Relativistic wave equations in momentum space

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Relativistic equal-time wave equations obtained from field theory which describe bound states of N Dirac particles inevitably involve Casimir-type positive-energy projection operators $\Lambda_+(i)$. For $N>2$, these operators are vital if the equations are to admit normalizable solutions. Such equations, which are of integro-differential form, have been used in the past to obtain relativistic corrections to, e.g., level shifts for a variety of simple atomic systems, and to provide a theoretical basis for the Dirac-Hartree-Fock type of equations for many-electron atoms. Here we initiate a study of such equations without making an expansion in powers of v/c. We work in momentum space, where the free-particle projection operators are simple functions of $\vec{p}$ and the wave equation is essentially no more complicated than in the nonrelativistic case. In the present paper we describe techniques for finding the eigenvalues of $h_+(1,2)=h_D(1)+h_D(2)+\Lambda_{++}V\Lambda_{++}$, where $h_D(i)$ is the free-particle Dirac Hamiltonian and V is a local potential with a $|\vec{r}_1-\vec{r}_2|^{-1}$ singularity. Numerical results are presented for the case of a pure Coulomb potential and a Coulomb-plus-Breit potential, for a wide range of mass ratios m_1/m_2 and coupling strength $e_1e_2/4\pi$. In the $m_2=\infty$ limit, comparison is made with the Dirac equation. The results are used to discuss the magnitude of level shifts associated with virtual-pair production in such two-body systems.

I. INTRODUCTION

The relativistic treatment of bound states in quantum theory is a problem of long standing. In this introductory section we first briefly review the old and relatively familiar approaches to the relativistic two-or-more–body problem for spin-$\frac{1}{2}$ particles. We then describe the advantages of more recent methods based on "no-pair equations," involving projection operators. Finally we state the purpose of this paper and give an outline of the following sections.

A. Historical review

A charged spin-$\frac{1}{2}$ fermion moving in an external electromagnetic field is well described by the Dirac equation. If the fermion is an electron and the field is the Coulomb potential provided by a point charge, this equation provides a highly accurate description of the spectrum of hydrogen and H-like ions. To take into account both radiative and nuclear-recoil effects, one can turn to the two-body Bethe-Salpeter (BS) equation, an integral equation which is an exact consequence of quantum field theory.[1] For the case of purely electromagnetic interactions, the kernel entering the BS equation is well approximated by the first few terms in an expansion in powers of $\alpha=e^2/4\pi$. Because of this the two-body BS equation has been extensively used in the calculation of energy levels of hydrogen, positronium, and muonium.[2]

Older and much simpler in form than the four-dimensional BS equation for two fermions is a two-body Dirac-type equation which, for a stationary state, has the form

$$h(1,2)\psi=E\psi\ , \tag{1.1a}$$

$$h(1,2)=\sum_{i=1}^{2}h_D(i)+V_{12}\ . \tag{1.1b}$$

Here

$$h_D(i)\equiv\vec{\alpha}_i\cdot\vec{p}_i^{\,\mathrm{op}}+\beta_i m_i \tag{1.2}$$

is the free Dirac Hamiltonian and V_{12} is a local interaction between particles 1 and 2, $V_{12}=V(r)$. In particular, suppose that V_{12} is taken to be the sum of the Coulomb interaction

$$V_{12}^{C}=\frac{e_1e_2}{4\pi}\frac{1}{r} \tag{1.3}$$

and the Breit operator representing exchange of a transverse photon,

$$V_{12}^{T}=B_{12}\equiv\frac{-e_1e_2}{4\pi}\frac{1}{2r}(\vec{\alpha}_1\cdot\vec{\alpha}_2+\vec{\alpha}_1\cdot\hat{r}\,\vec{\alpha}_2\cdot\hat{r})\ . \tag{1.4}$$

Then with 1 denoting an electron and 2 denoting a proton or muon, Eq. (1.1) is sufficiently accurate to give all the corrections of order α^4m_e to the nonrelativistic energy levels as well as some of the higher-order corrections. Such an equation was used long ago by Breit and coworkers to study recoil corrections in hydrogen.[3]

The first attack on the relativistic three-body problem in quantum theory appears also to have been made by

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Breit,[4] at least in the limiting case where one of the particle masses is regarded as infinite. Thus, he took as a starting point for the study of the spectrum of helium, the Hamiltonian

$$H(1,2)=\sum_{i=1}^{2} H_{D;\text{ext}}(i)+\frac{e^2}{r_{12}}\ , \tag{1.5a}$$

where

$$H_{D;\text{ext}}(i)=h_D(i)+V_{\text{ext}}(i)\ . \tag{1.5b}$$

Subsequently, the obvious generalization of (1.5a) to N-electron atoms was (implicitly) used to obtain the Dirac-Hartree-Fock (DHF) equations, as relativistic analogs of the Hartree-Fock equations.[5] With the advent of the computer age, the DHF type of equations became a major tool in the theoretical study of relativistic effects in many-electron atoms.[6]

Yet, it was pointed out over thirty years ago that Hamiltonians such as (1.5a) have no normalizable eigenfunctions.[7] This makes their use in the study of bound states suspect, to say the least, and obscures the physical significance of the DHF equations. These facts have been discussed extensively in recent years,[8,9] and proposals have been made for the use of equations which do not have the difficulties associated with (1.5a) and which, concomitantly, have a clear origin in quantum field theory.[10,11]

B. Relativistic equations with projection operators

Analysis based on quantum field theory shows that equal-time equations describing bound states of two or more fermions inevitably involve Hamiltonians which differ from (1.1) or (1.5a) in that the interaction term appears with Casimir-type positive-energy projection-operator factors. Although these factors make the Hamiltonian nonlocal they prevent the disease with which the natural looking equal-time equations are afflicted when there are more than two interacting particles.

For example, the two-body BS equation for two Dirac fermions interacting electromagnetically leads, in the ladder approximation and with neglect of transverse photons, to an equal-times equation of the form (1.1), with V_{12} given by[12]

$$(\Lambda_{++}-\Lambda_{--})V^c_{12}(\Lambda_{++}+\Lambda_{--})\ .$$

Here $\Lambda_{++}=\Lambda_+(1)\Lambda_+(2)$ and

$$\Lambda_\pm(i)=\frac{E_i^{\text{op}}\pm(\vec{\alpha}_i\cdot\vec{\mathrm{p}}_i^{\,\text{op}}+\beta_i m_i)}{2E_i^{\text{op}}}\ , \tag{1.6a}$$

with

$$E_i^{\text{op}}=E_i(\vec{\mathrm{p}}_i^{\,\text{op}}),\quad E_i(\vec{\mathrm{p}})\equiv(m_i^2+\vec{\mathrm{p}}^{\,2})^{1/2}\ . \tag{1.6b}$$

If we neglect the terms involving negative-energy projection operators, we are led to the equation

$$h^c_+\phi=E\phi\ , \tag{1.7a}$$

where h^c_+ is a "no-pair Hamiltonian" defined by

$$h^c_+=h_D(1)+h_D(2)+\Lambda_{++}V^c_{12}\Lambda_{++}\ . \tag{1.7b}$$

A similar approximation to the external-field BS equation describing two electrons moving in the electrostatic field provided by an infinitely heavy nucleus leads to the no-pair external-field Coulomb-ladder equation[13]

$$H_+\psi=E\psi\ , \tag{1.8a}$$

where

$$H_+(1,2)=H_{D;\text{ext}}(1)+H_{D;\text{ext}}(2)+L_{++}V^c_{12}L_{++}\ . \tag{1.8b}$$

Here $L_{++}=L_+(1)L_+(2)$ and $L_+(i)$ is the projection operator onto the space spanned by the positive-energy eigenstates of $H_{D;\text{ext}}(i)$. For two electrons ($e_1=e_2=-e$), the Hamiltonian $H_+(1,2)$ defined by (1.8b), in contrast to $H(1,2)$ defined by (1.5a), does have normalizable eigenstates which correspond physically to the discrete spectrum of helium or heliumlike ions. Moreover, its generalization to N electrons provides a suitable starting point for the derivation of relativistic Hartree-Fock-type equations.[10]

Although in the *pure* two-body case the projection operators are not necessary in order for normalizable solutions to exist, even in this case they are useful. Equation (1.7a) enjoys two properties not shared by Eq. (1.1): (i) it has a simple field-theoretic origin and (ii) it may be reduced to Pauli form without making any nonrelativistic approximations.[8]

The problem of "continuum dissolution" from which (1.5a) suffers is of relevance not only for the treatment of relativistic effects in atomic systems but also in hadronic systems. Thus, an attempt to study such effects in the quark model for the nucleon by replacing the nonrelativistic three-body Hamiltonian

$$h_{\text{nr}}=\sum_{i=1}^{3}(\vec{\mathrm{p}}_i^{\,\text{op}})^2/2m_i+\sum_{\substack{i,j=1\\ i<j}}^{3}V_{ij}\ ,$$

where V_{ij} is a local potential, by

$$h(1,2,3)=\sum_{i=1}^{3}h_D(i)+\sum_{\substack{i,j=1\\ i<j}}^{3}V_{ij} \tag{1.9}$$

is bound to fail because $h(1,2,3)$ has no bound states. In contrast, the Hamiltonian

$$h_+(1,2,3)=\sum_{i=1}^{3}h_D(i)+\Lambda_+^{\text{tot}}\sum_{\substack{i,j=1\\ i<j}}^{3}V_{ij}\Lambda_+^{\text{tot}}\ , \tag{1.10}$$

where $\Lambda_+^{\text{tot}}=\Lambda_+(1)\Lambda_+(2)\Lambda_+(3)$, has no such problem. In principle, one can try to use BS-type equations even for $N\geq 3$, but these are very complicated indeed[14] and few practical results have been obtained from them.

C. Outline

The purpose of this paper is to make a start on the numerical study of equations involving projection operators, such as (1.7) or (1.8). As a first example we shall study in Sec. II a modified external-field Dirac equation of the form[15]

$$h_+(1)\psi=E\psi\ , \tag{1.11a}$$

where

$$h_+(1)=h_D(1)+\Lambda_+(1)U(1)\Lambda_+(1)\ , \tag{1.11b}$$

with

$$U(1)=-Z\alpha/r_1\ . \tag{1.11c}$$

The eigenvalues of (1.11b) can be shown to differ from those of the ordinary Dirac equation only by terms of order $(Z\alpha)^6$ or higher for $l\neq 0$ states and for $l=0$ states by terms of order $(Z\alpha)^5 m$.[13] Study of (1.11) therefore provides a sensitive check on the accuracy of the numerical methods we shall employ. From a computational point of view, the main complication is that the projection operator $\Lambda_+(1)$ is a nonlocal operator in coordinate space. We therefore choose to study (1.11) in momentum space, where Λ_+ is a simple matrix function of $\vec{\mathrm{p}}$. The interaction U is then represented by a kernel $\tilde{U}(\vec{\mathrm{p}}-\vec{\mathrm{p}}\,')$ (i.e., by a nonlocal operator in $\vec{\mathrm{p}}$ space), but this is not different from the nonrelativistic case. Thus, at least when free-particle projection operators are involved, the relativistic $\vec{\mathrm{p}}$-space equation is almost as simple as its nonrelativistic counterpart,

$$\frac{\vec{\mathrm{p}}^{\,2}}{2m_1}\tilde{\phi}(\vec{\mathrm{p}})+\int \tilde{U}(\vec{\mathrm{p}}-\vec{\mathrm{p}}\,')\tilde{\phi}(\vec{\mathrm{p}}\,')d\vec{\mathrm{p}}\,'=W\tilde{\phi}(\vec{\mathrm{p}})\ . \tag{1.12}$$

In Sec. III we study the pure two-body no-pair equation

$$h_+(1,2)\psi=E\psi\ , \tag{1.13a}$$

where

$$h_+(1,2)=h_D(1)+h_D(2)+\Lambda_{++}V_{12}\Lambda_{++} \tag{1.13b}$$

and V_{12} is a local potential. For the classical two-body bound systems such as hydrogen and positronium, such a study is mainly of methodological interest. However, before one tackles the case of more than two particles, not to mention equations involving external-field projection operators,[8] it seems wise to study the simpler problem posed by (1.13). Moreover, by the use of equations such as (1.13) one can analyze the importance of relativistic effects in systems such as charmonium without resorting immediately to an expansion in powers of v/c. It is known that for some matrix elements relativistic corrections can be appreciable in this system, which makes a v/c expansion questionable. In the present paper we only consider the choices of V_{12} of most interest in pure electrodynamics: a Coulomb potential or a Coulomb potential plus the Breit operator. Our results are summarized in Sec. IV and used to discuss the magnitude of level shifts associated with virtual-pair production in two-body bound states.

II. NO-PAIR EXTERNAL-FIELD EQUATION

A. Reduction to Pauli form

We are interested in normalizable eigenfunctions of $h_+(1)$ [Eq. (1.11b)] which reduces to eigenfunctions of

$$h_{\mathrm{nr}}(1)=\frac{(\vec{\mathrm{p}}_1^{\,\mathrm{op}})^2}{2m_1}+U(1) \tag{2.1}$$

in the nonrelativistic limit. Since

$$[\Lambda_+(1),h_+(1)]=0 \tag{2.2}$$

we can and do restrict our attention to solutions of (1.11a) which satisfy

$$\Lambda_+(1)\psi(1)=\psi(1)\ . \tag{2.3}$$

The reduction of (1.11) to Pauli form is then straightforward, since (2.3) can be used to express the lower components ψ^- of ψ in terms of the upper components ψ^+. Thus, with $\beta_1^{\pm}=(1\pm\beta_1)/2$ and $\psi^{\pm}=\beta_1^{\pm}\psi$,

$$\psi=\psi^+ +\psi^-=(1+\xi_1^{\mathrm{op}})\psi^+,\quad \xi_1^{\mathrm{op}}=\frac{\vec{\alpha}_1\cdot\vec{\mathrm{p}}_1^{\,\mathrm{op}}}{E_1^{\mathrm{op}}+m_1}\ . \tag{2.4}$$

On setting[16]

$$\phi(1)\equiv(A_1^{\mathrm{op}})^{-1}\psi^+(1)\ , \tag{2.5a}$$

where

$$A_1^{\mathrm{op}}=\left[\frac{E_1^{\mathrm{op}}+m_1}{2E_1^{\mathrm{op}}}\right]^{1/2} \tag{2.5b}$$

and substituting (2.4) and (2.5) into (1.11a), one finds that $\phi(1)$ satisfies

$$h_{\mathrm{eff}}(1)\phi(1)=E\phi(1)\ , \tag{2.6a}$$

where the effective Hamiltonian h_{eff} is defined by

$$h_{\mathrm{eff}}(1)=E_1^{\mathrm{op}}+U_{\mathrm{eff}}(1)\ , \tag{2.6b}$$

with

$$U_{\mathrm{eff}}(1)=A_1^{\mathrm{op}}\beta_1^+(1+\xi_1^{\mathrm{op}})U(1)(1+\xi_1^{\mathrm{op}})\beta_1^+A_1^{\mathrm{op}}\ . \tag{2.6c}$$

If $U(1)$ is diagonal in Dirac indices, which is the case for a Coulomb potential, only even powers of $\vec{\alpha}_1$ contribute in (2.6c) and, acting on ϕ,

$$\begin{aligned} &U_{\mathrm{eff}}(1)\rightarrow A_1^{\mathrm{op}}[U(1)+\zeta_1^{\mathrm{op}}U(1)\zeta_1^{\mathrm{op}}]A_1^{\mathrm{op}}\ ,\\ &\zeta_1^{\mathrm{op}}\equiv\frac{\vec{\sigma}_1\cdot\vec{\mathrm{p}}_1^{\,\mathrm{op}}}{E_1^{\mathrm{op}}+m_1}\ , \end{aligned} \tag{2.7}$$

where $\vec{\sigma}_1$ is the doubled Pauli matrix vector. In the standard representation of the Dirac matrices, $\phi(1)$ has vanishing third and fourth components, so that *we henceforth regard $\phi(1)$ as a Pauli spinor and $\vec{\sigma}_1$ as the ordinary Pauli matrix vector,* without changing the notation. For U's of this type then, the $\vec{\mathrm{p}}$-space form of (2.6a) is

$$E_1(\vec{\mathrm{p}})\tilde{\phi}(\vec{\mathrm{p}})+\int d\vec{\mathrm{p}}\,'K(\vec{\mathrm{p}},\vec{\mathrm{p}}\,')\tilde{\phi}(\vec{\mathrm{p}}\,')=E\tilde{\phi}(\vec{\mathrm{p}})\ , \tag{2.8a}$$

where

$$\begin{aligned} K(\vec{\mathrm{p}},\vec{\mathrm{p}}\,')=A_1(\vec{\mathrm{p}})[&\tilde{U}(\vec{\mathrm{p}}-\vec{\mathrm{p}}\,')\\ &+\zeta_1(\vec{\mathrm{p}})\tilde{U}(\vec{\mathrm{p}}-\vec{\mathrm{p}}\,')\zeta_1(\vec{\mathrm{p}}\,')]A_1(\vec{\mathrm{p}}\,')\ . \end{aligned} \tag{2.8b}$$

Here

$$\tilde{U}(\vec{p}-\vec{p}\,')=\langle \vec{p} \mid U(1) \mid \vec{p}\,' \rangle = \frac{1}{(2\pi)^3}\int d\vec{r}\, e^{-i(\vec{p}-\vec{p}\,')\cdot\vec{r}}U(\vec{r}) \tag{2.9}$$

and A_1 and ζ are the $\vec{p}$-space forms of $A_1^{\rm op}$ and $\zeta_1^{\rm op}$:

$$A_1(\vec{p})=\left[\frac{E_1(\vec{p})+m_1}{2E_1(\vec{p})}\right]^{1/2}, \quad \zeta_1(\vec{p})=\frac{\vec{\sigma}_1\cdot\vec{p}}{E_1(\vec{p})+m_1}. \tag{2.10}$$

B. Radial equations for a Coulomb potential

For spherically symmetric $U(\vec{r})$, $\vec{j}_1^{\,\rm op}=\vec{l}_1^{\,\rm op}+\vec{\sigma}_1/2$ commutes with $h_{\rm eff}(1)$ so that we may look for $\vec{r}$-space eigenfunctions of the form

$$\phi(\vec{r})=R(r)Y^{j_z}_{j;l,1/2}(\hat{r}), \tag{2.11}$$

where Y is a two-component Pauli spinor, which is an eigenfunction of $(\vec{j}^{\,\rm op})^2$, $(\vec{l}^{\,\rm op})^2$, and $j_z^{\rm op}$ with eigenvalue $j(j+1)$, $l(l+1)$, and j_z, respectively. The corresponding $\vec{p}$-space function then has the form

$$\tilde{\phi}(\vec{p})=g(p)Y^{j_z}_{j;l,1/2}(\hat{p}), \tag{2.12a}$$

where $\hat{p}=\vec{p}/|\vec{p}|$ is a unit vector, the analog of $\hat{r}$, and $g(p)$ is a Bessel transform of $R(r)$:

$$g(p)=\sqrt{(2/\pi)}i^l\int_0^\infty dr\, r^2 j_l(pr)R(r). \tag{2.12b}$$

We shall concentrate on S states. For $l=0$, $j=\frac{1}{2}$, Y is a constant spinor and we may perform the angular integration over the $\hat{p}\,'$ angles in (2.8). We therefore define a simplified kernel by

$$K_0(p,p')=\int d\hat{p}\,' K(\vec{p},\vec{p}\,'). \tag{2.13}$$

Using the relation $\vec{\sigma}\cdot\vec{p}\,\vec{\sigma}\cdot\vec{p}\,'=\vec{p}\cdot\vec{p}\,'+i\vec{\sigma}\cdot\vec{p}\times\vec{p}\,'$, in (2.8b) and noting that for spherically symmetric $U(\vec{r})$ the $\vec{p}\times\vec{p}\,'$ term makes no contribution, we get

$$K_0(p,p')=A(p)\int d\hat{p}\,'\,\tilde{U}(\vec{p}-\vec{p}\,')\times\left[1+\frac{\vec{p}\cdot\vec{p}\,'}{(E_1+m_1)(E_1'+m_1)}\right]A(p'). \tag{2.14}$$

For a Coulomb potential, $U(1)=-\alpha Z/|\vec{r}_1|$, we have

$$\tilde{U}(\vec{k})=-\frac{\alpha Z}{2\pi^2}\frac{1}{|\vec{k}|^2}, \tag{2.15}$$

and (2.14) yields

$$K_0(p,p')=-\frac{\alpha Z}{\pi}k_0(p,p'),$$

with

$$k_0(p,p')=\frac{A(p)}{p}\frac{A(p')}{p'}\times\left[Q_0(z)+\frac{p}{E_1+m_1}\frac{p'}{E_1'+m_1}Q_1(z)\right], \tag{2.16}$$

where

$$z=(p^2+p'^2)/2pp'. \tag{2.17}$$

Here the $Q_l(z)$'s are Legendre functions of the second kind:

$$Q_0(z)=-\tfrac{1}{2}\ln\frac{z-1}{z+1}, \quad Q_1(z)=zQ_0(z)-1. \tag{2.18}$$

The equation to be studied then takes the form

$$E_1(p)g(p)-\frac{\alpha Z}{\pi}\int_0^\infty dp'\,p'^2k_0(p,p')g(p')=Eg(p). \tag{2.19}$$

C. Taming the Coulomb singularity

To obtain reasonable accuracy in the numerical solution of (2.19) it is vital to deal with the logarithmic singularity of the kernel at $p=p'$, corresponding to $z=1$. This singularity is the same which arises in the nonrelativistic counterpart of (2.19), viz.,

$$\frac{p^2}{2m_1}g(p)-\frac{\alpha Z}{\pi}\int_0^\infty dp'\,p'^2\frac{Q_0(z)}{pp'}g(p')=Wg(p). \tag{2.20}$$

We may therefore adapt a method due to Landé to the case at hand.[17] Thus, inside the integral in (2.20) we write

$$p'^2g(p')=[p'^2g(p')-p^2g(p)]+p^2g(p). \tag{2.21}$$

The integral arising from the difference term in (2.21) now has an integrand which is no longer divergent at $p'=p$ and the integral arising from the last term in (2.21) may, in this case, be carried out explicitly. Since

$$\int_0^\infty\frac{dp'}{p'}\ln\left[\frac{p-p'}{p+p'}\right]^2=-\pi^2, \tag{2.22}$$

Eq. (2.20) can be written

$$\left[\frac{p^2}{2m_1}-\frac{\alpha Z\pi p}{2}\right]g(p)+\frac{\alpha Z}{2\pi}\int_0^\infty\frac{dp'}{pp'}\ln\left[\frac{p-p'}{p+p'}\right]^2[p'^2g(p')-p^2g(p)]=Wg(p). \tag{2.23}$$

On introduction of a mesh $(p_1,p_2,\ldots,p_{\max})$ and associated integration weights $(w_1,w_2,\ldots,w_{\max})$ in p space, (2.23) reduces to a finite matrix eigenvalue problem which may be handled by standard techniques.

Essentially the same approach can be used for Eq. (2.19). We make the following repartition of the integrand:

$$p'^2k_0(p,p')g(p')=C(p,p')+N(p)\frac{Q_0(z)}{p'}g(p), \tag{2.24a}$$

where, with $b_1=p/(E_1+m_1)$, $b_1'=p'/(E_1'+m_1)$, we define

$$C(p,p')=\frac{A(p)}{pp'}[A(p')p'^2g(p')-A(p)p^2g(p)]Q_0(z)$$
$$+\frac{A(p)}{pp'}b_1[zA(p')b_1'p'^2g(p')$$
$$-A(p)b_1p^2g(p)]Q_0(z)$$
$$-\frac{A(p)}{p}\frac{A(p')}{p'}b_1b_1'p'^2g(p') \tag{2.24b}$$

and

$$N(p)=A^2(p)p(1+b_1^2)\ . \tag{2.24c}$$

The $C(p,p')$ term in (2.24a) is nonsingular at $p'=p$ and the contribution of the second term in (2.24a) to the integral in (2.19) can be evaluated analytically by use of (2.22). Substituting (2.24) into (2.19) we get

$$\left[E_1(p)-\frac{\alpha Z\pi}{2}N(p)\right]g(p)-\frac{\alpha Z}{\pi}\int_0^\infty dp'\,C(p,p')$$
$$=Eg(p)\ , \tag{2.25}$$

an equation whose eigenvalues may be found numerically just as in the case of (2.23),[18] for which, of course, an analytic solution is available.

For P waves and higher-angular-momentum states we can proceed in a similar manner. Thus, the equations analogous to (2.19) for the $l=1$, $j=l\pm\frac{1}{2}$ states are

$$E_1(p)g(p)-\frac{\alpha Z}{\pi}\int_0^\infty dp'\,p'^2k_1^{\pm}(p,p')g(p')=Eg(p)\ , \tag{2.26a}$$

where

$$k_1^{\pm}(p,p')=\frac{A(p)A(p')}{pp'}$$
$$\times\left[Q_1(z)+\frac{p}{(E_1+m_1)}\frac{p'}{(E_1'+m_1)}Q_{1\pm1}(z)\right]\ . \tag{2.26b}$$

Again the logarithmic singularities in the $Q_l(z)$'s can be extracted as before and the eigenvalues of (2.26) can be found just as for S states.

D. Numerical results and analysis of accuracy

1. Results for $h_+(1)$ and $h_D(1)$

To solve (2.19) we first scale the momentum variable p via

$$p=\gamma m_1k\ , \tag{2.27}$$

where

$$\gamma\equiv\alpha Z \tag{2.28}$$

controls the relativistic corrections to the nonrelativistic binding energy W. The resulting equation reduces to the S-wave Schrödinger equation (2.20) in the limit $\gamma\to0$, so that if we define

$$\epsilon(\gamma)=(E-m_1)/\gamma^2m_1\ , \tag{2.29}$$

then

$$\epsilon(0)=-0.5$$

for the ground state. Shown in Fig. 1 are the numerical values of $\epsilon(\gamma)$ for the S-wave ground state as a function of γ. For comparison, also shown in Fig. 1 are the corresponding eigenvalues of the Dirac equation

$$\epsilon_D(\gamma)=\frac{(1-\gamma^2)^{1/2}-1}{\gamma^2}\ . \tag{2.30}$$

As can be seen, the binding is always stronger for $h_+(1)$ than for $h_D(1)$.

To assess the accuracy of our numerical method we may make a number of checks. We first solve the nonrelativistic Schrödinger equation in momentum space, e.g., (2.20), using the techniques described above to handle the singularities; we find, for the ground state,

$$W^{\rm num}=0.500\,001\,85\gamma^2m_1\ .$$

This coincides with the exact value

$$W=-0.5\gamma^2m_1$$

to better than 1 part in 10^5.

To test the method in a relativistic context when the answer is known, we have also solved numerically the momentum space Dirac equation

$$(\vec\alpha\cdot\vec{\rm p}+\beta m_1)\tilde\psi(\vec{\rm p})-\frac{\alpha Z}{2\pi^2}\int\frac{d\vec{\rm p}\,'}{|\vec{\rm p}-\vec{\rm p}\,'|^2}\tilde\psi(\vec{\rm p}\,')=E_D\tilde\psi(\vec{\rm p})\ , \tag{2.31}$$

for the S-wave ground-state energy E_D. We then compare $\epsilon_D=(E_D-m_1)/\gamma^2m_1$, given by (2.30), with $\epsilon_D^{\rm num}=(E_D^{\rm num}-m_1)/\gamma^2m_1$. We find that the relative error in $\epsilon_D^{\rm num}(\gamma)$,

$${\rm Er}_D(\gamma)\equiv\frac{\epsilon_D^{\rm num}(\gamma)-\epsilon_D(\gamma)}{\epsilon_D(\gamma)}\ , \tag{2.32}$$

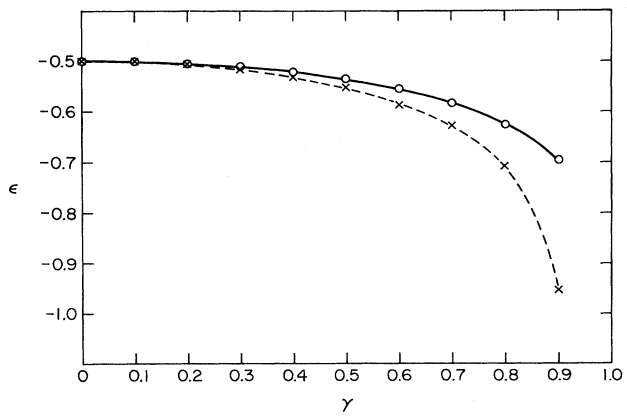

FIG. 1. Scaled eigenvalue $\epsilon(\gamma)$ for the ground state of $h_+(1)$, defined by Eqs. (1.11) and (2.29), shown as a function of $\gamma=\alpha Z$; the dashed line connecting the numerically obtained points is drawn as a guide to the eye. Also shown are the corresponding numerically obtained eigenvalues for the Dirac equation; the solid curve is the exact function $\epsilon_D(\gamma)$.

is of order 10^{-5} for $0\leq\gamma\leq 0.9$. Thus we can expect that the relative error in $\epsilon^{\rm num}(\gamma)$,

$$\mathrm{Er}(\gamma)\equiv\frac{\epsilon^{\rm num}(\gamma)-\epsilon(\gamma)}{\epsilon(\gamma)}\ , \tag{2.33}$$

also remains near its value for $\gamma=0$ (about 10^{-6}) when γ becomes larger. Furthermore, we find that, for $10^{-3}\lesssim\gamma\lesssim 10^{-2}$,

$$\mathrm{Er}_D(\gamma)\approx\mathrm{Er}_D(0)(1+a\gamma^2)\ , \tag{2.34}$$

with $a\approx 0.28$; this dependence of $\mathrm{Er}_D(\gamma)$ on γ for small γ is also expected on theoretical grounds.[19] Thus, we shall assume that a similar relation holds for $\mathrm{Er}(\gamma)$.

2. *Expansion in powers of αZ*

We now turn to a further analysis of the eigenvalues $\epsilon(\gamma)$ of the h_+ equation, shown in Fig. 1, and their relation to $\epsilon_D(\gamma)$. Clearly $\epsilon_D(\gamma)$ is analytic in γ for $|\gamma|<1$ and can be expanded in a power series

$$\epsilon_D(\gamma)=-\tfrac{1}{2}-\tfrac{1}{8}\gamma^2-\tfrac{1}{16}\gamma^4+\cdots\ . \tag{2.35}$$

It is therefore tempting to try a similar expansion for $\epsilon(\gamma)$,

$$\epsilon(\gamma)=c_0+c_1\gamma+c_2\gamma^2+c_3\gamma^3+c_4\gamma^4+\cdots\ .$$

It may be tempting, but it would be wrong. Indeed, it is straightforward from Eq. (1.11) to show that for the $1s$ state we have

$$c_0\equiv\epsilon(0)=-\tfrac{1}{2},\quad c_1\equiv\epsilon'(0)=0,\quad c_2\equiv\frac{1}{2!}\epsilon''(0)=-\tfrac{1}{8}\ , \tag{2.36}$$

in agreement with the first few terms of (2.35). However, this similarity fails when pushed farther. In particular, it can be shown that for S states,[13]

$$\epsilon(\gamma)=c_0+c_2\gamma^2+c_3\gamma^3+O(\gamma^4\ln\gamma)\ . \tag{2.37}$$

Thus, (i) $\epsilon(\gamma)$ is *not* analytic in γ near $\gamma=0$ and, further, (ii) a term of order γ^5 appears in the total energy $E=m_1+\epsilon(\gamma)\gamma^2 m_1$. The coefficient c_3 can be found explicitly in terms of the nonrelativistic wave function via

$$c_3\gamma^5 m_1=-\frac{4\gamma^2}{3m_1^2}\,|\,\langle\phi_{n0}\,|\,\delta(\vec{r})\,|\,\phi_{n0}\rangle\,|^2\ . \tag{2.38}$$

For the $1s$ state this implies that

$$c_3=-\frac{4}{3\pi}\approx-0.42441\ . \tag{2.39}$$

Armed with the theoretical results (2.37)—(2.39) we can see to what extent our numerically determined $\epsilon^{\rm num}(\gamma)$ can reproduce the values of c_2 and c_3; we have already seen that c_0 is reproduced to 1 part in 10^5. To find c_2 from our (numerical) data, we extrapolate values of the quantity

$$c_2^{\rm num}(\gamma)\equiv[\epsilon^{\rm num}(\gamma)-\epsilon^{\rm num}(0)]/\gamma^2$$

to $\gamma=0$ and find

$$c_2^{\rm num}=-0.125418\ ,$$

which agrees very well with the exact value $c_2=-\frac{1}{8}=-0.1250$. To find $c_3^{\rm num}$, we extrapolate

$$c_3^{\rm num}(\gamma)\equiv[c_2^{\rm num}(\gamma)-c_2^{\rm num}]/\gamma$$

to $\gamma=0$ and find

$$c_3^{\rm num}=-0.408\ ,$$

in good agreement with (2.39). A least-squares fit with a cubic polynomial in γ gives similar results.

It should be noted that the contributions to the level shift of the γ^3 term in the binding energy is, for $\gamma\sim 10^{-3}$, only 1 part in $\sim 10^9$ of the main term, whereas our calculation of $\epsilon^{\rm num}(\gamma)$ was only claimed to be accurate to 1 part in $\sim 10^5$. The reason that we have, nevertheless, been able to extract the coefficient of the γ^3 term by our extrapolation procedure is that the error $\mathrm{Er}(\gamma)$ defined by (2.33) indeed satisfies an equation of the form (2.34), with an a of order unity. Thus $\mathrm{Er}(\gamma)$ is constant to 1 part in 10^5 in the range $\gamma\sim 0.001$ to 0.005 and the quantity $\epsilon^{\rm num}(\gamma)-\epsilon^{\rm num}(0)$ is accurate to at least 1 part in 10^{11} for γ in the indicated range. We have obtained results of similar precision for P states. We can thus feel confident of the accuracy of the numerical methods employed and are ready to turn to the two-body problem.

III. NO-PAIR TWO-BODY EQUATIONS

A. Preliminaries

In this section we study the low-lying bound-state spectrum of the two-body Hamiltonian $h_+(1,2)$ discussed in Sec. I, viz.,

$$h_+(1,2)=h_D(1)+h_D(2)+\Lambda_{++}V_{12}\Lambda_{++}\ . \tag{3.1}$$

We consider only the choices

$$V_{12}=V_{12}^c \tag{3.2a}$$

and

$$V_{12}=V_{12}^c+V_{12}^T\ , \tag{3.2b}$$

where V_{12}^c and V_{12}^T are the Coulomb potential and Breit operator, respectively, given by Eqs. (1.3) and (1.4). The reduction of the equation

$$h_+(1,2)\psi=E\psi$$

to Pauli form proceeds as described in Ref. 16. We set, in the c.m. system and in momentum space,

$$\psi=S_1S_2\phi\ , \tag{3.3a}$$

where, with

$$\xi_i=\frac{\vec{\alpha}_i\cdot\vec{\mathrm{p}}_i}{E_i(p)+m_i},\quad A_i=\left[\frac{E_i(\vec{\mathrm{p}})+m_i}{2E_i(\vec{\mathrm{p}})}\right]^{1/2}\ ,$$
$$S_i=(1+\xi_i)\beta_i^+A_i\ , \tag{3.3b}$$

and

$$\vec{\mathrm{p}}_1=-\vec{\mathrm{p}}_2=\vec{\mathrm{p}}\ .$$

The resulting equation for ϕ has the form

$$h_{\rm rel}\phi(\vec{\rm p})=E\phi(\vec{\rm p})\ , \tag{3.4}$$

where

$$h_{\rm rel}=E_1(\vec{\rm p})+E_2(\vec{\rm p})+V_{\rm eff}^{\rm op} \tag{3.5a}$$

and the interaction operator $V_{\rm eff}^{\rm op}$ has a kernel

$$V_{\rm eff}(\vec{\rm p},\vec{\rm p}')=(S_1S_2)^{\dagger}\tilde{V}_{12}(\vec{\rm p},\vec{\rm p}')S_1S_2\ . \tag{3.5b}$$

For the choice (3.2a) V_{12} is diagonal in Dirac-matrix indices and (3.5b) reduces to

$$V_{\rm eff}(\vec{\rm p},\vec{\rm p}')=A_1(\vec{\rm p})A_2(\vec{\rm p})(\tilde{V}^c_{12}+\zeta_1\tilde{V}^c_{12}\zeta_1'+\zeta_2\tilde{V}^c_{12}\zeta_2' +\zeta_1\zeta_2\tilde{V}^c_{12}\zeta_1'\zeta_2')A_1(\vec{\rm p}')A_2(\vec{\rm p}')\ , \tag{3.6a}$$

where

$$\zeta_1=\frac{\vec{\sigma}_1\cdot\vec{\rm p}}{E_1(\vec{\rm p})+m_1},\quad \zeta_2=\frac{\vec{\sigma}_2\cdot\vec{\rm p}}{E_2(\vec{\rm p})+m_2}\ , \tag{3.6b}$$

and the ζ_1' are similarly defined, with $\vec{\rm p}\to\vec{\rm p}'$; $\tilde{V}^c_{12}$ is the Fourier transform of (1.3), given by

$$\tilde{V}^c_{12}(\vec{\rm p}-\vec{\rm p}')=-\alpha/(2\pi^2\,|\,\vec{\rm p}-\vec{\rm p}'\,|^2) \tag{3.6c}$$

for $e_1=-e_2=-e$. For the choice (3.2b) we must add the contribution from the Breit operator; to spare the reader we do not write it out explicitly.

For the choice (3.2a) there is no tensor-force term in $V_{\rm eff}(\vec{\rm p},\vec{\rm p}')$ and the bound-state wave function can be taken to be an eigenfunction of $\vec{\rm j}^{\,2}_{\rm op}$, $j^z_{\rm op}$, $\vec{\rm S}^2$, and $\vec{\rm l}^{\,2}_{\rm op}$, where $\vec{\rm S}=\vec{\sigma}_1/2+\vec{\sigma}_2/2$, $\vec{\rm l}_{\rm op}=i(\partial/\partial\vec{\rm p})\times\vec{\rm p}$, and $\vec{\rm j}_{\rm op}=\vec{\rm S}+\vec{\rm l}_{\rm op}$. Thus we may write, as in the one-body problem [Eq. (2.12)],

$$\phi(\vec{\rm p})=g(p)Y^{j_z}_{j,l,s}(\hat{p})\ , \tag{3.7}$$

where $s=1$ or 0 and Y is an angular momentum eigenfunction. The resulting equation for $g(p)$ may be solved in the same way as (2.19).

For the choice (3.2b) there is a tensor-force term in $V_{\rm eff}(\vec{\rm p},\vec{\rm p}')$ and l is, in general, not a good quantum number. Thus, there will be mixing between, e.g., ^3S and ^3D states, etc. For simplicity we therefore consider only ^1S states, which do not mix.

B. Numerical results

Before solving (3.4) we first scale the momentum variable, as in the one-particle case, via

$$p=\alpha m_1 k\ ,$$

where α, now regarded as variable, controls the relativistic corrections to the nonrelativistic binding energy W. We define the two-particle binding energy, scaled by α^2m_1,

$$\epsilon(\alpha)=(E-m_1-m_2)/\alpha^2m_1\ . \tag{3.8}$$

For $\alpha\to0$, the resulting equation then reduces to the Schrödinger equation for a particle of mass $\mu=m_1m_2/(m_1+m_2)$ and the scaled ground-state binding energy has the limiting value

$$\epsilon(0)=-\frac{1}{2}\frac{m_2}{m_1+m_2}\ .$$

Shown in Fig. 2 are the numerical values of $\epsilon(\alpha)$ for the singlet S-wave ground state as a function of α, for the choices (3.2a) and (3.2b), with $m_1=m_2=m$. As can be seen, for choice (3.2a) $\epsilon(\alpha)$ is almost independent of α in the range considered. This is surprising—it would be nice to understand it on physical grounds.

As a test of the numerical accuracy we compare our $\epsilon^{\rm num}(\alpha)$ in the region $|\alpha|\ll1$ with the first few terms of the expansion of $\epsilon(\alpha)$. For the choice (3.2a), with $m_1=m_2=m$, one can show that

$$\epsilon(\alpha)=c_0+c_2\alpha^2+c_3\alpha^3+O(\alpha^4\ln\alpha)\ , \tag{3.9}$$

with

$$c_0=-\tfrac{1}{4},\quad c_2=\tfrac{3}{64}=0.046\,875\ , \tag{3.10}$$

and

$$c_3=-\frac{\alpha^2}{m^2}\left[\frac{\pi}{2}+\frac{5}{3}\right]|\langle\phi_{n0}|\,\delta(\vec{\rm r})\,|\phi_{n0}\rangle|^2_{n=1}/\alpha^2m$$
$$=-\left[\frac{\pi}{2}+\frac{5}{3}\right]\Big/8\pi\approx-0.128\,81\ . \tag{3.11}$$

We expect our accuracy to be comparable to that obtained for the $m_2=\infty$ case in Sec. II, and indeed we find

$$c_0^{\rm num}=-0.250\,001\,4\ ,$$

so that our nonrelativistic solution is again reproduced to better than 1 part in 10^5. To get $c_2^{\rm num}$ and $c_3^{\rm num}$ we extrapolate to $\alpha=0$ the same expressions as in the one-particle case and get

$$c_2^{\rm num}=0.046\,746\ ,$$
$$c_3^{\rm num}=-0.127\ ,$$

in excellent agreement with the theoretical results (3.10) and (3.11).

For the choice (3.2b) the values of c_0 and c_2 in the expansion (3.9) are

$$c_0=-\tfrac{1}{4},\quad c_2=-\tfrac{21}{64}=-0.328\,125\ . \tag{3.12}$$

The numerical values found were

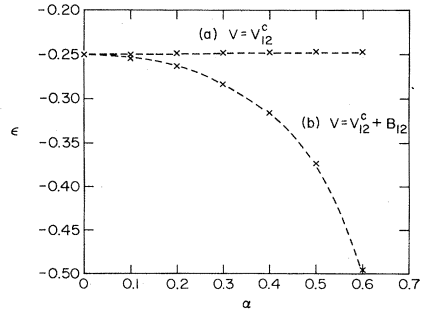

FIG. 2. Scaled eigenvalue $\epsilon(\alpha)$, defined by Eq. (3.8), for the $^1S_0$ ground state of $h_+(1,2)$ [Eq. (3.1)], as a function of α, regarded as variable, for $m_1=m_2$ and for two choices of V_{12}.

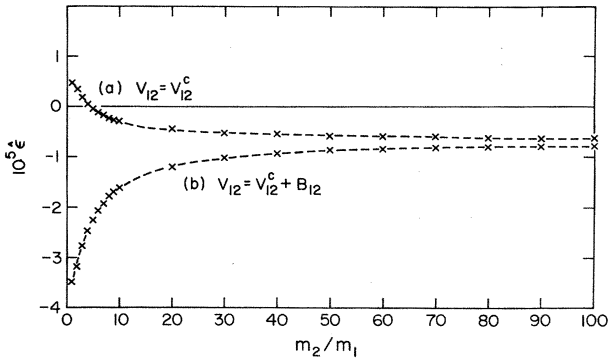

FIG. 3. Scaled fine-structure energy $\hat{\epsilon}$, defined by Eq. (3.13), for the $^1S_0$ ground state of $h_+(1,2)$, as a function of the mass ratio m_2/m_1, for two choices of V_{12}.

$$c_0^{\rm num}=-0.2500014,\quad c_2^{\rm num}=-0.327936\ ,$$

in good agreement with (3.12). We also find

$$c_3^{\rm num}=0.188\ ,$$

but have not calculated the theoretical value of c_3.

If $m_1\neq m_2$ there is still some interest in obtaining accurate solutions to Eq. (3.4). The numerical method can be used in this case just as easily as in the equal-mass case. Figure 3 shows the quantity

$$\hat{\epsilon}=[\epsilon(\alpha)-\epsilon(0)]m_1\mu^{-1} \tag{3.13}$$

as a function of the ratio m_2/m_1, for the choices (3.2a) and (3.2b), with $\alpha=\frac{1}{137}$. We have verified that in either case $\epsilon(\alpha)$ converges to the corresponding eigenvalue of $h_+(1)$ with $Z=1$, when $m_2\to\infty$, as expected. This figure can be used to read off some of the recoil corrections for μ-mesic hydrogen ($m_2/m_1\sim 9$).

IV. SUMMARY AND DISCUSSION

Three-dimensional relativistic wave equations derived from field theory which describe a system of N interacting Dirac particles inevitably involve projection operators. In this paper we have shown that the presence of these operators need not be a barrier to obtaining accurate eigenvalues for two-body bound states, even when the interactions involve $1/r$ singularities—as they do for most cases of physical interest. Although we have not stressed it, the method of solution also supplies wave functions of corresponding accuracy. This should provide encouragement for the use of such no-pair equations for the case when $N\geq 3$, e.g., even for moderately heavy atoms, where further approximations, of course, have to be made to reduce the problem of tractable form, but where free-particle projection operators can still be used. For very heavy atoms one must either deal with the external-field projection operators (which are nonlocal even in $\vec{p}$ space) or use an approach such as that described in Ref. 8.

Apart from this, the no-pair equations are of interest even for the relatively few-body problem, e.g., $N=3$, because of the absence of continuum dissolution. Their application to the quark model of the nucleon remains to be explored.

Even for the two-body problem the no-pair equations studied in Sec. III are of interest because of the physical insight they give on some aspects of level shifts in electromagnetically bound systems such as hydrogen, muonium, and positronium.

In this connection let us pursue a bit the question of contributions arising from intermediate states involving fermion-antifermion pairs. As we have seen earlier, in the one-particle case ($m_2=\infty$) there is a γ^5 contribution to the total energy $E=m_1+\epsilon(\gamma)\gamma^2 m_1$. However, no such term exists in the expansion of the exact Dirac eigenvalue $E_D=(1-\gamma^2)^{1/2}m_1$. For this one-particle case the γ^5 term coming from (2.19) can be shown to be precisely canceled by pair-correction terms, so that there is complete agreement among results obtained from the Dirac equation, the theoretical values obtained from $h_+(1)$ and the pair diagram, and our numerical results, at least to order γ^5.

It is interesting to analyze this problem for the case of $m_1\leq m_2<\infty$. The time-ordered diagrams which need to be considered are shown in Fig. 4. The α^5 contributions from these diagrams may be written in the form

$$\Delta E_j=\pi\alpha^2\,|\,\langle\phi_{n0}\,|\,\delta(\vec{r})\,|\,\phi_{n0}\rangle\,|^2\frac{F_j}{m_1^2}\ ,$$

where the F_j are integrals over algebraic functions, which we need not record here. For $n=1$ we have

$$\Delta E_j=\alpha^5\frac{\mu^3}{m_1^2}F_j\ . \tag{4.1}$$

Calculation shows that for $m_1=m_2$,

$$F_a=1,\quad F_b=1,\quad F_c=-\left[\frac{5}{3}-\frac{\pi}{2}\right],$$

whereas for $m_2=\infty$,

$$F_a=\tfrac{4}{3},\quad F_b=0,\quad F_c=0\ .$$

But there is also an α^5 contribution ΔE_d in the general case, coming from the power-series expansion of the eigenvalue E of h_+, of the same form as (4.1), with an integral F_d replacing F_j. We find

$$F_d=-\left[\frac{5}{3}+\frac{\pi}{2}\right]\ (m_1=m_2);\quad F_d=-\tfrac{4}{3}\ (m_2=\infty)\ .$$

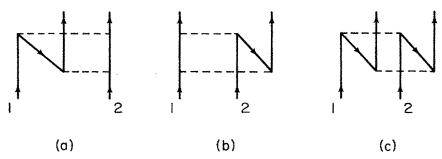

FIG. 4. Time-ordered Feynman diagrams associated with virtual-pair creation and annihilation arising from the Coulomb interaction.

It follows that for $m_1=m_2$,

$$\Sigma F_\alpha = 1+1-\left[\frac{5}{3}-\frac{\pi}{2}\right]-\left[\frac{5}{3}+\frac{\pi}{2}\right]=-\tfrac{4}{3} \tag{4.2}$$

and there is a *net* $\alpha^5 m$ term, whereas for $m_2=\infty$,

$$\Sigma F_\alpha = \tfrac{4}{3}+0+0-\tfrac{4}{3}=0 \tag{4.3}$$

and there is no net $\alpha^5 m$ term, as already mentioned in Sec. III. The analytic form of ΣF is given by

$$\Sigma F_\alpha = -\tfrac{4}{3}(m_1/m_2)\ ,$$

consistent with (4.2) and (4.3).

In conclusion, we hope to have demonstrated that the (free) positive-energy projection operators which make the no-pair equations look a bit daunting are not an impediment to the accurate numerical solution of such equations. The application of Hamiltonians such as $h_+(1,2)$ to bound states of $(q,\bar{q})$ systems *without* the use of a v/c expansion would seem to be a worthwhile extension of the techniques presented in this paper.[20]

ACKNOWLEDGMENTS

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