Singlet-Triplet Splitting of Positronium in Light-Front QED

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Abstract

We study the QED bound-state problem in a light-front hamiltonian approach. It is important to establish the equivalence (or not) of equal-time and light-front approaches in the well-understood arena of Quantum Electrodynamics. Along these lines, the singlet-triplet ground state spin splitting in positronium is calculated. The well-known result, $\frac{7}{6} \alpha^2 \text{Ryd}$, is obtained analytically, which establishes the equivalence between the equal-time and light-front approaches (at least to this order). The true equivalence of the two approaches can only be established after higher-order calculations. It was previously shown that this light-front result could be obtained analytically [1], but a simpler method is presented in this paper.

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I. INTRODUCTION

A calculation of the singlet-triplet ground state spin splitting in positronium is rather trivial from the viewpoint of a Coulomb gauge equal-time calculation (see for example §83–84 of [2]). This is not the case in a light-cone gauge light-front calculation (see for example [3]). We will briefly outline the derivation of the effective Hamiltonian, and then proceed with an analytic calculation of the singlet-triplet splitting.

II. EFFECTIVE HAMILTONIAN AND ITS ZEROTH ORDER SPECTRUM

A brief description of the approach will be given, and the resulting effective Hamiltonian which will be studied in this paper will be written. For details of the derivation of the effective Hamiltonian, and for the original references, see [4].

The starting point is the canonical QED Hamiltonian in the light-cone gauge. Then a regulator is introduced, $\Lambda$, which removes high energy exchanges from the theory. Proceeding, a unitary transformation is defined that acts on the regulated canonical Hamiltonian and produces an effective Hamiltonian at a lower energy scale, $\lambda$. The transformation is unitary, so the spectrum of the regulated canonical Hamiltonian and the effective Hamiltonian are equivalent (of course approximations can invalidate this conclusion). The $\Lambda \to \infty$ limit is studied, and the regulated canonical Hamiltonian is adjusted so that this limit can be taken. So far this is nothing but the old story of renormalization, but the procedure is far from trivial in a light-front approach since longitudinal locality is lost.\(^1\) Unfortunately a complete story of how the renormalization works out is not available, the study is very much a work in progress. However, to obtain the results of this paper consistently, only the one loop electron self-energy renormalization needs to be performed. This will not be shown explicitly in this paper, but is in [4]. The resulting effective Hamiltonian satisfies the Schrödinger equation written below, which is conveniently written in the notation of one body Quantum Mechanics. Note, to obtain this form of the second order effective Hamiltonian, we needed to place the scale in the following window, $m\alpha^2 \ll \lambda \ll m\alpha$. This lower bound is the nonperturbative energy scale of interest; if $\lambda$ is lowered below this bound, the Coulomb interaction does not arise from the second order effective interactions alone. This upper bound is the dominant energy of emitted and absorbed photons; placing $\lambda$ below this bound allows the leading order results to be obtained in the valence sector alone. Given this, the second order effective Hamiltonian satisfies the following Schrödinger equation

\[
(\hat{H}_o + \hat{V}) |\Phi_N\rangle = M_N^2 |\Phi_N\rangle,
\]

where $M_N$ is the mass of the state and

\[
\bullet \quad \langle \Phi_N | \Phi_{N'} \rangle = \delta_{NN'}.
\]

\(^1\) On a positive note, recall that there is an exact scale invariance of the theory under a longitudinal scaling; thus no nonperturbative longitudinal scale can arise through the process of renormalization.
\[ 1 = \sum s_1s_2 \int d^3p \, |ps_{1s_2}\rangle \langle ps_{1s_2}| = \sum s_1s_2 \int d^3x \, |xs_{1s_2}\rangle \langle xs_{1s_2}| = \sum \Phi_N \langle \Phi_N | (3) \]

\[ \langle p's_{3s_4}|\hat{V}|ps_{1s_2}\rangle = V(p's_{3s_4};ps_{1s_2}) \]

\[ \langle p's_{3s_4}|\hat{H}_o|ps_{1s_2}\rangle = 4(m^2 + p^2)\delta^3(p-p')\delta_{s_1s_3}\delta_{s_2s_4} - (4m)\frac{\alpha}{2\pi^2} \delta_{s_1s_3}\delta_{s_2s_4} \]

\[ M_N^2 = (2m + B_N)^2 \]  

\( m \) is the electron mass, \(-B_N\) is the binding energy, and \( N \) labels all the quantum numbers of the state. For notational purposes note that we label the final relative three-momentum with a prime, and that the initial and final electrons are labeled by “1” and “3” respectively, and the initial and final positrons are labeled by “2” and “4” respectively. Before proceeding to write \( \hat{V} \), it is convenient to discuss the spectrum of \( \hat{H}_o \).

In zeroth order \( \hat{V} \) is neglected and Eq. (1) becomes

\[ \hat{H}_o|\phi_N\rangle = M_N^2|\phi_N\rangle = (4m^2 + 4mB_N)|\phi_N\rangle \]

This last equality defines our zeroth order binding energy, \(-B_N\). Projecting this eigenvalue equation into momentum space gives

\[ \left(-B_N + \frac{p^2}{m}\right)\phi_N(p's_{3s_4}) = \frac{\alpha}{2\pi^2} \int \frac{d^3p}{(p-p')^2}\phi_N(ps_{3s_4}), \]

the familiar non-relativistic Schrödinger equation for positronium.

After a simplification detailed in the next Section and mentioned in the Abstract, like the Coulomb gauge equal-time calculation, to obtain the ground state singlet-triplet splitting, only the wave function at the origin is required, which we thus record:

\[ (\phi_N(x=0))^2 = \frac{1}{(2\pi)^3} \left( \int d^3p \, \phi_N(p) \right)^2 = \frac{1}{\pi} \left( \frac{m\alpha}{2n} \right)^3 \delta_{l,0}. \]

\( n \) is the principal quantum number, and \( l \) is the angular momentum quantum number.

Now we proceed to write \( \hat{V} \). Note that \( \hat{V} \) is not diagonal in momentum space, so if we define

\[ \hat{V} = \hat{V}^{(0)} + \hat{V}^{(1)} + \hat{V}^{(2)} + \cdots, \]

where the superscript implies the \( \alpha \)-scaling of a matrix element of the operator in momentum space, then in first order bound-state perturbation theory these operators contribute

\[ \langle \phi_N|\hat{V}^{(S)}|\phi_{N'}\rangle \sim m^2\alpha^{3+S}. \]

Note that Eq. (10) starts at \( S = 0 \); this is a result of the derivation of the effective Hamiltonian. Interestingly, note that in a Coulomb gauge equal-time calculation, this
series starts at \( S = 1 \). In summary, to be consistent to order \( \alpha^4 \), we need to look at all matrix elements \( \mathcal{V}^{(s)}(\mathbf{p}'s_3 s_4; \mathbf{p}s_1 s_2) \) with \( S \leq 1 \).

Before proceeding to write out these expressions for \( \mathcal{V}^{(s)} \), note that we only calculate spin splittings, so constants along the diagonal in spin space were neglected. Given this, to get the spin splittings correct to order \( \alpha^4 \) we need to consider

\[
\mathcal{V}^{(0)}(\mathbf{p}'s_3 s_4; \mathbf{p}s_1 s_2) = \frac{-c_{ex} e^2}{4\pi^3(\mathbf{p} - \mathbf{p}')^2} v^{(0)}(\mathbf{p}'s_3 s_4; \mathbf{p}s_1 s_2),
\]

where

\[
\begin{align*}
v^{(0)}(\mathbf{p}'s_3 s_4; \mathbf{p}s_1 s_2) &= \left( \delta_{s_1 s_3} \delta_{s_2 s_4} f_1(\mathbf{p}'s_3 s_4; \mathbf{p}s_1 s_2) + \delta_{s_1 s_3} \delta_{s_2 s_4} f_2(\mathbf{p}'s_3 s_4; \mathbf{p}s_1 s_2) \right), \\
f_1(\mathbf{p}'s_3 s_4; \mathbf{p}s_1 s_2) &= s_1(p_y - p'_y) - i(p_x - p'_x), \\
f_2(\mathbf{p}'s_3 s_4; \mathbf{p}s_1 s_2) &= s_4(p_y - p'_y) + i(p_x - p'_x).
\end{align*}
\]

\( s_i/2 \) is the spin quantum number of fermion “\( i \)”; \( s_i = \pm 1 \) \( (i = 1, 2, 3, 4) \) only; \( \bar{s}_i = -s_i \). The only other interaction that needs to be considered is

\[
\mathcal{V}^{(1)}(\mathbf{p}'s_3 s_4; \mathbf{p}s_1 s_2) = \frac{e^2}{4m^2 \pi^3} \left( c_{ex} \delta_{s_1 s_2} \delta_{s_1 s_4} \delta_{s_3 s_4} + c_{ex} \delta_{s_2 s_4} \delta_{s_2 s_4} \delta_{s_3 s_4} + \right.
\]

\[
+ \left. \left( \frac{1}{2} - c_{ex} \frac{(p_y - p'_y)^2}{(\mathbf{p} - \mathbf{p}')^2} \right) \delta_{s_1 \bar{s}_1} \delta_{s_3 \bar{s}_4} \right).
\]

The constants \( c_{ex} \) and \( c_{an} \) were introduced only to distinguish the terms that arise from the ‘exchange’ and ‘annihilation’ channels respectively; \( c_{ex} = c_{an} = 1 \).

### III. SINGLET-TRIPLET SPLITTING

Now we will calculate the ground state singlet-triplet splitting to order \( \alpha^4 \) using bound-state perturbation theory in \( \hat{\mathcal{V}} \). Perhaps the most straightforward approach is to just get busy and calculate, since the non-relativistic Coulomb spectrum is so well known. This is exactly what is done in [1]; however, as can be seen by the complexity of Appendix C in that paper, the calculation is complicated and at the level of a “Lamb shift calculation.” We will now present a simpler method to calculate this shift.\(^3\) This simpler method uses a unitary transformation to “remove” \( \mathcal{V}^{(0)} \) much in the spirit of Schwinger’s early QED calculations [4]. This simpler method now follows.

First, set up a general unitary transformation with hermitian generator \( \hat{Q} \):

\[
\begin{align*}
\hat{H} &= \hat{H}_0 + \hat{\mathcal{V}}^{(0)} + \hat{\mathcal{V}}^{(1)} + \hat{\mathcal{V}}^{(2)} + \cdots, \\
\hat{H}' &= e^{i\hat{Q}} \hat{H} e^{-i\hat{Q}} \\
&= \hat{H} + i \left[ \hat{Q}, \hat{H} \right] + \frac{i^2}{2!} \left[ \hat{Q}, \left[ \hat{Q}, \hat{H} \right] \right] + \cdots.
\end{align*}
\]

\(^2\) For example, \( \frac{m e^2 \mathbf{p}}{(\mathbf{p} - \mathbf{p}')^2} \sim \frac{\alpha^2}{\sigma^2} \implies S = 0 \).

\(^3\) The idea behind this simpler method originated with Brusudová and Perry [4].
Now define $\hat{Q}$ by requiring its commutator with $\hat{H}_o$ to cancel $\hat{V}^{(0)}$:

$$\hat{V}^{(0)} + i [\hat{Q}, \hat{H}_o] = 0.$$  \hspace{1cm} (19)

Putting this into Eq. (18) gives

$$\hat{H}' = \hat{H}_o + \left(1 - \frac{1}{2!}\right) [i\hat{Q}, \hat{V}^{(0)}] + e^{i\hat{Q}} \left(\hat{V}^{(1)} + \hat{V}^{(2)} + \cdots\right) e^{-i\hat{Q}}$$

$$+ \left(\frac{1}{2!} - \frac{1}{3!}\right) [i\hat{Q}, [i\hat{Q}, \hat{V}^{(0)}]] + \left(\frac{1}{3!} - \frac{1}{4!}\right) [i\hat{Q}, [i\hat{Q}, [i\hat{Q}, \hat{V}^{(0)}]]] + \cdots.$$  \hspace{1cm} (20)

Note that $\hat{H}$ and $\hat{H}'$ have equivalent lowest order spectrums given by $\hat{H}_o$; this can be seen easily by looking at matrix elements of the equations in Coulomb states, that is in states of $\hat{H}_o$. To summarize, we must diagonalize the following interaction in spin space to obtain the order $\alpha^4$ ground state singlet-triplet splitting in positronium:

$$\delta^{(1)} M^2 (s_3, s_4; s_1, s_2) = \langle \phi_{1,0,0,s_1,s_4} | \hat{V}^{(1)} + \frac{1}{2} [i\hat{Q}, \hat{V}^{(0)}] | \phi_{1,0,0,s_1,s_2} \rangle,$$  \hspace{1cm} (21)

where $\hat{Q}$ is a solution to Eq. (19). The superscript on $\delta^{(1)} M^2$ signifies that it is a first order bound-state perturbation theory shift. The quantum numbers are $N = (n, l, m_l, s_e, s_\tau) \rightarrow (1, 0, 0, s_e, s_\tau)$ for the ground state.

In what follows we will solve Eq. (19) for $\hat{Q}$ in the free basis in momentum space, and then calculate the shift defined by Eq. (21).

From the form of $\hat{V}^{(0)}$ and $\hat{H}_o$ we see that $\hat{Q}$ has the following general form

$$\langle p's_3s_4 | i\hat{Q} | p's_1s_2 \rangle = \delta^3(p - p') \langle p's_3s_4 | i\hat{R} | p's_1s_2 \rangle,$$  \hspace{1cm} (22)

where from Eq. (13), $\hat{R}$ satisfies

$$\frac{\delta^{(0)} (p's_3s_4; p's_1s_2)}{2m} = \langle p's_3s_4 | i\hat{R} | p's_1s_2 \rangle - \langle p's_3s_4 | i\hat{R} | p's_1s_2 \rangle.$$  \hspace{1cm} (23)

Recall Eq. (13) for the form of $\delta^{(0)}$. Thus, the general form of $\hat{R}$ is

$$\langle p's_3s_4 | i\hat{R} | p's_1s_2 \rangle = \frac{\delta_{s_1,s_3} \delta_{s_2,s_4}}{2m} (s_1p_y - ip_x) + \frac{\delta_{s_1,s_3} \delta_{s_2,s_4}}{2m} (s_4p_y + ip_x).$$  \hspace{1cm} (24)

Since $\hat{Q}$ is diagonal in momentum space it is a simple matter to calculate the contributions from Eq. (21). Define

$$\delta M_i^2 = \langle \phi_{1,0,0,s_3,s_4} | \hat{V}^{(1)} | \phi_{1,0,0,s_1,s_2} \rangle,$$  \hspace{1cm} (25)

$$\delta M_2^2 = \langle \phi_{1,0,0,s_3,s_4} | \frac{1}{2} [i\hat{Q}, \hat{V}^{(0)}] | \phi_{1,0,0,s_1,s_2} \rangle.$$  \hspace{1cm} (26)

\footnote{This is the trick, to solve for $\hat{Q}$ in the free basis; if $\hat{Q}$ is solved for in the Coulomb basis the calculation follows the one carried out in \cite{ref}.}
First, $\delta M_i^2$:
\[
\delta M_i^2 = \int d^3p d^3p' \langle \phi_{100} | p' \rangle \langle p | \phi_{100} \rangle V^{(i)} (p's_3 s_4; p s_1 s_2).
\]  
(27)

Using the rotational symmetry of the integrand, we can replace
\[
\frac{(p_\perp - p'_\perp)^2}{(p - p')^2} \to \frac{2}{3} \left( (p_x - p'_x)^2 + (p_y - p'_y)^2 + (p_z - p'_z)^2 \right) = \frac{2}{3}.
\]  
(28)

After this, the remaining integrals are trivial (recall Eq. (10)) and we have
\[
\frac{\delta M_i^2}{2m^2 \alpha^4} = \frac{1}{2} \delta_{s_1 s_2} \delta_{s_1 s_4} \delta_{s_2 s_4} - \frac{1}{12} \delta_{s_1 s_2} \delta_{s_3 s_4} + \frac{1}{2} \delta_{s_1 s_2} \delta_{s_1 s_4} \delta_{s_1 s_3}.
\]  
(29)

Next, $\delta M_2^2$:
\[
\delta M_2^2 = \langle \phi_{1,0,0,s_3 s_4} | \frac{1}{2} [iQ, \hat{V}^{(0)}] | \phi_{1,0,0,s_1 s_2} \rangle
\]  
(30)
\[
= \frac{1}{2} \sum_{s_c \in \pi} \int d^3p d^3p' \langle \phi_{100} | p' \rangle \langle p | \phi_{100} \rangle \left( \langle p's_3 s_4 | i \hat{R} | p's_c s_\pi \rangle \langle p's_c s_\pi | \hat{V}^{(0)} | p s_1 s_2 \rangle - \langle p's_3 s_4 | \hat{V}^{(0)} | p s_1 s_2 \rangle \langle p's_c s_\pi | i \hat{R} | p s_1 s_2 \rangle \right).
\]  
(31)

Recalling Eq. (12) and using Eq. (23) we have
\[
\delta M_2^2 = \frac{\alpha}{\pi^2} \int d^3p d^3p' \langle \phi_{100} | p' \rangle \langle p | \phi_{100} \rangle \frac{F}{(p - p')^2},
\]  
(32)
where
\[
F = \sum_{s_c \in \pi} \langle p s_c s_\pi | i \hat{R} | p s_1 s_2 \rangle \langle p's_3 s_4 | \hat{v}^{(0)} | p s_c s_\pi \rangle
\]  
(33)
\[
= \frac{1}{2} \sum_{s_c \in \pi} \left( \langle p s_c s_\pi | i \hat{R} | p s_1 s_2 \rangle - \langle p's_c s_\pi | i \hat{R} | p s_1 s_2 \rangle \right) \langle p's_3 s_4 | \hat{v}^{(0)} | p s_c s_\pi \rangle.
\]  
(34)

Using the fact that $\hat{v}^{(0)}$ is odd under $p \leftrightarrow p'$ in this last step. Using Eq. (23) this becomes
\[
F = \frac{1}{4m} \sum_{s_c \in \pi} \hat{v}^{(0)}(p's_3 s_4; p s_c s_\pi) \hat{v}^{(0)}(p's_c s_\pi; p s_1 s_2).
\]  
(35)

Using the even symmetry of the rest of the integrand under the operations $(p_x \to -p_x, p'_x \to -p'_x)$ and $(p_x \leftrightarrow p_y, p'_x \leftrightarrow p'_y)$ this sum can be simplified with result
\[
F = -\frac{1}{24m} (3g_1 + g_2) (p - p')^2,
\]  
(36)
where
\[ g_1 = s_1s_3 + s_2s_4 , \]  
\[ g_2 = 1 + s_1s_2 - s_2s_3 - s_1s_4 + s_3s_4 + s_1s_2s_3s_4 . \]  
(37)
(38)

Recall that \( s_i = \pm 1 \), \((i = 1, 2, 3, 4)\); the \( \frac{1}{2} \) has been factored out of these spins.\(^5\) The result was written in this form to show the equivalence with [1]. Combining the results we have
\[ \delta M^2_2 = -\frac{\alpha}{24\pi^2 m} (3g_1 + g_2) \int d^3p \int d^3p' \langle \phi_{100} | p' \rangle \langle p | \phi_{100} \rangle \]
\[ = -\frac{m^2 \alpha^4}{24} (3g_1 + g_2) , \]  
(39)
(40)

Combining the results we have
\[ \frac{\delta M^2_1 + \delta M^2_2}{2m^2\alpha^4} = \frac{1}{2} \delta_{s_1s_2} \delta_{s_3s_4} \delta_{s_5s_6} - \frac{1}{12} \delta_{s_1s_2} \delta_{s_3s_4} + \frac{1}{2} \delta_{s_2s_3} \delta_{s_4s_5} + \delta_{s_1s_2} \delta_{s_3s_4} \]
\[ - \frac{1}{48} (3g_1 + g_2) . \]  
(41)

The eigenvalues are
\[ \langle 1 | \delta M^2_1 + \delta M^2_2 | 1 \rangle = -\frac{5}{3} m^2 \alpha^4 , \]  
(42)
\[ \langle 2 | \delta M^2_1 + \delta M^2_2 | 2 \rangle = \frac{2}{3} m^2 \alpha^4 , \]  
(43)
\[ \langle 3 | \delta M^2_1 + \delta M^2_2 | 3 \rangle = \frac{2}{3} m^2 \alpha^4 , \]  
(44)
\[ \langle 4 | \delta M^2_1 + \delta M^2_2 | 4 \rangle = \frac{2}{3} m^2 \alpha^4 , \]  
(45)

with corresponding eigenvectors
\[ \left\{ | 1 \rangle = \frac{|++\rangle - |--\rangle}{\sqrt{2}} , | 2 \rangle = \frac{|++\rangle + |--\rangle}{\sqrt{2}} , | 3 \rangle = | -- \rangle , | 4 \rangle = | ++ \rangle \right\} . \]

These results translate to the well known answer, \( \frac{7}{6} \alpha^2 Ryd \), as can be seen by recalling the definition of our zeroth order and exact mass squared:
\[ (2m + B_N)^2 = 4m^2 + 4mB_N + \delta^{(1)} M^2 + \mathcal{O}(m^2 \alpha^5) , \]  
(46)
which gives
\[ B_{\text{triplet}} - B_{\text{singlet}} = \frac{7}{6} \alpha^2 Ryd + \mathcal{O}(m\alpha^5) , \]  
(47)
the desired result.

\(^5\) In order to get these simple forms for \( g_1 \) and \( g_2 \) it was useful to note the following simple relation:
\[ \delta_{ss'} = \frac{1}{2} s (s + s') \] (true because \( s^2 = 1 \)).
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