Application of the new fermion-antifermion equation to positronium and the numerical solution of its static-interaction limit, the Breit equation

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The fermion-antifermion equation derived recently is applied here to positronium with the aim of laying the groundwork for a systematic calculation of the higher-order corrections. An equation valid to the fourth order in the fine-structure constant is obtained which is equivalent to the corresponding equation derived within the Bethe-Salpeter formalism. The static-interaction limit of this equation, the Breit equation, is then decomposed into angular momentum states, whereby four second-order differential equations are obtained. The resulting eigenvalue equations are solved numerically using the appropriate boundary conditions at the origin. The resulting spectrum is in agreement with perturbative calculations.

I. INTRODUCTION

In previous publications[1,2] (hereafter referred to as Papers I and II, respectively) a new two-body formalism including a fermion-antifermion equation was derived within the context of quantum electrodynamics. This formalism was applied to a representative spectrum of quantum-electrodynamical bound-state calculations for the purpose of demonstrating its effectiveness in dealing with such problems.

In this paper, we take a preliminary step toward a systematic application of the fermion-antifermion equation of Paper II to the calculation of the positronium hyperfine structure. As is well known, on account of its great complexity, the theoretical calculation of this structure is lagging behind the experimental determination in accuracy. Indeed, calculations beyond the leading-order corrections are nontrivial, and those of sixth order (in the fine-structure constant α) constitute a delicate and challenging task.[3] Our task here, however, will be a limited one, consisting of an analysis of the positronium equation through fourth order as well as the decomposition and numerical solution of its static-interaction limit, the Breit equation.[4] That such a task is both necessary and worthwhile may be witnessed in similar calculations, including higher orders, within the customary Bethe-Salpeter bound-state formalism.[5] Specifically, we shall use the procedures of Papers I and II to reduce the exact system of functional-differential positronium equations to an ordinary equation valid to fourth order in α. As expected, this will be the Breit equation augmented by an effective potential representing the (corrected form of the) Breit interaction and the virtual annihilation contribution, both of which are of the fourth order. We will then proceed to an angular momentum decomposition of the Breit equation whereby we obtain four second-order differential equations, two of which are coupled. The appropriate boundary conditions at the origin are then found and the resulting eigenvalue problem solved by numerical integration. The spectrum thus obtained for the first two Bohr levels is in complete agreement with perturbative calculations. This establishes the Breit equation as a viable and physically well-behaved static-limit relativistic two-fermion equation. In the course of the above analyses, we also obtain the (known) effective potential representing all fourth-order corrections to the nonrelativistic (second-order) Hamiltonian.

The paper is organized as follows: Section II presents the derivation of the fourth-order positronium equation and the associated effective potential. Section III contains the angular momentum decomposition of the Breit equation, and Sec. IV continues with a consideration of boundary conditions at the origin and numerical solutions. Section V presents our concluding remarks.

II. DERIVATION OF THE FOURTH-ORDER POSITRONIUM EQUATION

In this section we shall start with the exact system of functional-differential equations describing positronium, Eqs. (7) of Paper II, and obtain therefrom an approximate equation valid to the fourth order in the fine-structure constant. Although our basic procedure will be the same as in Papers I and II, we shall here proceed in a more detailed manner as well as repeat some previous steps in order to facilitate a clear presentation of the derivations.

Let us briefly recall that the formalism involves an auxiliary vector potential A^μ which appears as a dummy functional variable upon which the various amplitudes depend and upon whose vanishing the physical values of these amplitudes obtain.

With the notation of Paper II (except for obvious minor alterations), the positronium equations in the center-of-mass frame and for equal times are

$$\left(i\frac{\partial}{\partial t}-h\right)\chi(x,y)=[U^{(e)}(x)+U^{(p)}(y)]\chi(x,y)+e[\beta^{(e)}\gamma_\mu^{(e)}F^\mu(x)-\beta^{(p)}\gamma_\mu^{(p)}F^\mu(y)]\times S(x,y)C\quad(x^0=y^0=t),\tag{1}$$

where

$$h=h^{(e)}(\vec{x})+h^{(p)}(\vec{y}),\tag{2}$$

$$h^{(e),(p)}(\vec{x})=\vec{\alpha}^{(e),(p)}\cdot\vec{p}_x+\beta^{(e),(p)}m,$$

$$U^{(e),(p)}(x)=\pm e\beta^{(e),(p)}\gamma_\mu^{(e),(p)}\phi^\mu(x),\tag{3}$$

$$\phi^\mu(x)=A^\mu(x)+i\int d^4z\,D^{\nu\mu}(z,x)\frac{\delta}{\delta A^\nu(z)},$$

$$F_\mu(x)=ie\int d^4z\,D^0_{\mu\nu}(x-z)\,\mathrm{tr}[\gamma^\nu\chi(z,z)C],\tag{4}$$

$$C=i\gamma^2\gamma^0.$$

Here we have employed the usual bispinor notation according to which a Dirac matrix labeled (e) $[(p)]$ operates on the first [second] spinor index of its operand, and one without a label effects an ordinary matrix multiplication. Moreover, the propagators S and D which appear above are to be obtained from the following Schwinger equations[6]:

$$D_{\mu\nu}(x,y)=D^0_{\mu\nu}(x-y)-ie\int d^4z\,d^4z'\,D^0_{\mu\lambda}(x-z)\times\mathrm{tr}\left(\gamma^\lambda\frac{\delta S(z,z)}{\delta A_\sigma(z')}\right)D_{\sigma\nu}(z',y),\tag{5}$$

$$S(x,y)=S^0(x-y)+e\int d^4z\,S^0(x-z)\gamma_\mu\phi^\mu(z)S(z,y),\tag{6}$$

where D^0 and S^0 are free propagators with an arbitrary choice of gauge for the former. For convenience, we shall adopt the Coulomb gauge in the present calculation. Note that Eqs. (5) and (6) constitute a closed set and are independent of the positronium equations.

The first step in the reduction of (1) is the extraction of the static Coulomb interaction. We shall do this by integrating the "electrostatic field" as in Papers I and II. We briefly recall that this is accomplished by means of the transformations

$$\chi(x,y)=e^{-iQ(x,y)}\hat{\chi}(x,y),\tag{7}$$

$$S(x,y)=e^{-iQ(x,y)}\hat{S}(x,y),\tag{8}$$

where

$$Q(x,y)=e\int dt'\Theta(t-t')[A^0(t',\vec{x})-A^0(t',\vec{y})].$$

The result is

$$\left(i\frac{\partial}{\partial t}-h\right)\hat{\chi}=[\hat{U}^{(e)}(x)+\hat{U}^{(p)}(y)+\mathcal{U}(x,y)]\hat{\chi}(x,y)+e[\beta^{(e)}\gamma_\mu^{(e)}F^\mu(x)-\beta^{(p)}\gamma_\mu^{(p)}F^\mu(y)]\times S(x,y)C\quad(x^0=y^0=t),\tag{9}$$

where

$$\mathcal{U}(x,y)=-e^2\int d^4z\,D_{00}(z,x)[\delta(\vec{z}-\vec{x})+\delta(\vec{z}-\vec{y})],$$

and

$$\hat{U}^{(e)}(x)=ie\int d^4z\,D_{00}(z,x)\frac{\delta}{\delta A_0(z)}-\vec{\alpha}^{(e)}\cdot\left(e\vec{\phi}(x)+e\vec{\nabla}\int dt'\,\theta(t-t')\,A^0(t',\vec{x})\right).$$

Here $\hat{S}$ and $\hat{U}^{(p)}$ are defined analogously to $\hat{\chi}$ and $\hat{U}^{(e)}$, respectively. Note that the "electrostatic field" A^0 has been integrated away and in its place have appeared the electrostatic potential $\mathcal{U}$ and the higher-order corrections thereto (represented by the $\vec{\nabla}A^0$ term).

Equation (9) is still exact. We now proceed to omit from consideration self-energy contributions and multiphoton exchanges, all of which contribute to $O(m\alpha^2)$ and higher. These simplifications will reduce the propagators D and $\hat{S}$ to their lowest-order terms D^0 and S^0, $\mathcal{U}(x,y)$ to the Coulomb potential $V_C(\vec{x}-\vec{y})$, $U^{(e),(p)}$ to

$$u^{(e)}(x)=-e\alpha_i^{(e)}\left(A^i(x)+i\int d^4z\,D^0_{ij}(z-x)\frac{\delta}{\delta B_j(z)}\right),$$

$$u^{(p)}(y)=e\alpha_i^{(p)}\left(B^i(y)+i\int d^4z\,D^0_{ij}(z-y)\frac{\delta}{\delta A_j(z)}\right),$$

and Eq. (9) to

$$\left(i\frac{\partial}{\partial t}-h-V_C(\vec{x}-\vec{y})\right)\hat{\chi}(x,y)=[u^{(p)}(x)+u^{(p)}(y)]\hat{\chi}(x,y)+e[\beta^{(e)}\gamma_\mu^{(e)}f^\mu(x)-\beta^{(p)}\gamma_\mu^{(p)}f^\mu(y)]\times S^0(x-y)C\quad(x^0=y^0=t),\tag{10}$$

where

$$f_\mu(x)=ie\int d^4x'\,D^0_{\mu\nu}(x-x')e^{-ip\cdot x'}\,\mathrm{tr}[\gamma^\nu\hat{\chi}(0,0)C].$$

Upon taking note of Eq. (8) of Paper II and the fact that the total momentum P^μ in the center-of-mass frame has only a time component equal to the mass of positronium E, we may convert the last equation into

$$f^i(x)=(-ie/E^2)e^{-iEx^0}\mathrm{tr}[\gamma^i\hat{\chi}(0,0)C],\tag{11}$$

with f^0 vanishing. Furthermore, to the desired order of accuracy, E in the denominator may be replaced by $2m$. Note that there are now two vec-

tors $\vec{A}$ and $\vec{B}$ which appear as functional variables; this change has the sole effect of preventing the emission and reabsorption of a photon by the same fermion. Also observe that the interaction terms appearing in the right-hand side of (10) originate in single (transverse) photon exchange in the forward (represented by the terms containing u) and crossed (represented by the terms containing f) channels.

We now proceed to convert the forward-exchange contribution into a potential to the leading order. This is most simply accomplished by considering the interaction operator whose expectation value will yield the first-order energy shift contributed by $u^{(e)}+u^{(p)}$. That operator according to Eq. (22) of Paper I is [see also Eq. (23) therein]

$$\lim_{\vec{A},\vec{B}\to 0} i\int dt'\{u^{(e)}(t')\exp[-i(h-E^0)(t-t')][\Theta(t-t')\Lambda^{+(p)}-\Theta(t'-t)\Lambda^{-(p)}]u^{(p)}(t)$$
$$+u^{(p)}(t')\exp[-i(h-E^0)(t-t')][\Theta(t-t')\Lambda^{+(e)}-\Theta(t'-t)\Lambda^{-(e)}]u^{(e)}(t)\}, \tag{12}$$

where $\Lambda^{\pm}$ are the customary energy projection operators, and E^0 is the energy of the unperturbed two-particle state. Note that in writing the above we have neglected the Coulomb binding in the unperturbed states. Upon carrying out the implied functional differentiations, we can write the above operator (in configuration space) as

$$-e^2\int dt'\{\exp[-i(\epsilon_i^{(e)}+\epsilon_f^{(p)}-E^0)(t-t')]D^{0ij}(t-t',\vec{x}-\vec{y}')\delta(\vec{x}-\vec{x}')$$
$$\times[\Theta(t-t')\Lambda^{+(p)}(\vec{y}-\vec{y}')-\Theta(t'-t)\Lambda^{-(p)}(\vec{y}-\vec{y}')]\alpha_i^{(e)}\alpha_j^{(p)}+\exp[-i(\epsilon_i^{(p)}+\epsilon_f^{(e)}-E^0)(t-t')]$$
$$\times D^{0ij}(t-t',\vec{x}'-\vec{y})\delta(\vec{y}-\vec{y}')[\Theta(t-t')\Lambda^{+(e)}(\vec{x}-\vec{x}')-\Theta(t'-t)\Lambda^{-(e)}(\vec{x}-\vec{x}')]\alpha_i^{(p)}\alpha_j^{(e)}\}, \tag{13}$$

where ϵ_i (ϵ_f) denotes an initial (final) energy. We now observe that the dominant contribution to (13) comes from photon momenta of the order of Bohr momentum $m\alpha$, for which the kinetic energies $[O(m\alpha^2)]$ involved in ϵ_i, ϵ_f, and E^0 may be neglected. Furthermore, only combinations which render energy differences occurring in the exponential terms negligible relative to the photon energy contribute to the desired order. This circumstance, together with the effect of the energy projection operators, reduces the four terms occurring in (13), respectively, to

$$\tfrac{1}{2}(\Lambda^{++}U_B\Lambda^{++}+\Lambda^{-+}U_B\Lambda^{-+}),$$
$$-\tfrac{1}{2}(\Lambda^{+-}U_B\Lambda^{+-}+\Lambda^{--}U_B\Lambda^{--}),$$
$$\tfrac{1}{2}(\Lambda^{++}U_B\Lambda^{++}+\Lambda^{+-}U_B\Lambda^{+-}),$$
$$-\tfrac{1}{2}(\Lambda^{-+}U_B\Lambda^{-+}+\Lambda^{--}U_B\Lambda^{--}),$$

whose sum, upon discarding the (negligible) terms involving Λ^{--}, yields the (correct form of the) Breit interaction

$$V_B(\vec{r})=\Lambda^{++}U_B(\vec{r})\Lambda^{++}, \tag{14}$$

where

$$\Lambda^{++}=\Lambda^{+(e)}\Lambda^{+(p)},$$

etc., and U_B is given by

$$U_B(\vec{r})=-2e^2\alpha_i^{(e)}\alpha_j^{(p)}\int_{-\infty}^{+\infty}dt'\,D^{0ij}(t',\vec{r})\,\Theta(\pm t')$$
$$=-\alpha_i^{(e)}\alpha_j^{(p)}(\delta^{ij}-\hat{\nabla}^i\hat{\nabla}^j)V_C(r)$$
$$=-\tfrac{1}{2}(\vec{\alpha}^{(e)}\cdot\vec{\alpha}^{(p)}+\vec{\alpha}^{(e)}\cdot\hat{r}\,\vec{\alpha}^{(p)}\cdot\hat{r})V_C(r). \tag{15}$$

As is well known, U_B is the interaction term obtained by Breit[4] on the basis of intuitive reasoning and known to be incorrect if treated beyond first order. V_B, on the other hand, is correct to order $m\alpha^4$ and agrees (to this order) with results obtained within the Bethe-Salpeter formalism.[7]

Finally we turn to the simplification of the virtual annihilation potential. To the desired accuracy, we may replace $S^0(0,\vec{x}-\vec{y})$ in (10) by $-\frac{1}{2}i\delta(\vec{x}-\vec{y})$, which turns the virtual annihilation term in (10) into (cf. Sec. IV of Paper II),

$$(\pi\alpha/m^2)e^{-iEt}\delta(\vec{x}-\vec{y})\,\mathrm{tr}[\vec{\gamma}\hat{\chi}(0,0)C]\cdot\vec{\alpha}C.$$

We are now in a position to assemble the time-independent, center-of-mass-frame positronium equation to $O(m\alpha^4)$:

$$E\chi(\vec{r})=[h^{(e)}(\vec{r})+h^{(p)}(-\vec{r})+V_C(r)+V_B(\vec{r})]\hat{\chi}(\vec{r})$$
$$+\int d\vec{r}'\,V_A(\vec{r},\vec{r}')\chi(\vec{r}'), \tag{16}$$

where

$$\int d\vec{r}'\,V_A(\vec{r},\vec{r}')\chi(\vec{r}')=\frac{\pi\alpha}{m^2}\delta(\vec{r})\vec{\alpha}C\cdot\mathrm{tr}[\vec{\gamma}\chi(0)C],$$

and $V_B(\vec{r})$ is defined by Eqs. (14) and (15).

As repeatedly mentioned above, Eq. (16) is accurate to order $m\alpha^4$, i.e., an order α^2 higher in accuracy than the nonrelativistic limit and the first correction thereto. One could therefore define an effective potential $V^{(4)\mathrm{eff}}$ accurate to $O(m\alpha^4)$. Clearly, $V^{(4)\mathrm{eff}}$ is the sum of the contributions of V_B, V_A, and whatever $O(m\alpha^4)$ correction is produced by the Breit equation. The latter is calcu-

lated in Sec. III where it is shown to be

$$\Delta^{\text{eff}} = -\frac{\vec{p}^4}{4m^3} + \frac{\pi\alpha\delta(\vec{r})}{m^2} + \frac{\alpha\vec{L}\cdot\vec{S}}{2m^2r^3}\,, \tag{45}$$

where $\vec{S}$ is the total spin operator. Similarly, the effective potential corresponding to V_A may be immediately obtained from its definition above (see also Sec. IV of Paper II); it is

$$V_A^{\text{eff}} = (\pi\alpha\vec{S}^2/m^2)\delta(\vec{r})\,.$$

The evaluation of V_B^{eff} may be achieved by multiplying out the Dirac matrices occurring in (14), and retaining the leading-order contributions which come from the even Dirac operators (i.e., terms containing an even number of $\vec{\alpha}$'s). This procedure and some algebra lead to the result

$$V_B^{\text{eff}} = -\frac{\alpha}{2m^2r}[\vec{p}^2 + (\hat{r}\cdot\vec{p})^2] + \frac{\alpha}{m^2r^3}\vec{L}\cdot\vec{S} + \frac{8\pi\alpha}{3m^2}\delta(\vec{r})\vec{s}^{(e)}\cdot\vec{s}^{(p)} + \frac{\alpha}{m^2r^3} \times [3\vec{s}^{(e)}\cdot\hat{r}\,\vec{s}^{(p)}\cdot\hat{r} - \vec{s}^{(e)}\cdot\vec{s}^{(p)}]\,,$$

where $\vec{s}$ represents a spin operator. Finally, the total $O(m\alpha^4)$ effective potential is given by[8]

$$V^{(4)\text{eff}} = \frac{-\vec{p}^4}{4m^3} - \frac{\alpha}{2m^2r}[\vec{p}^2 + (\hat{r}\cdot\vec{p})^2] + \frac{\pi\alpha\delta(\vec{r})}{m^2} \times\left(\frac{4}{3}\vec{s}^{(e)}\cdot\vec{s}^{(p)}\right) + \frac{3}{2}\frac{\alpha}{m^2r^3}\vec{L}\cdot\vec{S} + \frac{\alpha}{m^2r^3} \times (3\vec{s}^{(e)}\cdot\hat{r}\,\vec{s}^{(p)}\cdot\hat{r} - \vec{s}^{(e)}\cdot\vec{s}^{(p)})\,.$$

Returning to Eq. (16), we remark that the "range" of the annihilation term V_A, which reduced to zero as a consequence of our approximation, was originally finite and equal to $1/m$ as expected. If one wishes, one may make the reverse replacement

$$\delta(\vec{r}) \to \frac{m^2}{2\pi^2}\frac{K_1(r)}{r}\,,$$

where K is the modified Bessel function of the second kind, to obtain an interaction of finite range. Of course, the two are equivalent within $O(m\alpha^4)$.

We conclude this section by reminding the reader that the contributions to $V^{(4)\text{eff}}$ have long been known in one form or another; here we have derived them within the new formalism.

III. DECOMPOSITION OF THE BREIT EQUATION

In this and the following sections[9] we will present the decomposition and numerical solution of the Breit equation

$$E\chi(\vec{r}) = [h^{(e)}(\vec{r}) + h^{(p)}(-\vec{r}) + V(r)]\chi(\vec{r})\,, \tag{17}$$

where we are now denoting the Coulomb potential by V. Although we could equally well carry out the same for the complete fourth-order equation (16), we shall not do so, since the difference between the two represents $O(m\alpha^4)$ contributions and is not accurate beyond this order. Furthermore, the main objective of illustrating the procedure of solving a Breit-type equation is served equally well, as well as more simply, by considering Eq. (17).

It is convenient to revert to a matrix notation by setting

$$\chi = \psi\Sigma_2\,,$$

which leads to

$$E\psi = H\psi \equiv [\tfrac{1}{2}V + \vec{\alpha}\cdot\vec{p} + \beta m, \psi]_+\,, \tag{18}$$

where it is understood that

$$\psi\vec{p} \equiv \vec{p}\,\psi \equiv -i\vec{\nabla}_r\psi\,.$$

Let us record the standard symmetry properties associated with (18).[10] The operator H is Hermitian under the inner product

$$\langle\phi|\psi\rangle = \int d\vec{r}\,\mathrm{tr}[\phi^\dagger(\vec{r})\psi(\vec{r})]\,, \tag{19}$$

which is inherited from the bispinor inner product of Eq. (17). The (total) angular momentum operator $\vec{J}$ and its square are represented by

$$\vec{J}\psi = \vec{L}\psi + \tfrac{1}{2}[\vec{\Sigma}, \psi]\,, \tag{20}$$

$$\vec{J}^2\chi = \vec{L}^2\psi + \vec{L}\cdot[\vec{\Sigma}, \psi] + \tfrac{3}{2}\psi - \tfrac{1}{2}\vec{\Sigma}\cdot\psi\vec{\Sigma}\,, \tag{21}$$

where $\vec{L}$ is equal to $\vec{r}\times\vec{p}$ as usual. The parity operator P is defined by

$$P\psi(\vec{r}) = \beta\psi(-\vec{r})\beta\,. \tag{22}$$

In addition to the above, the exchange symmetry of the equation (induced by charge conjugation symmetry) may be represented by the operator Q, where

$$Q\psi = \beta\Sigma_2\psi^t\Sigma_2\beta\,. \tag{23}$$

It is now a matter of standard procedure to verify that the Hermitian operators H, $\vec{J}^2$, J_3, P, and Q constitute a commuting set. The latter four may therefore be used to classify the possible states in the usual way. As usual, it is convenient to use $\pi = (-1)^J P$ instead of P. We therefore denote by $\phi_{JM\pi Q}$ a wave function which is an eigenfunction of the set $\vec{J}^2$, J_3, π, and Q with the corresponding eigenvalues $J(J+1)$, M, π, Q [e.g., ϕ_{JM+-} has parity $(-1)^J$ and is odd under Q]. We will omit the steps involved in the construction of the ϕ's and directly state the results:

$$\phi_{JM++}=[\tfrac{1}{2}(f_1+f_2)+\tfrac{1}{2}\beta(f_1-f_2)+\vec{\alpha}\cdot(\vec{p}g_1+\vec{p}\times\vec{L}g_2)]y_{JM}(\hat{r}), \quad (24)$$

$$\phi_{JM+-}=[\tfrac{1}{2}\vec{\Sigma}\cdot\vec{L}(f_1+f_2)+\tfrac{1}{2}\beta\vec{\Sigma}\cdot\vec{L}(f_1-f_2)+\beta\vec{\alpha}\cdot(\vec{p}g_1+\vec{p}\times\vec{L}g_2)]y_{JM}(\hat{r}), \quad J\geq 1 \quad (25)$$

$$\phi_{JM-+}=(\beta\gamma_5 g_1+\vec{\alpha}\cdot\vec{L}g_2)y_{JM}(\hat{r}), \quad (26)$$

$$\phi_{JM--}=\{\tfrac{1}{2}\vec{\Sigma}\cdot[\vec{p}(f_1+g_1)+\vec{p}\times\vec{L}(f_2+g_2)]+\tfrac{1}{2}\beta\vec{\Sigma}\cdot[\vec{p}(f_1-g_1)+\vec{p}\times\vec{L}(f_2-g_2)]+\gamma_5 F_1+\beta\vec{\alpha}\cdot\vec{L}F_2\}Y_{JM}(\hat{r}), \quad (27)$$

where f_1, f_2, g_1, g_2, F_1, and F_2 are arbitrary functions of r, unrelated from one equation to another. In terms of the customary classification of the states of a pair of spin-$\frac{1}{2}$ particles, ϕ_{JM++} represents a singlet state, ϕ_{JM+-} a triplet state with $L=J$, and ϕ_{JM--} a triplet state with $J=L-1$ and $L+1$. As for ϕ_{JM-+}, we can easily verify that it is unphysical by verifying that it cannot satisfy (18). To see this, we obtain from (18) the easily derived constraint (cf. Appendix of Paper II)

$$\mathrm{tr}[\gamma^0\gamma^5\psi]=0, \quad (28)$$

and apply it to ϕ_{JM-+} to deduce that g_1 must vanish. The vanishing of g_2 is similarly ascertained upon insertion into (18).

The next stage in the decomposition of (18) is the insertion of the ϕ's above therein and the extraction of the resulting radial equations. Again we will omit the details and record the results. For singlet states we get

$$[(V-\epsilon)f_1+2\vec{p}^2 g_1]y_{JM}(\hat{r})=0,$$
$$[(-4m+V-\epsilon)f_2+2\vec{p}^2 g_1]y_{JM}(\hat{r})=0,$$
$$[\vec{p}(f_1+f_2)-(E-V)(\vec{p}g_1+\vec{p}\times\vec{L}g_2)]y_{JM}(\hat{r})=0, \quad (29)$$

where we have set $E=2m+\epsilon$, $-\epsilon$ being the binding energy. Some simple steps transform (29) into a single equation for $u^S_J\equiv f_1+f_2$:

$$\left[\frac{\vec{p}^2}{m}+4ma(1-a)-\frac{\alpha}{2m^2r^3(1-2a)}\vec{r}\cdot\vec{\nabla}\right]u^S_J=0, \quad (30)$$

where

$$\vec{p}^2=p_r^2+\frac{J(J+1)}{r^2}, \quad p_r^2=-\frac{d^2}{dr^2}-\frac{2}{r}\frac{d}{dr}, \quad a=\frac{V-\epsilon}{4m}.$$

Note that a is $O(\alpha^2)$ and that to $O(m\alpha^4)$, Eq. (30) reduces to

$$\left(\frac{\vec{p}^2}{m}+V-\epsilon\right)u^S_J-\left(4ma^2+\frac{\alpha}{2m^2r^3}\vec{r}\cdot\vec{\nabla}\right)u^S_J\simeq 0.$$

Thus the effective potential representing the $O(m\alpha^4)$ energy shift for this case is given by

$$V^{\mathrm{eff}}_{++}=-\frac{(V-\epsilon)^2}{4m}-\frac{\alpha}{2m^2r^3}\vec{r}\cdot\vec{\nabla}=-\frac{\vec{p}^4}{4m^3}+\frac{\pi\alpha\delta(\vec{r})}{m^2}. \quad (31)$$

Next we turn to ϕ_{JM+-} (corresponding to triplet states with $L=J$), where we obtain the equations

$$[(V-\epsilon)f_1+2i\vec{p}^2 g_2]Y_{JM}(\hat{r})=0,$$
$$[(4m+\epsilon-V)f_2+2i\vec{p}^2 g_2]y_{JM}(\hat{r})=0, \quad (32)$$
$$[i\vec{p}\times\vec{L}(f_2-f_1)-(E-V)(\vec{p}g_1+\vec{p}\times\vec{L}g_2)]y_{JM}(\hat{r})=0.$$

As before, Eqs. (32) may be reduced to a single one for $u^T_{J,J}\equiv f_2-f_1$;

$$\left(\frac{\vec{p}^2}{m}+4ma(1-a)-\frac{\alpha}{2m^2r^3(1-2a)}\times(1+\vec{r}\cdot\vec{\nabla})\right)u^T_{J,J}=0, \quad J\geq 1. \quad (33)$$

The corresponding equation to $O(m\alpha^4)$ is

$$\left(\frac{\vec{p}^2}{m}+V-\epsilon\right)u^T_{J,J}-\left(4ma^2+\frac{\alpha}{2m^2r^3}(1+\vec{r}\cdot\vec{\nabla})\right)u^T_{J,J}\simeq 0, \quad J\geq 1,$$

with the $O(m\alpha^4)$ effective potential given by

$$V^{\mathrm{eff}}_{+-}=-\frac{(V-\epsilon)^2}{4m}-\frac{\alpha}{2m^2r^3}(1+\vec{r}\cdot\vec{\nabla})=\frac{-\vec{p}^4}{4m^3}-\frac{\alpha}{2m^2r^3}, \quad (34)$$

where we have dropped an inconsequential δ-function term because $L=J\neq 0$ in this case.

Finally, we turn to ϕ_{JM--}, and define

$$\vec{\mathcal{F}}=\vec{p}f_1+\vec{p}\times\vec{L}f_2, \quad \vec{\mathcal{G}}=\vec{p}g_1+\vec{p}\times\vec{L}g_2, \quad \tilde{V}=E-V.$$

Using these definitions, we may write the equations resulting in this case as follows:

$$[(2m-\tilde{V})\vec{\mathcal{F}}+2\vec{p}F_1-2i\vec{p}\times\vec{L}F_2]y_{JM}(\hat{r})=0,$$
$$[-(2m+\tilde{V})\vec{\mathcal{G}}+2\vec{p}F_1+2i\vec{p}\times\vec{L}F_2]y_{JM}(\hat{r})=0,$$
$$[\tilde{V}F_1-\vec{p}(\vec{\mathcal{F}}+\vec{\mathcal{G}})]y_{JM}(\hat{r})=0, \quad (35)$$
$$[i\vec{L}^2\tilde{V}F_2-(\vec{L}\times\vec{p})\cdot(\vec{\mathcal{F}}-\vec{\mathcal{G}})]y_{JM}(\hat{r})=0.$$

As in the above, these equations may again be simplified, but this time to one in terms of the vector function $\vec{A}=\vec{\mathcal{F}}-\vec{\mathcal{G}}$;

$$[(\vec{p}^2+m^2-\tfrac{1}{4}\tilde{V}^2)\vec{A}-\vec{q}\vec{p}\cdot\vec{A}-(\vec{p}\times\vec{L})(1/\vec{L}^2)(\vec{L}\times\vec{q})\cdot\vec{A}]\times y_{JM}(\hat{r})=0, \quad (36)$$

where

$$\vec{q}=\vec{p}\ln\tilde{V}.$$

It is clear from the definition of $\vec{A}$ that $\vec{L}\cdot\vec{A}=0$. Using this property, we make the convenient resolution

$$\begin{aligned}
&\vec{A} = \vec{A}_{J-1} + \vec{A}_{J+1}, \\
&\vec{A}_{J-1} = (\hat{r} + i\alpha_1 \hat{r} \times \vec{L}) u^T_{J,J-1}(r), \\
&\vec{A}_{J+1} = (\hat{r} + i\alpha_2 \hat{r} \times \vec{L}) u^T_{J,J+1}(r), \\
&\alpha_1 = -\frac{1}{J}, \quad \alpha_2 = \frac{1}{J+1},
\end{aligned} \tag{37}$$

such that the two pieces of $\vec{A}$ represent the two orbital angular momentum components of $\vec{A}$;

$$\vec{L}^2 \vec{A}_{J-1} Y_{JM} = J(J-1) \vec{A}_{J-1} Y_{JM},$$
$$\vec{L}^2 \vec{A}_{J+1} Y_{JM} = (J+1)(J+2) \vec{A}_{J+1} Y_{JM}.$$

Let us also note in passing that the functions just defined are related to the original functions f_1, f_2, g_1, and g_2 according to

$$u^T_{J,J-1} + u^T_{J,J+1} = -i \frac{\partial}{\partial r}(f_1 + g_1) + \frac{J(J+1)}{r}(f_2 + g_2), \tag{38}$$

$$\alpha_1 u^T_{J,J-1} + \alpha_2 u^T_{J,J+1} = \frac{i}{r}(f_1 + g_1) - \frac{1}{r}\left(1 + r\frac{\partial}{\partial r}\right)(f_2 + g_2).$$

Equation (36) may now conveniently be resolved into a pair of coupled equations for $u^T_{J,J-1}$ and $u^T_{J,J+1}$. These are

$$\left(\frac{p_r^2}{m} + \frac{J(J-1)}{mr^2} + (V-\epsilon)\right) u^T_{J,J-1} - \left(4ma^2 + \frac{q(1+J+2J^2+\vec{r}\cdot\vec{\nabla})}{(2J+1)mr} + \frac{(1+J)rq'}{(2J+1)mr}\right) u^T_{J,J-1}$$
$$+ \left(\frac{qJ(3+2J+2\vec{r}\cdot\vec{\nabla})}{(2J+1)mr} + \frac{Jrq'}{(2J+1)mr}\right) u^T_{J,J+1} = 0, \tag{39}$$

$$\left(\frac{p_r^2}{m} + \frac{(J+1)(J+2)}{mr^2} + (V-\epsilon)\right) u^T_{J,J+1} - \left(4ma^2 - \frac{q(2+3J+2J^2+\vec{r}\cdot\vec{\nabla}}{(2J+1)mr} + \frac{Jrq'}{(2J+1)mr}\right) u^T_{J,J+1}$$
$$+ \left(\frac{q(J+1)(1-2J+2\vec{r}\cdot\vec{\nabla})}{(2J+1)mr} + \frac{(J+1)rq'}{(2J+1)mr}\right) u^T_{J,J-1} = 0, \tag{40}$$

where

$$q = \frac{\partial}{\partial r}\ln(1-2a), \quad q' = \frac{\partial}{\partial r} q.$$

To obtain the $O(m\alpha^4)$ equations, we first note that to the desired order of accuracy,

$$q \simeq \frac{-\alpha}{2mr^2} = \frac{\alpha}{2m}\frac{\partial}{\partial r}\frac{1}{r},$$
$$q' \simeq \frac{\alpha}{2m}\frac{\partial^2}{\partial r^2}\frac{1}{r} = \frac{\alpha}{2m}\left[-4\pi\delta(\vec{r}) + \frac{2}{r^3}\right].$$

Using these, we obtain the $O(m\alpha^4)$ equations as follows:

$$\left(\frac{p_r^2}{m} + \frac{J(J-1)}{mr^2} + (V-\epsilon)\right) u^T_{J,J-1} - \left(4ma^2 - \frac{(J-1)\alpha}{2m^2r^3} + \frac{\alpha\vec{r}\cdot\vec{\nabla}}{2m^2r^3}\right) u^T_{J,J-1} \simeq 0, \quad J \geq 1, \tag{41}$$

$$\left(\frac{p_r^2}{m} + \frac{(J+1)(J+2)}{mr^2} + (V-\epsilon)\right) u^T_{J,J+1} - \left(4ma^2 + \frac{(J+2)\alpha}{2m^2r^3} + \frac{\alpha\vec{r}\cdot\vec{\nabla}}{2m^2r^3}\right) u^T_{J,J+1} \simeq 0. \tag{42}$$

The corresponding $O(m\alpha^4)$ effective potentials are given by

$$V^{\text{eff}}_{--}(J-1) = -\frac{\vec{p}^4}{4m^3} + \frac{\pi\alpha\delta(\vec{r})}{m^2} + \frac{(J-1)\alpha}{2m^2r^3}, \quad J \geq 1 \tag{43}$$

$$V^{\text{eff}}_{--}(J+1) = -\frac{\vec{p}^4}{4m^3} + \frac{\pi\alpha\delta(\vec{r})}{m^2} - \frac{(J+2)\alpha}{2m^2r^3}, \tag{44}$$

where we recall that the (second) subscript on the functions u in all cases indicates the orbital angular momentum of the nonrelativistic limit of that function.

The last pair of equations may be further simplified by noting that the expectation value of the operator $\vec{L}\cdot\vec{S}$ is equal to $J-1$ and $-2-J$ for Eqs. (41) and (42) respectively. Therefore the above effective potentials may be unified as in

$$\Delta^{\text{eff}} = -\frac{\vec{p}^4}{4m^3} + \frac{\pi\alpha\delta(\vec{r})}{m^2} + \frac{\alpha\vec{L}\cdot\vec{S}}{2m^2r^3}. \tag{45}$$

Actually, Eq. (45) also represents the effective potentials of Eqs. (31) and (34), and it is therefore the $O(m\alpha^4)$ effective potential for the Breit equation (17).

We conclude this section by summarizing the re-

sults obtained above. The Breit equation (17) has been reduced to four second-order differential equations for four wave functions as follows: Eq. (30) for the wave function u_J^S describing singlet states, Eq. (33) for $u_{J,J}^T$ describing triplet states of orbital angular momentum equal to J, and the coupled equations (39) and (40) for the wave functions $u_{J,J-1}^T$ and $u_{J,J+1}^T$ describing triplet states of orbital angular momentum equal to $J-1$ and $J+1$ respectively. In all four equations the nonrelativistic limit is apparent, and the lowest-order energy shift, which is of order $m\alpha^4$, may be obtained from the effective potential given by Eq. (45).

IV. NUMERICAL INTEGRATION OF THE RADIAL EQUATIONS

In this section we shall briefly discuss the numerical integration of the equations obtained above. Actually, the only nontrivial aspect of this task is the singular behavior of the equations near the origin. This phenomenon is familiar within the context of the Dirac equation with a Coulomb potential, and it is simply a consequence of the union of first-order (second-order) differential equations with potentials behaving like r^{-1} (r^{-2}) or worse near the origin.[11] Again, as in the Dirac-Coulomb case, the smallness of α renders the situation harmless.

We shall start by considering the behavior of the equations near the origin:

$$\left(r^2\frac{\partial^2}{\partial r^2}+3r\frac{\partial}{\partial r}-J(J+1)+\frac{\alpha^2}{4}\right)u_J^S\simeq 0\,, \tag{46}$$

$$\left(r^2\frac{\partial^2}{\partial r^2}+3r\frac{\partial}{\partial r}-J(J+1)+\frac{\alpha^2}{4}+1\right)u_{J,J}^T\simeq 0,\quad J\geq 1, \tag{47}$$

$$\left(r^2\frac{\partial^2}{\partial r^2}+\frac{4J+1}{2J+1}r\frac{\partial}{\partial r}-\frac{J(J+1)(2J-1)}{2J+1}+\frac{\alpha^2}{4}\right)u_{J,J-1}^T - \frac{2J}{2J+1}\left(r\frac{\partial}{\partial r}+J+1\right)u_{J,J+1}^T\simeq 0,\quad J\geq 1\,, \tag{48}$$

$$\left(r^2\frac{\partial^2}{\partial r^2}+\frac{4J+3}{2J+1}r\frac{\partial}{\partial r}-\frac{J(J+1)(2J+3)}{2J+1}+\frac{\alpha^2}{4}\right)u_{J,J+1}^T - \frac{2(J+1)}{2J+1}\left(r\frac{\partial}{\partial r}-J\right)u_{J,J-1}^T\simeq 0\,. \tag{49}$$

The asymptotic behavior of the solutions of the above equations are then given by

$$u_{J,J}^S\to r^{-1\pm\mu_J}, \tag{50}$$

$$u_{J,J}^T\to r^{-1\pm\nu_J}, \tag{51}$$

$$\begin{pmatrix}u_{J,J-1}^T\\ u_{J,J+1}\end{pmatrix}\to\begin{pmatrix}1\\1\end{pmatrix}r^{\pm\nu_J}+\xi\begin{pmatrix}\beta_J^{\pm}\\1\end{pmatrix}r^{-1\pm\mu_J},\quad J\geq 1 \tag{52}$$

$$u_{0,1}^T\to r^{-1\pm\mu_0}, \tag{53}$$

where

$$\mu_J=\left[1+J(J+1)-\tfrac{1}{4}\alpha^2\right]^{1/2},\quad \nu_J=\left[J(J+1)-\tfrac{1}{4}\alpha^2\right]^{1/2},$$

$$\beta_J^{\pm}=\frac{J}{J+1}\,\frac{J\pm\mu_J}{J+1\mp\mu_J}.$$

Note the appearance of the mixing parameter ξ for the coupled equations. Clearly, as long as α is sufficiently small, the solutions with the upper choice of sign can be picked out as the regular one, and the others discarded. More precisely, for those values of α for which the choice of the lower sign leads to a non-square-integrable function at the origin, the corresponding Hamiltonian is self-adjoint, and one obtains a discrete bound-state spectrum.[12] In this way one arrives at the condition $\alpha^2<3$ by considering the $J=0$ states and imposing the condition just stated. Needless to say, this condition is well satisfied by the physical value of α.

With the boundary conditions at the origin given by the regular solutions of Eqs. (50)–(52), one is left with the straightforward task of the numerical solution of the eigenvalue equations (30), (33), and (39). Aside from the boundary conditions at the origin, the procedure is the same as with the ordinary Schrödinger equation. Omitting the details of the computations, we will only note that sample integrations carried out for several cases, including the first two Bohr levels, yielded energy shifts in agreement with the perturbative results obtained from Eq. (45) within the accuracy of the latter.

V. CONCLUDING REMARKS

In this paper we have presented a complete analysis of the new positronium equation to fourth order. This has entailed the rederivation of a number of known results, customarily obtained within the Bethe-Salpeter formalism, as well as the decomposition and numerical solution of the static-interaction Breit equation. The latter has demonstrated the proper physical behavior of the Breit equation, especially its short-distance properties, in some detail. This is of some importance, since the Breit equation is the only *simple*, static-interaction, relativistic, two-fermion equation which has been derived directly from field the-

ory. It is even of more significance for our work, since the treatment accorded the full fermion-antifermion equation (1) relies upon it as the zeroth-order approximation. We have therefore thought these results of basic importance in attempting a systematic application to the calculation of the spectrum of positronium, a task which we hope the present work has facilitated.

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