_{\hat{\mathfrak{b}}}(E)$ and $\hat{\mathscr{R}}^{(-)}_{\hat{\mathfrak{b}}}(E)$ are introduced. The operator $\hat{\mathscr{R}}^{(+)}_{\hat{\mathfrak{b}}}(E)$ is, to some extent, an analog of the nonrelativistic operator $\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}(E)$. The nonrelativistic limit of the operator $\hat{\mathscr{R}}^{(+)}_{\hat{\mathfrak{b}}}(E)$ is discussed in Sec. IV B. In Sec. IV C the explicit forms of the operators $\hat{\mathscr{R}}^{(\pm)}_{\hat{\mathfrak{b}}}(E)$ are found. Finally, conclusions are presented in Sec. V.

II. PRELIMINARIES

Before we proceed to the matter, we acquaint the reader with the notation used throughout the paper. In the following, we shall restrict our considerations to a finite volume $\mathscr{V}$ bounded by a surface $\mathscr{S}$. Everywhere in the paper $\mathbf{r}$ stands for a position vector of a point in the volume $\mathscr{V}$. If the point $\mathbf{r}$ lies on the boundary $\mathscr{S}$, we use the symbol $\boldsymbol{\rho}$ instead of $\mathbf{r}$. Moreover, $\mathbf{n}(\boldsymbol{\rho})$ means an outward unit vector normal to the surface $\mathscr{S}$ at the point $\boldsymbol{\rho}$. Since this should not cause any misunderstanding, we shall use the same symbols to denote inner products of scalar or spinor functions. Thus, if $\Phi(\mathbf{r})$ and $\Phi'(\mathbf{r})$ are two scalar functions (such functions appear in the nonrelativistic theory), their volume and surface scalar products are

$$\langle\Phi|\Phi'\rangle\equiv\int_{\mathscr{V}}d^3\mathbf{r}\;\Phi^*(\mathbf{r})\Phi'(\mathbf{r}),\quad(\Phi|\Phi')\equiv\int_{\mathscr{S}}d^2\boldsymbol{\rho}\;\Phi^*(\boldsymbol{\rho})\Phi'(\boldsymbol{\rho}), \tag{3}$$

respectively, where the asterisk denotes the complex conjugation. If, in turn, $\Phi(\mathbf{r})$ and $\Phi'(\mathbf{r})$ are two spinor functions (encountered in the Dirac theory), their volume and surface scalar products are

$$\langle\Phi|\Phi'\rangle \equiv \int_{\mathscr{V}} d^3\mathbf{r}\ \Phi^\dagger(\mathbf{r})\Phi'(\mathbf{r}), \quad (\Phi|\Phi') \equiv \int_{\mathscr{S}} d^2\boldsymbol{\rho}\ \Phi^\dagger(\boldsymbol{\rho})\Phi'(\boldsymbol{\rho}), \tag{4}$$

respectively, where the dagger denotes the matrix Hermitian conjugation. In Eqs. (3) and (4) $d^3\mathbf{r}$ is an infinitesimal volume element around the point $\mathbf{r}$ and $d^2\boldsymbol{\rho}$ is an infinitesimal scalar surface element around the point $\boldsymbol{\rho}$.

The following notation concerning the operators will be used: if $\hat{\mathscr{O}}$ is an integral operator on the surface $\mathscr{S}$ and if $\mathscr{O}(\boldsymbol{\rho},\boldsymbol{\rho}')$ is its integral kernel, then for any well behaving scalar or spinor function $\Phi(\boldsymbol{\rho})$ we have

$$\hat{\mathscr{O}}\Phi(\boldsymbol{\rho}) = \int_{\mathscr{S}} d^2\boldsymbol{\rho}'\ \mathscr{O}(\boldsymbol{\rho},\boldsymbol{\rho}')\Phi(\boldsymbol{\rho}'), \tag{5}$$

$$\Phi^\dagger(\boldsymbol{\rho})\hat{\mathscr{O}} = \int_{\mathscr{S}} d^2\boldsymbol{\rho}'\ \Phi^\dagger(\boldsymbol{\rho}')\mathscr{O}(\boldsymbol{\rho}',\boldsymbol{\rho}) \tag{6}$$

[here the dagger denotes either the complex or the matrix Hermitian conjugation according to the type of the function $\Phi(\boldsymbol{\rho})$ used].

We also define a family of delta functions, $\delta^{(1)}_{\mathscr{S}}(\mathbf{r})$, $\delta^{(2)}(\boldsymbol{\rho}-\boldsymbol{\rho}')$ and $\delta^{(3)}(\mathbf{r}-\mathbf{r}')$, such that for any reasonable function $\Phi(\mathbf{r})$, either scalar or spinor, one has

$$\int_{\mathscr{V}} d^3\mathbf{r}\ \delta^{(1)}_{\mathscr{S}}(\mathbf{r})\Phi(\mathbf{r}) = \int_{\mathscr{S}} d^2\boldsymbol{\rho}\ \Phi(\boldsymbol{\rho}), \tag{7}$$

$$\int_{\mathscr{S}} d^2\boldsymbol{\rho}'\ \delta^{(2)}(\boldsymbol{\rho}'-\boldsymbol{\rho})\Phi(\boldsymbol{\rho}') = \Phi(\boldsymbol{\rho}), \tag{8}$$

$$\int_{\mathscr{V}} d^3\mathbf{r}'\ \delta^{(3)}(\mathbf{r}'-\mathbf{r})\Phi(\mathbf{r}') = \Phi(\mathbf{r}), \quad \int_{\mathscr{V}} d^3\mathbf{r}'\ \delta^{(3)}(\mathbf{r}'-\boldsymbol{\rho})\Phi(\mathbf{r}') = \Phi(\boldsymbol{\rho}). \tag{9}$$

It may be inferred from Eqs. (7), (8) and the second of Eqs. (9) that, formally,

$$\delta^{(3)}(\mathbf{r}'-\boldsymbol{\rho}) = \delta^{(2)}(\boldsymbol{\rho}'-\boldsymbol{\rho})\delta^{(1)}_{\mathscr{S}}(\mathbf{r}'), \quad \delta^{(1)}_{\mathscr{S}}(\mathbf{r}) = \int_{\mathscr{S}} d^2\boldsymbol{\rho}'\ \delta^{(3)}(\boldsymbol{\rho}'-\mathbf{r}). \tag{10}$$

III. *R*-MATRIX THEORY FOR THE SCHRÖDINGER EQUATION

A. The operator $\hat{\mathscr{R}}_{\hat{b}}(E)$

In this section we shall be concerned with a nonrelativistic pointlike and spinless particle of mass m moving with energy E in the field of force described by a real, local, in general noncentral potential $V(\mathbf{r})$. We restrict our considerations to the volume $\mathscr{V}$ bounded by the surface $\mathscr{S}$. [It is to be emphasized that the particle's movement is not constrained to the volume $\mathscr{V}$. The particle may leave and enter this volume across the surface $\mathscr{S}$ freely but we focus our attention on its movement when it penetrates the domain $\mathscr{V}$.] The Schrödinger equation describing the dynamics of the particle is

$$[\hat{H}-E]\Psi(E,\mathbf{r}) = 0, \tag{11}$$

where the Hamiltonian $\hat{H}$ is

$$\hat{H}=-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2+V(\mathbf{r}). \tag{12}$$

It will be assumed hereafter that energy E is real.

Consider now two wave functions $\Psi(E,\mathbf{r})$ and $\Psi'(E,\mathbf{r})$ which are solutions to the wave equation (11) corresponding to the same energy E. Premultiplying the equation for $\Psi(E,\mathbf{r})$ by $\Psi'^*(E,\mathbf{r})$ and the complex conjugate of the equation for $\Psi'(E,\mathbf{r})$ by $\Psi(E,\mathbf{r})$, subtracting, integrating the result over the volume $\mathscr{V}$, and making use of the Green integration theorem, we obtain

$$\langle\hat{H}\Psi'|\Psi\rangle-\langle\Psi'|\hat{H}\Psi\rangle=\frac{\hbar^2}{2m}(\Psi'|\nabla_n\Psi)-\frac{\hbar^2}{2m}(\nabla_n\Psi'|\Psi), \tag{13}$$

where $\nabla_n\Psi(E,\boldsymbol{\rho})$ denotes the outward normal derivative of the function $\Psi(E,\mathbf{r})$ at the surface point $\boldsymbol{\rho}$. By virtue of Eq. (11) and the reality of E, the left-hand side of Eq. (13) is zero. Consequently, we have

$$(\Psi'|\nabla_n\Psi)=(\nabla_n\Psi'|\Psi). \tag{14}$$

Equation (14) may be formally interpreted that the normal derivative operator ∇_n, when acting on functions satisfying in the interior of the volume $\mathscr{V}$ the Schrödinger equation (11) at the fixed energy E, is Hermitian with respect to the surface scalar product $(|)$.

We shall introduce now an auxiliary energy-dependent linear Hermitian integral operator $\hat{\mathscr{B}}(E)$ defined on $L^2_{(|)}(\mathscr{S})$ such that

$$\nabla_n\Psi(E,\boldsymbol{\rho})=\hat{\mathscr{B}}(E)\Psi(E,\boldsymbol{\rho}) \tag{15}$$

for any solution to Eq. (11) at energy E. The operator $\hat{\mathscr{B}}(E)$ is represented by an integral kernel $\mathscr{B}(E,\boldsymbol{\rho},\boldsymbol{\rho}')$ in terms of which Eq. (15) may be rewritten in the form

$$\nabla_n\Psi(E,\boldsymbol{\rho})=\int_{\mathscr{S}}d^2\boldsymbol{\rho}'\ \mathscr{B}(E,\boldsymbol{\rho},\boldsymbol{\rho}')\Psi(E,\boldsymbol{\rho}'). \tag{16}$$

The existence of the operator $\hat{\mathscr{B}}(E)$ has been proved by Szmytkowski[19] who has demonstrated that the kernel $\mathscr{B}(E,\boldsymbol{\rho},\boldsymbol{\rho}')$ has the representation

$$\mathscr{B}(E,\boldsymbol{\rho},\boldsymbol{\rho}')=\sum_i\ \Psi_i(E,\boldsymbol{\rho})b_i(E)\Psi_i^*(E,\boldsymbol{\rho}'), \tag{17}$$

where $\{\Psi_i(E,\mathbf{r})\}$ are those solutions to the Schrödinger equation (11) at energy E which have constant normal derivatives on $\mathscr{S}$,

$$\nabla_n\Psi_i(E,\boldsymbol{\rho})=b_i(E)\Psi_i(E,\boldsymbol{\rho}) \tag{18}$$

and are normalized according to $(\Psi_i|\Psi_i)=1$ (notice that the surface, *not* volume, scalar product has been used for the normalization purposes). It has been shown[19] that the numbers $\{b_i(E)\}$ are real and that the surface functions $\{\Psi_i(E,\boldsymbol{\rho})\}$ are such that $(\Psi_i|\Psi_j)=\delta_{ij}$.

It should be emphasized that the operators ∇_n and $\hat{\mathscr{B}}(E)$ are not identical. If $\Phi(\mathbf{r})$ is any sufficiently regular function defined in the volume $\mathscr{V}$, in general one has

$$\nabla_n\Phi(\boldsymbol{\rho})\neq\hat{\mathscr{B}}(E)\Phi(\boldsymbol{\rho}) \tag{19}$$

unless $\Phi(\mathbf{r})$ obeys in $\mathscr{V}$ the Schrödinger equation (11) at energy E.

We are now prepared to introduce an integral operator $\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}(E)$ defined on $L^2_{(|)}(\mathscr{S})$, with the integral kernel $\mathscr{R}_{\hat{\mathfrak{b}}}(E,\boldsymbol{\rho},\boldsymbol{\rho}')$, a matrix representation of which plays the central role in the R-matrix theory. Let $\hat{\mathfrak{b}}$ be some linear Hermitian integral operator defined on $L^2_{(|)}(\mathscr{S})$, with the integral kernel $\mathfrak{b}(\boldsymbol{\rho},\boldsymbol{\rho}')$. The operator $\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}(E)$ is then defined as an operator reciprocal to the operator $\hat{\mathscr{B}}(E)-\hat{\mathfrak{b}}$ in the sense of

$$\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}(E)[\hat{\mathscr{B}}(E)-\hat{\mathfrak{b}}]\hat{\mathscr{P}}(E)=\hat{\mathscr{P}}(E), \tag{20}$$

where $\hat{\mathscr{P}}(E)$ is the projector on the manifold of surface parts of solutions to the Schrödinger equation (11) at energy E with the kernel

$$\mathscr{P}(E,\boldsymbol{\rho},\boldsymbol{\rho}')=\sum_i \Psi_i(E,\boldsymbol{\rho})\Psi_i^*(E,\boldsymbol{\rho}'). \tag{21}$$

The functions $\{\Psi_i(E,\mathbf{r})\}$ have been defined below Eq. (17). In principle, the operator $\hat{\mathfrak{b}}$ used in the definition (20) may be arbitrary and the only restriction we impose on $\hat{\mathfrak{b}}$ is that the operator $\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}(E)$ should exist. In terms of the operator $\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}(E)$ the surface relation (15) may be rewritten in the form

$$\Psi(E,\boldsymbol{\rho})=\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}(E)[\nabla_n-\hat{\mathfrak{b}}]\Psi(E,\boldsymbol{\rho}) \tag{22}$$

or, equivalently, in terms of the kernel $\mathscr{R}_{\hat{\mathfrak{b}}}(E,\boldsymbol{\rho},\boldsymbol{\rho}')$, in the form

$$\Psi(E,\boldsymbol{\rho})=\int_{\mathscr{S}} d^2\boldsymbol{\rho}'\ \mathscr{R}_{\hat{\mathfrak{b}}}(E,\boldsymbol{\rho},\boldsymbol{\rho}')[\nabla_n'-\hat{\mathfrak{b}}]\Psi(E,\boldsymbol{\rho}'). \tag{23}$$

To relate the operator and matrix formulations of the theory, we assume that some set of surface functions $\{\Phi_i(\boldsymbol{\rho})\}\in L^2_{(|)}(\mathscr{S})$ orthonormal under the surface scalar product $(|)$ and spanning the surface $\mathscr{S}$ is given. In this basis the kernel $\mathscr{R}_{\hat{\mathfrak{b}}}(E,\boldsymbol{\rho},\boldsymbol{\rho}')$ has a bilinear expansion

$$\mathscr{R}_{\hat{\mathfrak{b}}}(E,\boldsymbol{\rho},\boldsymbol{\rho}')=\sum_{i,j} \Phi_i(\boldsymbol{\rho})(\Phi_i|\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}\Phi_j)\Phi_j^*(\boldsymbol{\rho}'), \tag{24}$$

where the energy-dependent expansion coefficients

$$(\Phi_i|\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}\Phi_j)\equiv\int_{\mathscr{S}} d^2\boldsymbol{\rho}\int_{\mathscr{S}} d^2\boldsymbol{\rho}'\ \Phi_i^*(\boldsymbol{\rho})\mathscr{R}_{\hat{\mathfrak{b}}}(E,\boldsymbol{\rho},\boldsymbol{\rho}')\Phi_j(\boldsymbol{\rho}'), \tag{25}$$

matrix elements of the operator $\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}(E)$ between the basis functions $\{\Phi_i(\boldsymbol{\rho})\}$, form an R-matrix $\mathsf{R}_{\mathsf{b}}(E)$ in that particular representation. The matrix representation of Eq. (22), obtained by projecting the latter from the left on the basis functions $\{\Phi_i(\boldsymbol{\rho})\}$ is

$$\mathsf{P}(E)=\mathsf{R}_{\mathsf{b}}(E)[\mathsf{D}(E)-\mathsf{b}\mathsf{P}(E)], \tag{26}$$

where $\mathsf{P}(E)$ and $\mathsf{D}(E)$ are column matrices with elements $\{P_i(E)=(\Phi_i|\Psi)\}$ and $\{D_i(E)=(\Phi_i|\nabla_n\Psi)\}$, respectively, and b is a square matrix with elements $\{b_{ij}=(\Phi_i|\hat{\mathfrak{b}}\Phi_j)\}$. The relation (26) is identical with the relation (1) found by Teichmann and Wigner.[6] We have thus succeeded to formulate the R-matrix theory for the Schrödinger equation in terms of integral operators and to relate this formulation to the standard matrix approach to the theory. It remains to find the explicit form of the operator $\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}(E)$. In Sec. III B we shall construct its kernel following the method due to Kapur and Peierls and to Wigner.

B. Construction of the operator $\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}(E)$

In this section it will be our goal to find the operator $\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}(E)$ defined by Eq. (20) by constructing its integral kernel $\mathscr{R}_{\hat{\mathfrak{b}}}(E,\boldsymbol{\rho},\boldsymbol{\rho}')$. We shall follow, with improvements whenever they are necessary, an approach due to Kapur and Peierls[1] and to Wigner and co-workers.[2–6] For further purposes we shall need a set of functions $\{\Psi_{\hat{\mathfrak{b}}k}(\mathbf{r})\}$ defined as solutions of the boundary-value problem consisting of the Schrödinger differential equation

$$[\hat{H}-E_{\hat{\mathfrak{b}}k}]\Psi_{\hat{\mathfrak{b}}k}(\mathbf{r})=0 \tag{27}$$

and the boundary condition

$$\nabla_n \Psi_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho}) = \hat{\mathfrak{b}} \Psi_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho}) \tag{28}$$

with $\{E_{\hat{\mathfrak{b}}k}\}$ being eigenvalues. Because of the Hermicity of the operator $\hat{\mathfrak{b}}$ under the surface scalar product $(|)$, the boundary-value problem (27) and (28) is self-adjoint with respect to the volume scalar product $\langle|\rangle$ and therefore the eigenvalues $\{E_{\hat{\mathfrak{b}}k}\}$ are real and eigenfunctions belonging to different eigenvalues are orthogonal in the sense of

$$\langle \Psi_{\hat{\mathfrak{b}}k} | \Psi_{\hat{\mathfrak{b}}k'} \rangle = 0 \quad (E_{\hat{\mathfrak{b}}k} \neq E_{\hat{\mathfrak{b}}k'}). \tag{29}$$

In what follows, we shall assume that the functions belonging to degenerate eigenvalues (if there are any) have been also orthogonalized and that the normalization factors of the eigenfunctions have been chosen so that

$$\langle \Psi_{\hat{\mathfrak{b}}k} | \Psi_{\hat{\mathfrak{b}}k'} \rangle = \delta_{kk'} . \tag{30}$$

We assume also that the boundary condition operator $\hat{\mathfrak{b}}$ is such that the set of eigenfunctions $\{\Psi_{\hat{\mathfrak{b}}k}(\mathbf{r})\}$ is complete in the volume $\mathscr{V}$. The corresponding closure relation is then

$$\sum_k \Psi_{\hat{\mathfrak{b}}k}(\mathbf{r}) \Psi^*_{\hat{\mathfrak{b}}k}(\mathbf{r}') = \delta^{(3)}(\mathbf{r}-\mathbf{r}') \quad (\mathbf{r},\mathbf{r}' \in \mathscr{V} \setminus \mathscr{S}). \tag{31}$$

[Notice that, because the functions $\{\Psi_{\hat{\mathfrak{b}}k}(\mathbf{r})\}$ are constrained to obey the boundary condition (28), it is not known *a priori* whether the relation (31) holds also for the points $\mathbf{r}$ and $\mathbf{r}'$ lying on the surface $\mathscr{S}$ or not. We shall study this problem later in this section.]

By virtue of the assumed completeness of the set $\{\Psi_{\hat{\mathfrak{b}}k}(\mathbf{r})\}$, one may use these functions for expanding the wave function $\Psi(E,\mathbf{r})$ satisfying the Schrödinger equation (11). Denoting the expansion by $\overline{\Psi}_{\hat{\mathfrak{b}}}(E,\mathbf{r})$, one has

$$\overline{\Psi}_{\hat{\mathfrak{b}}}(E,\mathbf{r}) \equiv \sum_k \Psi_{\hat{\mathfrak{b}}k}(\mathbf{r}) \langle \Psi_{\hat{\mathfrak{b}}k} | \Psi \rangle \tag{32}$$

or, explicitly,

$$\overline{\Psi}_{\hat{\mathfrak{b}}}(E,\mathbf{r}) \equiv \int_{\mathscr{V}} d^3\mathbf{r}' \left\{ \sum_k \Psi_{\hat{\mathfrak{b}}k}(\mathbf{r}) \Psi^*_{\hat{\mathfrak{b}}k}(\mathbf{r}') \right\} \Psi(E,\mathbf{r}'). \tag{33}$$

The expansion coefficients $\langle \Psi_{\hat{\mathfrak{b}}k} | \Psi \rangle$ in Eq. (32) may be found in the standard way: One premultiplies Eq. (11) by $\Psi^*_{\hat{\mathfrak{b}}k}(\mathbf{r})$, postmultiplies the complex conjugate of Eq. (27) by $\Psi(E,\mathbf{r})$, subtracts and integrates the result over the volume $\mathscr{V}$ obtaining

$$\langle \hat{H} \Psi_{\hat{\mathfrak{b}}k} | \Psi \rangle - \langle \Psi_{\hat{\mathfrak{b}}k} | \hat{H} \Psi \rangle = [E_{\hat{\mathfrak{b}}k} - E] \langle \Psi_{\hat{\mathfrak{b}}k} | \Psi \rangle \tag{34}$$

which, after utilizing the explicit form (12) of the Hamiltonian $\hat{H}$ and the assumed Hermicity of the potential $V(\mathbf{r})$, becomes

$$\frac{\hbar^2}{2m} \langle \Psi_{\hat{\mathfrak{b}}k} | \boldsymbol{\nabla}^2 \Psi \rangle - \frac{\hbar^2}{2m} \langle \boldsymbol{\nabla}^2 \Psi_{\hat{\mathfrak{b}}k} | \Psi \rangle = [E_{\hat{\mathfrak{b}}k} - E] \langle \Psi_{\hat{\mathfrak{b}}k} | \Psi \rangle. \tag{35}$$

The left-hand side of Eq. (35) may be simplified by using the Green integration theorem which states that

$$\langle \Psi_{\hat{\mathfrak{b}}k} | \boldsymbol{\nabla}^2 \Psi \rangle - \langle \boldsymbol{\nabla}^2 \Psi_{\hat{\mathfrak{b}}k} | \Psi \rangle = (\Psi_{\hat{\mathfrak{b}}k} | \nabla_n \Psi) - (\nabla_n \Psi_{\hat{\mathfrak{b}}k} | \Psi). \tag{36}$$

Transforming the second surface integral on the right-hand side of Eq. (36) with the aid of the boundary condition (28) and substituting the resulting equation to Eq. (35) one arrives at

$$\langle \Psi_{\hat{\mathfrak{b}}k} | \Psi \rangle = \frac{\hbar^2}{2m} \frac{(\Psi_{\hat{\mathfrak{b}}k} | [\nabla_n - \hat{\mathfrak{b}}] \Psi)}{E_{\hat{\mathfrak{b}}k} - E}, \tag{37}$$

hence, it follows that

$$\overline{\Psi}_{\hat{\mathfrak{b}}}(E,\mathbf{r}) = \frac{\hbar^2}{2m} \sum_k \Psi_{\hat{\mathfrak{b}}k}(\mathbf{r}) \frac{(\Psi_{\hat{\mathfrak{b}}k} | [\nabla_n - \hat{\mathfrak{b}}] \Psi)}{E_{\hat{\mathfrak{b}}k} - E}. \tag{38}$$

For the sake of convenience, we shall rewrite the latter equation in the explicit form

$$\overline{\Psi}_{\hat{\mathfrak{b}}}(E,\mathbf{r}) = \int_{\mathscr{S}} d^2\boldsymbol{\rho}' \frac{\hbar^2}{2m} \sum_k \frac{\Psi_{\hat{\mathfrak{b}}k}(\mathbf{r}) \Psi^*_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho}')}{E_{\hat{\mathfrak{b}}k} - E} [\nabla'_n - \hat{\mathfrak{b}}] \Psi(E,\boldsymbol{\rho}'). \tag{39}$$

Equation (39) holds for an arbitrary point $\mathbf{r}$ in the volume $\mathscr{V}$ and in particular it is valid also for points on the surface $\mathscr{S}$, i.e., one has

$$\overline{\Psi}_{\hat{\mathfrak{b}}}(E,\boldsymbol{\rho}) = \int_{\mathscr{S}} d^2\boldsymbol{\rho}' \frac{\hbar^2}{2m} \sum_k \frac{\Psi_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho}) \Psi^*_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho}')}{E_{\hat{\mathfrak{b}}k} - E} [\nabla'_n - \hat{\mathfrak{b}}] \Psi(E,\boldsymbol{\rho}'). \tag{40}$$

To proceed further, we shall define an integral operator $\hat{\overline{\mathscr{R}}}_{\hat{\mathfrak{b}}}(E)$ relating the surface functions $\Psi(E,\boldsymbol{\rho})$ and $\overline{\Psi}_{\hat{\mathfrak{b}}}(E,\boldsymbol{\rho})$ in the following way:

$$\overline{\Psi}_{\hat{\mathfrak{b}}}(E,\boldsymbol{\rho}) = \hat{\overline{\mathscr{R}}}_{\hat{\mathfrak{b}}}(E) [\nabla_n - \hat{\mathfrak{b}}] \Psi(E,\boldsymbol{\rho}). \tag{41}$$

The operator $\hat{\overline{\mathscr{R}}}_{\hat{\mathfrak{b}}}(E)$ is represented by its integral kernel $\overline{\mathscr{R}}_{\hat{\mathfrak{b}}}(E,\boldsymbol{\rho},\boldsymbol{\rho}')$ which, from Eqs. (40) and (41), is found to be

$$\overline{\mathscr{R}}_{\hat{\mathfrak{b}}}(E,\boldsymbol{\rho},\boldsymbol{\rho}') = \frac{\hbar^2}{2m} \sum_k \frac{\Psi_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho}) \Psi^*_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho}')}{E_{\hat{\mathfrak{b}}k} - E}. \tag{42}$$

Consider now the problem of convergence of the expansion $\overline{\Psi}_{\hat{\mathfrak{b}}}(E,\mathbf{r})$. If the point $\mathbf{r}$ lies in the interior of the volume $\mathscr{V}$, by virtue of the closure relation (31) and Eq. (33) we have

$$\overline{\Psi}_{\hat{\mathfrak{b}}}(E,\mathbf{r}) \equiv \int_{\mathscr{V}} d^3\mathbf{r}' \left\{ \sum_k \Psi_{\hat{\mathfrak{b}}k}(\mathbf{r}) \Psi^*_{\hat{\mathfrak{b}}k}(\mathbf{r}') \right\} \Psi(E,\mathbf{r}') = \Psi(E,\mathbf{r}) \quad (\mathbf{r} \in \mathscr{V} \setminus \mathscr{S}). \tag{43}$$

On utilizing this result in Eq. (39) we obtain

$$\Psi(E,\mathbf{r}) = \int_{\mathscr{S}} d^2\boldsymbol{\rho}' \frac{\hbar^2}{2m} \sum_k \frac{\Psi_{\hat{\mathfrak{b}}k}(\mathbf{r}) \Psi^*_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho}')}{E_{\hat{\mathfrak{b}}k} - E} [\nabla'_n - \hat{\mathfrak{b}}] \Psi(E,\boldsymbol{\rho}') \quad (\mathbf{r} \in \mathscr{V} \setminus \mathscr{S}). \tag{44}$$

The relation (44) is valid for points $\mathbf{r}$ lying arbitrarily close to the surface $\mathscr{S}$. The function $\Psi(E,\mathbf{r})$ obeys the second-order differential equation (11) and therefore it is continuous across the surface $\mathscr{S}$. Hence, we must have

$$\Psi(E,\boldsymbol{\rho}) = \lim_{\mathbf{r} \to \boldsymbol{\rho}} \int_{\mathscr{S}} d^2\boldsymbol{\rho}' \frac{\hbar^2}{2m} \sum_k \frac{\Psi_{\hat{\mathfrak{b}}k}(\mathbf{r}) \Psi^*_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho}')}{E_{\hat{\mathfrak{b}}k} - E} [\nabla'_n - \hat{\mathfrak{b}}] \Psi(E,\boldsymbol{\rho}') \quad (\mathbf{r} \in \mathscr{V} \setminus \mathscr{S}) \tag{45}$$

and comparison of Eqs. (22) and (45) yields the following representation of the kernel $\mathscr{R}_{\hat{\mathfrak{b}}}(E,\boldsymbol{\rho},\boldsymbol{\rho}')$:

$$\mathscr{R}_{\hat{\mathfrak{b}}}(E,\boldsymbol{\rho},\boldsymbol{\rho}') = \lim_{\mathbf{r} \to \boldsymbol{\rho}} \left\{ \frac{\hbar^2}{2m} \sum_k \frac{\Psi_{\hat{\mathfrak{b}}k}(\mathbf{r}) \Psi^*_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho}')}{E_{\hat{\mathfrak{b}}k} - E} \right\}. \tag{46}$$

The question which arises now is: Can the operations $\underline{\lim}_{\mathbf{r}\to\boldsymbol{\rho}}$ and Σ_k be interchanged in Eq. (46)? Or, in other words, are the kernels $\mathscr{R}_{\hat{\mathfrak{b}}}(E,\boldsymbol{\rho},\boldsymbol{\rho}')$ and $\mathscr{R}_{\hat{\mathfrak{b}}}(E,\boldsymbol{\rho},\boldsymbol{\rho}')$ identical? We shall show now that in the nonrelativistic case discussed in the present section the answer is positive. To this end, we observe that the question posed is closely related to the following problem: How does the closure relation for the functions $\{\Psi_{\hat{\mathfrak{b}}k}(\mathbf{r})\}$ look whenever any of the points $\mathbf{r},\mathbf{r}'$ lies on the surface $\mathscr{S}$? On the ground of the analysis of the form of Eq. (31) and the first of Eqs. (10) we assume that the following relations hold:

$$\sum_k \Psi_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho})\Psi^*_{\hat{\mathfrak{b}}k}(\mathbf{r}')=\mathscr{A}_{\hat{\mathfrak{b}}}(\boldsymbol{\rho},\boldsymbol{\rho}')\,\delta^{(1)}_{\mathscr{S}}(\mathbf{r}') \quad (\mathbf{r}'\in\mathscr{V}), \tag{47}$$

$$\sum_k \Psi_{\hat{\mathfrak{b}}k}(\mathbf{r})\Psi^*_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho}')=\mathscr{A}_{\hat{\mathfrak{b}}}(\boldsymbol{\rho},\boldsymbol{\rho}')\,\delta^{(1)}_{\mathscr{S}}(\mathbf{r}) \quad (\mathbf{r}\in\mathscr{V}), \tag{48}$$

where the kernel $\mathscr{A}_{\hat{\mathfrak{b}}}(\boldsymbol{\rho},\boldsymbol{\rho}')$ defining the surface integral operator $\hat{\mathscr{A}}_{\hat{\mathfrak{b}}}$ is to be found. It stems from the definitions (33) and (47) that the kernel $\mathscr{A}_{\hat{\mathfrak{b}}}(\boldsymbol{\rho},\boldsymbol{\rho}')$ relates the surface functions $\overline{\Psi}_{\hat{\mathfrak{b}}}(E,\boldsymbol{\rho})$ and $\Psi(E,\boldsymbol{\rho})$ according to

$$\overline{\Psi}_{\hat{\mathfrak{b}}}(E,\boldsymbol{\rho})=\int_{\mathscr{S}} d^2\boldsymbol{\rho}'\ \mathscr{A}_{\hat{\mathfrak{b}}}(\boldsymbol{\rho},\boldsymbol{\rho}')\Psi(E,\boldsymbol{\rho}'). \tag{49}$$

Equivalently, in an abstract form Eq. (49) reads

$$\overline{\Psi}_{\hat{\mathfrak{b}}}(E,\boldsymbol{\rho})=\hat{\mathscr{A}}_{\hat{\mathfrak{b}}}\Psi(E,\boldsymbol{\rho}). \tag{50}$$

To determine $\mathscr{A}_{\hat{\mathfrak{b}}}(\boldsymbol{\rho},\boldsymbol{\rho}')$ we postmultiply the kernel

$$\sum_{k'} \Psi_{\hat{\mathfrak{b}}k'}(\boldsymbol{\rho})\Psi^*_{\hat{\mathfrak{b}}k'}(\mathbf{r}')$$

with an arbitrary eigenfunction from the basis set $\{\Psi_{\hat{\mathfrak{b}}k}(\mathbf{r}')\}$ and integrate the result over the volume $\mathscr{V}$. On one hand, from the orthogonality relation (30) one obtains

$$\int_{\mathscr{V}} d^3\mathbf{r}'\left\{\sum_{k'} \Psi_{\hat{\mathfrak{b}}k'}(\boldsymbol{\rho})\Psi^*_{\hat{\mathfrak{b}}k'}(\mathbf{r}')\right\}\Psi_{\hat{\mathfrak{b}}k}(\mathbf{r}')=\Psi_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho}). \tag{51}$$

On the other hand, from Eq. (47) one finds

$$\int_{\mathscr{V}} d^3\mathbf{r}'\left\{\sum_{k'} \Psi_{\hat{\mathfrak{b}}k'}(\boldsymbol{\rho})\Psi^*_{\hat{\mathfrak{b}}k'}(\mathbf{r}')\right\}\Psi_{\hat{\mathfrak{b}}k}(\mathbf{r}')=\hat{\mathscr{A}}_{\hat{\mathfrak{b}}}\Psi_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho}). \tag{52}$$

From Eqs. (51) and (52) one infers that

$$\hat{\mathscr{A}}_{\hat{\mathfrak{b}}}\Psi_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho})=\Psi_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho}). \tag{53}$$

This relation holds for an arbitrary scalar eigenfunction $\Psi_{\hat{\mathfrak{b}}k}$ and therefore we conclude that

$$\hat{\mathscr{A}}_{\hat{\mathfrak{b}}}=\hat{\mathscr{I}}\Leftrightarrow\mathscr{A}_{\hat{\mathfrak{b}}}(\boldsymbol{\rho},\boldsymbol{\rho}')=\delta^{(2)}(\boldsymbol{\rho}-\boldsymbol{\rho}') \tag{54}$$

(here $\hat{\mathscr{I}}$ denotes the unit operator) which, in conjunction with Eq. (50), implies that

$$\overline{\Psi}_{\hat{\mathfrak{b}}}(E,\boldsymbol{\rho})=\Psi(E,\boldsymbol{\rho}), \tag{55}$$

i.e., the eigenfunction expansion $\overline{\Psi}_{\hat{\mathfrak{b}}}(E,\mathbf{r})$ converges to the function $\Psi(E,\mathbf{r})$ also at the surface $\mathscr{S}$. From Eqs. (41) and (56) we infer that

$$\Psi(E,\boldsymbol{\rho})=\hat{\hat{\mathscr{R}}}_{\hat{\mathfrak{b}}}(E)[\nabla_n-\hat{\mathfrak{b}}]\Psi(E,\boldsymbol{\rho}), \tag{56}$$

hence it follows that the operators $\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}(E)$ and $\hat{\hat{\mathscr{R}}}_{\hat{\mathfrak{b}}}(E)$ are identical,

$$\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}(E)=\hat{\hat{\mathscr{R}}}_{\hat{\mathfrak{b}}}(E) \tag{57}$$

and therefore [cf. Eq. (42)] one has

$$\mathscr{R}_{\hat{\mathfrak{b}}}(E,\boldsymbol{\rho},\boldsymbol{\rho}')=\frac{\hbar^2}{2m}\sum_k \frac{\Psi_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho})\Psi^*_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho}')}{E_{\hat{\mathfrak{b}}k}-E}, \tag{58}$$

which means that the operations Σ_k and $\lim_{\mathbf{r}\to\boldsymbol{\rho}}$ in Eq. (46) do commute. We have thus completed the task of finding the kernel of the operator $\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}(E)$. It is to be noticed that, in virtue of the reality of the eigenvalues $\{E_{\hat{\mathfrak{b}}k}\}$, it follows from Eq. (58) that the kernel $\mathscr{R}_{\hat{\mathfrak{b}}}(E,\boldsymbol{\rho},\boldsymbol{\rho}')$ possesses the property

$$\mathscr{R}_{\hat{\mathfrak{b}}}(E,\boldsymbol{\rho},\boldsymbol{\rho}')=\mathscr{R}^*_{\hat{\mathfrak{b}}}(E,\boldsymbol{\rho}',\boldsymbol{\rho}), \tag{59}$$

which means that the operator $\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}(E)$ is Hermitian.

Once the kernel $\mathscr{R}_{\hat{\mathfrak{b}}}(E,\boldsymbol{\rho},\boldsymbol{\rho}')$ has been determined, the *R*-matrix $\mathsf{R}_{\mathfrak{b}}(E)$ may be found. Projecting Eq. (58) from the left and from the right on the surface basis functions $\{\Phi_i(\boldsymbol{\rho})\}$ we get the well known result for $\mathsf{R}_{\mathfrak{b}}(E)$ (cf., for instance, Ref. 9)

$$\mathsf{R}_{\mathfrak{b}}(E)=\frac{\hbar^2}{2m}\sum_k \frac{\mathsf{P}_{\mathfrak{b}k}\mathsf{P}^{\dagger}_{\mathfrak{b}k}}{E_{\mathfrak{b}k}-E}, \tag{60}$$

where $\{\mathsf{P}_{\mathfrak{b}k}\}$ are column vectors with elements $\{P_{i,\mathfrak{b}k}=(\Phi_i|\Psi_{\hat{\mathfrak{b}}k})\}$ and $\{\mathsf{P}^{\dagger}_{\mathfrak{b}k}\}$ are row vectors with elements $\{P^*_{i,\mathfrak{b}k}=(\Psi_{\hat{\mathfrak{b}}k}|\Phi_i)\}$. Equation (60) is to be used in Eq. (25). Thus, we have completed the task of finding the matrix $\mathsf{R}_{\mathfrak{b}}(E)$ using the integral operators formalism.

In addition, it is to be noticed that as a by-product of the determination of the operator $\hat{\mathscr{A}}_{\hat{\mathfrak{b}}}$, from Eqs. (47), (48) and the second of Eqs. (54) we obtain the following extensions of the closure relation (31) for the cases when the point $\mathbf{r}'$ lies on the surface $\mathscr{S}$,

$$\sum_k \Psi_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho}')\Psi^*_{\hat{\mathfrak{b}}k}(\mathbf{r})=\sum_k \Psi_{\hat{\mathfrak{b}}k}(\mathbf{r})\Psi^*_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho}')=\delta^{(3)}(\mathbf{r}-\boldsymbol{\rho}') \quad (\mathbf{r}\in\mathscr{V}). \tag{61}$$

IV. *R*-MATRIX THEORY FOR THE DIRAC EQUATION

A. The operators $\hat{\mathscr{R}}^{(\pm)}_{\hat{\mathfrak{b}}}(E)$

In this section we shall present an operator formulation of the *R*-matrix theory for a Dirac particle moving in a real, local, in general noncentral potential $V(\mathbf{r})$. As in the nonrelativistic case discussed above, we restrict our considerations to the closed volume $\mathscr{V}$ surrounded by the surface $\mathscr{S}$ [in this connection, see a remark preceding Eq. (11)]. The time-independent Dirac equation describing the particle is

$$[\hat{H}-E]\Psi(E,\mathbf{r})=0, \tag{62}$$

where E is the total energy of the particle (including its rest energy mc^2) and the Hamiltonian $\hat{H}$ is

$$\hat{H}=-ic\hbar\,\boldsymbol{\alpha}\cdot\boldsymbol{\nabla}+\beta mc^2+V(\mathbf{r}), \tag{63}$$

where the Hermitian 4×4 Dirac matrices $\boldsymbol{\alpha}$ and β are defined as usual.[20]

Before proceeding further, we have to define a matrix function

$$\alpha_n(\boldsymbol{\rho})=\mathbf{n}(\boldsymbol{\rho})\cdot\boldsymbol{\alpha} \tag{64}$$

and a set of matrices

$$\beta^{(\pm)}=\frac{I\pm\beta}{2},\quad \alpha_n^{(\pm)}(\boldsymbol{\rho})=\beta^{(\pm)}\alpha_n(\boldsymbol{\rho}), \tag{65}$$

where I is the unit 4×4 matrix. The matrices $\alpha_n^{(\pm)}(\boldsymbol{\rho})$ and $\beta^{(\pm)}$ satisfy the following relations:

$$\alpha_n^{(+)}(\boldsymbol{\rho})+\alpha_n^{(-)}(\boldsymbol{\rho})=\alpha_n(\boldsymbol{\rho}),\quad \beta^{(+)}+\beta^{(-)}=I, \tag{66}$$

$$\alpha_n^{(\pm)\dagger}(\boldsymbol{\rho})=\alpha_n^{(\mp)}(\boldsymbol{\rho}),\quad \beta^{(\pm)\dagger}=\beta^{(\pm)}. \tag{67}$$

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

$$\beta^{(\pm)}\beta^{(\pm)}=\beta^{(\pm)},\quad \beta^{(\pm)}\beta^{(\mp)}=0,\quad \alpha_n^{(\pm)}(\boldsymbol{\rho})\alpha_n^{(\pm)}(\boldsymbol{\rho})=0,\quad \alpha_n^{(\pm)}(\boldsymbol{\rho})\alpha_n^{(\mp)}(\boldsymbol{\rho})=\beta^{(\pm)}, \tag{68}$$

$$\alpha_n^{(\pm)}(\boldsymbol{\rho})\beta^{(\pm)}=0,\quad \beta^{(\pm)}\alpha_n^{(\pm)}(\boldsymbol{\rho})=\alpha_n^{(\pm)}(\boldsymbol{\rho}),\quad \beta^{(\pm)}\alpha_n^{(\mp)}(\boldsymbol{\rho})=0,\quad \alpha_n^{(\pm)}(\boldsymbol{\rho})\beta^{(\mp)}=\alpha_n^{(\pm)}(\boldsymbol{\rho}), \tag{69}$$

which may be easily derived from the definitions (64) and (65) and the anticommutation relations satisfied by the matrices $\boldsymbol{\alpha}$ and β.[20] Henceforth, whenever the matrices $\alpha_n^{(\pm)}(\boldsymbol{\rho})$ multiply an integral operator, we shall omit their argument $\boldsymbol{\rho}$ and assume that the following notational convention holds: If $\hat{\mathscr{O}}$ is an operator with a kernel $\mathscr{O}(\boldsymbol{\rho},\boldsymbol{\rho}')$, then $\alpha_n^{(\pm)}\hat{\mathscr{O}}$ and $\hat{\mathscr{O}}\alpha_n^{(\pm)}$ are operators with kernels $\alpha_n^{(\pm)}(\boldsymbol{\rho})\mathscr{O}(\boldsymbol{\rho},\boldsymbol{\rho}')$ and $\mathscr{O}(\boldsymbol{\rho},\boldsymbol{\rho}')\alpha_n^{(\pm)}(\boldsymbol{\rho}')$, respectively.

After that preparation we are now ready to attack the problem posed. Let $\Psi(E,\mathbf{r})$ and $\Psi'(E,\mathbf{r})$ be two solutions to Eq. (62) at the same energy E. On applying the Gauss divergence theorem we find

$$\langle\hat{H}\Psi'|\Psi\rangle-\langle\Psi'|\hat{H}\Psi\rangle=(\Psi'|ic\hbar\alpha_n\Psi). \tag{70}$$

By virtue of the reality of E, the left-hand side of this equation vanishes and we obtain

$$(\Psi'|i\alpha_n\Psi)=0. \tag{71}$$

On utilizing Eqs. (66) and (67) we may rewrite this relation in two equivalent forms,

$$(i\alpha_n^{(+)}\Psi'|\Psi)=(\Psi'|i\alpha_n^{(+)}\Psi),\quad (i\alpha_n^{(-)}\Psi'|\Psi)=(\Psi'|i\alpha_n^{(-)}\Psi). \tag{72}$$

Relations (72) may be formally interpreted that $i\alpha_n^{(\pm)}$, when acting on solutions of the Dirac equation (62) at fixed energy E, are Hermitian with respect to the surface scalar product $(|)$.

In the next step, we introduce two auxiliary energy-dependent linear Hermitian integral operators $\hat{\mathscr{B}}^{(\pm)}(E)$ defined on $L^2_{(|)}(\mathscr{S})$ such that

$$i\alpha_n^{(\pm)}(\boldsymbol{\rho})\Psi(E,\boldsymbol{\rho})=\gamma^{(\pm)}\hat{\mathscr{B}}^{(\pm)}(E)\Psi(E,\boldsymbol{\rho}) \tag{73}$$

for any solution of Eq. (62) at energy E. In Eq. (73) and hereafter

$$\gamma^{(\pm)}=\pm\left(\frac{\hbar}{2mc}\right)^{\pm 1} \tag{74}$$

are numerical constants introduced for later convenience, primarily to facilitate a later discussion of the nonrelativistic limit [notice that $\gamma^{(\mp)}=-(\gamma^{(\pm)})^{-1}$]. The operators $\hat{\mathscr{B}}^{(\pm)}(E)$ are represented by their integral kernels $\mathscr{B}^{(\pm)}(E,\boldsymbol{\rho},\boldsymbol{\rho}')$ and Eq. (73) may be equivalently rewritten in the form

$$i\alpha_n^{(\pm)}(\boldsymbol{\rho})\Psi(E,\boldsymbol{\rho})=\gamma^{(\pm)}\int_{\mathscr{S}}d^2\boldsymbol{\rho}'\ \mathscr{B}^{(\pm)}(E,\boldsymbol{\rho},\boldsymbol{\rho}')\Psi(E,\boldsymbol{\rho}'). \tag{75}$$

The existence of the operators $\hat{\mathscr{B}}^{(\pm)}(E)$ has been proved by Szmytkowski[21] who has shown that the kernels $\mathscr{B}^{(\pm)}(E,\boldsymbol{\rho},\boldsymbol{\rho}')$ may be written in the forms

$$\mathscr{B}^{(+)}(E,\boldsymbol{\rho},\boldsymbol{\rho}')=\sum_i \beta^{(+)}\Psi_i(E,\boldsymbol{\rho})b_i(E)\Psi_i^\dagger(E,\boldsymbol{\rho}')\beta^{(+)}, \tag{76}$$

$$\mathscr{B}^{(-)}(E,\boldsymbol{\rho},\boldsymbol{\rho}')=(\gamma^{(-)})^2\sum_i \beta^{(-)}\Psi_i(E,\boldsymbol{\rho})b_i^{-3}(E)\Psi_i^\dagger(E,\boldsymbol{\rho}')\beta^{(-)}, \tag{77}$$

where $\{\Psi_i(E,\mathbf{r})\}$ are those solutions to the Dirac equation (62) at energy E which on the surface $\mathscr{S}$ satisfy the relations

$$i\alpha_n^{(+)}(\boldsymbol{\rho})\Psi_i(E,\boldsymbol{\rho})=\gamma^{(+)}b_i(E)\beta^{(+)}\Psi_i(E,\boldsymbol{\rho}) \tag{78}$$

and are normalized according to $(\Psi_i|\beta^{(+)}\Psi_i)=1$. It may be shown[21] that, as in the nonrelativistic case, the numbers $\{b_i(E)\}$ are real and that the surface spinor functions $\{\Psi_i(E,\boldsymbol{\rho})\}$ are orthogonal in the sense of $(\Psi_i|\beta^{(+)}\Psi_j)=\delta_{ij}$.

It is to be noticed that Eqs. (76) and (77) imply the following property of the operators $\hat{\mathscr{B}}^{(\pm)}(E)$:

$$\beta^{(\pm)}\hat{\mathscr{B}}^{(\pm)}(E)\beta^{(\pm)}=\hat{\mathscr{B}}^{(\pm)}(E). \tag{79}$$

Moreover, the operators $\hat{\mathscr{B}}^{(+)}(E)$ and $\hat{\mathscr{B}}^{(-)}(E)$ are not independent. Indeed, operating on Eq. (73) from the left with $-i\alpha_n^{(\mp)}(\boldsymbol{\rho})$ yields

$$\beta^{(\mp)}\Psi(E,\boldsymbol{\rho})=-\gamma^{(\pm)}i\alpha_n^{(\mp)}\hat{\mathscr{B}}^{(\pm)}(E)\Psi(E,\boldsymbol{\rho}). \tag{80}$$

Operating then on this equation from the left with $\alpha_n^{(\pm)}\hat{\mathscr{B}}^{(\mp)}(E)$ and transforming the resulting equation with the aid of Eq. (80) gives

$$\beta^{(\pm)}\Psi(E,\boldsymbol{\rho})=\alpha_n^{(\pm)}\hat{\mathscr{B}}^{(\mp)}(E)\alpha_n^{(\mp)}\hat{\mathscr{B}}^{(\pm)}(E)\Psi(E,\boldsymbol{\rho}), \tag{81}$$

which implies that the operators $\hat{\mathscr{B}}^{(\pm)}(E)$ and $\alpha_n^{(\pm)}\hat{\mathscr{B}}^{(\mp)}(E)\alpha_n^{(\mp)}$ are reciprocal in the sense of

$$[\alpha_n^{(\pm)}\hat{\mathscr{B}}^{(\mp)}(E)\alpha_n^{(\mp)}]\hat{\mathscr{B}}^{(\pm)}(E)\hat{\mathscr{P}}^{(\pm)}(E)=\hat{\mathscr{P}}^{(\pm)}(E), \tag{82}$$

where the projectors $\hat{\mathscr{P}}^{(\pm)}(E)$ are related to the operator $\hat{\mathscr{P}}(E)$ projecting on the surface parts of solutions to the Dirac equation (62) at energy E in the following way:

$$\hat{\mathscr{P}}^{(\pm)}(E)=\beta^{(\pm)}\hat{\mathscr{P}}(E)\beta^{(\pm)}. \tag{83}$$

Integral kernels of the projectors $\hat{\mathscr{P}}^{(\pm)}(E)$ are

$$\mathscr{P}^{(+)}(E,\boldsymbol{\rho},\boldsymbol{\rho}')=\sum_i \beta^{(+)}\Psi_i(E,\boldsymbol{\rho})\Psi_i^\dagger(E,\boldsymbol{\rho}')\beta^{(+)}, \tag{84}$$

$$\mathscr{P}^{(-)}(E,\boldsymbol{\rho},\boldsymbol{\rho}')=(\gamma^{(-)})^2\sum_i \beta^{(-)}\Psi_i(E,\boldsymbol{\rho})b_i^{-2}(E)\Psi_i^\dagger(E,\boldsymbol{\rho}')\beta^{(-)}, \tag{85}$$

where the numbers $\{b_i(E)\}$ and the functions $\{\Psi_i(E,\mathbf{r})\}$ have been defined below Eqs. (76) and (77).

A note analogous to that remarked in the paragraph following Eq. (18) is in order here. Namely, we emphasize that the operators $i\alpha_n^{(\pm)}$ and $\gamma^{(\pm)}\hat{\mathscr{B}}^{(\pm)}(E)$ are not identical and for an arbitrary four-component spinor function $\Phi(\boldsymbol{\rho})$ defined on $\mathscr{S}$ in general one has

$$i\alpha_n^{(\pm)}(\boldsymbol{\rho})\Phi(\boldsymbol{\rho})\neq\gamma^{(\pm)}\hat{\mathscr{B}}^{(\pm)}(E)\Phi(\boldsymbol{\rho}) \tag{86}$$

unless $\Phi(\boldsymbol{\rho})$ coincides with a surface part of some solution to the Dirac equation (62) at energy E.

Let $\hat{\mathfrak{b}}^{(+)}$ and $\hat{\mathfrak{b}}^{(-)}$ be two linear Hermitian integral operators defined on $L^2_{(|)}(\mathscr{S})$, with the integral kernels $\mathfrak{b}^{(+)}(\boldsymbol{\rho},\boldsymbol{\rho}')$ and $\mathfrak{b}^{(-)}(\boldsymbol{\rho},\boldsymbol{\rho}')$, respectively. It will be assumed that the operators $\hat{\mathfrak{b}}^{(\pm)}$ are such that

$$\beta^{(\pm)}\hat{\mathfrak{b}}^{(\pm)}\beta^{(\pm)}=\hat{\mathfrak{b}}^{(\pm)} \tag{87}$$

[cf. Eq. (79)] and such that

$$\hat{\mathfrak{b}}^{(\pm)}\alpha_n^{(\pm)}\hat{\mathfrak{b}}^{(\mp)}\alpha_n^{(\mp)}=\alpha_n^{(\pm)}\hat{\mathfrak{b}}^{(\mp)}\alpha_n^{(\mp)}\hat{\mathfrak{b}}^{(\pm)}=\beta^{(\pm)} \tag{88}$$

[cf. Eq. (82)]. We define the operators $\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}^{(+)}(E)$ and $\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}^{(-)}(E)$, possessing the property

$$\beta^{(\pm)}\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}^{(\pm)}(E)\beta^{(\pm)}=\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}^{(\pm)}(E), \tag{89}$$

as the operators reciprocal to the operators $\hat{\mathscr{B}}^{(+)}(E)-\hat{\mathfrak{b}}^{(+)}$ and $\hat{\mathscr{B}}^{(-)}(E)-\hat{\mathfrak{b}}^{(-)}$, respectively, in the sense of

$$\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}^{(\pm)}(E)[\hat{\mathscr{B}}^{(\pm)}(E)-\hat{\mathfrak{b}}^{(\pm)}]\hat{\mathscr{I}}^{(\pm)}(E)=\hat{\mathscr{I}}^{(\pm)}(E). \tag{90}$$

In Sec. IV B we shall show how the operator $\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}^{(+)}(E)$ is related to the operator $\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}(E)$ encountered in the nonrelativistic theory.

In terms of the operators $\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}^{(\pm)}(E)$ the surface relation (73) may be rewritten as

$$\beta^{(\pm)}\Psi(E,\boldsymbol{\rho})=-\gamma^{(\mp)}\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}^{(\pm)}(E)[i\alpha_n^{(\pm)}-\gamma^{(\pm)}\hat{\mathfrak{b}}^{(\pm)}]\Psi(E,\boldsymbol{\rho}) \tag{91}$$

or, explicitly,

$$\beta^{(\pm)}\Psi(E,\boldsymbol{\rho})=-\gamma^{(\mp)}\int_{\mathscr{S}}d^2\boldsymbol{\rho}'\ \mathscr{R}_{\hat{\mathfrak{b}}}^{(\pm)}(E,\boldsymbol{\rho},\boldsymbol{\rho}')[i\alpha_n^{(\pm)}(\boldsymbol{\rho}')-\gamma^{(\pm)}\hat{\mathfrak{b}}^{(\pm)}]\Psi(E,\boldsymbol{\rho}'). \tag{92}$$

Assume now that a complete set of spinor functions $\{\Phi_i(\boldsymbol{\rho})\}\in L^2_{(|)}(\mathscr{S})$ orthonormal with respect to the surface scalar product $(|)$, spanning the surface $\mathscr{S}$, is given. In the basis $\{\Phi_i(\boldsymbol{\rho})\}$ the kernels $\mathscr{R}_{\hat{\mathfrak{b}}}^{(\pm)}(E,\boldsymbol{\rho},\boldsymbol{\rho}')$ have bilinear expansions

$$\mathscr{R}_{\hat{\mathfrak{b}}}^{(\pm)}(E,\boldsymbol{\rho},\boldsymbol{\rho}')=\sum_{i,j}\ \beta^{(\pm)}\Phi_i(\boldsymbol{\rho})(\Phi_i|\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}^{(\pm)}\Phi_j)\Phi_j^{\dagger}(\boldsymbol{\rho}')\beta^{(\pm)}, \tag{93}$$

where the coefficients

$$(\Phi_i|\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}^{(+)}\Phi_j)\equiv\int_{\mathscr{S}}d^2\boldsymbol{\rho}\int_{\mathscr{S}}d^2\boldsymbol{\rho}'\ \Phi_i^{\dagger}(\boldsymbol{\rho})\mathscr{R}_{\hat{\mathfrak{b}}}^{(+)}(E,\boldsymbol{\rho},\boldsymbol{\rho}')\Phi_j(\boldsymbol{\rho}') \tag{94}$$

and

$$(\Phi_i|\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}^{(-)}\Phi_j)\equiv\int_{\mathscr{S}}d^2\boldsymbol{\rho}\int_{\mathscr{S}}d^2\boldsymbol{\rho}'\ \Phi_i^{\dagger}(\boldsymbol{\rho})\mathscr{R}_{\hat{\mathfrak{b}}}^{(-)}(E,\boldsymbol{\rho},\boldsymbol{\rho}')\Phi_j(\boldsymbol{\rho}') \tag{95}$$

form *R*-matrices $\mathsf{R}_{\mathsf{b}}^{(+)}(E)$ and $\mathsf{R}_{\mathsf{b}}^{(-)}(E)$, respectively. To relate the matrix and operator formulations of the theory, we need a matrix representation of Eq. (91). Projecting the latter equation from the left on the basis spinor functions $\{\Phi_i(\boldsymbol{\rho})\}$ gives

$$\mathsf{P}^{(\pm)}(E)=\mathsf{R}_{\mathsf{b}}^{(\pm)}(E)\left[\pm\left(\frac{2mc}{\hbar}\right)^{\pm1}\mathsf{Q}^{(\pm)}(E)-\mathsf{b}^{(\pm)}\mathsf{P}^{(\pm)}(E)\right], \tag{96}$$

where $\mathsf{P}^{(\pm)}(E)$ and $\mathsf{Q}^{(\pm)}(E)$ are column matrices with elements $\{P_i^{(\pm)}(E)=(\Phi_i|\beta^{(\pm)}\Psi)\}$ and $\{Q_i^{(\pm)}(E)=(\Phi_i|i\alpha_n^{(\pm)}\Psi)\}$, respectively, and $\mathsf{b}^{(\pm)}$ are square matrices with elements

$\{b_{ij}^{(\pm)}=(\Phi_i|\hat{\mathfrak{b}}^{(\pm)}\Phi_j)\}$. Equations (96) are the counterparts of the nonrelativistic formula (1). The relation which corresponds to the choice of the upper sign in Eq. (96) was found before by Chang.[16]

In Sec. IV C we shall show how the integral kernels of the operators $\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}^{(\pm)}(E)$ may be constructed.

B. The nonrelativistic limit

It is of interest to investigate the nonrelativistic limit of Eq. (91) in order to relate the relativistic and nonrelativistic formulations of the operator versions of the *R*-matrix theory. To accomplish this goal, we proceed in the standard manner and express the relativistic four-component wave function $\Psi(E,\mathbf{r})$ in terms of two-component spinors $\psi_U(E,\mathbf{r})$ and $\psi_L(E,\mathbf{r})$ in the following way:

$$\Psi(E,\mathbf{r})=\begin{pmatrix}\psi_U(E,\mathbf{r})\\ \psi_L(E,\mathbf{r})\end{pmatrix}. \tag{97}$$

It is a standard problem in introductory quantum mechanics to show that in the nonrelativistic limit the function $\psi_U(E,\mathbf{r})$ obeys the Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2+V(\mathbf{r})-E\right]\psi_U(E,\mathbf{r})=0 \quad (c\to\infty) \tag{98}$$

[cf. Eqs. (11) and (12)] while

$$\psi_L(E,\mathbf{r}) \xrightarrow{c\to\infty} -\left(\frac{\hbar}{2mc}\right) i\boldsymbol{\sigma}\cdot\boldsymbol{\nabla}\,\psi_U(E,\mathbf{r}), \tag{99}$$

where $\boldsymbol{\sigma}$ is a vector composed of the Pauli matrices. The relation (99) holds for arbitrary $\mathbf{r}$, in particular it is also valid on the surface $\mathscr{S}$, i.e., for $\mathbf{r}=\boldsymbol{\rho}$. Next, we notice that, as a consequence of Eqs. (87) and (89), the operators $\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}^{(+)}(E)$ and $\hat{\mathfrak{b}}^{(+)}$ act on an arbitrary function

$$\Phi(\boldsymbol{\rho})=\begin{pmatrix}\phi_U(\boldsymbol{\rho})\\ \phi_L(\boldsymbol{\rho})\end{pmatrix} \tag{100}$$

from $L^2_{(|)}(\mathscr{S})$ in the following way:

$$\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}^{(+)}(E)\Phi(\boldsymbol{\rho})\equiv\begin{pmatrix}\hat{\mathscr{R}}'_{\hat{\mathfrak{b}}}(E)\,\phi_U(\boldsymbol{\rho})\\ 0\end{pmatrix}, \quad \hat{\mathfrak{b}}^{(+)}\Phi(\boldsymbol{\rho})\equiv\begin{pmatrix}\hat{\mathfrak{b}}'\,\phi_U(\boldsymbol{\rho})\\ 0\end{pmatrix}, \tag{101}$$

where $\hat{\mathscr{R}}'_{\hat{\mathfrak{b}}}(E)$ and $\hat{\mathfrak{b}}'$ are operators acting on two-component functions. Making use of Eq. (101), the surface relation (91) may be rewritten in terms of the upper component of $\Psi(E,\boldsymbol{\rho})$ and of the operators $\hat{\mathscr{R}}'_{\hat{\mathfrak{b}}}(E)$ and $\hat{\mathfrak{b}}'$ in the following way:

$$\psi_U(E,\boldsymbol{\rho})=\hat{\mathscr{R}}'_{\hat{\mathfrak{b}}}(E)\left[\left(\frac{2mc}{\hbar}\right) i\boldsymbol{\sigma}\cdot\mathbf{n}(\boldsymbol{\rho})\,\psi_L(E,\boldsymbol{\rho})-\hat{\mathfrak{b}}'\,\psi_U(E,\boldsymbol{\rho})\right]. \tag{102}$$

The relation (102) is exact. Passing in this relation to the nonrelativistic limit, making use of Eq. (99) and utilizing well-known properties of the Pauli matrices, which give

$$[\boldsymbol{\sigma}\cdot\mathbf{n}(\boldsymbol{\rho})][\boldsymbol{\sigma}\cdot\boldsymbol{\nabla}]=\nabla_n+i\boldsymbol{\sigma}\cdot[\mathbf{n}(\boldsymbol{\rho})\times\boldsymbol{\nabla}], \tag{103}$$

we obtain

$$\psi_U(E,\boldsymbol{\rho})=\hat{\mathscr{R}}'_{\hat{\mathfrak{b}}}(E)[\nabla_n+i\boldsymbol{\sigma}\cdot[\mathbf{n}(\boldsymbol{\rho})\times\boldsymbol{\nabla}]-\hat{\mathfrak{b}}']\,\psi_U(E,\boldsymbol{\rho}) \quad (c\to\infty). \tag{104}$$

It is understood that in Eq. (104) $\psi_U(E,\boldsymbol{\rho})$, $\hat{\mathscr{R}}'_{\hat{\mathfrak{b}}}(E)$ and $\hat{\mathfrak{b}}'$ stand for nonrelativistic limits of the quantities which have been denoted with the same symbols before the passage to the limit has been done. Comparison between Eqs. (22) and (104) shows that in the nonrelativistic limit

$$\hat{\mathscr{R}}'_{\hat{\mathfrak{b}}}(E) \xrightarrow{c\to\infty} \hat{\mathscr{R}}_{\hat{\mathfrak{b}}}(E)\hat{\mathscr{I}} \tag{105}$$

(here $\hat{\mathscr{I}}$ is the unit 2×2 operator) provided that the operator $\hat{\mathfrak{b}}^{(+)}$ is chosen so that

$$\hat{\mathfrak{b}}' \xrightarrow{c\to\infty} \hat{\mathfrak{b}}\hat{\mathscr{I}}+i\boldsymbol{\sigma}\cdot[\mathbf{n}(\boldsymbol{\rho})\times\boldsymbol{\nabla}], \tag{106}$$

where $\hat{\mathfrak{b}}$ is the operator used in the formulation of the theory for the Schrödinger equation (cf. Sec. III A). It is interesting and somewhat surprising that the operators $\hat{\mathfrak{b}}'$ and $\hat{\mathfrak{b}}\hat{\mathscr{I}}$ do not coincide. This observation is, however, consistent with earlier findings of Norrington and Grant[22,23] and of Thumm and Norcross[24] who investigated the nonrelativistic limit of the matrix formulation of the theory in the specific case of the spherically symmetric volume $\mathscr{V}$.

C. Construction of the operators $\hat{\mathscr{R}}^{(\pm)}_{\hat{\mathfrak{b}}}(E)$

Thus far we have discussed some properties of the operators $\hat{\mathscr{R}}^{(\pm)}_{\hat{\mathfrak{b}}}(E)$ but have not touched the problem of construction of integral kernels of these operators. This will be the subject of the present section.

To achieve the goal, we need a set of auxiliary spinor functions $\{\Psi_{\hat{\mathfrak{b}}k}(\mathbf{r})\}$ defined as eigenfunctions of the boundary value problem consisting of the differential equation [cf. Eq. (62)]

$$[\hat{H}-E_{\hat{\mathfrak{b}}k}]\Psi_{\hat{\mathfrak{b}}k}(\mathbf{r})=0 \tag{107}$$

and of the homogeneous boundary condition

$$i\alpha_n^{(\pm)}(\boldsymbol{\rho})\Psi_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho})=\gamma^{(\pm)}\int_{\mathscr{S}}d^2\boldsymbol{\rho}'\ \mathfrak{b}^{(\pm)}(\boldsymbol{\rho},\boldsymbol{\rho}')\Psi_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho}'). \tag{108}$$

In Eq. (107) $\hat{H}$ is the Dirac Hamiltonian defined by Eq. (63) and $E_{\hat{\mathfrak{b}}k}$ is an eigenvalue for the problem belonging to an eigenfunction $\Psi_{\hat{\mathfrak{b}}k}(\mathbf{r})$. In the more compact operator notation the boundary condition (108) reads

$$i\alpha_n^{(\pm)}(\boldsymbol{\rho})\Psi_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho})=\gamma^{(\pm)}\hat{\mathfrak{b}}^{(\pm)}\Psi_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho}). \tag{109}$$

At first sight it might seem that Eqs. (107) and (109) constitute two eigenvalue problems depending on which of the two possible signs is chosen in Eq. (109). Yet this is not the case: It is easy to verify that, because of relation (88), both boundary conditions (109) are essentially equivalent and consequently we have only one eigenvalue problem. For the sake of later applications, we notice also here that the boundary condition (109) may be equivalently rewritten, after operating on it from the left with $-i\alpha_n^{(\mp)}(\boldsymbol{\rho})$, in the form

$$\beta^{(\mp)}\Psi_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho})=-\gamma^{(\pm)}i\alpha_n^{(\mp)}\hat{\mathfrak{b}}^{(\pm)}\Psi_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho}) \tag{110}$$

hence, it follows that

$$\Psi_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho})\equiv\beta^{(\pm)}\Psi_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho})+\beta^{(\mp)}\Psi_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho})=[\beta^{(\pm)}-\gamma^{(\pm)}i\alpha_n^{(\mp)}\hat{\mathfrak{b}}^{(\pm)}]\Psi_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho}). \tag{111}$$

Henceforth we shall assume that the integral operators $\hat{\mathfrak{b}}^{(\pm)}$ are such that the eigenfunctions $\{\Psi_{\hat{\mathfrak{b}}k}(\mathbf{r})\}$ form a complete set in the interior of the volume $\mathscr{V}$. It may be inferred from Eqs. (107) and (109) and from properties of the operators $\hat{\mathfrak{b}}^{(\pm)}$ that eigenvalues $\{E_{\hat{\mathfrak{b}}k}\}$ are real and eigenfunctions $\{\Psi_{\hat{\mathfrak{b}}k}(\mathbf{r})\}$ belonging to different eigenvalues are orthogonal. Indeed, after premultiplying Eq. (107) (with k replaced by k') by $\Psi^{\dagger}_{\hat{\mathfrak{b}}k}(\mathbf{r})$, postmultiplying the matrix Hermitian conjugate of Eq.

(107) by $\Psi_{\hat{\mathfrak{b}}k'}(\mathbf{r})$, subtracting, integrating the result over the volume $\mathscr{V}$, employing the Gauss divergence theorem, making use of the boundary condition (107) and of the Hermicity of $\hat{\mathfrak{b}}^{(\pm)}$, one arrives at

$$[E_{\hat{\mathfrak{b}}k}^{*}-E_{\hat{\mathfrak{b}}k'}]\langle\Psi_{\hat{\mathfrak{b}}k}|\Psi_{\hat{\mathfrak{b}}k'}\rangle=0, \tag{112}$$

hence the validity of the assertion follows immediately. Hereafter we shall assume that functions belonging to degenerate eigenvalues (if there are any) have also been orthogonalized and that the functions $\{\Psi_{\hat{\mathfrak{b}}k}(\mathbf{r})\}$ have been normalized so that

$$\langle\Psi_{\hat{\mathfrak{b}}k}|\Psi_{\hat{\mathfrak{b}}k'}\rangle=\delta_{kk'}\,. \tag{113}$$

On the ground of the assumed completeness, the eigenfunctions $\{\Psi_{\hat{\mathfrak{b}}k}(\mathbf{r})\}$ obey the closure relation

$$\sum_{k}\ \Psi_{\hat{\mathfrak{b}}k}(\mathbf{r})\Psi_{\hat{\mathfrak{b}}k}^{\dagger}(\mathbf{r}')=\delta^{(3)}(\mathbf{r}-\mathbf{r}')I \quad (\mathbf{r},\mathbf{r}'\in\mathscr{V}\setminus\mathscr{S}) \tag{114}$$

[cf. the remark following Eq. (31)].

Consider now a problem of expanding the function $\Psi(E,\mathbf{r})$ satisfying the Dirac equation (62) in the series of eigenfunctions $\{\Psi_{\hat{\mathfrak{b}}k}(\mathbf{r})\}$. Denoting the expansion by $\overline{\Psi}_{\hat{\mathfrak{b}}}(E,\mathbf{r})$, we have

$$\overline{\Psi}_{\hat{\mathfrak{b}}}(E,\mathbf{r})\equiv\sum_{k}\ \Psi_{\hat{\mathfrak{b}}k}(\mathbf{r})\langle\Psi_{\hat{\mathfrak{b}}k}|\Psi\rangle \tag{115}$$

or equivalently

$$\overline{\Psi}_{\hat{\mathfrak{b}}}(E,\mathbf{r})\equiv\int_{\mathscr{V}}d^{3}\mathbf{r}'\left\{\sum_{k}\ \Psi_{\hat{\mathfrak{b}}k}(\mathbf{r})\Psi_{\hat{\mathfrak{b}}k}^{\dagger}(\mathbf{r}')\right\}\Psi(E,\mathbf{r}'). \tag{116}$$

The expansion coefficients $\langle\Psi_{\hat{\mathfrak{b}}k}|\Psi\rangle$ may be found in the routine way. We premultiply Eq. (62) by $\Psi_{\hat{\mathfrak{b}}k}^{\dagger}(\mathbf{r})$, postmultiply the matrix Hermitian conjugate of Eq. (107) by $\Psi(E,\mathbf{r})$, subtract and integrate over the volume $\mathscr{V}$ obtaining

$$ic\hbar\int_{\mathscr{V}}d^{3}\mathbf{r}\ \ \nabla\cdot[\Psi_{\hat{\mathfrak{b}}k}^{\dagger}(\mathbf{r})\boldsymbol{\alpha}\Psi(E,\mathbf{r})]=[E_{\hat{\mathfrak{b}}k}-E]\langle\Psi_{\hat{\mathfrak{b}}k}|\Psi\rangle. \tag{117}$$

Employing the Gauss divergence theorem, the volume integral on the left-hand side may be converted into a surface integral

$$\int_{\mathscr{V}}d^{3}\mathbf{r}\ \nabla\cdot[\Psi_{\hat{\mathfrak{b}}k}^{\dagger}(\mathbf{r})\boldsymbol{\alpha}\Psi(E,\mathbf{r})]=\int_{\mathscr{S}}d^{2}\boldsymbol{\rho}\ \Psi_{\hat{\mathfrak{b}}k}^{\dagger}(\boldsymbol{\rho})\alpha_{n}(\boldsymbol{\rho})\Psi(E,\boldsymbol{\rho}). \tag{118}$$

This yields

$$\langle\Psi_{\hat{\mathfrak{b}}k}|\Psi\rangle=\frac{(\Psi_{\hat{\mathfrak{b}}k}|ic\hbar\,\alpha_{n}\Psi)}{E_{\hat{\mathfrak{b}}k}-E}. \tag{119}$$

Making use of the properties of the matrices $\alpha_{n}(\boldsymbol{\rho})$ and $\alpha_{n}^{(\pm)}(\boldsymbol{\rho})$, of the boundary condition (109) and of the Hermicity property of the operators $\hat{\mathfrak{b}}^{(\pm)}$ we transform this expression to the form

$$\langle\Psi_{\hat{\mathfrak{b}}k}|\Psi\rangle=\frac{c\hbar(\Psi_{\hat{\mathfrak{b}}k}|[i\alpha_{n}^{(\pm)}-\gamma^{(\pm)}\hat{\mathfrak{b}}^{(\pm)}]\Psi)}{E_{\hat{\mathfrak{b}}k}-E} \tag{120}$$

and consequently we arrive at

$$\overline{\Psi}_{\hat{\mathfrak{b}}}(E,\mathbf{r})=\sum_k \Psi_{\hat{\mathfrak{b}}k}(\mathbf{r})\,\frac{c\hbar(\Psi_{\hat{\mathfrak{b}}k}|[i\alpha_n^{(\pm)}-\gamma^{(\pm)}\hat{\mathfrak{b}}^{(\pm)}]\Psi)}{E_{\hat{\mathfrak{b}}k}-E} \tag{121}$$

or equivalently

$$\overline{\Psi}_{\hat{\mathfrak{b}}}(E,\mathbf{r})=\int_{\mathscr{S}}d^2\boldsymbol{\rho}'\;c\hbar\sum_k\;\frac{\Psi_{\hat{\mathfrak{b}}k}(\mathbf{r})\Psi^{\dagger}_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho}')}{E_{\hat{\mathfrak{b}}k}-E}\,[i\alpha_n^{(\pm)}(\boldsymbol{\rho}')-\gamma^{(\pm)}\hat{\mathfrak{b}}^{(\pm)}]\Psi(E,\boldsymbol{\rho}'). \tag{122}$$

In particular, if the point $\mathbf{r}$ lies on the surface $\mathscr{S}$, then we have

$$\overline{\Psi}_{\hat{\mathfrak{b}}}(E,\boldsymbol{\rho})=\int_{\mathscr{S}}d^2\boldsymbol{\rho}'\;c\hbar\sum_k\;\frac{\Psi_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho})\Psi^{\dagger}_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho}')}{E_{\hat{\mathfrak{b}}k}-E}\,[i\alpha_n^{(\pm)}(\boldsymbol{\rho}')-\gamma^{(\pm)}\hat{\mathfrak{b}}^{(\pm)}]\Psi(E,\boldsymbol{\rho}'). \tag{123}$$

At that moment, it is convenient to define two integral operators $\hat{\overline{\mathscr{R}}}^{(\pm)}_{\hat{\mathfrak{b}}}(E)$ (notice the bar) such that [cf. Eq. (91)]

$$\beta^{(\pm)}\overline{\Psi}_{\hat{\mathfrak{b}}}(E,\boldsymbol{\rho})=-\gamma^{(\mp)}\hat{\overline{\mathscr{R}}}^{(\pm)}_{\hat{\mathfrak{b}}}(E)[i\alpha_n^{(\pm)}-\gamma^{(\pm)}\hat{\mathfrak{b}}^{(\pm)}]\Psi(E,\boldsymbol{\rho}). \tag{124}$$

Comparison of Eqs. (123) and (124) shows that the operators $\hat{\overline{\mathscr{R}}}^{(\pm)}_{\hat{\mathfrak{b}}}(E)$ have the integral kernels

$$\overline{\mathscr{R}}^{(\pm)}_{\hat{\mathfrak{b}}}(E,\boldsymbol{\rho},\boldsymbol{\rho}')=c\hbar\,\gamma^{(\pm)}\sum_k\;\frac{\beta^{(\pm)}\Psi_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho})\Psi^{\dagger}_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho}')\beta^{(\pm)}}{E_{\hat{\mathfrak{b}}k}-E}. \tag{125}$$

By virtue of the closure relation (114), in the interior of the volume $\mathscr{V}$ one has

$$\overline{\Psi}_{\hat{\mathfrak{b}}}(E,\mathbf{r})\equiv\int_{\mathscr{V}}d^3\mathbf{r}'\left\{\sum_k\;\Psi_{\hat{\mathfrak{b}}k}(\mathbf{r})\Psi^{\dagger}_{\hat{\mathfrak{b}}k}(\mathbf{r}')\right\}\Psi(E,\mathbf{r}')=\Psi(E,\mathbf{r})\quad(\mathbf{r}\in\mathscr{V}\setminus\mathscr{S}), \tag{126}$$

i.e., the expansion $\overline{\Psi}_{\hat{\mathfrak{b}}}(E,\mathbf{r})$ does converge to the function $\Psi(E,\mathbf{r})$ and consequently

$$\Psi(E,\mathbf{r})=\int_{\mathscr{S}}d^2\boldsymbol{\rho}'\;c\hbar\sum_k\;\frac{\Psi_{\hat{\mathfrak{b}}k}(\mathbf{r})\Psi^{\dagger}_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho}')}{E_{\hat{\mathfrak{b}}k}-E}\,[i\alpha_n^{(\pm)}(\boldsymbol{\rho}')-\gamma^{(\pm)}\hat{\mathfrak{b}}^{(\pm)}]\Psi(E,\boldsymbol{\rho}')\quad(\mathbf{r}\in\mathscr{V}\setminus\mathscr{S}). \tag{127}$$

This relation is valid for the point $\mathbf{r}$ laying as close to the boundary $\mathscr{S}$ as we please and therefore, in view of the continuity of the function $\Psi(E,\mathbf{r})$ across $\mathscr{S}$, one has

$$\Psi(E,\boldsymbol{\rho})=\lim_{\mathbf{r}\to\boldsymbol{\rho}}\int_{\mathscr{S}}d^2\boldsymbol{\rho}'\;c\hbar\sum_k\;\frac{\Psi_{\hat{\mathfrak{b}}k}(\mathbf{r})\Psi^{\dagger}_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho}')}{E_{\hat{\mathfrak{b}}k}-E}\,[i\alpha_n^{(\pm)}(\boldsymbol{\rho}')-\gamma^{(\pm)}\hat{\mathfrak{b}}^{(\pm)}]\Psi(E,\boldsymbol{\rho}')\quad(\mathbf{r}\in\mathscr{V}\setminus\mathscr{S}) \tag{128}$$

and consequently

$$\beta^{(\pm)}\Psi(E,\boldsymbol{\rho})=\lim_{\mathbf{r}\to\boldsymbol{\rho}}\int_{\mathscr{S}}d^2\boldsymbol{\rho}'\;c\hbar\sum_k\;\frac{\beta^{(\pm)}\Psi_{\hat{\mathfrak{b}}k}(\mathbf{r})\Psi^{\dagger}_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho}')\beta^{(\pm)}}{E_{\hat{\mathfrak{b}}k}-E}\,[i\alpha_n^{(\pm)}(\boldsymbol{\rho}')-\gamma^{(\pm)}\hat{\mathfrak{b}}^{(\pm)}]\Psi(E,\boldsymbol{\rho}')\quad(\mathbf{r}\in\mathscr{V}\setminus\mathscr{S}), \tag{129}$$

which, in conjunction with Eq. (92), implies

$$\mathscr{R}^{(\pm)}_{\hat{\mathfrak{b}}}(E,\boldsymbol{\rho},\boldsymbol{\rho}')=\lim_{\mathbf{r}\to\boldsymbol{\rho}}\left\{c\hbar\,\gamma^{(\pm)}\sum_k\;\frac{\beta^{(\pm)}\Psi_{\hat{\mathfrak{b}}k}(\mathbf{r})\Psi^{\dagger}_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho}')\beta^{(\pm)}}{E_{\hat{\mathfrak{b}}k}-E}\right\}. \tag{130}$$

This is to be compared with Eq. (125).

We now ask the question: Are the operations $\lim_{\mathbf{r}\to\boldsymbol{\rho}}$ and Σ_k in Eq. (130) interchangeable freely? Relying on the apparent similarity of the relativistic theory discussed here to the nonrelativistic theory exposed in Sec. III B one might expect that the answer to this question is positive. However, this is *not* the case. In the relativistic theory the operations $\lim_{\mathbf{r}\to\boldsymbol{\rho}}$ and Σ_k do *not* commute and accordingly one finds $\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}^{(\pm)}(E,\boldsymbol{\rho},\boldsymbol{\rho}')\neq\overline{\mathscr{R}}_{\hat{\mathfrak{b}}}^{(\pm)}(E,\boldsymbol{\rho},\boldsymbol{\rho}')$ and $\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}^{(\pm)}(E)\neq\hat{\overline{\mathscr{R}}}_{\hat{\mathfrak{b}}}^{(\pm)}(E)$. To show this (and find the consequences of interchanging the two operations) we need to find a direct relation between the surface functions $\overline{\Psi}_{\hat{\mathfrak{b}}}(E,\boldsymbol{\rho})$ and $\Psi(E,\boldsymbol{\rho})$. We begin with an observation that the closure relation (114) cannot hold whenever any of the points $\mathbf{r}$ or $\mathbf{r}'$ lies on the surface $\mathscr{S}$ since the upper and the lower components of the surface spinor functions $\{\Psi_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho})\}$ are related by the boundary condition (109). Therefore, we assume that

$$\sum_k \Psi_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho})\Psi_{\hat{\mathfrak{b}}k}^{\dagger}(\mathbf{r}')=\mathscr{A}_{\hat{\mathfrak{b}}}(\boldsymbol{\rho},\boldsymbol{\rho}')\,\delta_{\mathscr{S}}^{(1)}(\mathbf{r}') \quad (\mathbf{r}'\in\mathscr{V}), \tag{131}$$

$$\sum_k \Psi_{\hat{\mathfrak{b}}k}(\mathbf{r})\Psi_{\hat{\mathfrak{b}}k}^{\dagger}(\boldsymbol{\rho}')=\mathscr{A}_{\hat{\mathfrak{b}}}(\boldsymbol{\rho},\boldsymbol{\rho}')\,\delta_{\mathscr{S}}^{(1)}(\mathbf{r}) \quad (\mathbf{r}\in\mathscr{V}) \tag{132}$$

[cf. Eq. (114) and the first of Eqs. (9)] and hope that, in the course of the following considerations, we shall be able to find the surface kernel $\mathscr{A}_{\hat{\mathfrak{b}}}(\boldsymbol{\rho},\boldsymbol{\rho}')$. Substituting the relation (131) into the definition (116) we get

$$\overline{\Psi}_{\hat{\mathfrak{b}}}(E,\boldsymbol{\rho})=\int_{\mathscr{S}} d^2\boldsymbol{\rho}'\ \mathscr{A}_{\hat{\mathfrak{b}}}(\boldsymbol{\rho},\boldsymbol{\rho}')\Psi(E,\boldsymbol{\rho}'), \tag{133}$$

which implies that the kernel $\mathscr{A}_{\hat{\mathfrak{b}}}(\boldsymbol{\rho},\boldsymbol{\rho}')$ defines the integral operator $\hat{\mathscr{A}}_{\hat{\mathfrak{b}}}$ transforming the surface function $\Psi(E,\boldsymbol{\rho})$ into $\overline{\Psi}_{\hat{\mathfrak{b}}}(E,\boldsymbol{\rho})$,

$$\overline{\Psi}_{\hat{\mathfrak{b}}}(E,\boldsymbol{\rho})=\hat{\mathscr{A}}_{\hat{\mathfrak{b}}}\Psi(E,\boldsymbol{\rho}). \tag{134}$$

An important property of the operator $\hat{\mathscr{A}}_{\hat{\mathfrak{b}}}$ may be deduced from the definitions (131) and (132) and the relation (111). On one hand, it follows from Eq. (111) that

$$\sum_k \Psi_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho})\Psi_{\hat{\mathfrak{b}}k}^{\dagger}(\mathbf{r}')=[\hat{\mathscr{I}}-\gamma^{(\pm)}i\alpha_n^{(\mp)}\hat{\mathfrak{b}}^{(\pm)}]\beta^{(\pm)}\left\{\sum_k \Psi_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho})\Psi_{\hat{\mathfrak{b}}k}^{\dagger}(\boldsymbol{\rho}')\right\}, \tag{135}$$

where $\hat{\mathscr{I}}$ is the unit operator. On the other hand, if $\Phi(\boldsymbol{\rho})$ is any reasonable spinor function defined on the surface $\mathscr{S}$, from Eq. (132) and the Hermicity of the operators $\hat{\mathfrak{b}}^{(\pm)}$ under the surface scalar product $(|)$ we readily obtain

$$\begin{aligned}
&\int_{\mathscr{S}} d^2\boldsymbol{\rho}'\left\{\sum_k \Psi_{\hat{\mathfrak{b}}k}(\mathbf{r})\Psi_{\hat{\mathfrak{b}}k}^{\dagger}(\boldsymbol{\rho}')\right\}\Phi(\boldsymbol{\rho}')\\
&=\sum_k \Psi_{\hat{\mathfrak{b}}k}(\mathbf{r})\int_{\mathscr{S}} d^2\boldsymbol{\rho}'\{[\beta^{(\pm)}-\gamma^{(\pm)}i\alpha_n^{(\mp)}\hat{\mathfrak{b}}^{(\pm)}]\Psi_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho}')\}^{\dagger}\Phi(\boldsymbol{\rho}')\\
&=\int_{\mathscr{S}} d^2\boldsymbol{\rho}'\left\{\sum_k \Psi_{\hat{\mathfrak{b}}k}(\mathbf{r})\Psi_{\hat{\mathfrak{b}}k}^{\dagger}(\boldsymbol{\rho}')\right\}\beta^{(\pm)}[\hat{\mathscr{I}}+\gamma^{(\pm)}\hat{\mathfrak{b}}^{(\pm)}i\alpha_n^{(\pm)}]\Phi(\boldsymbol{\rho}').
\end{aligned} \tag{136}$$

Equations (131), (132), (135) and (136) imply that the operator $\hat{\mathscr{A}}_{\hat{\mathfrak{b}}}$ may be sought in any of the two equivalent forms

$$\hat{\mathscr{A}}_{\hat{\mathfrak{b}}}=[\hat{\mathscr{I}}-\gamma^{(+)}i\alpha_n^{(-)}\hat{\mathfrak{b}}^{(+)}]\hat{\mathscr{A}}_{\hat{\mathfrak{b}}}^{(+)}[\hat{\mathscr{I}}+\gamma^{(+)}\hat{\mathfrak{b}}^{(+)}i\alpha_n^{(+)}], \tag{137}$$

$$\hat{\mathscr{A}}_{\hat{\mathfrak{b}}}=[\hat{\mathscr{I}}-\gamma^{(-)}i\alpha_n^{(+)}\hat{\mathfrak{b}}^{(-)}]\hat{\mathscr{A}}_{\hat{\mathfrak{b}}}^{(-)}[\hat{\mathscr{I}}+\gamma^{(-)}\hat{\mathfrak{b}}^{(-)}i\alpha_n^{(-)}], \tag{138}$$

where the operators

$$\hat{\mathscr{A}}_{\hat{\mathfrak{b}}}^{(\pm)}=\beta^{(\pm)}\hat{\mathscr{A}}_{\hat{\mathfrak{b}}}\beta^{(\pm)} \tag{139}$$

have the integral kernels $\mathscr{A}_{\hat{\mathfrak{b}}}^{(\pm)}(\boldsymbol{\rho},\boldsymbol{\rho}')=\beta^{(\pm)}\mathscr{A}_{\hat{\mathfrak{b}}}(\boldsymbol{\rho},\boldsymbol{\rho}')\beta^{(\pm)}$ defined formally by

$$\sum_k \beta^{(\pm)}\Psi_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho})\Psi_{\hat{\mathfrak{b}}k}^{\dagger}(\mathbf{r}')\beta^{(\pm)}=\mathscr{A}_{\hat{\mathfrak{b}}}^{(\pm)}(\boldsymbol{\rho},\boldsymbol{\rho}')\delta_{\mathscr{S}}^{(1)}(\mathbf{r}') \quad (\mathbf{r}'\in\mathscr{V}). \tag{140}$$

The operators $\hat{\mathscr{A}}_{\hat{\mathfrak{b}}}^{(+)}$ and $\hat{\mathscr{A}}_{\hat{\mathfrak{b}}}^{(-)}$ are related; it is readily derivable from Eqs. (137) to (139) that

$$\hat{\mathscr{A}}_{\hat{\mathfrak{b}}}^{(\pm)}=(\gamma^{(\pm)})^2\alpha_n^{(\pm)}\hat{\mathfrak{b}}^{(\mp)}\hat{\mathscr{A}}_{\hat{\mathfrak{b}}}^{(\mp)}\hat{\mathfrak{b}}^{(\mp)}\alpha_n^{(\mp)}. \tag{141}$$

To find the explicit form of the operator $\hat{\mathscr{A}}_{\hat{\mathfrak{b}}}$, we postmultiply the kernel

$$\sum_{k'} \Psi_{\hat{\mathfrak{b}}k'}(\boldsymbol{\rho})\Psi_{\hat{\mathfrak{b}}k'}^{\dagger}(\mathbf{r}')$$

by any function $\Psi_{\hat{\mathfrak{b}}k}(\mathbf{r}')$ from the complete set $\{\Psi_{\hat{\mathfrak{b}}k}(\mathbf{r}')\}$ and integrate over the volume $\mathscr{V}$. From the orthogonality relation (113) we infer that

$$\int_{\mathscr{V}} d^3\mathbf{r}'\left\{\sum_{k'} \Psi_{\hat{\mathfrak{b}}k'}(\boldsymbol{\rho})\Psi_{\hat{\mathfrak{b}}k'}^{\dagger}(\mathbf{r}')\right\}\Psi_{\hat{\mathfrak{b}}k}(\mathbf{r}')=\Psi_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho}). \tag{142}$$

On the other hand, from Eq. (131) we have

$$\int_{\mathscr{V}} d^3\mathbf{r}'\left\{\sum_{k'} \Psi_{\hat{\mathfrak{b}}k'}(\boldsymbol{\rho})\Psi_{\hat{\mathfrak{b}}k'}^{\dagger}(\mathbf{r}')\right\}\Psi_{\hat{\mathfrak{b}}k}(\mathbf{r}')=\hat{\mathscr{A}}_{\hat{\mathfrak{b}}}\Psi_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho}). \tag{143}$$

Equating the right-hand sides of Eqs. (142) and (143) we find

$$\hat{\mathscr{A}}_{\hat{\mathfrak{b}}}\Psi_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho})=\Psi_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho}). \tag{144}$$

At first sight Eq. (144) might seem to imply that, as in the nonrelativistic theory, the operator $\hat{\mathscr{A}}_{\hat{\mathfrak{b}}}$ is the unit operator. Yet this is *not* the case. The reason is that in the relativistic theory the functions $\{\Psi_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho})\}$ are multicomponent and their upper and lower components are related by the algebraic condition (109). Rewriting Eq. (144) with the aid of Eqs. (137) and (138) we obtain

$$[\hat{\mathscr{I}}-\gamma^{(\pm)}i\alpha_n^{(\mp)}\hat{\mathfrak{b}}^{(\pm)}]\hat{\mathscr{A}}_{\hat{\mathfrak{b}}}^{(\pm)}[\hat{\mathscr{I}}+\gamma^{(\pm)}\hat{\mathfrak{b}}^{(\pm)}i\alpha_n^{(\pm)}]\Psi_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho})=\Psi_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho}). \tag{145}$$

Upon operating on both sides of this equation with $\beta^{(\pm)}$ and utilizing the boundary condition (109) we get

$$\hat{\mathscr{A}}_{\hat{\mathfrak{b}}}^{(\pm)}[\hat{\mathscr{I}}+(\gamma^{(\pm)})^2(\hat{\mathfrak{b}}^{(\pm)})^2]\Psi_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho})=\beta^{(\pm)}\Psi_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho}) \tag{146}$$

and accordingly

$$\hat{\mathscr{A}}_{\hat{\mathfrak{b}}}^{(\pm)}=\beta^{(\pm)}[\hat{\mathscr{I}}+(\gamma^{(\pm)})^2(\hat{\mathfrak{b}}^{(\pm)})^2]^{-1}\beta^{(\pm)} \tag{147}$$

since the relation (136) holds for an arbitrary eigenfunction $\Psi_{\hat{\mathfrak{b}}k}$. Hence, it follows that

$$\hat{\mathscr{A}}_{\hat{\mathfrak{b}}}=[\beta^{(\pm)}-\gamma^{(\pm)}i\alpha_n^{(\mp)}\hat{\mathfrak{b}}^{(\pm)}][\hat{\mathscr{I}}+(\gamma^{(\pm)})^2(\hat{\mathfrak{b}}^{(\pm)})^2]^{-1}[\beta^{(\pm)}+\gamma^{(\pm)}\hat{\mathfrak{b}}^{(\pm)}i\alpha_n^{(\pm)}] \tag{148}$$

and consequently Eq. (134) may be written in the form

$$\overline{\Psi}_{\hat{\mathfrak{b}}}(E,\boldsymbol{\rho})=[\beta^{(\pm)}-\gamma^{(\pm)}i\alpha_n^{(\mp)}\hat{\mathfrak{b}}^{(\pm)}][\hat{\mathscr{I}}+(\gamma^{(\pm)})^2(\hat{\mathfrak{b}}^{(\pm)})^2]^{-1}[\beta^{(\pm)}+\gamma^{(\pm)}\hat{\mathfrak{b}}^{(\pm)}i\alpha_n^{(\pm)}]\Psi(E,\boldsymbol{\rho}). \tag{149}$$

Substituting this relation to Eq. (124), after straightforward manipulations we arrive at

$$\beta^{(\pm)}\Psi(E,\boldsymbol{\rho})=-\gamma^{(\mp)}[\hat{\hat{\mathscr{R}}}_{\hat{\mathfrak{b}}}^{(\pm)}(E)-\hat{\mathfrak{b}}^{(\pm)}[(\gamma^{(\mp)})^2\hat{\mathscr{I}}+(\hat{\mathfrak{b}}^{(\pm)})^2]^{-1}][i\alpha_n^{(\pm)}-\gamma^{(\pm)}\hat{\mathfrak{b}}^{(\pm)}]\Psi(E,\boldsymbol{\rho}) \tag{150}$$

hence, on comparing Eqs. (91) and (150), we find the relationship between the operators $\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}^{(\pm)}(E)$ and $\hat{\hat{\mathscr{R}}}_{\hat{\mathfrak{b}}}^{(\pm)}(E)$,

$$\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}^{(\pm)}(E)=\hat{\hat{\mathscr{R}}}_{\hat{\mathfrak{b}}}^{(\pm)}(E)-\hat{\mathfrak{b}}^{(\pm)}[(\gamma^{(\mp)})^2\hat{\mathscr{I}}+(\hat{\mathfrak{b}}^{(\pm)})^2]^{-1}. \tag{151}$$

Equation (150) may be perceived as a set of two homogeneous coupled equations for the functions $\beta^{(+)}\Psi(E,\boldsymbol{\rho})$ and $\beta^{(-)}\Psi(E,\boldsymbol{\rho})$. Indeed, upon utilizing the properties of the matrices $\alpha_n^{(\pm)}(\boldsymbol{\rho})$ and $\beta^{(\pm)}$ the two relations constituting Eq. (150) may be explicitly rewritten in the form

$$\beta^{(+)}\Psi(E,\boldsymbol{\rho})=-\gamma^{(-)}\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}^{(+)}(E)\,i\alpha_n^{(+)}\beta^{(-)}\Psi(E,\boldsymbol{\rho})-\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}^{(+)}(E)\,\hat{\mathfrak{b}}^{(+)}\beta^{(+)}\Psi(E,\boldsymbol{\rho}), \tag{152}$$

$$\beta^{(-)}\Psi(E,\boldsymbol{\rho})=-\gamma^{(+)}\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}^{(-)}(E)\,i\alpha_n^{(-)}\beta^{(+)}\Psi(E,\boldsymbol{\rho})-\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}^{(-)}(E)\,\hat{\mathfrak{b}}^{(-)}\beta^{(-)}\Psi(E,\boldsymbol{\rho}), \tag{153}$$

where the operators $\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}^{(\pm)}(E)$ have been given by Eq. (151). The following problem arises now: Since Eqs. (152) and (153) are homogeneous and coupled, are they consistent? This should be the case if the relations (151) are correct; therefore seeking an answer to the question posed provides a test for correctness of the method of construction of the operators $\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}^{(\pm)}(E)$ presented above. [It is to be emphasized that testing the theory in that manner is by no means insipid. This is just the way in which Szmytkowski and Hinze[17,18] recognized an error in earlier attempts[15,16] to formulate the *R*-matrix theory for the Dirac equation within the framework of the matrix language.] To clear up the problem we solve Eq. (153) for $\beta^{(-)}\Psi(E,\boldsymbol{\rho})$ obtaining

$$\beta^{(-)}\Psi(E,\boldsymbol{\rho})=-\gamma^{(+)}\beta^{(-)}[\hat{\mathscr{I}}+\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}^{(-)}(E)\,\hat{\mathfrak{b}}^{(-)}]^{-1}\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}^{(-)}(E)\,i\alpha_n^{(-)}\beta^{(+)}\Psi(E,\boldsymbol{\rho}). \tag{154}$$

Substituting this relation into the right-hand side of Eq. (152), making use of Eq. (151) and of the relations

$$\hat{\hat{\mathscr{R}}}_{\hat{\mathfrak{b}}}^{(\pm)}(E)=-\alpha_n^{(\pm)}\hat{\mathfrak{b}}^{(\mp)}\hat{\hat{\mathscr{R}}}_{\hat{\mathfrak{b}}}^{(\mp)}(E)\,\hat{\mathfrak{b}}^{(\mp)}\alpha_n^{(\mp)} \tag{155}$$

which stem from the explicit form (125) of the kernels $\overline{\mathscr{R}}_{\hat{\mathfrak{b}}}^{(\pm)}(E,\boldsymbol{\rho},\boldsymbol{\rho}')$, the conditions (110) and the Hermicity of the operators $\hat{\mathfrak{b}}^{(\pm)}$ [please notice that the relations analogous to Eq. (155) but with $\hat{\hat{\mathscr{R}}}_{\hat{\mathfrak{b}}}^{(\pm)}(E)$ replaced by $\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}^{(\pm)}(E)$ do not hold], utilizing the properties of the matrices $\alpha_n^{(\pm)}(\boldsymbol{\rho})$ and $\beta^{(\pm)}$ and employing Eq. (88) transforms the right-hand side of Eq. (152) to $\beta^{(+)}\Psi(E,\boldsymbol{\rho})$. Similarly, determining $\beta^{(+)}\Psi(E,\boldsymbol{\rho})$ from Eq. (152)

$$\beta^{(+)}\Psi(E,\boldsymbol{\rho})=-\gamma^{(-)}\beta^{(+)}[\hat{\mathscr{I}}+\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}^{(+)}(E)\,\hat{\mathfrak{b}}^{(+)}]^{-1}\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}^{(+)}(E)\,i\alpha_n^{(+)}\beta^{(-)}\Psi(E,\boldsymbol{\rho}) \tag{156}$$

and substituting the result to the right-hand side of Eq. (153) transforms the latter, after some manipulations, to $\beta^{(-)}\Psi(E,\boldsymbol{\rho})$. Since in both cases the final results obtained are identical with the left-hand sides of the respective equations, one is led to the conclusion that Eqs. (152) and (153) are indeed consistent.

Given the relation (151) between the operators $\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}^{(\pm)}(E)$ and $\hat{\hat{\mathscr{R}}}_{\hat{\mathfrak{b}}}^{(+)}(E)$, one may find the matrix representation of the operators $\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}^{(\pm)}(E)$ in the surface basis $\{\Phi_i(\boldsymbol{\rho})\}$. Projecting Eq. (151) from the left and from the right onto the spinor functions from the set $\{\Phi_i(\boldsymbol{\rho})\}$ one obtains

$$\mathsf{R}_{\mathsf{b}}^{(\pm)}(E)=\frac{\hbar^2}{2m}\sum_k \frac{\mathsf{P}_{\mathsf{b}k}^{(\pm)}\mathsf{P}_{\mathsf{b}k}^{(\pm)\dagger}}{E_{\mathsf{b}k}-E}-\frac{\mathsf{b}^{(\pm)}}{(\gamma^{(\mp)})^2\mathsf{I}+(\mathsf{b}^{(\pm)})^2}, \tag{157}$$

where $\{\mathsf{P}_{\mathfrak{b}k}^{(\pm)}\}$ are column vectors with elements $\{P_{i,\mathfrak{b}k}^{(\pm)}=(\Phi_i|\beta^{(\pm)}\Psi_{\hat{\mathfrak{b}}k})\}$, $\{\mathsf{P}_{\mathfrak{b}k}^{(\pm)\dagger}\}$ are row vectors with elements $\{P_{i,\mathfrak{b}k}^{(\pm)*}=(\beta^{(\pm)}\Psi_{\hat{\mathfrak{b}}k}|\Phi_i)\}$, $\mathsf{b}^{(\pm)}$ are square matrices with elements $\{b_{ij}^{(\pm)}=(\Phi_i|\hat{\mathfrak{b}}^{(\pm)}\Phi_j)\}$ and I is the matrix of the unit operator with elements $\{I_{ij}=\delta_{ij}\}$. The result (157) is to be used in Eq. (96).

Let us examine somewhat closer the right-hand side of Eq. (157). Its first constituent is the matrix representation of the operators $\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}^{(\pm)}(E)$ in the basis $\{\Phi_i(\boldsymbol{\rho})\}$; its form is formally identical with that of the nonrelativistic matrix $\mathsf{R}_{\mathfrak{b}}(E)$ given by Eq. (61) (cf., however, Sec. IV B). To the contrary, the second term on the right-hand side of Eq. (157) does not have its counterpart in the nonrelativistic theory. The origin of the occurrence of this term is the structure of the Dirac equation which is the set of coupled first-order equations while the Schrödinger equation is the second-order equation. The additional term in the formula for the matrix $\mathsf{R}_{\mathfrak{b}}^{(+)}(E)$ vanishes in the event when $\gamma^{(+)}=0$ (i.e., $\gamma^{(-)}=\infty$, which corresponds to the nonrelativistic limit $c\rightarrow\infty$) and in the exceptional case $\mathsf{b}^{(+)}=0$. With regard to the matrix $\mathsf{R}_{\mathfrak{b}}^{(-)}(E)$, the second term in Eq. (157) vanishes in the case $\mathsf{b}^{(-)}=0$. It is to be mentioned that the particular case of Eq. (157) was obtained, in a different way, by Szmytkowski and Hinze[18] who considered a spherically symmetric volume $\mathscr{V}$ and used a very particular surface basis $\{\Phi_i(\boldsymbol{\rho})\}$.

Finally, it is to be noticed that once the operator $\hat{\mathscr{A}}_{\hat{\mathfrak{b}}}$ has been determined [cf. Eq. (148)], the explicit forms of the relations (131) and (132) may be given. We shall not discuss the general case when the operators $\hat{\mathfrak{b}}^{(\pm)}$ are arbitrary [but still related by Eq. (88)] and consider instead what happens if $\gamma^{(+)}=0$, $\hat{\mathfrak{b}}^{(+)}=\hat{0}$ or $\hat{\mathfrak{b}}^{(-)}=\hat{0}$ (here $\hat{0}$ denotes the null operator).

The first case, $\gamma^{(+)}=0$, corresponds to the nonrelativistic limit $c\rightarrow\infty$. From Eq. (148) one finds

$$\hat{\mathscr{A}}_{\hat{\mathfrak{b}}}=\beta^{(+)}\Rightarrow\mathscr{A}_{\hat{\mathfrak{b}}}(\boldsymbol{\rho},\boldsymbol{\rho}')=\delta^{(2)}(\boldsymbol{\rho}-\boldsymbol{\rho}')\beta^{(+)}\quad(c\rightarrow\infty)\tag{158}$$

and, after substitution to Eqs. (131) and (132),

$$\sum_k \Psi_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho}')\Psi_{\hat{\mathfrak{b}}k}^{\dagger}(\mathbf{r})=\sum_k \Psi_{\hat{\mathfrak{b}}k}(\mathbf{r})\Psi_{\hat{\mathfrak{b}}k}^{\dagger}(\boldsymbol{\rho}')=\delta^{(3)}(\mathbf{r}-\boldsymbol{\rho}')\beta^{(+)}\quad(\mathbf{r}\in\mathscr{V},c\rightarrow\infty).\tag{159}$$

This result is in accord with the relation (61) found in the nonrelativistic case.

In the event when $\hat{\mathfrak{b}}^{(+)}=\hat{0}$, from the boundary condition (109) and the properties of the matrices $\alpha_n^{(\pm)}(\boldsymbol{\rho})$ one infers that the basis functions $\{\Psi_{\hat{\mathfrak{b}}k}(\mathbf{r})\}$ possess the property

$$\beta^{(-)}\Psi_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho})=0\quad(\hat{\mathfrak{b}}^{(+)}=\hat{0}),\tag{160}$$

i.e., their lower components vanish identically on $\mathscr{S}$. From Eq. (148) one finds

$$\hat{\mathscr{A}}_{\hat{\mathfrak{b}}}=\beta^{(+)}\Rightarrow\mathscr{A}_{\hat{\mathfrak{b}}}(\boldsymbol{\rho},\boldsymbol{\rho}')=\delta^{(2)}(\boldsymbol{\rho}-\boldsymbol{\rho}')\beta^{(+)}\quad(\hat{\mathfrak{b}}^{(+)}=\hat{0})\tag{161}$$

and consequently

$$\sum_k \Psi_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho}')\Psi_{\hat{\mathfrak{b}}k}^{\dagger}(\mathbf{r})=\sum_k \Psi_{\hat{\mathfrak{b}}k}(\mathbf{r})\Psi_{\hat{\mathfrak{b}}k}^{\dagger}(\boldsymbol{\rho}')=\delta^{(3)}(\mathbf{r}-\boldsymbol{\rho}')\beta^{(+)}\quad(\mathbf{r}\in\mathscr{V},\hat{\mathfrak{b}}^{(+)}=\hat{0}).\tag{162}$$

It is to be emphasized that although the relations (159) and (162) are seemingly identical, they refer to completely different situations. In the case of Eq. (159) the operator $\hat{\mathfrak{b}}^{(+)}$ is arbitrary and $c=\infty$ while in the case of Eq. (162) the operator $\hat{\mathfrak{b}}^{(+)}$ is the null operator and the speed of light c is finite.

It remains to consider the third special case, namely that when $\hat{\mathfrak{b}}^{(-)}=\hat{0}$. Now one finds that the upper components of the functions $\{\Psi_{\hat{\mathfrak{b}}k}(\mathbf{r})\}$ vanish identically on $\mathscr{S}$,

$$\beta^{(+)}\Psi_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho})=0\quad(\hat{\mathfrak{b}}^{(-)}=\hat{0}),\tag{163}$$

and that

$$\hat{\mathscr{A}}_{\hat{\mathfrak{b}}}=\beta^{(-)}\Rightarrow \mathscr{A}_{\hat{\mathfrak{b}}}(\boldsymbol{\rho},\boldsymbol{\rho}')=\delta^{(2)}(\boldsymbol{\rho}-\boldsymbol{\rho}')\beta^{(-)} \quad (\hat{\mathfrak{b}}^{(-)}=\hat{0}) \tag{164}$$

and consequently

$$\sum_k \Psi_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho}')\Psi^{\dagger}_{\hat{\mathfrak{b}}k}(\mathbf{r})=\sum_k \Psi_{\hat{\mathfrak{b}}k}(\mathbf{r})\Psi^{\dagger}_{\hat{\mathfrak{b}}k}(\boldsymbol{\rho}')=\delta^{(3)}(\mathbf{r}-\boldsymbol{\rho}')\beta^{(-)} \quad (\mathbf{r}\in\mathscr{V},\hat{\mathfrak{b}}^{(-)}=\hat{0}). \tag{165}$$

The reader should compare the relations (159), (162) and (165) with the closure relation (114).

V. CONCLUDING REMARKS

In this paper we have formulated Wigner's *R*-matrix theory in the language of integral operators rather than matrices. In the first part of the work, following the ideas of Nesbet,[12,13] we have shown that in the nonrelativistic theory for particles described by the Schrödinger equation the central role is played by the integral operator $\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}(E)$ which relates function values to normal derivatives on a surface $\mathscr{S}$ of a closed volume $\mathscr{V}$ inside which the function satisfies the Schrödinger equation at energy *E*. Matrix elements of the operator $\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}(E)$ between functions from an orthonormal scalar basis set spanning the surface $\mathscr{S}$ form an *R*-matrix $\mathsf{R}_{\mathfrak{b}}(E)$. The method due to Kapur and Peierls[1] and to Wigner,[2–4,6] has been used, with necessary modifications and improvements, to construct an integral kernel of the operator $\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}(E)$.

In the second part of the work we have developed the operator formulation of Wigner's *R*-matrix theory for the Dirac equation. It has been found that in the relativistic theory a counterpart of the nonrelativistic operator $\hat{\mathscr{R}}_{\hat{\mathfrak{b}}}(E)$ is an integral operator $\hat{\mathscr{R}}^{(+)}_{\hat{\mathfrak{b}}}(E)$ relating on the enclosing surface $\mathscr{S}$ values of upper and lower components of spinor wave functions satisfying in the volume $\mathscr{V}$ the Dirac equation at energy *E*. Besides the operator $\hat{\mathscr{R}}^{(+)}_{\hat{\mathfrak{b}}}(E)$, another operator $\hat{\mathscr{R}}^{(-)}_{\hat{\mathfrak{b}}}(E)$ arises in the relativistic theory in the natural way. By generalizing Wigner's method,[2–4,6] we have constructed explicit forms of the operators $\hat{\mathscr{R}}^{(\pm)}_{\hat{\mathfrak{b}}}(E)$. It has been shown that although there are apparent similarities between the nonrelativistic and relativistic theories, the explicit form of the operator $\hat{\mathscr{R}}^{(+)}_{\hat{\mathfrak{b}}}(E)$ contains a component which does not have its counterpart in the nonrelativistic theory. This component vanishes in the nonrelativistic limit. This agrees with a result obtained earlier by Szmytkowski and Hinze[17,18] who found such a correction in the matrix representation of the operator $\hat{\mathscr{R}}^{(+)}_{\hat{\mathfrak{b}}}(E)$ in a particular case of the spherically symmetric volume $\mathscr{V}$ and for a very special choice of a spinor basis spanning the surface $\mathscr{S}$.

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