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BINARY BOOSTS

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Abstract

The relativistic motion of an isolated two–body system (bound or unbound) of given lab energy K^0 in QED is separated into *cms* motion and relative motion. The relative motion equation $\mathcal{K}_{\rm L}\psi_{\rm L}(\mathbf{r}_{\rm L}) = 0$ contains the momentum eigenvalue $\mathbf{K}$ of the *cms* motion. It is greatly simplified by a binary boost to the atomic rest frame, where K^0 and $\mathbf{K}$ appear only in a Lorentz–invariant combination. This boost is not a product of single–particle boosts, which are useful only for perturbative interactions. CPT–invariance is demonstrated, and orthogonality relations are derived.

I. INTRODUCTION

This paper is about the relativistic two–body problem in QED. It treats the separation of the *cms* motion from the relative motion in analogy with the nonrelativistic separation. The case of two spinless particles has been treated previously [1] but has no practical applications. When one of the two particles is a lepton (e, μ or τ) and the other is spinless, the two–body wave function contains an additional boost:

$$\mathrm{A} = (\gamma + \gamma_5 \mathbf{K}\boldsymbol{\sigma}_1/E)^{1/2}, \qquad \gamma = K^0/E, \qquad {K^0}^2 - \mathbf{K}^2 = E^2 \tag{1}$$

in units $\hbar = c = 1$. Here $K^\mu = (K^0, \mathbf{K})$ are the eigenvalues of $P^\mu = (i\partial_t, \mathbf{P})$ with $\mathbf{P} = \mathbf{p}_1 + \mathbf{p}_2$; $\boldsymbol{\sigma}_1$ are the Pauli matrices of particle 1, which are normally combined with the Dirac matrix γ_5 into $\boldsymbol{\alpha}_1 = \gamma_5\boldsymbol{\sigma}_1$. The *binary boost* A resembles the boost A_1 for a single free particle:

$$\mathrm{A}_1 = (\gamma_1 + \gamma_5 \mathbf{K}_1\boldsymbol{\sigma}_1/m_1)^{1/2}, \qquad \gamma_1 = K_1^0/m_1, \qquad {K_1^0}^2 - \mathbf{K}_1^2 = m_1^2. \tag{2}$$

(An alternative form of A_1 which avoids $\boldsymbol{\sigma}_1$ under the square root is $(2m_1)^{-1/2}\left(K_1^0 + m_1\right)^{-1/2}$ $(K_1^0 + m_1 + \boldsymbol{\alpha}_1\mathbf{K}_1)$, but (2) is in fact more elegant.) These points will be elaborated in section III. They are of interest for muonic helium $(\mu^-\alpha)$, mu–pionium $(\mu^-\pi^+)$ and also for precise recoil corrections in ordinary atoms.

Binary boosts are simplified by taking the z–axis along the total momentum $\mathbf{K}$, $\boldsymbol{\sigma}_1\mathbf{K} = \sigma_{1z}K$, and by abbreviating $K/E = \gamma v/c$ as $\widehat{K}$: $A = \left(\gamma + \gamma_5\widehat{K}\sigma_{1z}\right)^{1/2}$. The symbol β will denote the *parity Dirac matrix* which will be taken in diagonal form:

$$\beta = \gamma_0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad \gamma_5 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{3}$$

The boost which we find for two spinor particles contains $\sigma_z = \sigma_{1z} + \sigma_{2z}$ as well as a β–dependent mass ratio μ_β:

$$B = \left(1 + \frac{1}{2}\widehat{K}^2\sigma_z^2 + \mu_\beta\widehat{K}\sigma_z\gamma\gamma_5\right)^{1/2}, \quad \widehat{K} = K/E\,, \tag{4}$$

$$\mu_\beta = M_-/M_+\,, \quad M_\pm = m_2 \pm \beta m_1\,. \tag{5}$$

As σ_z^2 has only the two eigenvalues 4 and 0, an alternative form of B is

$$B = \tilde{\gamma} + \mu_\beta\widehat{K}\sigma_z\gamma_5/2\,, \quad \tilde{\gamma} = \sqrt{1 + \widehat{K}^2\sigma_z^2/4}\,. \tag{6}$$

Evidently, $\tilde{\gamma} = \gamma$ for $\sigma_z^2 = 4$ and $\tilde{\gamma} = 1$ for $\sigma_z^2 = 0$. B contains two Pauli matrices but only one β and one γ_5, i.e. B is an 8×8 matrix. For comparison, the two–body boost B_{12} used so far in perturbative QED is a 16×16–matrix,

$$B_{12} = A_1A_2 = (\gamma_1 + \mathbf{p}_1\boldsymbol{\alpha}_1/m_1)^{1/2}(\gamma_2 + \mathbf{p}_2\boldsymbol{\alpha}_2/m_2)^{1/2}\,. \tag{7}$$

It requires two separate conserved energies, K_1^0 and K_2^0, momentum operators $\mathbf{p}_1$ and $\mathbf{p}_2$ and Dirac matrices $\beta_1, \beta_2, \gamma_{51}, \gamma_{52}$. The main advantage of B is that it contains only the total momentum $\mathbf{K}$ instead of the individual momenta. It Lorentz transforms the asymptotic part of the *cms* spinorial wave function, the radial part of which is e^{ikr} in spherical coordinates (bound states have imaginary $k = i\kappa$; in QED, the ground state has $\kappa_0 = a_B^{-1}$, a_B being the relativistic Bohr radius). The boost B_{12}, on the other hand, requires asymptotic wave functions $e^{i\mathbf{k}_1\mathbf{r}_1}e^{i\mathbf{k}_2\mathbf{r}_2}$ and then by analogy also two different times, $e^{-iK_1^0t_1}e^{-iK_2^0t_2}$. The derivation of B is given in the next section. As in the nonrelativistic case, the shape of the potential $V(\mathbf{r}_\mathrm{L})$ is irrelevant in this derivation ($\mathbf{r}_\mathrm{L} = \mathbf{r}_1 - \mathbf{r}_2$). Anomalous magnetic moments can be included in the *cms* equation [2] but are as yet excluded from the boost. Thus the present treatment applies to the bound states of two charged leptons, which may be called leptonium (muonium $\mathrm{e}^-\mu^+$, antimuonium $\mathrm{e}^+\mu^-$, positronium $\mathrm{e}^-\mathrm{e}^+$), as well as to their scattering states up to $K^0 \to \infty$ and / or $E \to \infty$.

The relativistic separation of the *cms* coordinate $\mathbf{R}$ reads [1]

$$\mathbf{r}_1 = \mathbf{R} + \frac{1}{2}\left(1 - \Delta m^2/E^2\right)\mathbf{r}_\mathrm{L}, \qquad \mathbf{r}_2 = \mathbf{R} - \frac{1}{2}\left(1 + \Delta m^2/E^2\right)\mathbf{r}_\mathrm{L} \tag{8}$$

with $\Delta m^2 = m_1^2 - m_2^2 = -M_+M_-$. For loosely bound states, $E^2 \approx (m_1 + m_2)^2$ reduces (8) to the nonrelativistic transformation except for the index L in $\mathbf{r}_\mathrm{L}$ which still signifies the lab system. This additional index is necessary because $\mathbf{r}_\mathrm{L}$ is Lorentz–contracted in the direction $\mathbf{K}$. The uncontracted *cms* variable will be denoted by $\mathbf{r}^*$. In the following, the z–axis is taken along $\mathbf{K}$, such that x_L and y_L are not Lorentz–contracted, and

$$z_{\mathrm{L}} = z^*/\gamma, \qquad p_{\mathrm{L}z} = \gamma p_z^*. \tag{9}$$

The usual *cms* potential $V^* = -\alpha/r^*$ ($\alpha = e^2$) which is abstracted from the QED Born approximation is Lorentz–contracted in the lab system. In the 16–component Dirac–Breit equation which is applied successfully in atomic theory, this contraction is not evident, but a careful analysis shows that it is represented by the Breit operators [1]. With a simple $V(r) = -\alpha/r$, the *cms* equation is free of Breit operators. However, this form in fact requires a third variable transformation which affects only the distance, $r \to r^*$. In other words, the Fourier transform of the first Born approximation of the *cms* scattering amplitude produces a potential $V(r)$ where r is a *quasidistance* from the Dirac–Breit point of view. These procedures are up to now only approximately Lorentz–invariant and are not repeated here. We merely wish to reserve the index–free $\mathbf{r}$ for the quasiposition, which may or may not coincide with $\mathbf{r}^*$.

An important application of this 8–component formalism is to positronium. The relation $m_2 = m_1$ simplifies (8) to $\mathbf{r}_1 = \mathbf{R} + \mathbf{r}_{\mathrm{L}}/2$, $\mathbf{r}_2 = \mathbf{R} - \mathbf{r}_{\mathrm{L}}/2$. In this case, B can be used in the small components ($\beta = -1$, $\mu_\beta = \infty$) only for $\sigma_z^2 = 0$, in which case the large components have $\sigma_z^2 = 4$. The opposite case requires a γ_5–transformation, which will be explained in section II.

We have found in the literature a formula which resembles (4): Replacing $E \to m_1$ and $\mu_\beta \to 1$, (4) becomes identical with a boost for a single free particle of spin 1 [3].

II. DERIVATION OF THE 8–COMPONENT EQUATION

A convenient starting point in the lab system is at present the 16–component Dirac–Breit equation

$$\left(\pi_{\mathrm{L}}^0 - m_1\beta_1 - m_2\beta_2 - P_{\mathrm{B}}\right)\psi_{\mathrm{DL}} = 0\,, \quad \pi_{\mathrm{L}}^0 = i\partial_t - V_{12} \tag{10}$$

where P_{B} is the Dirac–Breit momentum operator [1], and the indices D and L stand for Dirac and lab system, respectively. It contains $\mathbf{p}_1$ and $\mathbf{p}_2$ multiplied by Breit corrections $1 - V_{12}\left(\boldsymbol{\alpha}_1\boldsymbol{\alpha}_2 + \alpha_{1r}\alpha_{2r}\right)/2$, which contain low–energy approximations. In the future, one would like to formulate the Feynman rules for the fermion–fermion scattering amplitudes in terms of 8–component spinors, both in the lab system and in the *cms*, and then derive the interactions via Fourier transformations. At present, this derivation is incomplete even in the *cms*. The *cms* equation has been abstracted from (10), but most of its scattering amplitudes have been checked against the Born approximation for arbitrary energies. For the present construction of the free two–particle boost, we only need three properties of (10): (i) it is translationally invariant in space and time,

$$i\partial_t\psi_{\mathrm{DL}} = K^0\psi_{\mathrm{DL}}\,, \quad (\mathbf{p}_1 + \mathbf{p}_2)\,\psi_{\mathrm{DL}} = \mathbf{K}\psi_{\mathrm{DL}}\,, \tag{11}$$

(ii) it is exact at all energies in the asymptotic region $V_{12} = 0$ and (iii) it contains only a single time t, which contributes a factor e^{-iK^0t} for stationary states. The resulting time–independent Dirac–Breit equation is again (10), but with $\pi_{\mathrm{L}}^0 = K^0 - V_{12}$. It contains the six variables $\mathbf{r}_1$ and $\mathbf{r}_2$, precisely as in the nonrelativistic case. For $V_{12} = 0$, we thus have

$$\left(K^0 - m_1\beta_1 - m_2\beta_2 - \mathbf{p}_1\boldsymbol{\alpha}_1 - \mathbf{p}_2\boldsymbol{\alpha}_2\right)\psi_{\mathrm{DL}} = 0\,. \tag{12}$$

In the parity basis in which β_1 and β_2 are diagonal, the components of $\psi_{\rm DL}$ may be labelled by the index g for a large component and f for a small component of either particle: ψ_{gg}, ψ_{gf}, ψ_{fg} and ψ_{ff}. In the following, these components are rearranged into sums and differences as follows:

$$\psi_{\rm DL} = \begin{pmatrix} \psi_g \\ \psi_f \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} \psi_{gg} + \psi_{ff} \\ \psi_{gf} + \psi_{fg} \end{pmatrix}, \quad \chi_{\rm DL} = \begin{pmatrix} \chi_g \\ \chi_f \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} \psi_{gg} - \psi_{ff} \\ \psi_{gf} - \psi_{fg} \end{pmatrix}. \tag{13}$$

The index D stands for Dirac, the index L for the lab system. The factor $2^{-1/2}$ makes the transformation unitary. The 16–component equation thus assumes the form of two coupled 8–component equations,

$$\left(K^0 - \gamma_5 p_+\right) \psi_{\rm DL} = \beta M_+ \chi_{\rm DL}\,, \quad \left(K^0 + \gamma_5 p_-\right) \chi_{\rm DL} = \beta M_+ \psi_{\rm DL}\,, \tag{14}$$

$$p_\pm = \mathbf{p}_1 \boldsymbol{\sigma}_1 \pm \mathbf{p}_2 \boldsymbol{\sigma}_2\,, \tag{15}$$

with β, γ_5 and M_+ defined in (3) and (5). In words, γ_5 exchanges the single index g with the single index f in ψ and χ, while β multiplies f by -1. The original matrices β_1, β_2, γ_{51} and γ_{52} are now obsolete. Elimination of $\chi_{\rm DL}$ by means of the first equation (14) yields

$$\left(K^0 + \gamma_5 p_-\right) \beta M_+^{-1} \left(K^0 - \gamma_5 p_+\right) \psi_{\rm DL} = \beta M_+ \psi_{\rm DL}\,. \tag{16}$$

Upon multiplication by βM_+, this becomes

$$\left(K^{0^2} - M_+^2 - K^0 p_- \mu_\beta^{-1} \gamma_5 - K^0 p_+ \gamma_5 + \mu_\beta^{-1} p_- p_+\right) \psi_{\rm DL} = 0. \tag{17}$$

The denominator $M_- = m_2 - \beta m_1$ appears here because of $\gamma_5 \beta = -\beta \gamma_5$. At this point, we replace $\mathbf{r}_1$ and $\mathbf{r}_2$ by $\mathbf{R}$ and $\mathbf{r}_{\rm L}$ according to (8), which leads to

$$\mathbf{p}_1 = \mathbf{p}_{\rm L} + \frac{1}{2}\left(1 + \Delta m^2/E^2\right) \mathbf{K}\,, \quad \mathbf{p}_2 = -\mathbf{p}_{\rm L} + \frac{1}{2}\left(1 - \Delta m^2/E^2\right) \mathbf{K} \tag{18}$$

where (11) has already been used, and $E^2 = K^{0^2} - \mathbf{K}^2$ as in (1). $\psi_{\rm DL}$ is now a function of the vector $\mathbf{r}_{\rm L}$ and of the parameters K^0 and K (with the z–axis along $\mathbf{K}$). We now show that $\psi_{\rm DL}$ can be reduced to a function of the components $\mathbf{r}_{{\rm L}t} = (x_{\rm L}, y_{\rm L})$ and $z^* = \gamma z_{\rm L}$ which contains K^0 and K only in the combination $K^{0^2} - K^2 = E^2$. This justifies the choice of the transformation (8), (9) a posteriori.

The combinations $p_\pm$ of (15) become

$$\begin{aligned} p_- &= \mathbf{p}_{\rm L} \boldsymbol{\sigma}_t + \left(\gamma p_z^* + \frac{\Delta m^2}{2E^2} K\right) \sigma_z + \frac{1}{2} K \Delta\sigma_z, \\ p_+ &= \mathbf{p}_{\rm L} \Delta\boldsymbol{\sigma}_t + \left(\gamma p_z^* + \frac{\Delta m^2}{2E^2} K\right) \Delta\sigma_z + \frac{1}{2} K \sigma_z, \end{aligned} \tag{19}$$

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2\,, \quad \Delta\boldsymbol{\sigma} = \boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_2\,, \quad \boldsymbol{\sigma}_t = (\sigma_x, \sigma_y)\,. \tag{20}$$

Here we have denoted $\mathbf{p}_{{\rm L}t} \boldsymbol{\sigma}_t = \mathbf{p}_{\rm L} \boldsymbol{\sigma}_t$ in order to save one index. The operators $\mathbf{p}_{{\rm L}t}$ and p_z^* refer to the *cms*, but we avoid the notation $\mathbf{p} = -i\nabla$ which is reserved for the quasimomentum.

In the Pauli spinor space $\chi_1\chi_2$, $\boldsymbol{\sigma}$ is symmetric in 1 and 2. It transforms spin triplets into triplets and annihilates spin singlets. $\Delta\boldsymbol{\sigma}$ is antisymmetric and exchanges singlets ($\psi_{\mathrm{L}s}$) with triplets ($\psi_{\mathrm{L}t}$). It turns out that the following separation of mass factors is useful:

$$\psi_{\mathrm{DL}} = \begin{pmatrix} \psi_{\mathrm{DL}t} \\ \psi_{\mathrm{DL}s} \end{pmatrix} = \begin{pmatrix} M_+\psi_{\mathrm{L}t} \\ M_-\psi_{\mathrm{L}s} \end{pmatrix}. \tag{21}$$

The index D disappears here; the new components $\psi_{\mathrm{L}t}$ and $\psi_{\mathrm{L}s}$ form an 8–component spinor ψ_{L}, which satisfies the following equation:

$$\Big\{K^{0^2} - M_+^2 + \mu_\beta^{-1}p_-p_+ - K^0\Big[2\mathbf{p}_{\mathrm{L}}\boldsymbol{\sigma}_{1t} + \Big(2\gamma p_z^* + \frac{\Delta m^2 K}{E^2}\Big)\sigma_{1z} + \\ + \frac{K}{2}\left(\mu_\beta^{-1}\Delta\sigma_z + \mu_\beta\sigma_z\right)\Big]\gamma_5\Big\}\psi_{\mathrm{L}} = 0. \tag{22}$$

Here we have used $\boldsymbol{\sigma} + \Delta\boldsymbol{\sigma} = 2\boldsymbol{\sigma}_1$. The expression p_-p_+ simplifies considerably,

$$p_-p_+ = \frac{\Delta m^2}{E^2}K^2 + 2K\gamma p_z^*. \tag{23}$$

Remembering $\Delta m^2 = -M_+M_-$, the form $M_+\Delta m^2K^2/E^2M_- = -M_+^2K^2/E^2$ is combined with $-M_+^2$ into $-M_+^2(1+K^2/E^2) = -M_+^2\gamma^2$, $\gamma = K^0/E$. One may thus remove one factor γ from (22). The result is $\mathcal{K}_{\mathrm{L}}\psi_{\mathrm{L}} = 0$, where

$$\mathcal{K}_{\mathrm{L}} = (E^2 - M_+^2)\gamma + 2K\mu_\beta^{-1}p_z^* - \Big[2E\mathbf{p}_{\mathrm{L}}\boldsymbol{\sigma}_{1t} + (2E\gamma p_z^* - M_+M_-\widehat{K})\sigma_{1z} + \\ + \frac{1}{2}\widehat{K}E^2\left(\mu_\beta^{-1}\Delta\sigma_z + \mu_\beta\sigma_z\right)\Big]\gamma_5\,, \tag{24}$$

with $\widehat{K} = K/E$ as before. In the *cms*, i.e. $\widehat{K} = 0$, $\gamma = 1$, this reduces to

$$\mathcal{K}\psi = 0\,, \quad \mathcal{K} = E^2 - M_+^2 - 2E(\mathbf{p}_{\mathrm{L}}\boldsymbol{\sigma}_{1t} + p_z^*\sigma_{1z})\gamma_5\,. \tag{25}$$

The operator $\mathcal{K}$ is independent of $\boldsymbol{\sigma}_2$ and well–behaved for $m_1 = m_2$, where $M_+^2 = 2m_1^2(1+\beta)$ annihilates the small components. It remains to find a transformation $\psi_{\mathrm{L}} = B\psi$ which reduces $\mathcal{K}_{\mathrm{L}}$ to $\mathcal{K}$ after multiplication by another matrix $\bar{B}$ from the left

$$\bar{B}\mathcal{K}_{\mathrm{L}}B\psi = \mathcal{K}\psi = 0\,, \quad \mathcal{K} = \bar{B}\mathcal{K}_{\mathrm{L}}B\,. \tag{26}$$

As the operator $-2E\mathbf{p}_{\mathrm{L}}\boldsymbol{\sigma}_{1t}$ occurs in (25) in the same form as in (24), one needs

$$\bar{B}\,\boldsymbol{\sigma}_{1t}\,\gamma_5 = \boldsymbol{\sigma}_{1t}\,\gamma_5\,B^{-1}. \tag{27}$$

The form (24) suggests that B may not contain $\boldsymbol{\sigma}_{1t}$ and $\boldsymbol{\sigma}_{2t}$. Next, one may note that

$$\sigma_{1z}\boldsymbol{\sigma}_{1t} = -\boldsymbol{\sigma}_{1t}\sigma_{1z}\,, \quad \Delta\sigma_z\boldsymbol{\sigma}_{1t} = -\boldsymbol{\sigma}_{1t}\sigma_z. \tag{28}$$

After a few fruitless attempts, one solves (26) with

$$B = \left(1 + \frac{1}{2}\widehat{K}^2\sigma_z^2 + \mu_\beta \widehat{K}\sigma_z\gamma\gamma_5\right)^{1/2}, \quad B^{-1} = \left(1 + \frac{1}{2}\widehat{K}^2\sigma_z^2 - \mu_\beta \widehat{K}\sigma_z\gamma\gamma_5\right)^{1/2}, \tag{29}$$

$$\bar{B} = \left(1 + \frac{1}{2}\widehat{K}^2\Delta\sigma_z^2 + \mu_\beta^{-1}\widehat{K}\Delta\sigma_z\gamma\gamma_5\right)^{1/2}. \tag{30}$$

It remains to show how the eigenvalue ∞ of μ_β (5) is avoided for positronium. When the large components have $\sigma_z^2 = 4$, $\sigma_z = \pm 2$ implies $m_l = m_j \pm 1$ (m_l and m_j are the eigenvalues of L_z and $J_z = L_z + \sigma_z/2$). These states have parity $(-1)^{j+1}$ ($J^2 = j(j+1)$). The orbital parity of the small components is opposite, i.e. $(-1)^j$. The spin function can be either singlet or triplet, and in either case $m_l = m_j$ ensures $\sigma_z = 0$, i.e. the combination $\mu_\beta\sigma_z$ can be taken to vanish in (6). Thus in the application to positronium, one must discuss the spin structure for $m_1 \neq m_2$ and then take $m_1 = m_2$ in the final forms. When the large components have $\sigma_z = 0$, a chiral transformation $\psi_{\rm DL} = \gamma_5\psi_{{\rm DL},ch}$ transforms μ_β into μ_β^{-1}, such that the above argument applies again.

III. THE KLEIN–DIRAC BOOST

The 4–component Dirac–Klein–Gordon–Breit equation for systems such as $\mu^-\pi^+$ reads [1]

$$\left(\pi_{\rm L}^{0\,2} + \mathcal{K}_1 - \mathcal{K}_2 - 2m_1\pi_{\rm L}^0\beta\right)\psi_{\rm L}' = \gamma_5\left(\{\mathbf{p}_1, \pi_{\rm L}^0\}\boldsymbol{\sigma}_1 + b_1\right)\psi_{\rm L}' \tag{31}$$

where b_1 is the Breit modification of the momentum operator,

$$b_1 = -V_{12}\left(\boldsymbol{\sigma}_1\mathbf{p}_2 + \sigma_{1r}p_{2r}\right), \tag{32}$$

and $\mathcal{K}_i = m_i^2 + p_i^2$. The coordinate transformations (8) and (9) give

$$\mathcal{K}_1 - \mathcal{K}_2 = \gamma^2\Delta m^2 + 2\gamma p_z^* K. \tag{33}$$

Setting now $V_{12} = 0$ and extracting one factor γ, one obtains $\mathcal{K}_{\rm L}'\psi_{\rm L}' = 0$, with

$$\mathcal{K}_{\rm L}' = \left(E^2 + \Delta m^2\right)\left(\gamma - \gamma_5\widehat{K}\sigma_{1z}\right) + 2Kp_z^* - 2\gamma_5 E\left(\gamma p_z^*\sigma_{1z} + \mathbf{p}_{\rm L}\boldsymbol{\sigma}_{1t}\right) - 2m_1\beta E. \tag{34}$$

Writing the lab spinor $\psi_{\rm L}$ as a boost A times the *cms* spinor ψ', $\psi_{\rm L}' = A\psi'$, one finds

$$\mathcal{K}'\psi' = 0, \quad \mathcal{K}' = A\,\mathcal{K}_{\rm L}'\,A, \quad A = \left(\gamma + \gamma_5\widehat{K}\sigma_{1z}\right)^{1/2}, \tag{35}$$

$$\mathcal{K}' = E^2 + \Delta m^2 - 2Em_1\beta - 2E\left(p_z^*\alpha_z + \mathbf{p}_{\rm L}\boldsymbol{\alpha}_t\right). \tag{36}$$

The asymptotic energy E_1 of the spinor particle is $E_1 = (E^2 + \Delta m^2)/2E$, such that the first two terms in (36) arise from $2EE_1$. As $\mathcal{K}'$ has the Dirac operator structure, it is clear that its eigenvalues depend on $E^2 + \Delta m^2$ and $-2Em_1\beta$ only via $(E^2 + \Delta m^2)^2 - 4m_1^2E^2$. Setting now

$$\psi' = \left(2k^2E\right)^{-1/2}(E_1 - \beta m_1)^{1/2}\left(E^2 - M_-^2\right)^{1/2}\psi, \quad k^2 = E_1^2 - m_1^2 \tag{37}$$

one finds that $\mathcal{K}'$ is transformed into $\mathcal{K}$ as given in (25) (the resulting boost is rather different, however). The point $k^2 = 0$ comprises two thresholds at $E^2 = (m_1 + m_2)^2$ and two at $E^2 = (m_1 - m_2)^2$. In our example of a $\mu^-\pi^+$ system, $E = m_1 + m_2$ is the $\mu^-\pi^+$ threshold, $E = -m_1 - m_2$ the $\mu^+\pi^-$ threshold, $E = m_2 - m_1$ the $\mu^+\pi^+$ threshold and $E = m_1 - m_2$ the $\mu^-\pi^-$ threshold. For $m_1 = m_2$, one factor E can be separated from (36), leading to $\mathcal{K}' = E - 2m_1\beta - 2(p_z^*\alpha_z + \mathbf{p}_{\mathrm{L}}\boldsymbol{\alpha}_t)$. This completely eliminates the doubly–charged channels, which now require a separate equation. A similar decoupling occurs in the double–Dirac case for $m_1 = m_2$, which is discussed below.

IV. ORTHOGONALITY RELATIONS

A single 4–component Dirac spinor has components ψ_{R} and ψ_{L} in the chiral basis, where γ_5 is diagonal. β and γ_5 simply change their places in (3), i.e. β exchanges ψ_{R} and ψ_{L}. As β is part of the parity transformation, ψ_{R} and ψ_{L} are not parity eigenstates. They do form separate representations of the Lorentz group, however.

In the present case, both ψ and χ can have β diagonal and remain separate under Lorentz transformations. Elimination of ψ_{DL} from (14) leads to an equation for χ_{DL} in which the two brackets of (16) are interchanged, which is equivalent to the substitution $p_+ \longleftrightarrow -p_-$. The equation corresponding to (17) for χ_{DL} is thus

$$\left(K^{0\,2} - M_+^2 + \left(\mu_\beta^{-1}p_+ + p_-\right) K^0\gamma_5 + \mu_\beta^{-1}p_+p_-\right)\chi_{\mathrm{DL}} = 0\,. \tag{38}$$

It will be shown in the following that the orthogonality relations require both ψ and χ. The mass separation analogous to (21) is

$$\chi_{\mathrm{DL}} = \beta\begin{pmatrix}\chi_{\mathrm{L}t}\\ \mu_\beta^{-1}\chi_{\mathrm{L}s}\end{pmatrix}. \tag{39}$$

The relation analogous to (24) is $\mathcal{K}_{\chi\mathrm{L}}\chi_{\mathrm{L}} = 0$, with

$$\begin{aligned}\mathcal{K}_{\chi\mathrm{L}} = (E^2 - M_+^2)\gamma + 2K\mu_\beta^{-1}p_z^* - \Big[&2E\mathbf{p}_{\mathrm{L}}\boldsymbol{\sigma}_{1t} + (2E\gamma p_z^* - M_+M_-\widehat{K})\sigma_{1z} + \\ &+\frac{1}{2}\widehat{K}E^2\left(\mu_\beta\Delta\sigma_z + \mu_\beta^{-1}\sigma_z\right)\Big]\gamma_5\,,\end{aligned} \tag{40}$$

The boost is now different, $\chi_{\mathrm{L}} = B_\chi\chi$, where

$$B_\chi = \left(1 + \frac{1}{2}\widehat{K}^2\Delta\sigma_z^2 + \mu_\beta\widehat{K}\Delta\sigma_z\gamma\gamma_5\right)^{1/2} = \bar{B}^\dagger \tag{41}$$

where $\bar{B}$ has been given in (30). The hermitian conjugation of $\bar{B}$ in (30) merely exchanges the positions of μ_β^{-1} and γ_5. Observing $\left(\mu_\beta^{-1}\gamma_5\right)^\dagger = \gamma_5\mu_\beta^{-1} = \mu_\beta\gamma_5$, one readily verifies (41). The coordinate transformation (8) implies $d^3r_1\,d^3r_2 = d^3r_{\mathrm{L}}\,d^3R$, and the orthogonality of states with different momenta $\mathbf{K}$ follows simply from $\int d^3R\,\exp\{-i(\mathbf{K}-\mathbf{K}')\mathbf{R}\} = (2\pi)^3\delta(\mathbf{K}-\mathbf{K}')$. A subsequent boost allows one to discuss the orthogonality of the functions $\psi(\mathbf{r}_{\mathrm{L}})$ in the *cms*. The relevant equations here are $\mathcal{K}\psi = 0$ and $\mathcal{K}\chi = 0$, with $\mathcal{K}$ given by (25). The latter equation follows from $\mathcal{K}_{\chi\mathrm{L}}\chi_{\mathrm{L}} = 0$ for $\widehat{K} = 0$, $\gamma = 1$, i.e. $\mathcal{K}_\chi = \mathcal{K}$ in the *cms*.

In the ordinary Dirac equation, neither the potential $V(r)$ nor the momentum $\mathbf{p} = -i\nabla$ appear in the orthogonality relations. Both properties are also achieved here, but the details are surprising. The general operator form of $\mathcal{K}$ will be needed for all values of r, not just for $r \to \infty$ where $V(r) = 0$. This form can be derived from the Fourier transform of the QED Born approximation for elastic scattering $1 + 2 \to 1' + 2'$ in the *cms*:

$$\mathcal{K} = E^2 - M_+^2 - 2E\boldsymbol{\alpha}\mathbf{p} - 2EV(r) - \Lambda V'(r)\,, \tag{42}$$

$$\boldsymbol{\alpha} = \gamma_5\boldsymbol{\sigma}_1\,, \quad \Lambda = i\alpha_r\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2 = (\boldsymbol{\alpha}\times\boldsymbol{\sigma}_2)_r + i\gamma_5\sigma_{2r}\,, \tag{43}$$

and $V' = dV/dr$, $\sigma_r = \boldsymbol{\sigma}\hat{\mathbf{r}}$ as usual. The derivation from the Dirac–Breit equation leads to a more complicated form in the variable $\mathbf{r}^* = (z^*, x_{\mathrm{L}}, y_{\mathrm{L}})$, which involves Breit operators and also $V^2(r^*)$. However, it turns out that the substitution

$$r^* \approx r + \alpha/2E \tag{44}$$

does reduce the Dirac–Breit expression to (42) at low energies. As the QED Born approximation is free of low–energy approximations, (42) is much more practical than the Dirac–Breit equation.

To derive the orthogonality relations for the solution of a Hamiltonian equation $H\psi = E\psi$, one writes $H\psi_j = E_j\psi_j$, $(H\psi_i)^\dagger = E_i\psi_i^\dagger$, multiplies the first equation by $\psi_i^\dagger$, the second one by ψ_j , subtracts the second product from the first one, and integrates over all configuration space: $(E_i - E_j)\int\psi_i^\dagger\psi_j = 0$. The method can also be applied to the Klein–Gordon equation, $[(E - V(r))^2 + \nabla^2 - m^2]\psi = 0$ (in units $\hbar = c = 1$), but the square of $E - V$ produces a weight $w_{ij} = E_i + E_j - 2V$, i.e. $\int\psi_i^* w_{ij}\,\psi_j = \delta_{ij}$. The case at hand is more complicated because Λ is not hermitian. Its hermitian part is the recoil–corrected hyperfine operator. Its antihermitian part has zero expectation values in fine structure eigenstates; it is needed in positronium where fine and hyperfine structures are comparable (the energy eigenvalues remain real). Fortunately, the equation $\mathcal{K}_\chi\chi = 0$ has Λ replaced by $\Lambda^\dagger$:

$$\mathcal{K}_\chi = E^2 - M_+^2 - 2E\boldsymbol{\alpha}\mathbf{p} - 2EV(r) - \Lambda^\dagger V'(r)\,. \tag{45}$$

One may thus envisage orthogonality relations $\int\chi_i^\dagger w_{ij}\,\psi_j = \delta_{ij}$, where the antihermitian component disappears with $\Lambda^{\dagger\dagger} - \Lambda = 0$. However, the factor E multiplies not only $V(r)$ as in the Klein–Gordon equation, but also $\boldsymbol{\alpha}\mathbf{p}$. To avoid $\mathbf{p}$ in the orthogonality relations, E must be divided off. But then Λ/E is both non–hermitian and energy–dependent, in which case V' will remain in the orthogonality relations.

For $V = -\alpha/r$, one may introduce a dimensionless scaled variable,

$$\tilde{r} = Er \quad \partial/\partial\tilde{r} = E^{-1}\partial/\partial r \quad \tilde{\mathbf{p}} = \mathbf{p}/E\,, \tag{46}$$

and divide $\mathcal{K}$ by $E^2 = s$:

$$\left(2\boldsymbol{\alpha}\tilde{\mathbf{p}} + 2V(\tilde{r}) + \Lambda V'(\tilde{r}) - 1 + M_+^2/s\right)\psi(\tilde{r}) = 0\,. \tag{47}$$

Using the corresponding equation for $\chi^\dagger$, one arrives at

$$(s_i^{-1} - s_j^{-1}) \int \chi_i^\dagger\, M_+^2\, \psi_j\, d^3\tilde{r} = 0\,, \quad s_i = E_i^2\,, \tag{48}$$

$$\int \chi_i^\dagger\, M_+^2\, \psi_j\, d^3\tilde{r} = \delta_{ij}\,. \tag{49}$$

Remembering $M_+^2 = m_1^2 + m_2^2 + 2m_1 m_2 \beta$, this is a simple generalization of the static limit $m_1/m_2 = 0$. For positronium, the small components do not contribute to (49).

Equation (48) is explicitly CPT–invariant: Every bound state s_i has two different eigenvalues E_i, namely $E_i = \sqrt{s_i} \equiv m_{\mathrm{A}i}$ and $E_i = -\sqrt{s_i} \equiv -m_{\mathrm{A}i}$, where $m_{\mathrm{A}i}$ denotes the atomic mass in the state i (an excited atom is heavier than its ground state). Returning now to the time–dependent *cms* equation with $i\partial_t = E$, one finds that $E_i = -m_{\mathrm{A}i}$ belongs to the antiatom of mass $m_{\bar{\mathrm{A}}i}$, i.e. $m_{\bar{\mathrm{A}}i} = m_{\mathrm{A}i}$. Positronium is its own antiatom, of course.

Vacuum polarization introduces an extra scale into $V(r)$. The equation remains CPT–invariant, but (48) becomes more complicated. In the Klein–Dirac case of section III, the spinless particle normally has an extended charge distribution, leading to $V(r) \neq -\alpha/r$ for small r. The simplest way out is of course to take $V(\tilde{r})$ as an arbitrary function of $\tilde{r}$ in (47). In any case, finite charge distribution models need some tuning in order to conform with CPT.

It should be stated that the range of the dimensionless radial variable $\tilde{r}$ is $0 < \tilde{r} < \infty$ both for atoms and for antiatoms. In the old variable r, antiatoms have *negative distances*. Of course, this makes as little sense as the claim that antiatoms *fly backwards in time*.

We conclude with two comments on possible applications of the new equations: A vector potential $\mathbf{A}(\mathbf{r}, t)$ is included in (12) by replacing $\mathbf{p}_i \to \boldsymbol{\pi}_i = \mathbf{p}_i + q_i \mathbf{A}(\mathbf{r}_i, t)$. This allows one to calculate relativistic recoil effects in positronium de–excitation, or in the e^+e^-–recombination into positronium. In addition, the Lamb shift may be calculated from these processes via a dispersion integral.

The second comment concerns the case $m_1 = m_2$. Here M_+^2/s vanishes for the small components ψ_f of ψ. Calling for brevity

$$\tilde{V} = V(\tilde{r})\,, \quad \tilde{\boldsymbol{\pi}} = \tilde{\mathbf{p}} + \frac{i}{2} \widetilde{\nabla}\, \tilde{V} \boldsymbol{\sigma}_1 \boldsymbol{\sigma}_2\,, \tag{50}$$

one has $\psi_f = (1 - 2\tilde{V})^{-1}\, 2\boldsymbol{\sigma}_1 \tilde{\boldsymbol{\pi}}\, \psi_g$. The large components satisfy the equation

$$\left[4m_1^2/s - 1 + 2\tilde{V} + 4\boldsymbol{\sigma}_1 \tilde{\boldsymbol{\pi}}\, (1 - 2\tilde{V})^{-1}\, \boldsymbol{\sigma}_1 \tilde{\boldsymbol{\pi}}\right] \psi_g = 0\,. \tag{51}$$

For $\tilde{V} = +\,\alpha/\tilde{r}$, it has only scattering states, which would be e^-e^- and e^+e^+ in the case of two electrons. If it were possible to extend the present formalism to an external Coulomb potential, one would arrive at a theory which isolates the e^-e^-– and e^+e^+–channels from the e^-e^+–channel. This would dispense with *positive–energy projectors* and simplify the relativistic variational calculation of atomic ground states.

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