# Eight-component two-fermion equations

Ruth Häckl, Viktor Hund, and Hartmut Pilkuhn

Institut für Theoretische Teilchenphysik, Universität Karlsruhe, D-76128 Karlsruhe, Germany

(Received 17 November 1997)

An eight-component formalism is proposed for the relativistic two-fermion problem. In QED it extends the applicability of the Dirac equation with hyperfine interaction to the positronium case. The use of exact relativistic two-body kinematics entails a *CP*-invariant spectrum that is symmetric in the total center-of-mass system energy. It allows the extension of recent  $\alpha^6$  recoil corrections to the positronium case and implies recoil corrections to the fine and hyperfine structures and to the Bethe logarithm. [S1050-2947(98)04705-2]

PACS number(s): 03.65.Pm

### I. INTRODUCTION

The relativistic two-body problem for two spin-1/2 particles is based on 16-component wave functions that transform as the direct product of two four-component Dirac spinors  $\psi^{(16)} \sim \psi_1 \otimes \psi_2$ . For unequal masses  $m_2 > m_1$ , the equations are simplified by the elimination of the small components of particle 2 and by a subsequent power-series expansion about the nonrelativistic limit of this particle. One thus obtains an effective Dirac equation for particle 1, with a hyperfine interaction that contains the Pauli matrices  $\sigma_2$  of particle 2. Such an equation has  $4 \times 2 = 8$  components. It is very powerful for hydrogen and muonium [1-4]. More recently, a nonrelativistic quantum electrodynamics has been elaborated that allows one to eliminate the small components of both particles, which is particularly useful for the equalmass case  $m_1 = m_2$  as in positronium [5,6]. One thus arrives at an effective Schrödinger equation, in which the Pauli matrices  $\sigma_1$  and  $\sigma_2$  produce a four-component spin structure. However, the fact that the power-series expansions in  $\alpha$  are rapidly converging does not prevent technical difficulties, presently at order  $\alpha^6$  in the binding energies. These  $\alpha^6$  terms have only been calculated by the above eight-component strategy and only to first order in  $m_1/m_2$ .

In this paper a different eight-component equation is derived that does not eliminate small components and dispenses with nonrelativistic expansions. It exploits the fact that the chirality operator  $\gamma_1^5 \gamma_2^5$  commutes with the matrix  $\gamma_1^0 \gamma_2^0$  of the parity transformation; a corresponding separation of components does not exist for a single Dirac particle. We begin with the rederivation of an eight-component equation for two free spin-1/2 particles, in which the spin operator of particle 2 is removed in the center-of-mass (c.m.) system ( $\mathbf{p}_1 = -\mathbf{p}_2 = \mathbf{p}$ ) [7–9] by means of a matrix c, given in Eq. (20) below. The spin dependence in the laboratory system is generated by a boost, to be discussed in Sec. V. The removal matrix c also mixes large and small components via a Dirac matrix  $\beta = \gamma^0$ . For the total c.m. system energy E, the result is an effective single-particle Dirac equation, for a free particle of reduced mass  $\mu$  and reduced energy  $\epsilon$ :

$$\mu = m_1 m_2 / E, \quad \epsilon = (E^2 - m_1^2 - m_2^2) / 2E,$$

$$E = m_1 + m_2 + E_b, \qquad (1)$$

In Sec. III the QED Born amplitude for c.m. system scattering will be used to derive the interaction for this equation. The equation with interaction is for two leptons (no anomalous magnetic moments)

$$(\boldsymbol{\epsilon} - \boldsymbol{\mu}\boldsymbol{\beta} - \boldsymbol{V})\boldsymbol{\psi} = \boldsymbol{\gamma}_5(\boldsymbol{\sigma}_1 - i\boldsymbol{\sigma}^{\times}\boldsymbol{V}/\boldsymbol{E})\mathbf{p}\boldsymbol{\psi}, \quad \boldsymbol{\sigma}^{\times} = \boldsymbol{\sigma}_1 \times \boldsymbol{\sigma}_2.$$
(2)

Setting  $\gamma_5 \sigma_1 = \alpha = \gamma^0 \gamma$ , the equation has the appearance of the usual Dirac equation with hyperfine interaction, particularly as  $\alpha \times \sigma_2 / E$  may be approximated by  $\alpha \times \sigma_2 / (m_1 + m_2)$  to order  $\alpha^4$ . However, the complete operator  $-i\alpha \times \sigma_2 V \mathbf{p}/E$  contains an anti-Hermitian part that ensures exact relativistic two-body kinematics; for  $m_1 = m_2$ , it produces the correct spin structure to order  $\alpha^4$  [9]. A previous derivation from the 16-component Dirac-Breit equation produced a different hyperfine operator, which is equivalent to the present one only near threshold,  $-E_b/E \ll 1$ . The present hyperfine operator is left invariant by the *c* transformation. (The previous derivation also had to assume a point Coulomb potential  $V = -Z\alpha/r$ ,  $\alpha = e^2$ , and Ze the nuclear charge.)

The relativistic on-shell two-body kinematics has long been well known. One has  $\epsilon^2 - \mu^2 = E_1^2 - m_1^2 = E_2^2 - m_2^2 = k^2$ in the c.m. system, where  $k^2 = -\kappa^2$  is negative for bound states, and the asymptotic form  $e^{-\kappa r}$  of  $\psi$  displays  $\kappa^{-1}$  as a multiple of the Bohr radius. The incorporation of relativistic two-body kinematics results in a spectrum that expresses  $E^2$ in terms of  $m_1^2$  and  $m_2^2$ . The combination  $E\mu = m_1m_2$  is allowed in front of a square root (and possibly also with odd powers of  $Z\alpha$ , beginning with  $Z^5\alpha^5$ ). Our main nonperturbative result is

$$E^{2} - m_{1}^{2} - m_{2}^{2} = 2m_{1}m_{2}(1 + Z^{2}\alpha^{2}/n^{*2})^{-1/2}, \quad n^{*} = n - \beta_{d},$$
(3)

where  $n^*$  is an effective principal quantum number and  $\beta_d$  is a quantum defect. Except for the details of  $\beta_d$ , Eq. (3) applies to any combinations of spins. It had been derived for two spinless particles [10], where also its empirical applicability to parapositronium was noticed. It was then extended to the case of one spin-1/2 and one spinless particle [11]. The angular momentum defect  $\beta_l = -\delta l = -(l'-l)$  has been discussed for two fermions of arbitrary magnetic moments to order  $Z^4 \alpha^4$  [9]. It will be used in Sec. VIII to derive a "Barker-Glover" term in the fine structure. In Sec. IV a rather general formula for  $Z^6 \alpha^6$  recoil terms will be derived that includes several different effects. In Sec. VI a vector potential is included in Eq. (2) and evaluated in the dipole approximation. It leads to two additional quantum defects

$$n^* = n + \delta l - \beta_B - \beta' \,\delta_{l0}, \qquad (4)$$

where  $\beta_B$  is caused by the Bethe logarithm and  $\beta'$  is an additional quantum defect in *s* states. Parts of the Salpeter correction [2] are not included in Eq. (4); their mass dependence is examined in Sec. VII. Vacuum polarization and nuclear charge distributions are also discussed in that section. For antiprotonic atoms, vacuum polarization must be included as a part of *V* for low-*l* states. A method is proposed that extends the validity of Eq. (3) to such states. However, also in cases where Eq. (2) must be solved numerically, the  $E^2$  dependence remains and adds "recoil" corrections to the binding energies  $E_b$  of Eq. (1).

It may be worth mentioning that the  $E^2$  dependence of the spectrum is a very general consequence of the *CPT* theorem. With the separate validity of *C*, *P*, and *T* in QED, one may also say that the  $E^2$  dependence follows from *C* invariance, but in the relativistic case the *CP* transformation is slightly more convenient than *C* alone. Of course, the states that we calculate are *CP* eigenstates only in the case of positronium. Muonium is transformed into antimuonium under *CP*.

#### **II. FREE EIGHT-COMPONENT EQUATIONS**

Let particles i(=1,2) satisfy the free Dirac equations, in units  $\hbar = c = 1$ :

$$(i\partial_{i}^{0} - \boldsymbol{\alpha}_{i}\mathbf{p}_{i} - m_{i}\beta_{i})\psi_{i} = 0, \quad \boldsymbol{\alpha}_{i} = \gamma_{i}^{5}\boldsymbol{\sigma}_{i}, \quad \beta_{i} = \gamma_{i}^{0},$$
$$\partial_{i}^{0} = \partial/\partial t_{i}. \tag{5}$$

The  $\sigma_i$  are Pauli matrices and  $\gamma_i^5 \beta_i + \beta_i \gamma_i^5 = 0$ . The direct product  $\psi^{(16)} = \psi_1 \otimes \psi_2$  satisfies both Eqs. (5) and thus also their sum, in which  $i\partial_1^0 + i\partial_2^0$  will be replaced by its eigenvalue  $K^0$ , which is the total laboratory energy:

$$(K^{0} - \gamma_{1}^{5}\mathbf{p}_{1}\boldsymbol{\sigma}_{1} - \gamma_{2}^{5}\mathbf{p}_{2}\boldsymbol{\sigma}_{2} - m_{1}\boldsymbol{\beta}_{1} - m_{2}\boldsymbol{\beta}_{2})\psi^{(16)} = 0.$$
(6)

 $\psi^{(16)}$  is now divided into two octets  $\psi_{LP}$  and  $\chi_{LP}$ , which have  $\gamma_1^5 = \gamma_2^5 \equiv \gamma_5$  and  $\gamma_1^5 = -\gamma_2^5 = \gamma_5$ , respectively:

$$(K^0 - \gamma_5 \mathbf{p}_1 \boldsymbol{\sigma}_1 - \gamma_5 \mathbf{p}_2 \boldsymbol{\sigma}_2) \psi_{LP} = (m_1 \beta_1 + m_2 \beta_2) \chi_{LP}, \quad (7)$$

$$(K^0 - \gamma_5 \mathbf{p}_1 \boldsymbol{\sigma}_1 + \gamma_5 \mathbf{p}_2 \boldsymbol{\sigma}_2) \chi_{LP} = (m_1 \beta_1 + m_2 \beta_2) \psi_{LP}.$$
(8)

The coupling between  $\psi_{LP}$  and  $\chi_{LP}$  arises because each  $\beta_i$  reverses the eigenvalue of  $\gamma_i^5$ . In the chiral basis,  $\gamma_1^5$  and  $\gamma_2^5$  are diagonal:

$$\gamma_{i}^{5} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \beta_{i} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \psi_{i} = \begin{pmatrix} \psi_{ir} \\ \psi_{il} \end{pmatrix},$$
$$\psi_{LP} = \begin{pmatrix} \psi_{rr} \\ \psi_{ll} \end{pmatrix}, \quad \chi_{LP} = \begin{pmatrix} \psi_{rl} \\ \psi_{lr} \end{pmatrix}, \quad (9)$$

where the indices r and l (denoting right-handed and lefthanded, respectively) refer to the eigenvalues  $\pm 1$  of  $\gamma_1^5$  and  $\gamma_2^5$ . In the parity basis, the  $\beta_i$  are diagonal, with eigenvalues  $\pm 1$  for the large and small components g and f, respectively:

$$\boldsymbol{\gamma}_{i}^{5} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \boldsymbol{\beta}_{i} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \boldsymbol{\psi}_{i} = \begin{pmatrix} \boldsymbol{\psi}_{ig} \\ \boldsymbol{\psi}_{if} \end{pmatrix}, \quad (10)$$

$$\psi_{LP} = \begin{pmatrix} \psi_{gg} + \psi_{ff} \\ \psi_{fg} + \psi_{gf} \end{pmatrix}, \quad \chi_{LP} = \begin{pmatrix} \psi_{gg} - \psi_{ff} \\ \psi_{fg} - \psi_{gf} \end{pmatrix}.$$
(11)

In this eight-component space, we also define a matrix  $\beta$ :

$$\beta = \beta_1 \beta_2 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \beta \gamma_5 + \gamma_5 \beta = 0$$
(12)

(unit matrices are suppressed). Whereas  $\beta_i$  and  $\gamma_i^5$  do not commute,  $\beta$  does commute with  $\gamma_1^5 \gamma_2^5$  and both operators are diagonal in the representation (11). As Lorentz transformations commute with  $\gamma_i^5$  and parity transformations commute with  $\beta_i$ , the decomposition of  $\psi^{(16)}$  into  $\psi_{LP}$  and  $\chi_{LP}$  is invariant under the extended group of Lorentz (*L*) and parity (*P*) transformations. In the following  $\chi_{LP}$  will be eliminated. We introduce a compact notation

$$p_{\pm} = \mathbf{p}_1 \boldsymbol{\sigma}_1 \pm \mathbf{p}_2 \boldsymbol{\sigma}_2, \quad m_{\pm} = m_2 \pm \beta m_1$$
(13)

and observe  $\beta_2 \psi_{LP} = \chi_{LP}$  and  $\beta_2 \chi_{LP} = \psi_{LP}$  in the basis (11) such that we may effectively set  $\beta_2 = 1$  and  $\beta_1 = \beta$  in Eqs. (7) and (8) in this basis:

$$(K^{0} - \gamma_{5}p_{+})\psi_{LP} = m_{+}\chi_{LP}, \quad (K^{0} - \gamma_{5}p_{-})\chi_{LP} = m_{+}\psi_{LP}.$$
(14)

Using the first equation for the elimination of  $\chi_{LP}$ , one obtains for the second

$$(K^{0} - \gamma_{5}p_{-})(m_{+})^{-1}(K^{0} - \gamma_{5}p_{+})\psi_{LP} = m_{+}\psi_{LP}.$$
 (15)

Multiplying this equation by  $m_+$  and using

$$m_{+}m_{-}=m_{2}^{2}-m_{1}^{2}, \quad m_{+}\gamma_{5}=\gamma_{5}m_{-},$$
 (16)

one arrives at

$$\mathcal{K}_{0}\psi_{LP} = 0, \quad \mathcal{K}_{0} = (K^{0} - \gamma_{5}p_{-}m_{-}/m_{+})(K^{0} - \gamma_{5}p_{+}) - m_{+}^{2}.$$
(17)

Equation (14) or (17) can be Lorentz transformed to the c.m. system, where one has  $K^0 = E$  and  $p_-p_+ = p_1^2 - p_2^2 = 0$ . The constants of Eq. (17) are combined into  $E^2 - m_1^2 - m_2^2 = 2E\epsilon$ , with  $\epsilon$  defined by Eq. (1):

$$[2E\epsilon - E\gamma_5(\mathbf{p}\boldsymbol{\sigma}\boldsymbol{m}_-/\boldsymbol{m}_+ + \mathbf{p}\Delta\boldsymbol{\sigma})]\psi_{LP} = 2m_1m_2\beta\psi_{LP},$$
  
$$\boldsymbol{\sigma} = \boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2, \quad \Delta\boldsymbol{\sigma} = \boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_2, \quad (18)$$

where  $m_1m_2$  may also be written as  $E\mu$  according to Eq. (1). If  $\mathbf{p}\boldsymbol{\sigma}$  were present without the factor  $m_-/m_+$ , one would use  $\mathbf{p}\boldsymbol{\sigma}+\mathbf{p}\Delta\boldsymbol{\sigma}=2\mathbf{p}\boldsymbol{\sigma}_1$  and Eq. (18) would be identical to Eq. (2) for V=0, multiplied by 2*E*.

It is in fact possible to remove  $m_{-}/m_{+}$  from Eq. (18), by a transformation

$$\psi_{LP} = c \psi, \quad c^{-1} \gamma_5 = \gamma_5 c, \quad c \sigma c = \sigma m_+ / m_-,$$
  
 $c \Delta \sigma c = \Delta \sigma.$  (19)

Explicit forms of c are

$$c = (m_{+}m_{-})^{-1/2} [m_{2} + \frac{1}{2}m_{1}\beta(1 + \boldsymbol{\sigma}_{1}\boldsymbol{\sigma}_{2})]$$
  
=  $(m_{+}m_{-})^{-1/2} (m_{+} - 2m_{1}\Lambda_{s}),$  (20)

where  $\Lambda_s = (1 - \boldsymbol{\sigma}_1 \boldsymbol{\sigma}_2)/4$  is the projector on singlet spin states. To verify Eq. (19), one notices  $\Lambda_s \boldsymbol{\sigma} = \boldsymbol{\sigma} \Lambda_s = 0$ . In summary, the 16-component equation (6) is now transformed into a single free-Dirac equation  $(\boldsymbol{\epsilon} - \boldsymbol{\mu}\boldsymbol{\beta} - \gamma_5 \boldsymbol{\sigma}_1 \mathbf{p}) \psi_{free} = 0$ , with no trace of the spin operators of particle 2. In the next section it will be seen that the interaction for this equation contains no mass factors at all.

#### **III. ONE-PHOTON EXCHANGE INTERACTION**

A connection between bound states and perturbative QED rests on the *S* matrix S = 1 + iT and the Born series for the *T* matrix,  $T = T^{(1)} + T^{(2)} + \cdots$ . When this series is summed by appropriate differential or integral equations, the bound states appear as poles of *T*. In detail, one takes plane waves  $\psi_i = u_i e^{i\phi_i}$  with  $\phi_i = \mathbf{k}_i \mathbf{r}_i - E_i t$  for the initial states,  $\phi'_i$  $= \mathbf{k}'_i \mathbf{r}_i - E'_i t$  for the final states, and extracts the resulting energy-momentum-conserving  $\delta$  function from the *T*-matrix elements  $S_{if} = i(2\pi)^4 \delta(E - E') \delta(\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}'_1 - \mathbf{k}'_2) T_{if}$ . In analogy, we set  $\psi_{LP} = v e^{i\phi}$  and  $\chi_{LP} = w e^{i\phi}$ , with  $\phi = \phi_1$  $+ \phi_2$ . The first Born approximation to  $T^{(1)}_{if}$  of the matrix elements  $T_{if}$  is (with  $q_1 = -e$ ,  $q_2 = Ze$ , and  $e^2 = \alpha$ )

$$T_{if}^{(1)} = \frac{4\pi Z\alpha}{t} u_1^{\prime\dagger} u_2^{\prime\dagger} (1 - \alpha_1 \alpha_2) u_1 u_2$$
$$= \frac{4\pi Z\alpha}{t} [v^{\prime\dagger} (1 - \sigma_1 \sigma_2) v + w^{\prime\dagger} (1 + \sigma_1 \sigma_2) w], \qquad (21)$$

with  $t = q^{0^2} - \mathbf{q}^2$ ,  $q^0 = K_1^0 - K_1^{0'}$ , and  $\mathbf{q} = \mathbf{k}_1 - \mathbf{k}_1'$ . Using Eq. (14) for the elimination of  $v'^{\dagger}$  in one term and of *w* in the other,  $T_{if}^{(1)}$  is expressed in terms of an 8×8 matrix *M*:

$$w = \frac{1}{m_{+}} (K^{0} - \gamma_{5} k_{+}) v, \quad v'^{\dagger} = w'^{\dagger} (K^{0} - \gamma_{5} k'_{-}) \frac{1}{m_{+}},$$
$$T_{if}^{(1)} = w'^{\dagger} M v.$$
(22)

In the differential equation approach based on Eq. (5), the potential *V* is the Fourier transform of  $T^{(1)}$ , apart from corrections from the Hermitian part of  $T^{(2)}$  [12]. Unitarity  $S^{\dagger}S = 1$  implies  $T^{(1)\dagger} = T^{(1)}$  and thus  $V = V^{\dagger}$ , i.e., a Hermitian potential. However, the asymmetric form  $w'^{\dagger}Mv$  implies a non-Hermitian interaction  $\mathcal{K}_I$  in our differential equation  $(\mathcal{K}_0 + \mathcal{K}_I)\psi = 0$ . The simultaneous validity of  $(\mathcal{K}_0 + \mathcal{K}_I^{\dagger})\chi = 0$  guarantees real eigenvalues, though. The ordinary Dirac equation fails to order  $Z^4 \alpha^4$  in the states with l = f(l denotes the orbital and *f* the total angular momentum) due to hyperfine mixing.

We now restrict ourselves to the c.m. system,  $\mathbf{k}_1 + \mathbf{k}_2 = \mathbf{k}'_1 + \mathbf{k}'_2 = 0$  and call  $\mathbf{k}_1 = \mathbf{k}$  and  $\mathbf{p}_1 = \mathbf{p} = -i\nabla$ . The total phase  $\phi$  contains  $\mathbf{k}(\mathbf{r}_1 - \mathbf{r}_2) = \mathbf{k}\mathbf{r}$ , such that one has  $\mathbf{p}_2 = -\mathbf{p}$ . Moreover,  $K^0 = K^{0'} = E$ . To order  $Z^4 \alpha^4$ , one also has  $q^0 = 0$  and  $t = -\mathbf{q}^2$ :

$$-\mathbf{q}^{2}M/4\pi Z\alpha = (E - \gamma_{5}k'_{-})m_{+}^{-1}(1 - \boldsymbol{\sigma}_{1}\boldsymbol{\sigma}_{2}) + m_{+}^{-1}(1 + \boldsymbol{\sigma}_{1}\boldsymbol{\sigma}_{2})(E - \gamma_{5}k_{+}).$$
(23)

With  $k'_{-} = \mathbf{k}' \boldsymbol{\sigma}$ , one has  $k'_{-}(1 - \boldsymbol{\sigma}_1 \boldsymbol{\sigma}_2) = 4\mathbf{k}' \boldsymbol{\sigma} \Lambda_s = 0$ , as  $1 - \boldsymbol{\sigma}_1 \boldsymbol{\sigma}_2$  vanishes for triplet states, while  $\boldsymbol{\sigma}$  annihilates the singlet state. Consequently,

$$-\mathbf{q}^{2}M/4\pi Z\alpha = m_{+}^{-1}[2E - \gamma_{5}(1 + \boldsymbol{\sigma}_{1}\boldsymbol{\sigma}_{2})\mathbf{k}\Delta\boldsymbol{\sigma}]$$
$$= 2m_{+}^{-1}(E - i\gamma_{5}\mathbf{k}\boldsymbol{\sigma}^{\times}).$$
(24)

Combining now  $m_+^{-1}$  with  $w'^+$ , the Fourier transform of  $m_+M$  will be  $\mathcal{K}_I$ :

$$\mathcal{K}_I = EV - i \gamma_5 V \mathbf{p} \boldsymbol{\sigma}^{\times}, \quad V = -Z \alpha / r.$$
 (25)

This is to be added to  $\mathcal{K}_0$  [Eq. (17)] and used in Eq. (18). To arrive at the form (2) of the differential equation,  $\mathcal{K}_I$  must be replaced by  $c^{-1}\mathcal{K}_I c$  according to Eq. (19). Fortunately, one finds

$$c \boldsymbol{\sigma}^{\times} c = \boldsymbol{\sigma}^{\times}, \quad c^{-1} \mathcal{K}_{I} c = \mathcal{K}_{I}$$
 (26)

such that the same operator appears in fact in Eq. (2). To order  $Z^4 \alpha^4$  in E,  $\mathcal{K}_I$  is equivalent to the operator  $\mathcal{K}_{IB} = EV - \gamma_5 (i \sigma^{\times} - \sigma_2) [V, \mathbf{p}]/2$  of the Dirac-Breit approach [8,9], the transformation being

$$\psi_{B} = e^{\sigma_{1}\sigma_{2}V/2E}\psi \tag{27}$$

after the transformation c (notice  $c^{-1}\mathcal{K}_{IB}c \neq \mathcal{K}_{IB}$ ).

For the orders  $Z^5 \alpha^5$  and  $Z^6 \alpha^6$ , the condition  $q^0 = 0$ should be replaced by the current conservation conditions  $q_{\mu}J_i^{\mu} = 0$  (*i*=1,2). This produces the spin operator  $\boldsymbol{\sigma}_1^{\perp} \boldsymbol{\sigma}_2^{\perp} = \boldsymbol{\sigma}_1 \boldsymbol{\sigma}_2 - (\boldsymbol{\sigma}_1 \mathbf{q})(\boldsymbol{\sigma}_2 \mathbf{q})/\mathbf{q}^2$ , which is equivalent to using the Coulomb gauge. However, we have not yet performed this calculation. The  $Z^6 \alpha^6$  terms of Eq. (42) below result from the use of relativistic kinematics in Eq. (2).

### IV. SOLVING THE EQUATION NONPERTURBATIVELY

The total angular momentum  $\mathbf{F} = \mathbf{L} + (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2)/2 = \mathbf{J}_1 + \boldsymbol{\sigma}_2/2$  is conserved. All eight components of  $\psi$  have the same eigenvalues  $f(f+1) = F^2$  of  $\mathbf{F}^2$  and  $m_f$  of  $F_z$ ; factors 1/r and i/r are extracted from  $\psi_g$  and  $\psi_f$  as usual:

$$\psi_{gk} = \chi_k^{fm_f} \frac{1}{r} u_{gk}(r), \quad \psi_{fk} = \chi_k^{fm_f} \frac{i}{r} u_{fk}(r), \quad (28)$$

$$(\boldsymbol{\epsilon} - \boldsymbol{\mu} - \boldsymbol{V})u_g = i\,\widetilde{\boldsymbol{\pi}}u_f, \quad (\boldsymbol{\epsilon} + \boldsymbol{\mu} - \boldsymbol{V})u_f = -\,i\,\widetilde{\boldsymbol{\pi}}u_g,$$
  
$$\widetilde{\boldsymbol{\pi}} = (\boldsymbol{\sigma}_1 - i\,\boldsymbol{\sigma}^{\times}\boldsymbol{V}/\boldsymbol{E})r\mathbf{p}/r. \tag{29}$$

The index k assumes the four values k=s=(f,0) (singlet), k=1=(f,1) (triplet with orbital angular momentum l=f) and  $k = +_1 k = -$  (triplets with  $l \neq f$  and eigenvalues  $\mp 1$  of  $\sigma_{1r}\sigma_{2r} = \sigma_1 \hat{\mathbf{r}} \sigma_2 \hat{\mathbf{r}}$ ) [8]. We arrange the radial wave functions as

$$u_{g}(r) = \begin{pmatrix} u_{g+} \\ u_{g-} \\ u_{g1} \\ u_{gs} \end{pmatrix}, \quad u_{f}(r) = \begin{pmatrix} u_{f+} \\ u_{f-} \\ u_{f1} \\ u_{fs} \end{pmatrix},$$
$$\frac{\tilde{\pi}}{i} = \begin{pmatrix} 0 & 0 & -F/r & f_{-}\partial_{-} \\ 0 & 0 & \partial_{r} & -f_{-}F/r \\ F/r & \partial_{r} & 0 & 0 \\ f_{+}\partial_{+} & f_{+}F/r & 0 & 0 \end{pmatrix}, \quad (30)$$

with  $\partial_{\pm} = \partial_r \pm 1/r$  and  $f_{\pm} = 1 \pm 2V/E$ . The states  $k = \pm$  with  $l = f \pm 1$  have  $j_1 = j_2 = f \pm 1/2$  to order  $\alpha^2$ . An analytic solution of the equations is obtained when the hyperfine operator is replaced by an equivalent  $r^{-2}$  operator. At this level of precision, the equation becomes equivalent to the one derived from the Dirac-Breit equation [8,9], where the replacement was achieved by the substitution  $r = r' - Z\alpha a/2\mu$  (see Sec. VIII for *a*):

$$[\epsilon^2 - \mu^2 - 2\epsilon V - \tilde{L}^2/r^2 + \partial_r^2]u = 0.$$
(31)

 $\tilde{L}^2 = L^2 - Z^2 \alpha^2 (1+a)$  comprises all  $r^{-2}$  operators. Its eigenvalues will be denoted by l'(l'+1) to profit from the analogy with the Schrödinger equation. Defining moreover

$$\epsilon^2 - \mu^2 = -\kappa^2, \quad z = -2ikr = 2\kappa r, \quad \alpha_Z = Z\alpha,$$
  
 $\alpha_Z \epsilon / \kappa \equiv n^*, \quad (32)$ 

and  $u = e^{-z/2} z^{l'} F(z)$ , the equation becomes as usual an equation for the confluent hypergeometric function *F*,

$$[l'+1-z\partial_z^2 - (2l'+2-z)\partial_z]F = n^*F.$$
 (33)

For unbound states,  $\eta = -in^*$  is called the Sommerfeld parameter. For bound states,  $n^* - l' - 1$  must be a non-negative integer  $n_r$ . With l' near an integer l, one defines

$$\delta l = l' - l, \quad n^* = n_r + l' + 1 = n + \delta l,$$
 (34)

where  $n = n_r + l + 1$  is the principal quantum number and  $\delta l$  is always negative. All four eigenvalues  $\lambda$  of  $\tilde{L}^2 - F^2 + \alpha_Z^2$  are given by

$$\lambda^{2} [\lambda^{2} - 2\lambda - 4(F^{2} - \alpha_{Z}^{2}\epsilon/E) + 2\alpha_{Z}^{2}] - 2\alpha_{Z}^{2}\lambda$$
$$-\alpha_{Z}^{4}(1 - 4\epsilon/E) = 0.$$
(35)

It contains the Dirac eigenvalues with recoil-corrected hyperfine structure and hyperfine mixing near both static limits [9]. For equal masses, the equation is reliable only to order  $\alpha^2$ , but for l = f we nevertheless quote the result for  $\delta l$  to order  $\alpha^4$ . With  $1 - 4\epsilon/E = \alpha^2/4n^2$ , one solution of Eq. (35) is  $\lambda = -\alpha^4/8n^2$ . It belongs to parapositronium, as we shall see. The value of l' follows from  $l' + \frac{1}{2} = \sqrt{F^2 + 1/4 + \lambda - \alpha^2} = \sqrt{(l + \frac{1}{2})^2 + \lambda - \alpha^2}$ ,

$$-\delta l_{para} = \frac{\alpha^2}{2l+1} + \frac{\alpha^4}{(2l+1)^3} + \frac{\alpha^4}{8n^2(2l+1)}.$$
 (36)

For orthopositronium with l=f, one factor  $\lambda$  is divided off and  $\lambda^3$  can be neglected to order  $\alpha^4$ :

$$-\delta l_{ortho}(l=f) = \frac{\alpha^2}{2l+1} \left[ 1 - \frac{1}{2F^2} - \frac{\alpha^2}{2F^6} - \alpha^2 \left( \frac{1 - 1/2F^2}{2l+1} \right)^2 \right] - \frac{\alpha^4}{8n^2(2l+1)}.$$
(37)

We now arrive at our main point, namely, the calculation of  $E^2$ . From Eq. (32) and the definition (1) of  $\mu$  and  $\epsilon$ , one finds Eq. (3). Expansion of the square root leads to a more practical series, which to order  $\alpha_Z^8$  is

$$\frac{E^2 - m^2}{m_1 m_2} = -\frac{\alpha_Z^2}{n^{*2}} \left[ 1 - \frac{3}{4} \frac{\alpha_Z^2}{n^{*2}} + \frac{5}{8} \frac{\alpha_Z^4}{n^{*4}} \left( 1 - \frac{7}{8} \frac{\alpha_Z^2}{n^{*2}} \right) \right],$$
$$m = m_1 + m_2.$$
(38)

Insertion of  $n^* = n + \delta l$  yields, to order  $\alpha_Z^6$ ,

$$\frac{E^2 - m^2}{m_1 m_2} = -\frac{\alpha_Z^2}{n^2} \left(1 + \alpha_Z^2 \frac{b}{n}\right),$$
  
$$b = -\frac{2\delta l}{\alpha_Z^2} - \frac{3}{4n} + \frac{\alpha_Z^2}{n} \left(\frac{5}{8n^2} + 3\frac{\delta l}{\alpha_Z^2 n} + 3\frac{\delta l^2}{\alpha_Z^4}\right).$$
(39)

This expression is still quite compact, in view of the fact that  $\delta l$  contains both fine and hyperfine interactions. The result for *E* is, again to order  $\alpha_Z^6$ ,

$$E = [m^{2} - m_{1}m_{2}\alpha_{Z}^{2}(1 + \alpha_{Z}^{2}b/n)/n^{2}]^{1/2}$$
  
$$= m - \mu_{nr}\alpha_{Z}^{2}(1 + \alpha_{Z}^{2}b/n)/2n^{2}$$
  
$$- \mu_{nr}^{2}\alpha_{Z}^{4}(1 + \alpha_{Z}^{2}b/n)^{2}/8n^{4}m - \mu_{nr}^{3}\alpha_{Z}^{6}/16n^{6}m^{2},$$
  
(40)

where  $\mu_{nr} = m_1 m_2 / m$  is the nonrelativistic reduced mass and the expression (39) for *b* remains to be inserted. The third term of Eq. (40), with the approximation b = 0, is known as the Bechert-Meixner recoil correction [8]. To order  $\alpha_Z^6$ , *b* may be approximated by  $-2 \delta l / \alpha_Z^2 - 3/4n$ . For comparison with the literature [13,4], we split the reduced mass  $\mu_{nr}$  in a rather unusual way,

$$\mu_{nr} = \mu_{nr}(1 + \mu_{nr}/m) - \mu_{nr}^2/m \approx m_1^2(1 - m_1^2/m^2) - \mu_{nr}^2/m.$$
(41)

In the order  $\alpha_Z^6$ , we may then combine all contributions from Eq. (40) with that of an additional operator  $\sim L^2/r^4$  [13], which makes the expression complete for l > 0:

$$\Delta E(\alpha_Z^6) = \frac{\mu_{nr}^2 \alpha_Z^6}{2mn^6} \left( \frac{4n\,\delta l}{\alpha_Z^2} + 1 - \frac{\mu_{nr}}{8m} \right) + \frac{\alpha_Z^2}{2\mu_{nr}^2 m} \left\langle \frac{L^2}{r^4} \right\rangle. \tag{42}$$

1

$$\delta l_D / \alpha_Z^2 = (\gamma - j - \frac{1}{2}) / \alpha_Z^2 \approx -[1 + \alpha_Z^2 / (2j + 1)^2] / (2j + 1)$$
(43)

reproduces the known result [13]. Equation (42) generalizes this result to arbitrary masses and hyperfine interactions (Sec. VIII). However, we would like to advocate the direct use of formula (39) for  $(E^2 - m^2)/m_1m_2$  because it is more compact for calculations and less mass dependent for measurements.

### V. BOOSTS AND COORDINATE TRANSFORMATIONS

Lorentz transformations can be constructed directly for  $\psi$  and  $\psi_{LP}$ , but it is more convenient to use the known transformations of the single free-particle spinors  $\psi_1$  and  $\psi_2$ . We only need the boosts from the c.m. system to the laboratory system (*l*), where the system has a total four-momentum  $K^{\mu}$ :

$$\psi_{i,l} = A_i \psi_{i,cm},$$

$$A_i = (\gamma + \gamma_i^5 \mathbf{\hat{K}} \boldsymbol{\sigma}_i)^{1/2} = (2\gamma + 2)^{-1/2} (\gamma + 1 + \gamma_i^5 \mathbf{\hat{K}} \boldsymbol{\sigma}_i),$$
(44)

$$\hat{\mathbf{K}} = \mathbf{K}/E, \quad \gamma = K^0/E = (1 + \hat{K}^2)^{1/2}.$$
 (45)

We also take the z axis along **K**,  $\hat{\mathbf{K}}\boldsymbol{\sigma}_i = \hat{K}\boldsymbol{\sigma}_{iz}$ . Suppressing the index  $_{LP}$ , the eight-component laboratory spinor is

$$\psi_{l} = A \psi_{cm},$$

$$A = (\gamma + \gamma_{5} \hat{K} \sigma_{2z})^{1/2} (\gamma + \gamma_{5} \hat{K} \sigma_{1z})^{1/2}$$

$$= (1 + \frac{1}{2} \hat{K}^{2} \sigma_{z}^{2} + \hat{K} \sigma_{z} \gamma \gamma_{5})^{1/2},$$
(46)

$$A = \gamma + \frac{1}{2}\hat{K}\gamma_5\sigma_z - \frac{1}{2}\hat{K}^2\Delta\sigma_z^2/(2\gamma+2)$$
(47)

[in checking Eq. (47) by squaring Eq. (46), use  $\sigma_z \Delta \sigma_z = 0$ ,  $(\Delta \sigma_z)^2 = 2(1 - \sigma_{1z}\sigma_{2z})$ ,  $(\Delta \sigma_z)^4 = 4(\Delta \sigma_z)^2$ , and  $\hat{K}^4 = \hat{K}^2(\gamma^2 - 1)$ ]. The boost  $\bar{A}$  for  $\chi$  follows from A by replacing  $\gamma_5 \sigma_2$  by  $-\gamma_5 \sigma_2$ :

$$\chi_l = \bar{A}\chi_{cm}, \quad \bar{A} = \gamma + \frac{1}{2}\hat{K}\gamma_5 \Delta \sigma_z - \frac{1}{2}\hat{K}^2 \sigma_z^2 / (2\gamma + 2).$$
(48)

The inverse boost has **K** replaced by  $-\mathbf{K}$ , which is equivalent to a sign change of  $\gamma_5$ :

$$A\beta = \beta A^{-1}, \quad \bar{A}\beta = \beta \bar{A}^{-1}. \tag{49}$$

Insertion of Eq. (19),  $\psi_{cm} = c \psi$ , gives, in the laboratory system,  $\psi_l = A c \psi$ , and for the *c*-transformed  $\psi_l$ ,

$$\psi_{lc} = c^{-1} \psi_l = c^{-1} A c \psi = A_c \psi, \quad A_c = c^{-1} A c, \quad (50)$$

$$A_{c} = \gamma + \frac{1}{2} \gamma_{5} \hat{K} \sigma_{z} m_{+} / m_{-} - \frac{1}{2} \hat{K}^{2} \Delta \sigma_{z}^{2} / (2 \gamma + 2).$$
(51)

The corresponding boost for  $\chi$ , on the other hand, has a factor  $m_+$  extracted:

$$\bar{A}_{c} = m_{+}^{-1} A m_{+} = \gamma + \frac{1}{2} \gamma_{5} \hat{K} \Delta \sigma_{z} m_{+} / m_{-} - \frac{1}{2} \hat{K}^{2} \sigma_{z}^{2} / (2 \gamma + 2).$$
(52)

The desired boosts for  $\psi$  and  $\chi$  are  $A_c$  and  $\overline{A}_c$ , respectively. They are needed for the construction of Dirac-Breit equations in the presence of external potentials.

In a covariant treatment, the interaction between two particles at distance  $\mathbf{r}_l = \mathbf{r}_1 - \mathbf{r}_2$  depends also on a time difference  $x^0 = t_1 - t_2$  such that  $x^{\mu} = (x^0, \mathbf{r}_l)$  is a four-vector. A second independent four-vector  $X^{\mu}$  is defined such that  $P^{\mu} = i\partial_X^{\mu}$  becomes the total four-momentum  $p_1^{\mu} + p_2^{\mu}$ , which is conserved:

$$x^{\mu} = x_{1}^{\mu} - x_{2}^{\mu}, \quad X^{\mu} = \hat{E}_{1}x_{1}^{\mu} + \hat{E}_{2}x_{2}^{\mu}, \quad p_{1}^{\mu} = p^{\mu} + \hat{E}_{1}P^{\mu},$$

$$p_{2}^{\mu} = -p^{\mu} + \hat{E}_{2}P^{\mu}, \quad (53)$$

$$\hat{E}_1 + \hat{E}_2 = 1, \quad P^{\mu} = p_1^{\mu} + p_2^{\mu}, \quad P^{\mu}\psi = K^{\mu}\psi.$$
 (54)

The as yet open value of  $\hat{E}_1 - \hat{E}_2$  is chosen such that  $p^0 = i\partial/\partial x^0$  vanishes at asymptotic distances in the c.m. system where particles 1 and 2 are on their mass shells,  $E_1^2 - k^2 = m_1^2$  and  $E_2^2 - k^2 = m_2^2$ , i.e.,  $E_2^2 - E_1^2 = m_2^2 - m_1^2 = m_+ m_-$ . Using in addition  $E_1 + E_2 = E$ , one obtains

$$E_1 = (E^2 - m_+ m_-)/2E, \quad E_2 = (E^2 + m_+ m_-)/2E.$$
 (55)

Extracting now from Eq. (53)

$$p^{\mu} = \hat{E}_2 p_1^{\mu} - \hat{E}_1 p_2^{\mu} \tag{56}$$

and inserting the asymptotic values  $E_i$  of  $p_i^0$  in the c.m. system, one finds that  $p^0$  vanishes here for

$$\hat{E}_i = E_i / E = \frac{1}{2} (1 + \hat{m}_+ \hat{m}_-), \quad \hat{m}_{\pm} = m_{\pm} / E.$$
 (57)

In the interaction region,  $p^0$  does not vanish, but in the context of a single integral equation (Bethe-Salpeter equation) it cannot be treated as a dynamical variable. Instead, integrals involving  $p^0$  are treated as perturbations on  $\delta(p^0)$  integrals (Sec. VII).

The space coordinate transformation of Eq. (53) is

$$\mathbf{r}_1 = \mathbf{R} + \hat{E}_2 \mathbf{r}_l, \quad \mathbf{r}_2 = \mathbf{R} - \hat{E}_1 \mathbf{r}_l, \tag{58}$$

where  $z_i$  is Lorentz contracted,  $z_i = z/\gamma$ . The nonrelativistic approximation yields the familiar  $\hat{E}_i = m_i/m$ .

# VI. VECTOR POTENTIAL AND BETHE LOGARITHM

In the presence of a four-potential  $A^{\mu}$ ,  $p_1^{\mu}$ , and  $p_2^{\mu}$  are replaced by

$$\pi_1^{\mu} = p_1^{\mu} + eA^{\mu}(x_1), \quad \pi_2^{\mu} = p_2^{\mu} - ZeA^{\mu}(x_2).$$
(59)

The coefficients  $\hat{E}_1$  and  $\hat{E}_2$  of the transformation (53) to  $\pi^{\mu}$ and  $\Pi^{\mu}$  remain unchanged in a perturbative treatment of  $A^{\mu}$ . In the dipole approximation  $\mathbf{A}(x_1) = \mathbf{A}(x_2)$ , Eq. (56) leads to

$$\boldsymbol{\pi} = \hat{\boldsymbol{E}}_2 \boldsymbol{\pi}_1 - \hat{\boldsymbol{E}}_1 \boldsymbol{\pi}_2 = \mathbf{p} + re\mathbf{A}, \tag{60}$$

where  $re = r \times e$  is the dipole radiation charge [8],

$$r = \frac{1}{2} (Z+1) - \frac{1}{2} (Z-1) \hat{m}_{+} \hat{m}_{-}$$
  
= 1 +  $\frac{1}{2} (Z-1) (1 - \hat{m}_{+} \hat{m}_{-}).$  (61)

In the following, we use the Coulomb gauge in the c.m. system and replace **p** by  $\pi$  in Eq. (2). To exhibit its  $E^2$  dependence, we also multiply the equation by E:

$$(E\boldsymbol{\epsilon} - EV - m_1 m_2 \boldsymbol{\beta}) \boldsymbol{\psi} = \boldsymbol{\gamma}_5(\boldsymbol{\sigma}_1 - i \boldsymbol{\sigma}^{\times} V/E) E \boldsymbol{\pi} \boldsymbol{\psi}. \quad (62)$$

The substitution

$$\mathbf{r} = E \boldsymbol{\rho}, \quad \mathbf{p} = \mathbf{p}_{\boldsymbol{\rho}} / E, \quad \boldsymbol{\pi} = \boldsymbol{\pi}_{\boldsymbol{\rho}} / E$$
 (63)

puts Eq. (62) into a form that contains only even powers of *E*. For the moment, we assume  $V = -Z\alpha/r$  and  $EV = -Z\alpha/\rho = V(\rho)$ . Deviations will be discussed in Sec. VII. For the Lamb shift calculation, one neglects the hyperfine operator and obtains an explicit eigenvalue equation for  $E\epsilon = (E^2 - m_1^2 - m_2^2)/2$ ,

$$h\psi = E \epsilon \psi, \quad h = m_1 m_2 \beta + V(\rho) + \alpha \pi_{\rho}.$$
 (64)

Its Coulomb Green's function G satisfies the usual equation [2], taken in the variables  $\rho, \rho'$ :

$$[\nabla_{\rho}^{2} + (E\epsilon)^{2} - m_{1}^{2}m_{2}^{2} + 2E\epsilon Z\alpha/\rho + (Z\alpha + i\alpha\hat{\rho})Z^{2}\alpha^{2}/\rho^{2}]G(\rho,\rho', E\epsilon) = \delta(\rho - \rho').$$
(65)

Evidently, it is also independent of the signs of  $m_1$  and  $m_2$ . The same remark applies to r [Eq. (61)], but that expression uses the low-energy dipole approximation. Apart from that, the Bethe logarithm can depend only on  $E^2$ ,  $m_1^2$ , and  $m_2^2$ . Its proportionality to  $r^2$  has been noted previously [14,15]. Inspection of the formulas collected in [2] reveals another small *s* state correction, which is also proportional to  $r^2$ . Moreover, both corrections are proportional to  $m_1m_2$  and therefore pushed under the square root in Eq. (3), where they appear as quantum defects:

$$\beta_{B} = \frac{4\alpha^{3}}{3\pi} r^{2} \ln k_{0}(n,l), \quad \beta' = -\frac{4\alpha^{3}}{3\pi} r^{2} \left(\frac{5}{6} - \ln \alpha^{2}\right).$$
(66)

After the extraction of  $\beta_B$  and  $\beta'$ , there remains a somewhat reduced Salpeter shift

$$\Delta E'_{Sal} = -\frac{\mu_{nr}^2 Z^5 \alpha^5}{m \pi n^3} \left[ \frac{7}{3} a'_n + \frac{1}{m_+ m_-} \delta_{l0} \right] \\ \times \left( m_2^2 \ln \frac{m^2}{m_2^2} - m_1^2 \ln \frac{m^2}{m_1^2} \right), \qquad (67)$$

$$a_{n}^{\prime} = -2\,\delta_{l0} \left[ \ln \frac{2\,\alpha}{n} + \sum_{i=1}^{n} \frac{1}{i} + \frac{1}{2} - \frac{1}{2n} \right] + \frac{1 - \delta_{l0}}{l(l+1)(2l+1)},\tag{68}$$

with  $a'_1 = -2\ln(2\alpha)-2$ . The denominator  $m_+m_-$  in Eq. (67) will be discussed in the next section. The factor 1/m in front disappears in the expression for  $E^2$ , as  $E^2 \approx m^2 + 2mE_b$  according to Eq. (1).

# VII. BETHE-SALPETER EQUATION, VACUUM POLARIZATION, AND FORM FACTOR

Continuing with the *T* matrix of Sec. III, the two-photon exchange part  $T^{(2)}$  may be used to derive corrections to the main interaction, including the Salpeter shift (67). However, here we consider instead the more commonly used Bethe-Salpeter (BS) equation. It is formulated in the c.m. system, where Eq. (53) reduces to

$$p_1^{\mu} = p^{\mu} + E_1 g_{\mu 0}, \quad p_2^{\mu} = -p^{\mu} + E_2 g_{\mu 0}, \tag{69}$$

and  $p^{\mu}$  is an integration variable. Suppressing the integration, the BS equation applies to the two-fermion Green's function  $G = G^{(16)}$ ,

$$G^{(16)} = S^{(16)} + S^{(16)} K^{(16)} G^{(16)}, \tag{70}$$

where  $S^{(16)}$  is the product of two free fermion propagators in momentum space

$$S^{(16)} = (\not p_1 - m_1)^{-1} \otimes (\not p_2 - m_2)^{-1}$$
  
=  $(\not p_1 + m_1) \otimes (\not p_2 + m_2) / D_1 D_2$ , (71)  
$$D_1 = p_1^2 - m_1^2 + i\varepsilon = p^2 + 2E_1 p^0 + k^2 + i\varepsilon,$$
  
$$D_2 = p_2^2 - m_2^2 + i\varepsilon = p^2 - 2E_2 p^0 + k^2 + i\varepsilon,$$
 (72)

and the kernel  $K^{(16)}$  is the sum of all irreducible Feynman diagrams. Our proposed eight-component formalism simplifies *S* at the expense of *K*. Taking *K* from the matrix elements  $\chi^{\dagger}K\psi$  analogous to the 8×8 matrix *M* in Eq. (22), one has

$$S^{(16)}K^{(16)} = S^{(8)}K^{(8)}, \quad S^{(8)} = \sum v_{LP}w_{LP}^{\dagger}/D_1D_2.$$
 (73)

In a matrix notation where  $\gamma^0 = \beta$  and  $\gamma_5$  are identical for particles 1 and 2, the spin summation is now

$$\sum v_{LP} w_{LP}^{\dagger} = m_2 E_1 + m_1 \beta E_2 - m_- p^0$$
$$- \gamma_5 \mathbf{p} (m_2 \boldsymbol{\sigma}_1 - m_1 \beta \boldsymbol{\sigma}_2). \tag{74}$$

It is only a first-order polynomial in  $p_1$ ,  $p_2$ . Consequently, the numerator of  $S^{(8)}$  is linear in the integration variables, whereas  $S^{(16)}$  is quadratic. One may in fact go one step further and use irreducible representations of the Lorentz group, in which case one arrives at  $S^{(4)} = 1/D_1D_2$ . This amounts to the elimination of the dotted spinor components from  $\psi$  [16]; it is widely used in QCD calculations [17]. For bound states, however, it has the disadvantage of suppressing explicit parity invariance.

The term in parentheses in Eq. (74) is  $(m_-\sigma + m_+\Delta\sigma)/2$ in the notation of Eq. (18) and  $m_-\sigma$  may be converted into  $m_+\sigma$  by the transformation (20),

$$v_{LP} = cv, \quad w_{LP} = c^{-\gamma}w,$$

$$\sum vw^{\dagger} = (\epsilon - \gamma_5 \sigma_1 \mathbf{p} + \mu\beta + p^0 m_- / m_+)m_+. \quad (75)$$

- 1

To handle the  $p^0$  integration, one may use the formula  $1/(x - i\varepsilon) = P/x + i\pi \delta(x)$  (*P* is the principal value),

$$2E/D_1D_2 = 2i\pi\delta(p^0)/(\mathbf{p}^2 - k^2) - 1/D_1(p^0 + i\varepsilon) + 1/D_2(p^0 - i\varepsilon),$$
(76)

and treat all  $p^0$  integrals except the first one as perturbations of the Green's function. In these integrals, the spin summation (75) reduces to  $\Sigma v w^{\dagger}/m_{+} = \epsilon - \alpha \mathbf{p} + \mu \beta$ , which is simply the expression for a single-particle spin summation. In the remaining integrals, the complete two-fermion propagator has the more explicit numerator

$$2E\sum vw^{\dagger}/m_{+} = E^{2} - (m_{1}^{2} + m_{2}^{2} - 2m_{1}m_{2}\beta) \times (1 - Ep^{0}/m_{+}m_{-}) - 2\gamma_{5}\mathbf{p}_{\rho}\boldsymbol{\sigma}_{1}.$$
(77)

After integration, this  $p^0$  dependence produces factors  $(m_1^2 + m_2^2)/m_+m_-$  and  $m_1m_2\beta/m_+m_-$ . Such factors may also arise from the denominators  $1/D_1D_2^X$  of the crossed graph, which contain the combination  $p^0(E_1-E_2) = Ep^0\hat{m}_+\hat{m}_-$ . To check the mass dependence in the  $\delta_{l0}$  piece of  $\Delta E'_{Sal}$  [Eq. (67)], notice  $m_2^2 \ln(m^2/m_2^2) - m_1^2 \ln(m^2/m_1^2) = m_+m_- \ln(m_1m_2/m^2) + (m_1^2 + m_2^2) \ln(m^2/m_1m_2)$ .

We conclude with a discussion of the potential  $EV(r) \rightarrow V(\rho)$  in the presence of vacuum polarization and nuclear charge distribution. For a heavy particle 1 ( $\mu^-$  or  $\bar{p}$ ), electronic vacuum polarization is so large in low-*l* states that it must be added to the Coulomb potential  $V_C$ , in the form of the Uehling potential

$$V = V_C + V_U, \quad V_U = -\frac{Z\alpha^2}{3\pi r} \int_0^\infty d\lambda^2 e^{-\lambda r} S(\lambda^2), \quad (78)$$

with  $S_e = (1 - 4m_e^2/\lambda^2)^{1/2}(1 + 2m_e^2/\lambda^2)/\lambda^2\Theta(4m_e^2)$  in the electronic part of  $V_U$ . At fixed  $\lambda$ , the *r* dependence is easily converted to a  $\rho$  dependence  $(E/r)e^{-\lambda r} = \rho^{-1}e^{-\lambda E\rho}$ :

$$V_U(\rho) = -\frac{Z\alpha^2}{3\pi\rho} \int_0^\infty d\lambda^2 e^{-\lambda E\rho} S(\lambda^2).$$
(79)

The substitution  $\lambda E = \lambda'$  shows that the integral depends only on  $E^2$ . There is also a second-order recoil correction  $V_{Ur}^{(2)}$  which is spin independent [18]. For antiprotonic atoms, the radius of the vacuum polarization cloud is much larger than the Bohr radius  $(Z\alpha\mu)^{-1}$ : Below a critical value  $l_c$  of the orbital angular momentum l, vacuum polarization exceeds all relativistic effects (protonium  $\bar{p}p$  and  $\bar{p}^3$ He have  $l_c=3$  and 7, respectively) for all values of n [19]. For these orbitals, V is best constructed numerically from Eq. (79), particularly for the calculation of annihilation that is localized at very small  $\rho$ . However, for the calculation of the fine and hyperfine structure of these inner orbitals, the form (79) suggests the introduction of a running electric coupling constant  $\alpha_e$ :

$$V = V_e + \delta V_U, \quad V_e = -Z\alpha_e/\rho,$$
  
$$\delta V_U = V_U + Z(\alpha_e - \alpha)/\rho, \quad \langle \delta V_U \rangle = 0. \tag{80}$$

In this manner, the nonperturbative result (3) remains applicable, with  $\alpha_e > \alpha$ .

Recoil corrections to an extended nuclear charge distribution  $\rho_c(r)$  are particularly large for muonic atoms:

$$W(\rho) = -Z\alpha \int d^{3}r |\boldsymbol{\rho} - \mathbf{r}/E|^{-1} \rho_{c}(r),$$
  
$$\rho_{c}(r) = \int d^{3}q e^{-i\mathbf{q}\cdot\mathbf{r}} F(q^{2}).$$
(81)

Again,  $V(\rho)$  is  $E^2$  dependent.

# VIII. ANGULAR-MOMENTUM DEFECTS AND BARKER-GLOVER TERM

To order  $\alpha_Z^2 = Z^2 \alpha^2$ ,  $\delta l$  is easily found for particles of arbitrary masses  $m_i$  and g factors  $g_i = 2(1 + \kappa_i)$ .  $\delta l$  is conveniently expressed as

$$\delta l/\alpha_Z^2 = -(1+a)/(2l+1).$$
(82)

With the abbreviations  $\hat{m}_i = m_i/E$  and  $\hat{\epsilon} = \epsilon/E$  and the combinations

$$c_{1}^{2} = 1 - \hat{m}_{1}^{2} - \hat{\epsilon} + 2\kappa_{1}\hat{m}_{2}, \quad c_{2}^{2} = 1 - \hat{m}_{2}^{2} - \hat{\epsilon} + 2\kappa_{2}\hat{m}_{1},$$
(83)

$$c^{2} = 1 + 2\kappa_{1}\hat{m}_{2} + 2\kappa_{2}\hat{m}_{1} + 2\hat{\epsilon}(1 - g_{1}g_{2}/4), \qquad (84)$$

one finds

$$a(l=f\pm 1) = \pm c^2/(2j+1) \pm g_1 g_2 \hat{\epsilon}/(4f+2)$$
(85)

(where a sign error of [9] for l = f + 1 is corrected) and

$$a(l=f) = \pm \frac{c^2}{4F^2} \left[ \sqrt{(2f+1)^2 - 16F^2 \frac{c_1^2 c_2^2}{c^4}} \mp 1 \right]$$
  
$$\approx \pm \frac{c^2}{2j+1} \mp \frac{2c_1^2 c_2^2}{c^2 (2f+1)} \left[ 1 + \frac{4F^2 c_1^2 c_2^2}{c^4 (2f+1)^2} \right].$$
(86)

In Eq. (85),  $l=f\pm 1$  implies  $j=j_1=f\pm \frac{1}{2}=l\pm \frac{1}{2}$ . For  $g_1=g_2=2$ , c=1 leads exactly to the Dirac fine structure component (43) of  $\delta l$  for all values of  $m_1$  and  $m_2$ , including  $m_1=m_2$  as in positronium. The case l=f is more complicated because the two values  $j=l+\frac{1}{2}$  and  $j=l-\frac{1}{2}$  are mixed by the hyperfine interaction. We therefore define j as that value in the integer 2j+1 that appears in the main term  $c^2/(2j+1)$  of a(l=f) after expansion of the square root. It is frequently said that the fine structure contains the "Barker-Glover" term (for l>0) [2,3]



This is true for a spinless nucleus, except that the electron's anomalous magnetic moment frequently reverses the effect [11]. On the other hand, the weighted average over the hyperfine structure produces a more complicated expression

$$\bar{a} = (l-j)\{2c^2 + g_1g_2\hat{\epsilon}/2 - 2(c_1^2c_2^2/c^2) \\ \times [1 + 4L^2c_1^2c_2^2/c^4 \\ \times (2l+1)^2]\}/(2j+1).$$
(88)

This is the final result and as a rule it is much larger than the

Barker-Glover term. For  $g_1 = g_2 = 2$ , however,  $c_1^2 c_2^2 \approx \mu/m \approx \hat{\epsilon}$  to this order in  $\alpha$  and the main terms cancel in Eq. (88). There remains a small rest

$$\Delta \bar{E} = \alpha_Z^2 \mu_{nr} \bar{\delta} l/(2l+1) n^3 = -\mu_{nr} \alpha_Z^4 \bar{a}/n^3$$
  
=  $4\mu_{nr}^3 \alpha_Z^4 (l-j) L^2 / (2l+1)^3 (2j+1) m^2 n^3$ , (89)

which replaces  $E_{BG}$  in the case of muonium.

#### ACKNOWLEDGMENTS

The authors would like to thank S. Karshenboim and A. Yelkhovsky for helpful comments. This work was supported by the Deutsche Forschungsgemeinschaft.

- [1] H. Grotch and D. R. Yennie, Rev. Mod. Phys. 41, 350 (1969).
- [2] J. R. Sapirstein and D. Yennie, *Quantum Electrodynamics* (World Scientific, Singapore, 1990).
- [3] K. Pachucki et al., J. Phys. B 29, 177 (1996).
- [4] A. Yelkhovsky, JETP 83, 230 (1996).
- [5] W. E. Caswell and G. E. Lepage, Phys. Lett. **167B**, 437 (1986).
- [6] P. Labelle, S. M. Zebarjad, and C. P. Burgess, Phys. Rev. D 56, 8053 (1977); A. H. Hoang, P. Labelle, and S. M. Zebarjad, Phys. Rev. Lett. 79, 3387 (1997).
- [7] H. Pilkuhn, J. Phys. B 25, 289 (1992); H. Pilkuhn and F. Stäudner, Phys. Lett. A 178, 156 (1993).
- [8] M. Malvetti and H. Pilkuhn, Phys. Rep. 248, 1 (1994).
- [9] H. Pilkuhn, J. Phys. B 28, 4421 (1995).
- [10] E. Brezin, C. Itzykson, and J. Zinn-Justin, Phys. Rev. D 1,

2349 (1970).

- [11] H. Pilkuhn, J. Phys. B 17, 4061 (1984).
- [12] S. N. Gupta, *Quantum Electrodynamics* (Gordon and Breach, New York, 1977); S. N. Gupta, W. W. Repko, and C. J. Suchyta III, Phys. Rev. D 40, 4100 (1989).
- [13] K. Pachucki and H. Grotch, Phys. Rev. A 51, 1854 (1995); E.
   A. Golosov *et al.*, JETP 80, 208 (1995).
- [14] G. W. Erickson, J. Phys. Chem. Ref. Data 6, 833 (1977).
- [15] S. G. Karshenboim, JETP 80, 593 (1995).
- [16] L. M. Brown, Phys. Rev. 111, 957 (1958); M. Tonin, Nuovo Cimento 14, 1108 (1959).
- [17] G. Chalmers and W. Siegel, e-print hep-ph/9708251.
- [18] J. Fröhlich and H. Pilkuhn, J. Phys. B 17, 147 (1984).
- [19] S. Barmo, H. Pilkuhn, and H. G. Schlaile, Z. Phys. A 301, 283 (1981).