VARIATIONAL TWO FERMION WAVE EQUATIONS
IN QED: MUONIUM LIKE SYSTEMS

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Abstract We consider a reformulation of QED in which covariant Green functions are used to solve for the electromagnetic field in terms of the fermion fields. The resulting modified Hamiltonian contains the photon propagator directly. A simple Fock-state variational trial function is used to derive relativistic two-fermion equations variationally from the expectation value of the Hamiltonian of the field theory. The interaction kernel of the equation is shown to be, in essence, the invariant $M$ matrix in lowest order. Solutions of the two-body equations are presented for muonium like system for small coupling strengths. The results compare well with the observed muonium spectrum, as well as that for hydrogen and muonic hydrogen. Anomalous magnetic moment effects are discussed.

1. Introduction

It has been pointed out in previous publications that various models in Quantum Field Theory (QFT), including QED, can be reformulated, using mediating-field Green functions, into a form that is particularly convenient for variational calculation [1,2]. This approach was applied to the study of relativistic two-body eigenstates in the scalar Yukawa (Wick-Cutkosky) theory [3,4,5]. We shall implement such an approach to two-fermion states in QED in this paper.

The Lagrangian of two fermion fields interacting electromagnetically is ($\hbar = c = 1$)

\[ \mathcal{L} = \bar{\psi}(x) \left( i \gamma^\mu \partial_\mu - m_1 - q_1 \gamma^\mu A_\mu(x) \right) \psi(x) + \bar{\phi}(x) \left( i \gamma^\mu \partial_\mu - m_2 - q_2 \gamma^\mu A_\mu(x) \right) \phi(x) - \frac{1}{4} \left( \partial_\alpha A_\beta(x) - \partial_\beta A_\alpha(x) \right) \left( \partial^\alpha A^\beta(x) - \partial^\beta A^\alpha(x) \right). \] (1)

The corresponding Euler-Lagrange equations of motion are the coupled Dirac-Maxwell equations,

\[ (i \gamma^\mu \partial_\mu - m_1) \psi(x) = q_1 \gamma^\mu A_\mu(x) \psi(x), \] (2)

\[ (i \gamma^\mu \partial_\mu - m_2) \phi(x) = q_2 \gamma^\mu A_\mu(x) \phi(x), \] (3)

and

\[ \partial_\alpha \partial^\alpha A^\nu(x) - \partial^\nu \partial_\mu A^\mu(x) = j^\nu(x), \] (4)

where

\[ j^\nu(x) = q_1 \bar{\psi}(x) \gamma^\nu \psi(x) + q_2 \bar{\phi}(x) \gamma^\nu \phi(x). \] (5)

Equations (2)-(3) can be decoupled in part by using the well-known formal solution [6,7] of the Maxwell equation (4), namely

\[ A^\mu_\nu(x) = A^0_\nu(x) + \int d^4x' D_{\mu\nu}(x - x') j^\nu(x'), \] (6)

where $D_{\mu\nu}(x - x')$ is a Green function (or photon propagator in QFT terminology), defined by

\[ \partial_\alpha \partial^\alpha D_{\mu\nu}(x - x') - \partial_\mu \partial^\nu D_{\alpha\nu}(x - x') = g_{\mu\nu} \delta^4(x - x'), \] (7)
and \(A_\mu^0(x)\) is a solution of the homogeneous (or “free field”) equation (4) with \(j^\mu(x) = 0\).

We recall that equation (7) does not define the covariant Green function \(D_{\mu\nu}(x - x')\) uniquely. For one thing, one can always add a solution of the homogeneous equation (eq. (7) with \(g_{\mu\nu} \to 0\)). This allows for a certain freedom in the choice of \(D_{\mu\nu}\), as is discussed in standard texts (e.g. ref. \([6,7]\)). In practice, the solution of eq. (7), like that of eq. (4), requires a choice of gauge. However, we do not need to specify one at this stage.

Substitution of the formal solution (6) into equations (2) and (3) yields the “partly reduced” equations,

\[
(i\gamma^\mu \partial_\mu - m_1) \psi(x) = q_1 \gamma^\mu \left( A_\mu^0(x) + \int d^4 x' D_{\mu\nu}(x - x') j^\nu(x') \right) \psi(x), \tag{8}
\]

\[
(i\gamma^\mu \partial_\mu - m_2) \phi(x) = q_2 \gamma^\mu \left( A_\mu^0(x) + \int d^4 x' D_{\mu\nu}(x - x') j^\nu(x') \right) \phi(x). \tag{9}
\]

These are coupled nonlinear Dirac equations. To our knowledge no exact (analytic or numeric) solution of equations (8)-(9) for classical fields have been reported in the literature, though approximate (perturbative) solutions have been discussed by various authors, particularly Barut and his co-workers (see ref. \([8,9]\) and citations there in). However, our interest here is in the quantized field theory.

The partially reduced equations (8)-(9) are derivable from the stationary action principle

\[
\delta S[\psi] = \delta \int d^4 x \mathcal{L}_R = 0 \tag{10}
\]

with the Lagrangian density

\[
\mathcal{L}_R = \bar{\psi}(x) \left( i\gamma^\mu \partial_\mu - m_1 - q_1 \gamma^\mu A_\mu^0(x) \right) \psi(x) + \bar{\phi}(x) \left( i\gamma^\mu \partial_\mu - m_2 - q_2 \gamma^\mu A_\mu^0(x) \right) \phi(x) \\
- \frac{1}{2} \int d^4 x' j^\mu(x') D_{\mu\nu}(x - x') j^\nu(x) \tag{11}
\]

provided that the Green function is symmetric in the sense that

\[
D_{\mu\nu}(x - x') = D_{\mu\nu}(x' - x) \quad \text{and} \quad D_{\mu\nu}(x - x') = D_{\nu\mu}(x - x'). \tag{12}
\]

The interaction part of (11) has a somewhat modified structure from that of the usual formulation of QED. Thus, there are two interaction terms. The last term of (11) is a “current-current” interaction which contains the photon propagator sandwiched between the fermionic currents. We shall use this modified formulation together with a variational approach to obtain relativistic few-fermion equations, and to study their bound state solutions.

2. Hamiltonian

We shall consider the quantized theory in the equal-time formalism. To this end we write down the Hamiltonian density corresponding to the Lagrangian (11), namely

\[
\mathcal{H}_R = \mathcal{H}_0 + \mathcal{H}_I + \mathcal{H}_{II}, \tag{13}
\]

where

\[
\mathcal{H}_0 = \bar{\psi}(x) \left( -i \alpha^\mu \cdot \nabla + m_1 \beta \right) \psi(x) + \bar{\phi}(x) \left( -i \alpha^\mu \cdot \nabla + m_2 \beta \right) \phi(x), \tag{14}
\]

\[
\mathcal{H}_I = \frac{1}{2} \int d^4 x' j^\mu(x') D_{\mu\nu}(x - x') j^\nu(x), \tag{15}
\]

\[
\mathcal{H}_{II} = q_1 \bar{\psi}(x) \gamma_\mu A_\mu^0(x) \psi(x) + q_2 \bar{\phi}(x) \gamma_\mu A_\mu^0(x) \phi(x), \tag{16}
\]

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and where we have suppressed the kinetic-energy term of the free photon field. We construct a quantized theory by imposing equal-time anticommutation rules for the fermion fields, namely

\[ \{ \psi_\alpha(x, t), \psi^\dagger_\beta(y, t) \} = \{ \phi_\alpha(x, t), \phi^\dagger_\beta(y, t) \} = \delta_{\alpha\beta} \delta^3(x - y), \]

and all other vanish. In addition, there are the usual commutation rules for the \( A_0^\mu \) field, and commutation of the \( A_0^\mu \) field operators with the \( \psi \) and \( \phi \) field operators.

To specify our notation, we quote the Fourier decomposition of the field operators, namely

\[ \psi(x) = \sum_s \int \frac{d^3p}{(2\pi)^{3/2}} \left( \frac{m_1}{\Omega_p} \right)^{1/2} \left[ b_{ps} u_p(p, s) e^{-ip \cdot x} + d^\dagger_{ps} v_p(p, s) e^{ip \cdot x} \right], \quad \text{with} \quad p = p_m = (\omega_p, \mathbf{p}), \quad \omega_p = \sqrt{m_1^2 + p^2} \]

\[ \phi(x) = \sum_s \int \frac{d^3p}{(2\pi)^{3/2}} \left( \frac{m_2}{\Omega_p} \right)^{1/2} \left[ B_{ps} U_p(p, s) e^{-ip \cdot x} + D^\dagger_{ps} V_p(p, s) e^{ip \cdot x} \right], \quad \text{with} \quad p = p_m = (\Omega_p, \mathbf{p}), \quad \Omega_p = \sqrt{m_2^2 + p^2}. \]

Note that the mass-\( m_1 \) free-particle Dirac spinors \( u_p(p, s), v_p(p, s) \) where \((\gamma^\mu p_\mu - m_1) u_p(p, s) = 0, (\gamma^\mu p_\mu + m_1) v_p(p, s) = 0, \) are normalized such that

\[ u^\dagger(p, s) u_p(p, \sigma) = \delta_{\sigma\sigma}, \]

\[ u^\dagger(p, s) v_p(p, \sigma) = v^\dagger(p, s) v_p(p, \sigma) = 0. \]

The creation and destruction operators \( b^\dagger, b, d^\dagger, d \) of the (free) particles of mass \( m_1 \), and \( d^\dagger, d \) for the corresponding antiparticles, satisfy the usual anticommutation relations. The non-vanishing ones are

\[ \{ b_{ps}, b^\dagger_{qs} \} = \{ d_{ps}, d^\dagger_{qs} \} = \delta_{s\sigma} \delta^3(p - q). \]

Again, the analogous properties apply to the mass-\( m_2 \) spinors \( U, V \). The creation and destruction operators \( B^\dagger, B, D^\dagger, D \) for a concrete example, we can think of the mass-\( m_1 \) particles as electrons, and the mass-\( m_2 \) particles as muons, through any pairs of charged fermions could be considered.

3. Variational principle, two-fermion trial states and equations

The Hamiltonian formalism of QFT is based on the covariant eigenvalue equation

\[ \hat{P}^\mu | \psi \rangle = Q^\mu | \psi \rangle, \quad \text{with} \quad Q^\mu = (E, \mathbf{P}), \quad \text{and} \quad \hat{P}^\mu = (\hat{H}, \hat{P}) \]

where \( \hat{P}^\mu = (\hat{H}, \hat{P}) \) is the energy momentum operator, \( Q^\mu = (E, \mathbf{P}) \) is the 4-vector of energy and momentum, with \( E^2 - \mathbf{P}^2 = M^2 \), where \( M \) is the invariant mass of the system. There are very few problem in QFT for which exact solution of the \( \mu = 0 \) equation (22) can be written down. In practice, it is necessary to use approximation methods to solve it, such as the widely used covariant perturbation theory or lattice methods. Here we concentrate on the variational approach, which is based on the variational principle

\[ \delta \langle \psi | \hat{H} - E | \psi \rangle_{t=0} = 0, \]

which we shall consider in the rest frame i.e. \( \mathbf{P} = 0 \). Variational solutions are only as good as the trial states that are used. Thus, it is important that the trial states possess as many features of the exact solution as
possible. For a system like $\mu^+ e^-$, the simplest Fock-space trial state that can be written down in the rest frame is

$$|\psi_{\text{trial}}\rangle = \sum_{s_1 s_2} \int d^3 p F_{s_1 s_2}(p) \hat{b}_{ps_1} \hat{b}_{ps_2}^\dagger |0\rangle,$$

where $F_{s_1 s_2}$ are four adjustable functions. We use this trial state to evaluate the matrix elements needed to implement the variational principle (23), that is

$$\langle \psi_{\text{trial}} | : \hat{H}_0 - E : |\psi_{\text{trial}}\rangle = \sum_{s_1 s_2} \int d^3 p F^*_{s_1 s_2}(p) F_{s_1 s_2}(p) (\omega_p + \Omega_p - E)$$

and

$$\langle \psi_{\text{trial}} | : \hat{H}_I : |\psi_{\text{trial}}\rangle = -\frac{g_1 g_2 m_1 m_2}{(2\pi)^3} \sum_{\sigma_1 \sigma_2 s_1 s_2} \int \frac{d^3 p d^3 q}{\sqrt{\omega_p \omega_q \Omega_p \Omega_q}} F^*_{s_1 s_2}(p) F_{\sigma_1 \sigma_2}(q) \times \bar{\pi}(p, s_1) \gamma^\mu u(q, \sigma_1) D_{\mu\nu}(p - q) \bar{V}(-q, \sigma_2) \gamma^\nu V(-p, s_2),$$

where the Fourier transform of the Green function was used:

$$D_{\mu\nu}(x - x') = \int \frac{d^4 k}{(2\pi)^4} D_{\mu\nu}(k) e^{-ik(x-x')}.$$

For a particle-antiparticle system like positronium an additional virtual-annihilation interaction term,

$$\bar{\pi}(p, s_1) \gamma^\mu u(-p, s_2) D_{\mu\nu}(\omega_p) \bar{\pi}(-q, \sigma_2) \gamma^\nu u(q, \sigma_1)$$

appears in (26) [10]. Note that we have normal-order the entire Hamiltonian, since this circumvents the need for mass renormalization which would otherwise arise. Not that there is a difficulty with handling mass renormalization in the present formalism (as shown in various earlier papers; see, for example, ref. [11] and citations therein). It is simply that we are not interested in mass renormalization here, since it has no effect on the two-body bound state energies that we obtain in this paper. Furthermore, the approximate trial state (24), which we use in this work, is incapable of sampling loop effects. Thus, the normal-ordering of the entire Hamiltonian does not “sweep under the carpet” loop renormalization effects, since none arise at the present level of approximation. Note, also, that $\langle \psi_{\text{trial}} | : \hat{H}_I : |\psi_{\text{trial}}\rangle = 0$, that is the variational trial state (24) is insensitive to that part of the interaction Hamiltonian which is linear in $A_0^\mu(x)$. This means that, with the simple anzatz (24) only stable bound states and elastic scattering can be described, but not processes that involve radiation.

The variational principle (23) leads to the following equation

$$\sum_{s_1 s_2} \int d^3 p (\omega_p + \Omega_p - E) F_{s_1 s_2}(p) \delta F^*_{s_1 s_2}(p)$$

$$-\frac{m_1 m_2}{(2\pi)^3} \sum_{\sigma_1 \sigma_2 s_1 s_2} \int \frac{d^3 p d^3 q}{\omega_p \omega_q} F^*_{\sigma_1 \sigma_2}(q) (-i) M^{\text{opt}}_{s_1 s_2 \sigma_1 \sigma_2}(p, q) \delta F^*_{s_1 s_2}(p) = 0,$$

where $M^{\text{opt}}_{s_1 s_2 \sigma_1 \sigma_2}(p, q)$ is the usual invariant matrix element corresponding to the one-photon exchange Feynman diagram:

$$M^{\text{opt}}_{s_1 s_2 \sigma_1 \sigma_2}(p, q) = -\bar{\pi}(p, s_1) (-i q_1 \gamma^\mu) u(q, \sigma_1) iD_{\mu\nu}(p - q) \bar{V}(-q, \sigma_2) (-i q_2 \gamma^\nu) V(-p, s_2),$$

As mentioned above, for a fermion-antifermion system like positronium we obtain [10] the additional virtual-annihilation term ($q_1 = q_2 \equiv e$)

$$M^{\text{ann}}_{s_1 s_2 \sigma_1 \sigma_2}(p, q) = \bar{\pi}(p, s_1) (-ie\gamma^\mu) v(-p, s_2) iD_{\mu\nu}(\omega_p) \bar{\pi}(-q, \sigma_2) (-ie\gamma^\nu) u(q, \sigma_1).$$
Note that the $\mathcal{M}$-matrix arises naturally in this formalism, that is $\mathcal{M}$ is not put in by hand, nor does its derivation require additional Fock-space terms in the variational trial state (24), as is the case in traditional formulations (e.g. [12], [13]).

In the non-relativistic limit, the functions $F_{s_1 s_2}$ can be written as

$$F_{s_1 s_2}(p) = F(p)\Lambda_{s_1 s_2},$$

where the non-zero elements of $\Lambda_{ij}$ for total spin singlet $(S = 0)$ states are $\Lambda_{12} = -\Lambda_{21} = \frac{1}{\sqrt{2}}$, while for the spin triplet $(S = 1)$ states the non-zero elements are $\Lambda_{11} = 1$ for $m_s = +1$, $\Lambda_{12} = \Lambda_{21} = \frac{1}{\sqrt{2}}$ for $m_s = 0$, and $\Lambda_{22} = 1$ for $m_s = -1$. We use the notation that the subscripts 1 and 2 of $\Lambda$ correspond to $m_s = 1/2$ and $m_s = -1/2$ (or $\uparrow$ and $\downarrow$) respectively. Substituting (32) into (29), multiplying the result by $\Lambda_{s_1 s_2}$ and summing over $s_1$ and $s_2$, gives the equation

$$(\omega(p) + \Omega(p) - E)F(p) = \frac{1}{(2\pi)^3}\int d^3q\mathcal{K}(p, q)F(q),$$

where

$$\mathcal{K}(p, q) = -i \sum_{s_1 s_2 \sigma_1 \sigma_2} \Lambda_{s_1 s_2} M_{s_1 s_2 \sigma_1 \sigma_2} (p, q) \Lambda_{\sigma_1 \sigma_2}.$$  

To lowest-order in $(|p|, |q|)/(m_1, m_2)$ (i.e. in the non-relativistic limit), the kernel (34) reduces to $\mathcal{K} = q_1 q_2/|p - q|^2$, and so (33) reduces to the (momentum-space) Schrödinger equation

$$\left(\frac{p^2}{2m_r} - \varepsilon\right)F(p) = \frac{q_1 q_2}{(2\pi)^3}\int d^3q \frac{1}{|p - q|^2}F(q),$$

where $\varepsilon = E - M$ and $m_r = m_1 m_2/M, M = m_1 + m_2$. This verifies that the relativistic two-fermion equation (29) has the required non-relativistic limit.

4. Partial-wave decomposition and classification of states

In the relativistic case we shall not complete the variational procedure in (29) at this stage to get final equations for the four functions $F_{s_1 s_2}$, because they are not independent in general. We require that the trial state must be an eigenstate of the relativistic total angular momentum operator, its projection, and parity. Namely

$$\begin{bmatrix} \hat{J}^2 \\ \hat{J}_3 \\ \hat{P} \end{bmatrix} |\psi_{\text{trial}}\rangle = \begin{bmatrix} J(J + 1) \\ m_J \\ P \end{bmatrix} |\psi_{\text{trial}}\rangle.$$

For a system like positronium charge conjugation invariance is an additional requirement, that is

$$\hat{C} |e^+e^-\rangle = C |e^+e^-\rangle,$$

however this does not apply for $m_1 \neq m_2$. Explicit forms for the operators $\hat{J}^2, \hat{J}_3$ are given in Appendix A. The functions $F_{s_1 s_2}(p)$ can be written in the general form

$$F_{s_1 s_2}(p) = \sum_{\ell_{s_1 s_2}} \sum_{m_{s_1 s_2}} f_{s_1 s_2}^{\ell_{s_1 s_2} m_{s_1 s_2}} (p) Y_{\ell_{s_1 s_2}}^{m_{s_1 s_2}}(\hat{p}),$$

where $Y_{\ell_{s_1 s_2}}^{m_{s_1 s_2}}(\hat{p})$ are the usual spherical harmonics. Here and henceforth we will use the notation $p = |p|$ etc. (four-vectors will be written as $p^\mu$). The orbital indices $\ell_{s_1 s_2}$ and $m_{s_1 s_2}$ depend on the spin indices $s_1$ and $s_2$ and are specified by equations (36). The radial coefficients of expansion (38) $f_{s_1 s_2}^{\ell_{s_1 s_2} m_{s_1 s_2}} (p)$ also
depend on the spin variables. Substitution of (38) into (24) and then into (36) leads to two categories of relations among the adjustable functions.

**Mixed-spin states**

In this case \( \ell_{s_{1}s_{2}} \equiv \ell = J \) and the general solution of the system (36) is

\[
F_{s_{1}s_{2}}(\mathbf{p}) = C_{1}F_{s_{1}s_{2}}^{(sg)}(\mathbf{p}) + C_{2}F_{s_{1}s_{2}}^{(tr)}(\mathbf{p}),
\]

where \( C_{1} \) and \( C_{2} \) are arbitrary constants. \( F_{s_{1}s_{2}}^{(sg)}(\mathbf{p}) \) and \( F_{s_{1}s_{2}}^{(tr)}(\mathbf{p}) \) are functions, which correspond to pure singlet states with the total spin \( S = 0 \) and triplet states with \( S = 1 \) respectively. The singlet functions have the form

\[
F_{s_{1}s_{2}}^{(sg)}(\mathbf{p}) = f_{s_{1}s_{2}}^{(sg)}(\mathbf{p})Y_{\ell}^{m_{s_{1}s_{2}}}(\mathbf{\hat{p}}),
\]

where \( m_{11} = m_{22} = 0 \) and \( m_{12} = m_{21} = m_{J} \). The relations between \( f_{s_{1}s_{2}}^{(sg)}(\mathbf{p}) \) and \( f_{s_{1}s_{2}}^{(sg)}(\mathbf{p}) \) involve the Clebsch-Gordan (C-G) coefficients \( C^{(sg)m_{s_{1}s_{2}}} \), that is

\[
f_{s_{1}s_{2}}^{(sg)}(\mathbf{p}) = C^{(sg)m_{s_{1}s_{2}}}f(\mathbf{p}),
\]

as it shown in Appendix A. We see that the spin and radial variables separate in the sense that the factors \( f_{s_{1}s_{2}}^{(j)}(\mathbf{p}) \) have a common radial function \( f(\mathbf{p}) \), that is for the singlet functions we obtain

\[
F_{s_{1}s_{2}}^{(sg)}(\mathbf{p}) = C^{(sg)m_{s_{1}s_{2}}}f(\mathbf{p})Y_{J}^{m_{s_{1}s_{2}}}(\mathbf{\hat{p}}).
\]

The C-G coefficients \( C^{(sg)m_{s_{1}s_{2}}} \) have a simple form: \( C^{(sg)m_{11}} = C^{(sg)m_{22}} = 0 \), \( C^{(sg)m_{12}} = -C^{(sg)m_{21}} = 1 \) (see Appendix A). Thus the nonzero components of \( F_{s_{1}s_{2}}^{(sg)}(\mathbf{p}) \) are \( F_{s_{1}s_{2}}^{(sg)}(\mathbf{p}) \equiv F_{12}^{(sg)}(\mathbf{p}) \), \( F_{12}^{(sg)}(\mathbf{p}) \equiv F_{21}^{(sg)}(\mathbf{p}) \).

The triplet functions have the form

\[
F_{s_{1}s_{2}}^{(tr)}(\mathbf{p}) = f_{s_{1}s_{2}}^{(tr)}(\mathbf{p})Y_{J}^{m_{s_{1}s_{2}}}(\mathbf{\hat{p}}),
\]

where

\[
m_{11} = m_{J} - 1, \quad m_{12} = m_{21} = m_{J}, \quad m_{22} = m_{J} + 1.
\]

The expressions for \( f_{s_{1}s_{2}}^{(j)}(\mathbf{p}) \) involve the C-G coefficients \( C^{(tr)Jm_{s}} \) for \( S = 1 \) listed in Appendix A, that is

\[
f_{s_{1}s_{2}}^{(tr)}(\mathbf{p}) = C^{(tr)Jm_{s}}f^{(j)}(\mathbf{p}),
\]

where the index \( m_{s} \) is defined as

\[
m_{s} = +1, \quad \text{when} \quad m_{s_{1}s_{2}} = m_{11},
\]

\[
m_{s} = 0, \quad \text{when} \quad m_{s_{1}s_{2}} = m_{12} = m_{21},
\]

\[
m_{s} = -1, \quad \text{when} \quad m_{s_{1}s_{2}} = m_{22}.
\]

Thereupon, the triplet function is

\[
F_{s_{1}s_{2}}^{(tr)}(\mathbf{p}) = C^{(tr)Jm_{s}}f^{(j)}(\mathbf{p})Y_{J}^{m_{s_{1}s_{2}}}(\mathbf{\hat{p}}).
\]

We need to note that (42) is true for \( J \geq 0 \), while (47) is true for \( J \geq 1 \). Thus the coefficient \( C_{2} \) in (39) is zero when \( J = 0 \). In other words, for \( J = 0 \), only the pure singlet state arises. For a system like positronium the requirement (37) decouples the singlet and triplet states for all \( J \). Indeed, the charge conjugation eigenstates are

\[
|sg\rangle = \sum_{s_{1}s_{2}}C^{(sg)m_{s_{1}s_{2}}}\int d^{3}\mathbf{p}f^{(j)}(\mathbf{p})Y_{J}^{m_{s_{1}s_{2}}}(\mathbf{\hat{p}})b_{\mathbf{ps}_{1}}^\dagger D_{-\mathbf{ps}_{2}}^\dagger |0\rangle
\]

with \( C = (-1)^{J} \) for the pure singlet states, and

\[
|tr\rangle = \sum_{s_{1}s_{2}}C^{(tr)Jm_{s_{1}s_{2}}}\int d^{3}\mathbf{p}f^{(j)}(\mathbf{p})Y_{J}^{m_{s_{1}s_{2}}}(\mathbf{\hat{p}})b_{\mathbf{ps}_{1}}^\dagger D_{-\mathbf{ps}_{2}}^\dagger |0\rangle
\]
with \( C = (-1)^{J+1} \) for the pure triplet states, as it discussed in Appendix A.

The states (48) and (49) diagonalize the Hamiltonian (13) only for particle-antiparticle systems when \( m_1 = m_2 \). Thus, for positronium-like systems, the states can be characterized by the spin quantum number \( S \), and the mixed states (39) separate into singlet states (parastates) and triplet states (orthostates) \( S = 0 \) and triplet states \( S = 1 \). For distinct particles \( m_1 \neq m_2 \) \( C \) is not conserved and there is no separation into pure singlet and triplet states in general. Thus for arbitrary mass ratios we need to diagonalize the expectation value of the Hamiltonian (13) (Appendix E). This can be achieved by the following linear transformation

\[
\begin{bmatrix}
|s_{g_q}\rangle \\
|t_{r_q}\rangle
\end{bmatrix} = \tilde{U}
\begin{bmatrix}
|sg_j\rangle \\
|tr_j\rangle
\end{bmatrix},
\]

where \( \tilde{U} \) is the unimodular matrix

\[
\tilde{U} = \begin{bmatrix} a & -b \\ b & a \end{bmatrix}
\]

with components

\[
a = \sqrt{\frac{1 + \xi}{2}}, \quad b = \sqrt{\frac{1 - \xi}{2}},
\]

where

\[
\xi = \left(4 \left(\frac{m_1 - m_2}{m_1 + m_2}\right)^2 J (J + 1) + 1\right)^{-1/2}.
\]

The new states, which diagonalize the expectation value of \( \tilde{H} \), shall be called quasi-singlet \( |sg_q\rangle \) and quasi-triplet \( |tr_q\rangle \) states

\[
|sg_q\rangle = \sum_{s_1 s_2} C_{J m_j}^{(s_1),J m_{s_1 s_2}} \int d^3 p f^d (p) Y_{j m_j}^m (\hat{p}) b_1^m D_1^{s_1} D_2^{s_2} |0\rangle,
\]

\[
|tr_q\rangle = \sum_{s_1 s_2} C_{J m_j}^{(s_1),J m_{s_1 s_2}} \int d^3 p f^d (p) Y_{j m_j}^m (\hat{p}) b_1^m D_1^{s_1} D_2^{s_2} |0\rangle,
\]

where the coefficients \( C_{J m_j}^{(s_1),J m_{s_1 s_2}} \) and \( C_{J m_j}^{(s_1),J m_{s_1 s_2}} \) are listed in Table 1, and satisfy the following condition

\[
\sum_{\nu_1 \nu_2 m_j} \left(C_{J m_j}^{s_1, J m_{s_1 s_2}}\right)^2 = \sum_{\nu_1 \nu_2 m_j} \left(C_{J m_j}^{s_1, J m_{s_1 s_2}}\right)^2 = 2(2J + 1).
\]

Table 1. The quasi-state coefficients \( C_{J m_j}^{(s_1),J m_{s_1 s_2}} \) for \( s = s_s, s_t \).

| \( s_s \) | \( m_{11} = m_J - 1 \) | \( m_{12} = m_J \) | \( m_{21} = m_J \) | \( m_{22} = m_J + 1 \) |
|---|---|---|---|---|
| \( \frac{b \left(J + m_J\right)\left(m_J - m_J + 1\right)}{J(J + 1)} \) \( 1/2 \) | \(-b\frac{m_J}{J(J + 1)} + a\) | \(-b\frac{m_J}{J(J + 1)} + a\) | \(-b\frac{\left(J + m_J\right)\left(m_J + m_J + 1\right)}{J(J + 1)} \) \( 1/2 \) |
| \( -a \frac{\left(J + m_J\right)\left(m_J - m_J + 1\right)}{J(J + 1)} \) \( 1/2 \) | \(a\frac{m_J}{J(J + 1)} + b\) | \(a\frac{m_J}{J(J + 1)} + b\) | \(a \frac{\left(J + m_J\right)\left(m_J + m_J + 1\right)}{J(J + 1)} \) \( 1/2 \) |

Note that these coefficients differ from C-G coefficients, because of the coupled system we are dealing with. Remember that these coupled quasi-states arise only for \( J > 0 \). For \( J = 0 \) purely \( S = 0 \) states occur. Quasi-singlet and quasi-triplet states are both characterized by the same quantum numbers \( J, m_J \) and \( P = (-1)^{J+1} \). Because of the unimodularity of matrix (51) we can identify quasi-singlet and quasi-triplet states by quasi-spin (like isospin) \( t = 1/2 \) with \( t_3 = \mp 1/2 \), which is a new quantum number (or label). However, for our purpose it is more convenient to use the value \( s = t_3 + 1/2 \), which gives \( s = s_s = 0 \) or \( s = s_t = 1 \) for quasi-singlet and quasi-triplet states respectively. In this case the labels \( s_s \) and \( s_t \) reflect better the meaning of the indicated quasi-states. It is easy to see from (54) and Table 1 that for positronium the quasi states become true singlet \( (b = 0) \) and triplet \( (a = 0) \) states with different charge conjugation.
quantum numbers. It is useful to note for subsequent calculations that the coefficients $C_1$ and $C_2$ in (39) are $C_1 = a$, $C_2 = -b$ for quasi-singlet states $s = s_8 = 0$, and $C_1 = b$, $C_2 = a$ for quasi-triplet states $s = s_t = 1$.

The triplet $\ell$-mixing states

These states occur for $\ell_{s_1,s_2} \equiv \ell = J \mp 1$ (see Appendix A). The adjustable functions have the form

$$F_{s_1s_2}(p) = C_{Jm_j}^{(tr)J(J-1)m_{s_1s_2}} f_{J-1}^p \left( \begin{array}{c} \vec{m}_{s_1s_2} \\ \vec{p} \end{array} \right) + C_{Jm_j}^{(tr)J(J+1)m_{s_1s_2}} f_{J+1}^p Y_{m_{s_1s_2}} \left( \begin{array}{c} \vec{p} \end{array} \right),$$

(56)

where $m_{s_1s_2}$ are defined in (46), while the coefficients $C_{Jm_j}^{(tr)J(J\pm1)m_{s_1s_2}}$, which are precisely the C-G coefficients, can be found in Appendix A. Expression (56) involves two radial functions $f^J_{-1}(p)$ and $f^J_{+1}(p)$ which correspond to $\ell = J - 1$ and $\ell = J + 1$. This reflects the fact that the orbital angular momentum is not conserved and $\ell$ is not a good quantum number. The system in these states is characterized by $J$, $m_j$, and $P = (-1)^J$. In spectroscopic notation, these states are a mixture of $^3(J - 1)$ and $^3(J + 1)$ states. The exception is the state with $J = 0$, for which the orbital angular momentum is a good quantum number. Indeed, for $J = 0$ the function $f^J_{-1}(p)$ does not exist (see Appendix A), thus the function $F_{s_1s_2}(p)$ is defined only by the second term in (56). Note that $\ell$-mixing states appear for principal quantum number $n \geq 3$ only.

5. The relativistic radial equations for two fermion systems

It is not possible to write an universal two fermion wave equation, because the adjustable functions have different form for different states. Thus it was important to classify all states of the system before deriving final radial equations. Now we return to the variational equation (29) and replace the functions $F_{s_1s_2}(p)$ by the expression (39) for the quasi-states and by (56) for the triplet states. After completing the variational procedure we obtain the following results:

For the states with $\ell = J$, $P = (-1)^J \pm 1$ the radial equations are

$$(\omega_p + \Omega_p - E) f^J_{\mp 1}(p) = \frac{m_{s_{s_1}}m_{s_{s_2}}}{(2\pi)^{\frac{3}{2}}} \int d^3q \frac{q^2 dq}{\omega_p \omega_q \sqrt{p_{\|}} \Omega_q} K(p,q) f^J_{\pm 1}(q),$$

(57)

where the kernel $K(p,q)$ is defined by invariant $\mathcal{M}$-matrices as follows from (29). For the pure singlet states with $J = 0$, according to (42), (48) and (147), the kernel $K(p,q)$ is

$$K(p,q) = -\frac{i}{4\pi} \int d\vec{p} d\vec{q} (\mathcal{M}_{1212}(p,q) - \mathcal{M}_{1221}(p,q) - \mathcal{M}_{2112}(p,q) + \mathcal{M}_{2121}(p,q)), \quad (58)$$

For quasi-singlet and quasi-triplet states ($J \geq 1$) we have

$$K(p,q) = -i \sum_{s_{s_1} s_{s_2} \sigma_{1} \sigma_{2} m_{j}} \int d\vec{p} d\vec{q} C_{Jm_j}^{(s)s_{s_1} s_{s_2} \sigma_{1} \sigma_{2}} \mathcal{M}_{s_{s_1}s_{s_2}\sigma_{1}\sigma_{2}}(p,q) Y_{Jm_{j}}^{*}(\vec{p}) Y_{Jm_{j}}(\vec{q}),$$

(59)

where the coefficients $C_{Jm_j}^{(s)s_{s_1} s_{s_2} \sigma_{1} \sigma_{2}}$ are expressed through the coefficients $C_{Jm_j}^{(s)s_{s_1} s_{s_2}}$

$$C_{Jm_j}^{(s)s_{s_1} s_{s_2} \sigma_{1} \sigma_{2}} = C_{Jm_j}^{(s)s_{s_1} s_{s_2}} C_{Jm_j}^{(s)s_{s_1} s_{s_2}} / \sum_{m_{j}'m_{j}'} \left( C_{Jm_j}^{(s)s_{s_1} s_{s_2}} \right)^2,$$

(60)

where $s = s_8, s_t$. In (60) we have summed over $m_j$, because of the $2J + 1$ energy degeneracy.

For the triplet states with $\ell = J \mp 1$, we have two independent radial functions $f^J_{-1}(p)$ and $f^J_{+1}(p)$. Thus the variational equation (29) leads to a system of coupled equations for $f^J_{-1}(p)$ and $f^J_{+1}(p)$. It is convenient to write them in matrix form,

$$(\omega_p + \Omega_p - E) \mathbb{F}(p) = \frac{m_{s_{s_1}}m_{s_{s_2}}}{(2\pi)^{\frac{3}{2}}} \int \frac{q^2 dq}{\omega_p \omega_q \sqrt{p_{\|}} \Omega_q} K(p,q) \mathbb{F}(q),$$

(61)
We shall do the calculation in the Coulomb gauge, in which the photon propagator has the form
\[ \frac{1}{k^2} \begin{bmatrix} f^j_{j+1}(p) \\ f^j_{j+1}(p) \end{bmatrix}, \]
(62)
and
\[ \mathbb{K}(p, q) = \begin{bmatrix} K_{11}(p, q) & K_{12}(p, q) \\ K_{21}(p, q) & K_{22}(p, q) \end{bmatrix}. \]
(63)
The kernels \( K_{ij} \) are similar in form to (59), that is
\[ K_{ij}(p, q) = -i \sum_{s_1, s_2} C_{s_1 s_2}^{s_1 s_2} \int \mathcal{D} \hat{p} \mathcal{D} \hat{q} \mathcal{M}_{s_1 s_2}^{s_1 s_2}(p, q) Y_{\ell_1}^{m_1} (\hat{p}) Y_{\ell_2}^{m_2} (\hat{q}). \]
(64)
However the coefficients \( C_{s_1 s_2}^{s_1 s_2} \) are defined by the expression
\[ C_{s_1 s_2}^{s_1 s_2} = C_{F}^{(tr) \ell m s} C_{F}^{(tr) \ell m s} / \sum_{s_1, s_2} \left( C_{F}^{(tr) \ell m s} \right)^2, \]
(65)
where \( \ell_1 = J - 1, \ell_2 = J + 1 \). The system (61) reduces to a single equation for \( f_{J+1}(p) \) when \( J = 0 \), since \( f_{J-1}(p) = 0 \) in that case.

To our knowledge, it is not possible to obtain analytic solution of the relativistic radial momentum-space equations (57) and (61). Thus one must resort to numerical or other approximation methods. Numerical solutions of such equations are discussed, for example, in [11], while a variational approximations have been employed in [5]. However, in this paper we shall resort to perturbative approximations, in order to verify that our equations agree with known results for positronium to \( O(\alpha^4) \). We expect that this must be so, given that the interaction kernels (i.e. momentum-space potentials) of our equations involve the “tree-level” Feynman diagrams only.

Beyond \( O(\alpha^4) \) our equations are evidently incomplete. One could, of course, augment them by the addition of invariant matrix elements corresponding to one-loop Feynman diagrams to the existing \( \mathcal{M} \)-matrices in the kernels of our equations. Indeed such an approach has been used in a similar though not variational treatment of positronium and muonium by Zhang and Koniuk [14, 15]. These authors show that the inclusion of single-loop diagrams yields positronium energy eigenstates which are accurate to \( O(\alpha^5, \alpha^5 \ln \alpha) \). However such ad-hoc augmentation of the kernels would be contrary to the spirit of the present variational treatment, and we shall not pursue it in this work.

6. The kernels in semi-relativistic expansion and the non-relativistic limit

For perturbative solutions of our radial equations, it is necessary to work out expansions of the relevant expressions to first order beyond the non-relativistic limit. This shall be summarized in the present section. We shall do the calculation in the Coulomb gauge, in which the photon propagator has the form [16]
\[ D_{00}(k) = \frac{1}{k^2}, \quad D_{01}(k) = 0, \quad D_{ij}(k^\mu) = \frac{1}{k^\mu k^\nu} \left( \delta_{ij} - \frac{k_i k_j}{k^2} \right), \]
(66)
where \( k^\mu = (\omega_p - \omega_q, p - q) \).

To expand the amplitudes \( \mathcal{M} \) of (30), (31) up to the lowest non-trivial order of \( (p/m)^2 \), we take the free-particle spinors to be
\[ u(p, i) = \left[ \begin{array}{c} 1 + \frac{(p/m)^2}{2m} \\ \frac{(p/m)}{2m} \end{array} \right] \varphi_i, \quad v(p, i) = \left[ \begin{array}{c} (\frac{(p/m)}{2m}) \\ 1 + \frac{(p/m)^2}{8m^2} \end{array} \right] \chi_i, \]
(67)
as discussed in Appendix C. Analogously, the photon propagator takes on the form
\[ D_{00}(p - q) = \frac{1}{(p - q)^2}, \quad D_{kl}(p - q) \simeq -\frac{1}{(p - q)^2} \left( \delta_{kl} - \frac{(p - q)_k (p - q)_l}{(p - q)^2} \right), \]
(68)
The annihilation contribution, which arises for a particle-antiparticle system [10], is given by the term

$$\mathcal{M}_{s_1s_2\sigma_1\sigma_2}^{\text{ann}}(q, p) = \frac{iq_1q_2}{m_1m_2} \left( \frac{1}{\langle p - q \rangle^2} + \frac{1}{m_1m_2} \left( \frac{1}{2} \left( \frac{m_1}{m_2} + \frac{m_2}{m_1} \right) \left( \frac{1}{4} + \frac{q \cdot p}{(p - q)^2} \right) + \frac{(q \times p)^2}{(p - q)^4} \right) \right) \delta_{s_1\sigma_1} \delta_{s_2\sigma_2}. \quad (69)$$

The linear spin terms, which are responsible for spin-orbit interaction, become

$$\mathcal{M}_{s_1s_2\sigma_1\sigma_2}^{\text{ope}(s-o)}(q, p) = -\frac{q_1q_2}{4m_1m_2} \varphi_{s_1}^{\dagger} \chi_{s_2} \left( \left( \frac{m_2}{m_1} + 2 \right) \varphi_{s_1} \chi_{s_2} \right). \quad (70)$$

The quadratic spin terms or spin-spin interaction terms are

$$\mathcal{M}_{s_1s_2\sigma_1\sigma_2}^{\text{ope}(s-s)}(q, p) = \frac{iq_1q_2}{4m_1m_2} \varphi_{s_1}^{\dagger} \chi_{s_2} \left\{ \left( \frac{\varphi_{s_1} \cdot (p - q)}{(p - q)^2} \right) \varphi_{s_1} \chi_{s_2} \right\}. \quad (71)$$

The annihilation contribution, which arises for a particle-antiparticle system [10], is given by the term

$$\mathcal{M}_{s_1s_2\sigma_1\sigma_2}^{\text{ann}}(p, q) = -\frac{ie^2}{4m^2} \varphi_{s_1}^{\dagger} \chi_{s_2} \varphi_{s_1} \chi_{s_2}, \quad (72)$$

where we have excluded a divergent term, which appears in the Coulomb gauge. Here $m_1 = m_2 \equiv m$ and $q_1 = q_2 \equiv e$. The kernels are calculated from (58), (59), (64) with (69)-(71). They consist of three parts, namely

$$\mathcal{K}(p, q) = \mathcal{K}^{(s-gl)(or)}(p, q) + \mathcal{K}^{(s-o)}(p, q) + \mathcal{K}^{(s-s)}(p, q). \quad (73)$$

The singlet state ($\ell = J = 0, P = -1$)

Details of the calculations can be found in Appendix D. We use the notation: $z = (p^2 + q^2)/2pq$, and $Q_{\lambda}(z)$ are the Legendre functions of the second kind [17]. The contributions of the various terms to the kernel are as follows:

Orbital term

$$\mathcal{K}^{(s-gl)(or)}(p, q) = \frac{2\pi q_1q_2}{pq} Q_0(z) + \frac{\pi q_1q_2}{2m_1m_2} \left( \frac{m_1}{m_2} + \frac{m_2}{m_1} + 1 \right) \left( \frac{p + q}{p} \right) Q_0(z) + 2Q_1(z) - \left( \frac{m_1}{m_2} + \frac{m_2}{m_1} + 2 \right), \quad (74)$$

Spin-orbit interaction

$$\mathcal{K}^{(s-gl)(s-o)}(p, q) = 0, \quad (75)$$

Spin-spin interaction

$$\mathcal{K}^{(s-gl)(s-s)}(p, q) = \frac{2\pi q_1q_2}{m_1m_2} \quad (76)$$

The quasi-states ($\ell = J (J \geq 1), P = (-1)^{J+1}, s = 0, 1$)

The contributions of the various terms to the kernel are as follows:
Orbital term

\[ K^{(\text{orb})} (p, q) = \frac{\pi q_1 q_2}{pq} Q_J(z) + \frac{\pi q_1 q_2}{2m_1 m_2} \left( \frac{m_1}{m_2} + \frac{m_2}{m_1} - (J - 1) \right) \left( \frac{p}{q} + \frac{q}{p} \right) Q_J(z) + 2 (J + 1) Q_{J+1}(z) \]  

(77)

Spin-orbit interaction

\[ K^{(s-o)} (p, q) = \frac{\pi q_1 q_2}{2m_1 m_2} \left( -c_2^2 \left( \frac{m_1}{m_2} + \frac{m_2}{m_1} + 4 \right) + 2c_1 c_2 J (J + 1) \right) \left( \frac{p}{q} + \frac{q}{p} \right) Q_J(z) \]

\[ \times \frac{1}{2J + 1} (Q_{J+1}(z) - Q_{J-1}(z)) \]  

(78)

Spin-spin interaction

\[ K^{(s-s)} (p, q) = C_2^2 \frac{\pi q_1 q_2}{m_1 m_2} \left( \frac{p}{q} + \frac{q}{p} \right) Q_J(z) - C_2^2 \frac{\pi q_1 q_2}{2m_1 m_2} \frac{1}{2J + 1} \{ J Q_{J+1}(z) + (J + 1) Q_{J-1}(z) \} \]  

(79)

where \( C_1 \) and \( C_2 \) are defined in section 4.

The triplet states \((\ell = J - 1 \ (J \geq 1)), \ \ell = J + 1 (J \geq 0) \ P = (-1)^\ell \)

From (64), it follows that the kernels \( K_{12} \) and \( K_{21} \) are responsible for mixing of states with \( \ell = J - 1 \) and \( \ell = J + 1 \). These kernels have the form

\[ K_{12} (p, q) = K_{21} (p, q) = \frac{\pi q_1 q_2}{5m_1 m_2} \frac{\sqrt{J (J + 1)}}{(2J + 1)} \left( \frac{p}{q} Q_{J+1}(z) + \frac{q}{p} Q_{J-1}(z) - 2Q_J(z) \right), \]  

(80)

where only spin-spin interactions contribute. For kernels \( K_{11} \) and \( K_{11} \) we have from (64):

Orbital terms

\[ K^{(o)}_{11} (p, q) = \frac{2\pi q_1 q_2}{pq} Q_{J-1}(z) + \frac{\pi q_1 q_2}{2m_1 m_2} \left( \frac{m_1}{m_2} + \frac{m_2}{m_1} + 2 - J \right) \left( \frac{p}{q} + \frac{q}{p} \right) Q_{J-1}(z) \]

\[ + \frac{\pi q_1 q_2}{m_1 m_2} J Q_J(z) - \frac{\pi q_1 q_2}{2m_1 m_2} \left( \frac{m_1}{m_2} + \frac{m_2}{m_1} + 2 \right) \delta_{J,1}, \]  

(81)

Spin-orbit interaction

\[ K^{(s-o)}_{11} (p, q) = -\frac{\pi q_1 q_2}{2m_1 m_2} \frac{J - 1}{2J - 1} \left( \frac{m_2}{m_1} + \frac{m_1}{m_2} + 4 \right) (Q_J(z) - Q_{J-2}(z)) \]  

(83)

\[ K^{(s-o)}_{22} (p, q) = \frac{\pi q_1 q_2}{2m_1 m_2} \left( \frac{m_1}{m_2} + \frac{m_2}{m_1} + 4 \right) \frac{J + 2}{2J + 3} (Q_{J+2}(z) - Q_J(z)) \]  

(84)

Spin-spin interaction

\[ K^{(s-s)}_{11} (p, q) = \frac{\pi q_1 q_2}{2m_1 m_2} \frac{1}{2J + 1} \left( \frac{p}{q} + \frac{q}{p} \right) Q_{J-1}(z) - 2Q_J(z) \]  

(85)
\[ K^{(s-s)}_{22}(p,q) = \frac{\pi q_1 q_2}{2 m_1 m_2} \frac{1}{2J + 3} \left( \frac{p}{q} + \frac{q}{p} \right) Q_{J+1}(z) - 2Q_{J+2}(z) \]  
(86)

Annihilation term (particle-antiparticle system only, with \( m_1 = m_2 = m, q_1 = q_2 = e \))

\[ K^{ann}(p,q) = -\frac{2\pi e^2}{m^2} \delta_{J,1}. \]  
(87)

We note that in the non-relativistic limit the only terms that survive are the first terms of the orbital part of the kernels. They have the common form 2\( \pi q_1 q_2 Q_1(z)/pq \), where

\[ Q_l(z) = \frac{pq}{2\pi} \int \frac{d\tilde{q}d\tilde{p}}{(p-q)^2} Y^{m'_l}(\tilde{p}) Y^{m_l}(\tilde{q}). \]  
(88)

Thus, equations (57), (61) reduce to the form

\[(\omega_p + \Omega_p - E) f^\ell(p) = \frac{m_1 m_2 q_1 q_2}{\pi \sqrt{\omega_p \Omega_p} p} \int_0^\infty dq \frac{q}{\sqrt{\Omega_q}} Q_l(z) f^\ell(q). \]  
(89)

If we expand the relativistic free-particle energy

\[ \omega_p \simeq m_1 \left( 1 + \frac{1}{2} \left( \frac{p}{m_1} \right)^2 \right), \quad \Omega_p \simeq m_2 \left( 1 + \frac{1}{2} \left( \frac{p}{m_2} \right)^2 \right), \]  
(90)

we obtain the two particle Schrödinger radial equation in momentum space [18]

\[ \left( \frac{p^2}{2m_r} - \varepsilon \right) f^\ell(p) = \frac{\alpha}{\pi p} \int_0^\infty dq \, q Q_l(z) f^\ell(q), \]  
(91)

where \( \alpha = q_1 q_2 / 4\pi \). The solutions of these equations are well known. They are given in Appendix D (formula (201)).

7. Energy eigenvalues and relativistic corrections to \( O(\alpha^4) \) for arbitrary mass ratio

The energy eigenvalues \( E_{n,J} \) for the states, when \( \ell = J \), can be calculated from the equation

\[ E \int_0^\infty dp \, p^2 f^\ell(p) f^J(p) = \int_0^\infty dp \, p^2 (\omega_p + \Omega_p) f^\ell(p) f^J(p) + \]
\[- \frac{m_1 m_2}{(2\pi)^2} \int_0^\infty dp \frac{p^2}{\sqrt{\omega_p \Omega_p}} \int_0^\infty dq \frac{q^2}{\sqrt{\Omega_q}} K(p,q) f^\ell(p) f^J(q). \]  
(92)

For the \( \ell = J + 1 \) triplet states we have the matrix equation

\[ E \int_0^\infty dp \, p^2 \Xi(p) \Xi^\ell(p) = \int_0^\infty dp \, p^2 (\omega_p + \Omega_p) \Xi^{\ell}(p) \Xi(p) + \]
\[- \frac{m_1 m_2}{(2\pi)^2} \int_0^\infty dp \frac{p^2}{\sqrt{\omega_p \Omega_p}} \int_0^\infty dq \frac{q^2}{\sqrt{\Omega_q}} K(p,q) \Xi^{\ell}(p) \Xi(p). \]  
(93)

To obtain results for \( E \) to \( O(\alpha^4) \) we use the forms of the kernels expanded to \( O(p^2/m^2) \) (expressions (74)-(87)) and replace \( f^\ell(p) \) by their non-relativistic (Schrödinger) form (201) (see Appendix D). The most important integrals, which we used for calculating (92) and (93), are given in Appendix D. In Appendix F
respectively.

The total energy corrections are common for quasi-singlet and quasi-triplet states:

\[ \Delta \epsilon = E + \frac{\alpha^2 m_r}{2n^2} - M, \quad M = m_1 + m_2, \quad m_r = m_1 m_2 / (m_1 + m_2). \]

**Singlet states** \((\ell = J = 0, \quad P = -1)\) (which include the ground state)

The kinetic energy corrections

\[ \Delta \epsilon_n^{(sg)(k)} = -\frac{\alpha^4 m_r}{n^3} \left( 1 - \frac{3}{8n} \right) \left( 1 - \frac{3m_r}{M} \right), \quad (94) \]

Orbital energy corrections

\[ \Delta \epsilon_n^{(sg)(o)} = -\frac{\alpha^4 m_r}{n^3} \left( \frac{1}{2} + \frac{3m_r}{M} - \frac{m_r}{M} - \frac{1}{n} \right), \quad (95) \]

Spin-orbit energy corrections

\[ \Delta \epsilon_n^{(sg)(s-o)} = 0, \quad (96) \]

Spin-spin energy corrections

\[ \Delta \epsilon_n^{(sg)(s-s)} = -\frac{\alpha^4 m_r}{n^3} \frac{2m_r}{M}. \quad (97) \]

The total energy corrections

\[ \Delta \epsilon_n^{(sg)} = -\frac{\alpha^4 m_r}{n^3} \left( \frac{1}{2} + \frac{2m_r}{M} - \frac{1}{8n} \left( 3 - \frac{m_r}{M} \right) \right). \quad (98) \]

**Quasi-singlet, quasi-triplet states** \((\ell = J (J \geq 1), \quad P = (-1)^{J+1})\)

The kinetic energy and orbital energy corrections are common for quasi-singlet and quasi-triplet states:

\[ \Delta \epsilon_n^{(k)} = -\frac{\alpha^4 m_r}{2n^3} \left( 1 - \frac{3m_r}{M} \right) \left( \frac{2}{2J+1} - \frac{3}{4n} \right), \quad (99) \]

Orbital energy corrections

\[ \Delta \epsilon_n^{(orb)} = -\frac{\alpha^4 m_r m_r}{n^3} \left( \frac{3}{2J+1} - \frac{1}{n} \right), \quad (100) \]

Spin-orbit energy corrections

\[ \Delta \epsilon_n^{(s-o)} = \frac{\alpha^4 m_r}{2n^3} \frac{1}{M^2} \frac{-C_2^2 \left( (m_1 + m_2)^2 + 2m_1 m_2 \right) + 2C_1 C_2 \sqrt{J (J+1) (m_2^2 - m_1^2)}}{(2J+1) (J+1) J}. \quad (101) \]

Spin-spin energy corrections

\[ \Delta \epsilon_n^{(s-s)} = \frac{\alpha^4 m_r}{n^3} \frac{m_r}{M (2J+1) (J+1) J}. \quad (102) \]

The coefficients \(C_1\) and \(C_2\) are defined here in the same way as in formulas \((78), (79)\).

Thus, the total energy corrections are

\[ \Delta \epsilon_{n,J,s} = -\frac{\alpha^4 m_r}{n^3} \left( \frac{1}{2J+1} \left( 1 + \frac{1}{4J (J+1)} \right) - \frac{1}{8n} \left( 3 - \frac{m_r}{M} \right) \right), \quad (103) \]

where upper and lower signs correspond to quasi-singlet \(s = s_s = 0\) and quasi-triplet \(s = s_t = 1\) states respectively.

**Triplet states** \((\ell = J - 1 (J \geq 1), \quad P = (-1)^{J})\)
Kinetic energy corrections
\[ \Delta \varepsilon_{n,J}^{(tr)(k)} = -\frac{\alpha^4 m_r}{n^3} \left( \frac{1}{2J - 1} - \frac{3}{8n} \right) \left( 1 - \frac{3m_r}{M} \right), \]  
(104)

Orbital energy corrections
\[ \Delta \varepsilon_{n,J}^{(tr)(o)} = -\frac{\alpha^4 m_r}{n^3} \left( \frac{3}{2J - 1} - \frac{\delta_{J,1}}{2} - \frac{1}{n} \right) m_r, \]  
(105)

Spin-orbit energy corrections
\[ \Delta \varepsilon_{n,J}^{(tr)(s-o)} = \frac{\alpha^4 m_r}{n^3} \frac{1 - \delta_{J,1}}{2(2J - 1)} \left( 1 + \frac{2m_r}{M} \right), \]  
(106)

Spin-spin energy corrections
\[ \Delta \varepsilon_{n,J}^{(tr)(s-s)} = -\frac{\alpha^4 m_r}{n^3} \left( \frac{1 - \delta_{J,1}}{J(2J + 1)(2J - 1)} - \frac{2}{3} \delta_{J,1} \right) \frac{m_r}{M}. \]  
(107)

The total energy corrections
\[ \Delta \varepsilon_{n,J}^{tr} = -\frac{\alpha^4 m_r}{n^3} \left( \frac{1}{2J - 1} \left( 1 - \frac{1}{2J} - \frac{2m_r}{M} \frac{1}{2J + 1} \right) - \frac{1}{8n} \left( 3 - \frac{m_r}{M} \right) \right). \]  
(108)

The annihilation term for positronium-like systems is
\[ \Delta \varepsilon_{n}^{(anh)} = \frac{\alpha^4 m}{4n^3} \delta_{J,1}. \]  
(109)

**Triplet states** \((\ell = J + 1 \ (J \geq 0), \ P = (-1)^J)\)
The kinetic energy corrections
\[ \Delta \varepsilon_{n,J}^{(tr)(k)} = -\frac{\alpha^4 m_r}{n^3} \left( \frac{1}{2J + 3} - \frac{3}{8n} \right) \left( 1 - \frac{3m_r}{M} \right), \]  
(110)

Orbital energy corrections
\[ \Delta \varepsilon_{n,J}^{(tr)(o)} = -\frac{\alpha^4 m_r}{n^3} \left( \frac{3}{2J + 3} - \frac{1}{n} \right) m_r, \]  
(111)

Spin-orbit energy corrections
\[ \Delta \varepsilon_{n,J}^{(tr)(s-o)} = -\frac{\alpha^4 m_r}{n^3} \frac{1}{2(J + 1)(2J + 3)} \left( 1 + \frac{2m_r}{M} \right), \]  
(112)

Spin-spin energy corrections
\[ \Delta \varepsilon_{n,J}^{(tr)(s-s)} = -\frac{\alpha^4 m_r}{n^3} \frac{1}{(J + 1)(2J + 3)(2J + 1)} \frac{m_r}{M}. \]  
(113)

The total energy corrections
\[ \Delta \varepsilon_{n,J}^{tr} = -\frac{\alpha^4 m_r}{n^3} \left( \frac{1}{2J + 3} \left( 1 + \frac{1}{2(J + 1)} + \frac{2m_r}{M} \frac{1}{2J + 1} \right) - \frac{1}{8n} \left( 3 - \frac{m_r}{M} \right) \right). \]  
(114)

For two equal masses our calculations agree with positronium results [19]. In the limit when one of the masses becomes infinite, say \(m_2 \to \infty\), the above results reduce to those obtained for a one-electron Dirac equation in a static Coulomb potential (to \(O(\alpha^4)\)), namely
\[ \Delta \varepsilon_{n,J} = -\frac{\alpha^4 m_1}{n^3} \left( \frac{1}{2j + 1} - \frac{3}{8n} \right). \]  
(115)
Indeed, when \( m_2 \to \infty \) not only the total angular momentum, but also \( J_f^2 = (L_1 + S_1)^2 \) and \( S_2^2 \) are independently conserved. Thus, in this case, we can replace the quantum number \( J \) by \( j - 1/2 \) in \( (99)-(103) \)(when \( s = 0 \)) and \( (110)-(114) \), and by \( j + 1/2 \) in expressions \( (99)-(103) \)(when \( s = 1 \)) and \( (104)-(108) \). In other words

\[
J \to j - 1/2 \quad \text{for} \quad |sg_q\rangle \quad \text{and} \quad |tr_{\ell=J+1}\rangle, \quad (116)
\]

\[
J \to j + 1/2 \quad \text{for} \quad |tr_q\rangle \quad \text{and} \quad |tr_{\ell=J-1}\rangle.
\]

The quantum number \( j = |\ell \pm 1/2| \) belongs here to the particle with mass \( m_1 \).

The results \( (98), (103), (108) \) and \( (114) \) agree with the calculations of Connell, based on a quasipotential reduction of the Bethe-Salpeter equation \( [20] \), those of Hersbach, who used a relativistic Lippman-Schwinger formulation \( [21] \), and those of Duviryak and Darewych based on a two-fermion Breit equation \( [22] \). Grandy [8] obtained the same results from a perturbative solution of the coupled, nonlinear Dirac equations \( (8) \) and \( (9) \).

8. Fine and hyperfine structure. Recoil effects.

In this section we shall analyze the formulas obtained in the previous section and we shall apply them to the energy spectra of some exotic atoms. To compare our calculations with experimental data we shall use the standard spectroscopical notation. First of all, it follows from \( (94)-(96) \) and \( (104)-(106) \) that the difference between energy levels of \( 2S \) and \( 1S \) states is given by formula

\[
E(2S) - E(1S) = \frac{3\alpha^2 m_r}{8} + \frac{\alpha^4 m_r}{128} \left( 11 + 15 \frac{m_r}{M} \right). \quad (117)
\]

Note that the formula \( (117) \) ignores hyperfine splitting, that is we exclude the spin-spin interaction. The fine structure of \( 2P \)-state follows similarly from \( (104)-(106) \) and \( (110)-(112) \), provided that we exclude the spin-spin interaction \( (107) \) and \( (113) \)

\[
\Delta E_{fs}(2P) = E(2P_{3/2}) - E(2P_{1/2}) = \frac{\alpha^4 m_r}{32} \left( 1 + \frac{2m_r}{M} \right). \quad (118)
\]

The HFS of \( 1S_{1/2} \) and \( 2S_{1/2} \) is obtained from \( (98) \) and \( (108) \):

\[
\Delta E_{hfs}(1S_{1/2}) = \alpha^4 m_r \frac{8m_r}{3M}, \quad (119)
\]

\[
\Delta E_{hfs}(2S_{1/2}) = \alpha^4 m_r \frac{m_r}{3M}. \quad (120)
\]

Actually this hyperfine splitting, expressions \( (119) \) and \( (120) \), arises from the difference of spin-spin terms \( (97) \) and \( (107) \). The formulae \( (119) \) and \( (120) \) give the usual Fermi splitting \( [18] \).

The HFS of states with \( \ell > 0 \) is more complicated. For each \( \ell > 0 \) we have two sorts of states with different \( J \) and \( s \): states with \( J = \ell + 1 \) and \( J = \ell, s = s_s \) and states with \( J = \ell - 1 \) and \( J = \ell, s = s_t \). From \( (103),(108) \) and \( (114) \) we obtain the general HFS formulae for all quantum numbers \( n, \ell \) and for any mass ratio.

\[
\Delta E_{hfs}(n, \ell, s_s) \equiv \Delta \xi_{n,J=\ell+1}^{s_{tr}} - \Delta \xi_{n,J=\ell,s_s} = \frac{\alpha^4 m_r}{n^3} \frac{1}{2\ell + 1} \left( \frac{2\ell + 1 - \xi^{-1}}{4\ell (\ell + 1) + 2m_r} \frac{1}{M} \frac{1}{2\ell + 3} \right), \quad (121)
\]

\[
\Delta E_{hfs}(n, \ell, s_t) \equiv \Delta \xi_{n,J=\ell,s_t}^{s_{tr}} - \Delta \xi_{n,J=\ell-1}^{s_{tr}} = \frac{\alpha^4 m_r}{n^3} \frac{1}{2\ell + 1} \left( \frac{2\ell + 1 - \xi^{-1}}{4\ell (\ell + 1) + 2m_r} \frac{1}{M} \frac{1}{2\ell - 1} \right). \quad (122)
\]

The quantity \( \xi \) is defined by \( (53) \), but with the quantum number \( J \) replaced by \( \ell \).
For the particular case when $m_2 >> m_1$ we obtain from (121) and (122)

$$
\Delta E_{hfs} (n, \ell, s_s) = \frac{\alpha^4 m_1 n^3}{96} \frac{8 (\ell + 1)}{(2\ell + 1)^2} \frac{m_1}{(2\ell + 3) m_2}
$$

(123)

$$
\Delta E_{hfs} (n, \ell, s_t) = \frac{\alpha^4 m_1 n^3}{96} \frac{8\ell}{(2\ell + 1)^2} \frac{m_1}{(2\ell - 1) m_2}
$$

(124)

to leading order in $m_1/m_2$.

The approximate results (123) and (124) are the HFS formulae usually quoted in the literature (e.g. [18] p. 110, and [24] p. 836). As mentioned in section 7, in the one-body limit ($m_2 \to \infty$), states with labels $s_s$ and $s_t$ can be characterized by the quantum numbers $j = \ell + 1/2$ and $j = \ell - 1/2$ respectively. In this one-body picture, the labels $s_s$ and $s_t$ should be replaced by $j$ in the formulas (121), (124). Note here that, because of the mixed nature of the states $n\ell_{\ell-1/2}$ ($\ell = J, s_s = 1$) and $n\ell_{\ell+1/2}$ ($\ell = J, s_s = 0$), the spin-orbit interaction contributes to the splitting as well. The splitting is largest when $m_1 = m_2$ and disappears for all states in the one-body limit.

It is easy to get the HFS of $2P_{1/2}$, $2P_{3/2}$ states from (121) and (122):

$$
\Delta E_{hfs} (2P_{1/2}) = \alpha^4 m_r \left( \frac{1}{64} - \frac{\xi^{-1}}{192} + \frac{1}{12 M} \right)
$$

(125)

$$
\Delta E_{hfs} (2P_{3/2}) = \alpha^4 m_r \left( \frac{1}{64} - \frac{\xi^{-1}}{192} + \frac{1}{60 M} \right)
$$

(126)

where $\xi^{-1} = \sqrt{8 \left( \frac{m_1 - m_2}{M} \right)^2 + 1}$. Note that, if we use the pure triplet state instead of the mixed states, we get the following expressions for hyperfine splitting: $E_{hfs} (2P_{1/2}) = \alpha^4 m_r \left( \frac{1}{72} + \frac{m_1}{12M} \right)$, $E_{hfs} (2P_{3/2}) = \alpha^4 m_r \left( \frac{1}{72} + \frac{m_1}{12M} \right)$. These give the correct results only for $m_1 = m_2$ (positronium).

The results of our calculations and comparison with experimental data for muonium, hydrogen and muonic hydrogen are summarized in Tables 2-4. In each table the first two entries reflect, primary, fine-structure splittings, while $\Delta E_k$ corresponds to the $O (\alpha^3)$ recoil contribution to the Lamb shift, $E (2S_{1/2}) - E (2P_{1/2})$. Note that except for the hyperfine splitting of the ground state, which has been measured very accurately, the experimental results are quoted in the tables to the number of significant digits available. The calculated results, we must remember, are accurate to $O (\alpha^4)$ only, where as the experimental results are exact except for experimental error, that is they contain all orders in $\alpha$.

Although hydrogen and muonic hydrogen are not strictly leptonic atoms, we can take into account the proton anomalous magnetic moment in the hyperfine splitting in the same phenomenological manner as was done in [23]. Thus, to get the corrected result for HFS in hydrogen and muonic hydrogen, we multiply the expression for $\Delta E_{hfs}$ by the factor $(1 + k_p)$, where $k_p = 1.792847$ is the anomalous magnetic moment of the proton. The last columns in tables 3, 4 give the HFS corrected by the factor $(1 + k_p)$. The anomalous magnetic moment of the muon is very small, nevertheless for the sake of completeness, we provide the same corrections for muonium, where we use the factor $(1 + a_\mu)$ ($a_\mu = 0.001166$) to get the result of the last column in Table 2 from those of the third column. We note that doing so improves the agreement between the calculated and the experimental HFS results in most cases, and dramatically so for hydrogen and muonic hydrogen.

Table 2. Energy shifts, fine and hyperfine structure in muonium for $n = 1, 2$. 




From tables 2-4 we see that the $O(\alpha^4)$ calculated results agree with observation remarkably well, except, of course, for the Lamb shift, which is dominated by corrections of higher-order that $\alpha^3$. The present theoretical results for $\Delta E_L$ reflect only the $O(\alpha^4)$ recoil effects, and these provide a small, though not insignificant, contribution. Note that if we use the approximate $m_1/m_2$ expansion formulas (123) and (124), for example for HFS of $2P_{1/2}$ and $2P_{3/2}$ states we get the result (with $a_u$ and $k_p$ corrections) $\Delta E_{hfs}(2P_{1/2}) = 188.50$ MHz for muonium, and $\Delta E_{hfs}(2P_{3/2}) = 10.47$ meV for muonic hydrogen. These approximate results do not agree as well with observation as the values calculated without the $m_1/m_2$ expansion, and hence they differ from what we give in last columns of tables 2 and 4. Note that this difference can be of the same order as the contribution of higher order in $\alpha$ for HFS. The $m_1/m_2$ expansion approximation is not significant for hydrogen for which the mass ratio is very small, but it is appreciable for muonium and particularly for muonic hydrogen.

Since our results are true for arbitrary mass ratios we can speak here about recoil effects rather than about recoil corrections. The recoil effect contributes to the Lamb shift (shift between $2S_{1/2}$ and $2P_{1/2}$ levels). However the states $2S_{1/2}$ and $2P_{1/2}$ are split (hyperfine splitting as discussed below) because of the spin-spin interaction, so to calculate the Lamb shift we have to take the energy corrections for each state without spin-spin terms. For the state $2S_{1/2}$ it is the sum of the energy corrections (94) and (95), while for the $2P_{1/2}$ state we take the sum of (110), (111), and (112). Thus, the formula for the $O(\alpha^4)$ contribution to the Lamb shift produced by the recoil effect is

$$\Delta E_L^{(rc)} = E(2S_{1/2}) - E(2P_{1/2}) = \frac{\alpha^4 m_r}{24} \frac{m_e}{M}.$$ (127)
It is easy to see that the shift (127) is largest when \( m_1 = m_2 \), and disappears in the one-body limit, when \( m_2 \to \infty \).

There is a well known formula for the recoil correction of order \( \alpha^4 \) obtained on the basis of the Breit interaction [29], [30]

\[
\Delta \varepsilon_{n,\ell,j}^{(r)} = \frac{\alpha^4 m_r}{m_2^2} \left( 1 - \frac{1}{\ell + 1/2} \right) \left( 1 - \delta_{\ell,0} \right),
\]

which predicts the following contribution to the Lamb shift:

\[
\Delta E_L^{(rcl)} = \Delta \varepsilon_{2,0,1/2} - \Delta \varepsilon_{2,1,1/2} = -\frac{\alpha^4 m_r}{48} m_2^2.
\]

Comparison of the formulas (127) and (129) shows that the total recoil effect (127) is larger in magnitude than (129), and has opposite sign. The difference between (127) and (129) stems from the spin-orbit interaction:

If we ignore the term \( \left( \frac{m_1}{m_2} + 2 \right) \sigma_2 \) in expression (70), we get instead of (106) and (112) the following result for the spin-orbit contribution:

\[
\Delta \varepsilon^{(so)}_{n,j} = \frac{\alpha^4 m_r}{m_2^2} \frac{1 - \delta_{j,1}}{2J(2J - 1)} \left( 1 - \frac{m_2^2}{m_2^2} \right),
\]

for \( \ell = J - 1 \),

\[
\Delta \varepsilon^{(so)}_{n,J} = -\frac{\alpha^4 m_r}{m_2^2} \frac{1}{2(J+1)(2J+3)} \left( 1 - \frac{m_2^2}{m_2^2} \right).\]

The relevant terms are the second ones in (130), (131). We can replace the “J”-quantum numbers in (130) and (131) using (116):

\[
\frac{1}{J(2J - 1)} = -\left( \frac{1}{J} - \frac{2}{2J - 1} \right) \rightarrow -\left( \frac{1}{j + 1/2} - \frac{1}{\ell + 1/2} \right),
\]

and

\[
\frac{1}{(J + 1)(2J + 3)} = \frac{1}{J + 1} - \frac{2}{2J + 3} \rightarrow \frac{1}{j + 1/2} - \frac{1}{\ell + 1/2}.
\]

It is now easy to see that the second terms in (130) and (131) give the formula (128) which, therefore, must be regarded as incomplete. As already mentioned, the proper recoil contribution to the Lamb shift of muonium, hydrogen and muonic hydrogen, based on our result (127), is given in Tables 2-4.

9. Concluding remarks

We have used the variational method within the Hamiltonian formalism of QED to derive relativistic momentum-space wave equations for two-fermion systems like muonium. The trial states are chosen to be eigenstates of the total angular momentum operators \( \hat{J}_z \), \( \hat{J}_3 \), and parity, as well as charge conjugation for particle-antiparticle systems. A general relativistic reduction of the wave equations to radial form is given for arbitrary masses of the two fermions. For given \( J \) there is a single radial equation for total spin zero singlet states, but for spin triplet states there are, in general coupled equations. We have shown how classification of the states follows naturally from the system of eigenvalue equations (36), given our trial state.

It is not possible, as far as we know, to obtain analytic solutions of our relativistic radial equations nor the resulting eigenvalues of the two fermion system that they describe. However, it is possible to obtain \( O(\alpha^4) \) corrections to the energy eigenvalues analytically for all states using perturbation theory.

We have compared our calculated results with experiment for fine and hyperfine splitting of low-lying levels in muonium, hydrogen and muonic hydrogen. We find good agreement for muonium, as well as for hydrogen and muonic hydrogen provided that we take into account the anomalous magnetic moment of the proton in the later two cases.
The method presented here can be generalized to include effects higher order in $\alpha$ by using dressed propagators in place of the bare propagators. This shall be the subject of a forthcoming work.

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Appendix A: Total angular momentum operator in relativistic form

The total angular momentum operator is defined by the expression

\[ \mathbf{J} = \int d^3x \psi^\dagger(x) (\mathbf{\hat{L}} + \mathbf{\hat{S}}) \psi(x) + \int d^3x \phi^\dagger(x) (\mathbf{\hat{L}} + \mathbf{\hat{S}}) \phi(x), \]

(134)

where \( \mathbf{\hat{L}} \) is the orbital angular momentum and \( \mathbf{\hat{S}} \) - the spin operator: \( \mathbf{\hat{L}} = \mathbf{\hat{x}} \times \mathbf{\hat{p}} \) and \( \mathbf{\hat{S}} = \frac{1}{2} \mathbf{\hat{\sigma}} \). We use the standard representation for the Pauli matrices

\[ \mathbf{\hat{\sigma}} = \begin{bmatrix} \sigma_1 & 0 \\ 0 & \sigma_2 \end{bmatrix}, \]

(135)

\[ \sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \]

(136)

Using the field operators \( \psi(x) \) and \( \phi(x) \) in the form (17), (18), after tedious calculations we obtain the expression for operator \( \mathbf{\hat{J}} \). It consists of three parts: two total angular momentum operators of each particle-antiparticle system [10] and the following part, relevant to our considerations

\[ \mathbf{\hat{J}}_1 = \int d^3q \left( \mathbf{\hat{L}}_q \left( \mathbf{b}_{q\uparrow}^\dagger \mathbf{b}_{q\uparrow} + \mathbf{b}_{q\downarrow}^\dagger \mathbf{b}_{q\downarrow} + \mathbf{D}_{q\uparrow}^\dagger \mathbf{D}_{q\uparrow} + \mathbf{D}_{q\downarrow}^\dagger \mathbf{D}_{q\downarrow} \right) + \frac{i}{2} \left( \mathbf{b}_{q\uparrow}^\dagger \mathbf{b}_{q\downarrow} - \mathbf{b}_{q\downarrow}^\dagger \mathbf{b}_{q\uparrow} \right) \right) \]

(137)

\[ \mathbf{\hat{J}}_2 = \int d^3q \left( \mathbf{\hat{L}}_q \left( \frac{1}{2} \left( \mathbf{b}_{q\uparrow}^\dagger \mathbf{b}_{q\uparrow} - \mathbf{b}_{q\downarrow}^\dagger \mathbf{b}_{q\downarrow} \right) = \mathbf{D}_{q\uparrow}^\dagger \mathbf{D}_{q\uparrow} + \mathbf{D}_{q\downarrow}^\dagger \mathbf{D}_{q\downarrow} \right) \right) \]

\[ \mathbf{\hat{J}}_3 = \int d^3q \left( \mathbf{\hat{L}}_q \left( \frac{1}{2} \left( \mathbf{b}_{q\uparrow}^\dagger \mathbf{b}_{q\uparrow} + \mathbf{b}_{q\downarrow}^\dagger \mathbf{b}_{q\downarrow} \right) = \mathbf{D}_{q\uparrow}^\dagger \mathbf{D}_{q\uparrow} + \mathbf{D}_{q\downarrow}^\dagger \mathbf{D}_{q\downarrow} \right) \right) \]

Here \( \mathbf{\hat{L}}_q \) is the orbital angular momentum operator in momentum representation:

\[ (\mathbf{\hat{L}}_q)_{ij} = \mathbf{\hat{L}}_{q_{ij}} = -i (q \times \mathbf{\nabla}_q)_{ij}. \]

(138)

Note that these expressions are valid for any \( t \), since the time-dependent phase factors of the form \( e^{i\omega_q t} \)
cancel out. For the operator $\mathcal{J}^2 = \mathcal{J}_1^2 + \mathcal{J}_2^2 + \mathcal{J}_3^2$ we have

\[
\mathcal{J}^2 = \int d^3q \left( \begin{array}{c}
\mathcal{L}_q + \frac{2}{\pi} \left( b_{q\uparrow}^\dagger b_{q\uparrow} + b_{q\downarrow}^\dagger b_{q\downarrow} + D_{q\uparrow}^\dagger D_{q\uparrow} + D_{q\downarrow}^\dagger D_{q\downarrow} \right) \\
\mathcal{L}_q - b_{q\uparrow}^\dagger b_{q\downarrow} + L_q b_{q\uparrow} b_{q\downarrow} + L_q D_{q\uparrow}^\dagger D_{q\downarrow} + L_q + D_{q\uparrow}^\dagger D_{q\downarrow} \\
\mathcal{L}_q - b_{q\uparrow}^\dagger b_{q\downarrow} + D_{q\uparrow}^\dagger D_{q\downarrow} - D_{q\uparrow} D_{q\downarrow} \end{array} \right)
\]

\[
+ \frac{1}{2} \int d^3q' d^3q \left( \begin{array}{c}
2\mathcal{L}_{q'} \cdot \mathcal{L}_q \left( b_{q\uparrow}^\dagger b_{q\uparrow}^\dagger D_{q\uparrow}^\dagger D_{q\uparrow} + b_{q\downarrow}^\dagger b_{q\downarrow}^\dagger D_{q\downarrow}^\dagger D_{q\downarrow} \\
+ b_{q\uparrow}^\dagger b_{q\downarrow}^\dagger D_{q\uparrow}^\dagger D_{q\downarrow} + b_{q\downarrow}^\dagger b_{q\uparrow}^\dagger D_{q\downarrow}^\dagger D_{q\uparrow} \\
+ \frac{1}{2} \left( b_{q\uparrow}^\dagger b_{q\uparrow}^\dagger D_{q\downarrow}^\dagger D_{q\downarrow} - b_{q\uparrow}^\dagger b_{q\downarrow}^\dagger D_{q\downarrow}^\dagger D_{q\downarrow} \\
- \frac{1}{2} \left( b_{q\uparrow}^\dagger b_{q\uparrow}^\dagger D_{q\uparrow}^\dagger D_{q\downarrow} - b_{q\downarrow}^\dagger b_{q\uparrow}^\dagger D_{q\uparrow}^\dagger D_{q\downarrow} \\
+ b_{q\uparrow}^\dagger b_{q\downarrow}^\dagger D_{q\uparrow}^\dagger D_{q\downarrow} + b_{q\downarrow}^\dagger b_{q\uparrow}^\dagger D_{q\downarrow}^\dagger D_{q\uparrow} \right) \right) \\
+ \mathcal{L}_{q'} - b_{q\uparrow}^\dagger b_{q\downarrow}^\dagger D_{q\uparrow}^\dagger D_{q\downarrow} + b_{q\downarrow}^\dagger b_{q\uparrow}^\dagger D_{q\downarrow}^\dagger D_{q\uparrow} \\
+ \mathcal{L}_{q'} - b_{q\uparrow}^\dagger b_{q\downarrow}^\dagger D_{q\uparrow}^\dagger D_{q\downarrow} + b_{q\downarrow}^\dagger b_{q\uparrow}^\dagger D_{q\downarrow}^\dagger D_{q\uparrow} \right) \\
\end{array} \right), \quad (139)
\]

where

\[
\tilde{L}_{q+} = \tilde{L}_{q1} + i\tilde{L}_{q2}, \quad \tilde{L}_{q-} = \tilde{L}_{q1} - i\tilde{L}_{q2}.
\]

The formulae (137) and (139) apply to the particle-antiparticle system [10] as well if the operators $D^\dagger$ and $D$ are formally replaced by $d^\dagger$ and $d$.

The requirements (36) with trial state in the form of (24) lead to the system of equations ($F_{s_1 s_2}(\mathbf{p}) \equiv F_{s_1 s_2}$):

\[
\begin{align*}
(\tilde{L}_1 + 1)F_{11} &= m_J F_{11} \\
\tilde{L}_3 F_{12} &= m_J F_{12} \\
\tilde{L}_3 F_{21} &= m_J F_{21} \\
(\tilde{L}_3 - 1) F_{22} &= m_J F_{22}
\end{align*}
\]

\[
\begin{align*}
\left( J(J+1) - \tilde{L}_3^2 - 2 - 2\tilde{L}_3 \right)F_{11} &= \tilde{L}_- (F_{12} + F_{21}) \\
\left( J(J+1) - \tilde{L}_3^2 - 1 \right)F_{12} &= F_{21} + \tilde{L}_+ F_{11} + \tilde{L}_- F_{22} \\
\left( J(J+1) - \tilde{L}_3^2 - 1 \right)F_{21} &= F_{12} + \tilde{L}_+ F_{11} + \tilde{L}_- F_{22} \\
\left( J(J+1) - \tilde{L}_3^2 - 2 + 2\tilde{L}_3 \right)F_{22} &= \tilde{L}_+ (F_{12} + F_{21})
\end{align*}
\]

After substitution of the functions $F_{s_1 s_2}$, Eq. (38), into the system (141) and (142) we get

\[
m_{12} = m_{21} = m_J, \quad m_{11} = m_J - 1, \quad m_{22} = m_J + 1,
\]

\[
\ell_{11} = \ell_{22} = \ell_{12} = \ell_{21} \equiv \ell,
\]
and

\[
\begin{align*}
(J(J+1) - \ell(\ell+1) - 2m_J) f^1_{11}(p) &= \sqrt{(\ell-m_J+1)(\ell+m_J)} f^1_{12}(p) \\
&+ \sqrt{(\ell-m_J+1)(\ell+m_J)} f^1_{21}(p) \\
(J(J+1) - \ell(\ell+1) - 1) f^1_{12}(p) &= f^1_{21}(p) \\
&+ \sqrt{\ell+m_J}(\ell-m_J+1) f^1_{11}(p) \\
&+ \sqrt{\ell-m_J}(\ell+m_J+1) f^1_{22}(p) \\
(J(J+1) - \ell(\ell+1) - 1) f^1_{21}(p) &= f^1_{12}(p) \\
&+ \sqrt{\ell+m_J}(\ell-m_J+1) f^1_{11}(p) \\
&+ \sqrt{\ell-m_J}(\ell+m_J+1) f^1_{22}(p) \\
(J(J+1) - \ell(\ell+1) - 2m_J) f^1_{22}(p) &= \sqrt{(\ell+m_J+1)(\ell-m_J)} f^1_{12}(p) \\
&+ \sqrt{(\ell-m_J+1)(\ell+m_J)} f^1_{21}(p) \\
&+ \sqrt{(\ell-m_J+1)(\ell+m_J)} f^1_{22}(p)
\end{align*}
\]

(145)

The solution of this system leads to two categories of relations among the functions \(f^\ell_{s_1 s_2}(p)\). The first category, which we call the trivial one, is obtained when \(f^1_{11}(p) = f^1_{22}(p) = 0\). In this case, as it easy to see from (145) and (148), we get \(f^1_{12}(p) = -f^1_{21}(p)\). This solution corresponds to the singlet states of the system with \(\ell = J\) (\(J \geq 0\)) (as follows from (146) or (147)). This simple relation allows us to write the general formula for the components \(f^\ell_{s_1 s_2}(p)\) in the following form

\[
f^\ell_{s_1 s_2}(p) = C^{(s)} m_{s_1 s_2} f^J(p),
\]

(149)

where the radial function \(f^J(p)\) is common for all components, and the coefficients \(C^{(s)} m_{s_1 s_2}\) have the following properties

\[
C^{(s)} m_{11} = C^{(s)} m_{22} = 0, \quad C^{(s)} m_{21} = -C^{(s)} m_{12} = 1.
\]

(150)

The formulas (149) and (150) with the notation \(f^\ell_{s_1 s_2}(p) \equiv f^{(s)}_{s_1 s_2}(p)\) make eq. (41) evident.

The second category corresponds to the triplet states. First of all, it is not difficult to see from (146) and (147) that \(f^\ell_{12}(p) = f^\ell_{21}(p) \equiv f^\ell(p),\) and after some simple calculations we get:

for \(\ell = J - 1\) (\(J \geq 1\)

\[
\begin{align*}
(J-m_J) f^{J-1}_{11}(p) &= \sqrt{(J-m_J)(J+m_J-1)} f^{J-1}(p) \\
(J+m_J) f^{J-1}_{22}(p) &= \sqrt{(J+m_J)(J-m_J-1)} f^{J-1}(p),
\end{align*}
\]

(151)

(152)

for \(\ell = J\) (\(J \geq 1\)

\[
\begin{align*}
m_J f^J_{11}(p) &= -\sqrt{(J+m_J)(J-m_J+1)} f^J(p) \\
m_J f^J_{22}(p) &= \sqrt{(J-m_J)(J+m_J+1)} f^J(p),
\end{align*}
\]

(153)

(154)

for \(\ell = J + 1\) (\(J \geq 0\)

\[
\begin{align*}
(J+1-m_J) f^{J+1}_{11}(p) &= -\sqrt{(J-m_J+2)(J+m_J+1)} f^{J+1}(p) \\
(J+1-m_J) f^{J+1}_{22}(p) &= -\sqrt{(J-m_J+1)(J+m_J+2)} f^{J+1}(p).
\end{align*}
\]

(155)

(156)

It is convenient to introduce the table of coefficients \(C^{(tr)} m_{s_1}\), which represent the relations in (151)-(156).

Table 5. The C-G coefficients for triplet states (total spin \(S = 1\)).
Thus, we can write the relations between the components $f_{s_1s_2}^\ell (p)$ in the compact form

$$f_{s_1s_2}^\ell (p) = C_{Jm_j}^{(tr)\ell m_s} f^\ell (p). \quad (157)$$

The coefficients $C_{Jm_j}^{(tr)\ell m_s}$ coincide with the usual Clebsch-Gordan coefficients for total spin $S = 1$ except for a factor 2 in the denominator. The expression (38) can now be written in an explicit form

$$F_{s_1s_2} (p) = C_{Jm_j}^{(tr)(J-1)m_s} f^{J-1} (p) Y_{J-1}^{m_{s_1}m_{s_2}} (\hat{p}) + C_{Jm_j}^{(tr)Jm_s} f^J (p) Y_J^{m_{s_1}m_{s_2}} (\hat{p}) + C_{Jm_j}^{(tr)(J+1)m_s} f^{J+1} (p) Y_{J+1}^{m_{s_1}m_{s_2}} (\hat{p}). \quad (158)$$

However, as is shown in Appendix B, the first and third terms have parity $P = (-1)^J$, while the second term has parity $P = (-1)^{J+1}$. Thus, we get the result (56) by suppressing the second term in (158). The second term in (158) is associated with the singlet solution (42) for the mixed-spin states, which have the same parity.

**Appendix B: Parity and charge conjugation**

We consider the application of the parity operator to the trial state (24):

$$\hat{P} |\psi_{\text{trial}}\rangle = \sum_{s_{1s_2}} \int d^3p F_{s_{1s_2}} (p) \hat{P} b_{ps_1}^\dagger D_{ps_2}^\dagger |0\rangle = \sum_{s_{1s_2}} \int d^3p F_{s_{1s_2}} (p) \hat{P} b_{ps_1}^\dagger \hat{P}^{-1} D_{ps_2}^\dagger \hat{P}^{-1} |0\rangle. \quad (159)$$

Making use of the properties

$$\hat{P} b_{ps_1}^\dagger \hat{P}^{-1} = \eta^P b_{ps_1}^\dagger, \quad \hat{P} D_{ps_2}^\dagger \hat{P}^{-1} = -\eta^P D_{ps_2}^\dagger, \quad \hat{P} |0\rangle = |0\rangle, \quad (160)$$

where $\eta^P$ is the intrinsic parity ($\langle \eta^P \rangle^2 = 1$), it follows that

$$\hat{P} |\psi_{\text{trial}}\rangle = \sum_{s_{1s_2}} \int d^3p F_{s_{1s_2}} (p) \hat{P} b_{ps_1}^\dagger D_{ps_2}^\dagger |0\rangle = -\sum_{s_{1s_2}} \int d^3p F_{s_{1s_2}} (-p) b_{ps_1}^\dagger D_{ps_2}^\dagger |0\rangle = P \sum_{s_{1s_2}} \int d^3p F_{s_{1s_2}} (p) b_{ps_1}^\dagger D_{ps_2}^\dagger |0\rangle, \quad (161)$$

where the parity eigenvalue $P$ depends on the symmetry of $F_{s_{1s_2}} (p)$ in different states. For the singlet states ($\ell = J$) we get from (36) $F_{s_{1s_2}} (-p) = (-1)^J F_{s_{1s_2}} (p)$, so $P = (-1)^{J+1}$. For the triplet states with $\ell = J$ we get from (47) $F_{s_{1s_2}} (-p) = (-1)^J F_{s_{1s_2}} (p)$, so $P = (-1)^{J+1}$. For the triplet states with $\ell = J \pm 1$ we get from (56) $F_{s_{1s_2}} (-p) = (-1)^{J+1} F_{s_{1s_2}} (p)$, so $P = (-1)^{J+1}$.

Charge conjugation is associated with the interchange of the particle and antiparticle. Applying the charge conjugation operator to the trial state of the form (24) we get

$$\hat{C} |\psi_{\text{trial}}\rangle = \sum_{s_{1s_2}} \int d^3p F_{s_{1s_2}} (p) \hat{C} b_{ps_1}^\dagger D_{ps_2}^\dagger |0\rangle = \sum_{s_{1s_2}} \int d^3p F_{s_{1s_2}} (p) \hat{C} b_{ps_1}^\dagger \hat{C}^{-1} D_{ps_2}^\dagger \hat{C}^{-1} |0\rangle. \quad (162)$$
Using the relations
\[ \hat{C} b_{ps1}^\dagger \hat{C}^{-1} = \eta^C d_{ps1}^\dagger, \quad \hat{C} d_{ps2}^- \hat{C}^{-1} = \eta^C b_{ps2}^\dagger, \quad \hat{C} |0\rangle = |0\rangle, \] (163)
where \((\eta^C)^2 = 1\), we obtain
\[ \hat{C} |\psi_{\text{trial}}\rangle = \sum_{s_1s_2} \int d^3p F_{s_1s_2}(p) \hat{C} b_{ps1}^\dagger d_{ps2}^- |0\rangle = -\sum_{s_1s_2} \int d^3p F_{s_2s_1}(p) b_{ps1}^\dagger d_{ps2}^- |0\rangle \]
where the charge conjugation quantum number \(C\) depends on the symmetry of \(F_{s_1s_2}(p)\) in different states.
For the singlet states \((\ell = J)\) we get from (42) \(F_{s_1s_2}(-p) = (-1)^{J+1} F_{s_1s_2}(p)\), so \(C = (-1)^J\).
For the triplet states with \(\ell = J\) we get from (47) \(F_{s_1s_2}(-p) = (-1)^J F_{s_1s_2}(p)\), so \(C = (-1)^{J+1}\).
For the triplet states with \(\ell = J \pm 1\) we get from (56) \(F_{s_1s_2}(-p) = (-1)^{J+1} F_{s_1s_2}(p)\), so \(C = (-1)^J\).

**Appendix C: Expansion of the spinors and \(\mathcal{M}\)-matrix elements**

We recall the form of the particle spinors:
\[ u(p,i) = N_p \left[ \frac{1}{\omega_p + \sigma_p} \right] \varphi_i, \] (165)
where
\[ \varphi_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad \varphi_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \quad N_p = \sqrt{\frac{\omega_p + m_1}{2m_1}}. \] (166)
The antiparticle or “positron” representation for the \(v_i(p)\) spinors has the form
\[ v(p,i) = N_p \left[ \frac{\omega_p - m_1}{\omega_p + \sigma_p} \right] \chi_i; \] (167)
where
\[ \chi_1 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \quad \chi_2 = -\begin{bmatrix} 1 \\ 0 \end{bmatrix}. \] (168)
The normalization is
\[ \overline{v}(p,i) u(p,j) = \delta_{ij}, \quad \overline{v}(p,i) v(p,j) = -\delta_{ij}. \] (169)
Expanding in powers of \(p/m_1\) and keeping the lowest order non-trivial terms,
\[ \frac{(\sigma^2 p)}{\omega_p + m_1} \approx \frac{(\sigma^2 p)}{2m_1}, \] (170)
\[ N_p = \sqrt{\frac{\omega_p + m_1}{2m_1}} \approx 1 + \frac{p^2}{8m_1^2}, \] (171)
we obtain the result
\[ u(p,i) \approx \left(1 + \frac{p^2}{8m_1^2}\right) \left[ \frac{1}{\sigma^2 p} \right] \varphi_i = \left[ \frac{1}{\sigma^2 p} \left(\frac{1 + \frac{p^2}{8m_1^2}}{2m_1}\right)\right] \varphi_i, \] (172)
\[ v(p,i) \approx \left(1 + \frac{p^2}{8m_1^2}\right) \left[ \frac{\sigma^2 p}{2m_1} \right] \chi_i = \left[ \frac{\sigma^2 p}{2m_1} \left(1 + \frac{p^2}{8m_1^2}\right)\right] \chi_i. \] (173)
The \( M \)- matrix elements (69)-(72) have the following nonzero components:

**Orbital**

\[
M_{1111}^{(orb)}(q, p) = \left( \frac{1}{m_1 m_2} \right)^2 \left( \frac{1}{m_1} + \frac{m_1}{m_2} \right) \frac{(p - q)^2}{(p - q)^2},
\]

\[
M_{1212}^{(orb)}(q, p) = M_{2112}^{(orb)}(q, p) = M_{2222}^{(orb)}(q, p) = \left( \frac{1}{m_1 m_2} \right)^2 \left( \frac{1}{m_1} + \frac{m_1}{m_2} \right) \frac{(p - q)^2}{(p - q)^2},
\]

**Spin-orbit**

\[
M_{1111}^{(s-o)}(q, p) = \left( \frac{1}{m_1 m_2} \right)^2 \left( \frac{1}{m_1} + \frac{m_1}{m_2} \right) \frac{(p - q)^2}{(p - q)^2},
\]

\[
M_{1222}^{(s-o)}(q, p) = \left( \frac{1}{m_1 m_2} \right)^2 \left( \frac{1}{m_1} + \frac{m_1}{m_2} \right) \frac{(p - q)^2}{(p - q)^2},
\]

**Spin**

\[
M_{1111}^{(s-s)}(q, p) = \left( \frac{1}{m_1 m_2} \right)^2 \left( \frac{1}{m_1} + \frac{m_1}{m_2} \right) \frac{(q - q)^2}{(q - q)^2},
\]

\[
M_{1112}^{(s-s)}(q, p) = \left( \frac{1}{m_1 m_2} \right)^2 \left( \frac{1}{m_1} + \frac{m_1}{m_2} \right) \frac{(q - q)^2}{(q - q)^2},
\]

\[
M_{1212}^{(s-s)}(q, p) = \left( \frac{1}{m_1 m_2} \right)^2 \left( \frac{1}{m_1} + \frac{m_1}{m_2} \right) \frac{(q - q)^2}{(q - q)^2},
\]
Here \( p = (p_1, p_2, p_3) \) and

\[
\begin{align*}
p_+ &= p_1 + i p_2 = -\frac{\sqrt{8\pi}}{3} p Y_1^1 (\theta, \varphi), \\
p_- &= p_1 - i p_2 = \frac{\sqrt{8\pi}}{3} p Y_1^{-1} (\theta, \varphi), \\
p_3 &= \sqrt{\frac{4\pi}{3}} p Y_1^0 (\theta, \varphi).
\end{align*}
\]

(186)

For a particle-antiparticle system the annihilation components are

\[
\mathcal{M}^{anh}_{1111} = \mathcal{M}^{anh}_{2222} = \frac{ie^2}{2m^2},
\]

(188)

\[
\mathcal{M}^{anh}_{1212} = \mathcal{M}^{anh}_{1221} = \mathcal{M}^{anh}_{2112} = \mathcal{M}^{anh}_{2121} = \frac{ie^2}{4m^2}.
\]

(189)

**Appendix D: Some useful expressions, identities and integrals**

The following expressions and identities are useful for evaluating the \( \mathcal{M} \)-matrix:

\[
\frac{1}{(q - p)^2} = \frac{2\pi}{|p||q|} \sum_{\lambda} Q_{\lambda}(z) \sum_{m_{\lambda} = -\lambda}^+ \frac{Y_{\lambda}^{m_{\lambda}}(\hat{p}) Y_{\lambda}^{m_{\lambda}}(\hat{q})}{2},
\]

(190)

where \( z = (p^2 + q^2)/2pq \), and \( Q_{\lambda}(z) \) is the Legendre function of the second kind of order \( \lambda \) [17]. Then

\[
\frac{((p - q) \cdot p)^2}{(p - q)^4} = \frac{p^2}{(p - q)^2} - \frac{(p \times q)^2}{(p - q)^4}.
\]

(191)

The angular integration in (58), (59), (64) involves the following integrals

\[
\int d\hat{p} d\hat{q} f (\hat{p} \cdot \hat{q}) Y_{J}'^{m_J} (\hat{q}) Y_{J'}^{m_{J'}} (\hat{p}) = 2\pi \delta_{J,J'} \delta_{m_{J},m_{J'}} \int d\hat{p} d\hat{q} f (\hat{p} \cdot \hat{q}) P_J (\hat{p} \cdot \hat{q}),
\]

(192)

\[
\int d\hat{p} d\hat{q} \frac{\hat{p} \cdot \hat{q}}{(p - q)^2} P_J (\hat{p} \cdot \hat{q}) = \frac{1}{|p||q|} \left( \frac{J+1}{2J+1} Q_{J+1} (z) + \frac{J}{2J+1} Q_{J-1} (z) \right),
\]

(193)

\[
\int d\hat{p} d\hat{q} \frac{(p \times q)^2}{(p - q)^2} P_J (\hat{p} \cdot \hat{q}) = \frac{(J+1)(J+2)}{2(2J+1)} Q_{J+1} (z) - \frac{J(J-1)}{2(2J+1)} Q_{J-1} (z).
\]

(194)

Here \( f (\hat{p} \cdot \hat{q}) \) is an arbitrary function of \( \hat{p} \cdot \hat{q} \), \( P_J (x) \) is the Legendre polynomial of order \( J \).

The integrals in the form

\[
\int d\hat{p} Y_{J}^{m_J,*,*} (\hat{p}) Y_{J'}^{m_{J''}} (\hat{p}) Y_{J'''}^{m_{J'''}} (\hat{p})
\]

(195)

can be calculated using the Wigner-Eckart theorem [17].

The calculation of the relativistic energy corrections involves the integrals

\[
\int_0^\infty \int_0^\infty dp dq p^2 q^2 f^{\prime}(p)f^{\prime}(q) = 2\pi \left( \frac{\alpha m_e}{n} \right)^3 \delta_{J,0},
\]

(196)

\[
\int_0^\infty \int_0^\infty dp dq pf^{\prime}(p)f^{\prime}(q)Q_{J}(z_1) = \frac{\pi\alpha m_e}{n^2},
\]

(197)
\[
\int_0^\infty \int_0^\infty dp dq p^2 q^2 f^J(p)f^J(q)Q_J(z_1) = \\
\int_0^\infty \int_0^\infty dp dq p^3 q f^J(p)f^J(q)Q_J(z_1) = \frac{\pi}{n} \left( \frac{4}{2J+1} - \frac{1}{n} \right),
\]
\[
\int_0^\infty \int_0^\infty dp dq p^2 q^2 f^J(p)f^J(q)Q_J-1(z_1) = \frac{\pi}{n} \left( \frac{2}{J} - \frac{1}{n} \right),
\]
\[
\int_0^\infty \int_0^\infty dp dq p^2 q f^J(p)f^J(q)Q_J+1(z_1) = \frac{\pi}{n} \left( \frac{2}{J+1} - \frac{1}{n} \right).
\]

Here \( f^J \) is the nonrelativistic hydrogen-like radial wave function in momentum space [18]

\[
f^J(p) = \frac{2}{\pi} \frac{(n-J-1)!}{(n+J)!} \left( \frac{n^2 p^2 - 1}{(n^2 p^2 + 1)} \right)^{1/2} G_n^{J+1}(x),
\]

where \( G_n^{J+1}(x) \) are the Gegenbauer functions.

**Appendix E: Diagonalization of the expectation value of the Hamiltonian**

The matrix representation of the perturbing Hamiltonian \( \Delta \hat{H} = \hat{H} - \hat{H}_{NR} - M \), in the basis of the states \( | sg \rangle, | tr \rangle \) (48), (49), is \((J \neq 0)\)

\[
\langle \psi | \Delta \hat{H} | \psi \rangle_{t=0} = |a_{ij}| \quad (i, j = 1, 2),
\]

where the matrix elements \( a_{ij} \) are

\[
a_{11} = \langle sg | \Delta \hat{H} | sg \rangle = -\frac{\alpha^4 m_r}{n^3} \left( \frac{1}{2J+1} - \left( \frac{m_r}{M} \right) \frac{1}{8n} \right),
\]

\[
a_{22} = \langle tr | \Delta \hat{H} | tr \rangle = \frac{\alpha^4 m_r}{n^3} \left( \frac{1}{2J+1} - \frac{1}{8n} \right),
\]

\[
a_{12} = a_{21} = \langle sg | \Delta \hat{H} | tr \rangle = \langle tr | \Delta \hat{H} | sg \rangle = \frac{\alpha^4 m_r (m_1 - m_2)}{n^3} \frac{1}{2M} \frac{1}{2J+1} \frac{1}{\sqrt{J(J+1)}},
\]

Note that, in the case of positronium, the elements \( a_{11} \) and \( a_{22} \) give the energy corrections for pure singlet and triplet states respectively. Diagonalization of this matrix leads to (103) with eigenvectors (54).

**Appendix F: \( K_{12}, \ K_{21} \) kernels for \( l=J \neq 1 \) states**

The contribution to the energy correction due to the kernel \( K_{12} \) is

\[
\int dp dq p^2 q^2 K_{12}(p, q) f^{J-1}(p)f^{J+1}(q),
\]

where

\[
K_{12}(p, q) = \sum_{\sigma_1 \sigma_2 \sigma_1' \sigma_2'} C_{Jm_{j12}}^{\sigma_1 \sigma_2 \sigma_1' \sigma_2'} \int d\tilde{p} d\tilde{q} M_{Jm_{j12}}^{opc(s-s)}(\tilde{p}, \tilde{q}) Y_{J+1}^{m_{J12}}(\tilde{q}) Y_{J-1}^{-m_{J12}}(\tilde{p}).
\]
This requires the following integral

$$
\sum_{\sigma_1 \sigma_2 \sigma_1 \sigma_2} C_{\sigma_1 \sigma_2 \sigma_1 \sigma_2}^{J_m J_{m_2}} \int d^3p \, d^3q \, f^{J-1}(p)Y_{J_{m_2}}^{\dagger} \cdot (p) \mathcal{M}_{\sigma_1 \sigma_2 \sigma_1 \sigma_2}^{\text{pec}(s-s)} \cdot (p, q) \, f^{J+1}(q)Y_{J_{m_1}}^{\dagger} \cdot (q). \tag{208}
$$

We calculate this form in coordinate space. The Fourier transforming of $\mathcal{M}_{\sigma_1 \sigma_2 \sigma_1 \sigma_2}^{\text{pec}(s-s)} (p, q)$ is

$$
\mathcal{M}_{\sigma_1 \sigma_2 \sigma_1 \sigma_2}^{\text{pec}(s-s)} (p, q) = \int d^3r d^3r' \, \mathcal{M}_{\sigma_1 \sigma_2 \sigma_1 \sigma_2} (r, r') \, e^{-i(p \cdot q)(r-r')}, \tag{209}
$$

where the $\mathcal{M}_{\sigma_1 \sigma_2 \sigma_1 \sigma_2} (r, r')$ matrix in general is a local operator [16]

$$
\mathcal{M}_{\sigma_1 \sigma_2 \sigma_1 \sigma_2} (r, r') = \mathcal{M}_{\sigma_1 \sigma_2 \sigma_1 \sigma_2} (r) \, \delta (r-r'). \tag{210}
$$

We apply this transformation to the $\mathcal{M}_{\sigma_1 \sigma_2 \sigma_1 \sigma_2}^{\text{pec}(s-s)} (p, q)$-matrix (see (71)). Because of the angular integration in (207), only the first term of (71) contributes. The Fourier transformation of that term is

$$
\frac{(\vec{\sigma_2} \cdot (p - q)) (\vec{\sigma_1} \cdot (p - q))}{4(p - q)^2} \rightarrow \frac{3}{16 \pi r^2} \left( \frac{\vec{\sigma_2} \cdot r}{r} \right) \left( \frac{\vec{\sigma_1} \cdot r}{r} \right). \tag{211}
$$

Furthermore,

$$
\int d^3p \, f^{J-1}(p)Y_{J_{m_2}}^{\dagger} \cdot (p) e^{-ip \cdot r} = R_n^{J-1}(r)Y_{J_{m_2}}^{\dagger}(r), \tag{212}
$$

$$
\int d^3q \, f^{J+1}(q)Y_{J_{m_1}}^{\dagger} \cdot (q) e^{-iq \cdot r} = R_n^{J+1}(r)Y_{J_{m_1}}^{\dagger}(r), \tag{213}
$$

where

$$
R_n^\ell (r) = - \frac{2}{n^2} \sqrt{n - \ell - 1}! \ell! \left( \frac{2r}{n} \right)^{\ell} r^\ell \left( \frac{2r}{n} \right)^{\ell}. \tag{214}
$$

The associated Laguerre functions $L_\lambda^\mu (\rho)$ are related to the confluent hypergeometric functions by

$$
L_\lambda^\mu (\rho) = (-1)^\mu \frac{\lambda!}{\mu!(\lambda - \mu)!} F (-\lambda + \mu, \mu + 1; \rho). \tag{215}
$$

The generating function for the Laguerre functions is

$$
U_\mu (\rho, u) \equiv (-1)^\mu \frac{u^\mu}{(1 - u)^{\mu+1}} \exp \left( - \frac{u \rho}{1 - u} \right) = \sum_{\lambda=\mu}^\infty \frac{L_\lambda^\mu (\rho)}{\lambda!} u^\lambda, \tag{216}
$$

hence

$$
\sum_{\sigma_1 \sigma_2 \sigma_1 \sigma_2} C_{\sigma_1 \sigma_2 \sigma_1 \sigma_2}^{J_m J_{m_2}} \int d^3p \, d^3q \, f^{J-1}(p)Y_{J_{m_2}}^{\dagger} \cdot (p) \mathcal{M}_{\sigma_1 \sigma_2 \sigma_1 \sigma_2}^{\text{pec}(s-s)} \cdot (p, q) \, f^{J+1}(q)Y_{J_{m_1}}^{\dagger} \cdot (q)
\begin{align*}
&= \sum_{\sigma_1 \sigma_2 \sigma_1 \sigma_2} C_{\sigma_1 \sigma_2 \sigma_1 \sigma_2}^{J_m J_{m_2}} \int d^3r \, R_n^{J-1}(r)Y_{J_{m_2}}^{\dagger}(r) \left( 3\alpha \frac{(\vec{\sigma_2} \cdot r)}{16 \pi m_1 m_2 r^2} \right) R_n^{J+1}(r)Y_{J_{m_1}}^{\dagger}(r) \\
&= \frac{3\alpha}{16 \pi m_1 m_2} \int dr \, (\vec{r} \cdot \vec{r}) \left( \frac{1}{r^3} R_n^{J-1}(r) \right) R_n^{J+1}(r) \times \\
&\quad \times \sum_{\sigma_1 \sigma_2 \sigma_1 \sigma_2} C_{\sigma_1 \sigma_2 \sigma_1 \sigma_2}^{J_m J_{m_2}} \int d\vec{r} \, Y_{J_{m_2}}^{\dagger}(\vec{r}) \left( \vec{\sigma_2} \cdot \vec{r} \right) \left( \vec{\sigma_1} \cdot \vec{r} \right) Y_{J_{m_1}}^{\dagger}(\vec{r}).
\end{align*} \tag{217}
$$
We can show, that
\[ \sum_{\sigma_1 \sigma_2} C_{J m_{j_1 j_2}}^{s_1 s_2 \sigma_1 \sigma_2} \int d\mathbf{r} Y_{j_1 j_2}^{m_{j_1 j_2}}(\hat{\mathbf{r}}) (\mathbf{\sigma}_2 \cdot \hat{\mathbf{r}}) (\mathbf{\sigma}_1 \cdot \hat{\mathbf{r}}) Y_{J+1}^{m_{j_1 j_2}}(\hat{\mathbf{r}}) = \frac{1}{15} \sqrt{J(J+1)} \frac{J}{2J+1}, \] (218)
but
\[ \int_0^\infty dr r^2 \frac{1}{r} R_{n\ell}^{J-1}(r) R_{n\ell}^{J+1}(r) = 0. \] (219)
The last expression can be proved in the following way. Let us consider the more general case
\[ \int_0^\infty dr r^{\beta+2} R_{n\ell}^\beta(r) R_{n\ell}^\beta(r). \] (220)
The generating function for $R_{n\ell}^\beta(r)$ is
\[ G_{n\ell}(r, u) = -2 \frac{2}{n} \sqrt{\frac{(n-\ell-1)!}{((n+\ell)!)} e^{-\pi/n}} \left( \frac{2r}{n} \right)^\ell (-1)^{2\ell+1} \frac{u^{2\ell+1}}{(1-u)^{2\ell+2}} \exp \left\{ - \frac{u}{1-u} \frac{2r}{n} \right\}. \] (221)
Then we consider an expression
\[
\int_0^\infty dr r^{\beta+2} G_{n\ell}(r, u) G_{n\ell'}(r, v) = \int_0^\infty dr r^{\beta+2} \frac{4}{n^2} \sqrt{\frac{(n-\ell-1)!(n-\ell'-1)!}{((n+\ell)!)^2 ((n+\ell')!)^2}} e^{-2r/n} \left( \frac{2r}{n} \right)^{\ell+\ell'} \times \\
\times \frac{u^{2\ell+1}v^{2\ell'+1}}{(1-u)^{2\ell+2} (1-v)^{2\ell'+2}} \exp \left\{ - \left( \frac{u}{1-u} + \frac{v}{1-v} \right) \frac{2r}{n} \right\} \\
= \frac{4}{n^2} \sqrt{\frac{(n-\ell-1)!(n-\ell'-1)!}{((n+\ell)!)^2 ((n+\ell')!)^2}} \frac{u^{2\ell+1}v^{2\ell'+1}}{(1-u)^{2\ell+2} (1-v)^{2\ell'+2}} \times \\
\times \int_0^\infty dr \left( \frac{2r}{n} \right)^{\beta+2+\ell+\ell'} \exp \left\{ - \left( \frac{1+u}{1-u} + \frac{v}{1-v} \right) \frac{2r}{n} \right\}. \] (222)
It is well known that
\[ \int_0^\infty d\rho \rho^\beta e^{-\rho} = \Gamma(\beta+1). \] (223)
Hence
\[
\int_0^\infty dr \left( \frac{2r}{n} \right)^{\beta+2+\ell+\ell'} \exp \left\{ - \left( \frac{1+u}{1-u} + \frac{v}{1-v} \right) \frac{2r}{n} \right\} = \left( \frac{u}{2} \right)^{\beta+3} \left( \frac{(1-u)(1-v)}{1-uv} \right)^{\beta+3+\ell+\ell'} \Gamma(\beta+3+\ell+\ell'). \] (224)
and
\[
\int_0^\infty dr r^{\beta+2} G_{n\ell}(r, u) G_{n\ell'}(r, v) = \frac{2^{\beta-1}}{n^{\beta+1}} \sqrt{\frac{(n-\ell-1)!(n-\ell'-1)!}{((n+\ell)!)^2 ((n+\ell')!)^2}} \times \\
\times \frac{u^{2\ell+1}v^{2\ell'+1}(1-u)^{\beta+1+\ell+\ell'}(1-v)^{\beta+1+\ell-\ell'}}{(1-uv)^{\beta+3+\ell+\ell'}} \Gamma(\beta+3+\ell+\ell'). \] (225)
We expand this expression in a series:

\[ \int_0^\infty dr r^{\beta+2} G_{n\ell} (r, u) G_{n\ell'} (r, v) = \sum_{\eta \eta'} C_{\eta \eta'} (n, \beta, \ell, \ell') u^\eta v^{\eta'}. \]  

(226)

It is not difficult to show [31], that the coefficient \( C_{n+\ell, n+\ell'} \) are given by the integral

\[ C_{n+\ell, n+\ell'} (n, \beta, \ell, \ell') = \int_0^\infty dr r^{\beta+2} R^\ell_n (r) R^{\ell'}_n (r). \]  

(227)

Simple but tedious calculations show that this coefficient is zero for \( \beta = -3, \ell = J - 1, \ell' = J + 1 \). Thus the kernel \( K_{12} \) does not contribute to the energy corrections at \( O(\alpha^4) \). The same result is obtained for the kernel \( K_{21} \).

References

1. J. W. Darewych, Annales Fond. L. de Broglie (Paris) 23, 15 (1998).
2. J. W. Darewych, in Causality and Locality in Modern Physics, G Hunter et al. (eds.), p. 333, (Kluwer 1998).
3. J. W. Darewych, Can. J. Phys. 76, 523 (1998).
4. M. Barham and J. W. Darewych, J. Phys. A 31, 3481 (1998).
5. B. Ding and J. Darewych, J. Phys. G 26, 907 (2000).
6. J. D. Jackson, Classical Electrodynamics (John Wiley, New York, 1975).
7. A. O. Barut, Electrodynamics and Classical Theory of Fields and Particles (Dover, New York, 1980).
8. W. T. Grandy, Relativistic Quantum Mechanics of Leptons and Fields (Kluwer, 1991).
9. A. O. Barut, in Geometrical and Algebraic Aspects of Nonlinear Field Theory, edited by S. De Filippo, M. Marinaro, G. Marmo and G. Vilasi, (Elsevier New York, 1989), p. 37.
10. A. G. Terekidj, J. W. Darewych, Preprint: arxiv,[hep-th/0303250]
11. J. W. Darewych and L. Di Leo, J. Phys. A: Math. Gen. 29, 6817 (1996).
12. J. W. Darewych and M. Horbatsch, J. Phys. B: At. Mol. Opt. 22, 973 (1989); 23, 337 (1990).
13. W. Dykshoorn and R. Konik, Phys. Rev. A 41, 64 (1990).
14. T. Zhang and R. Konik, Can. J. Phys. 70, 683 (1992).
15. T. Zhang and R. Konik, Can. J. Phys. 70, 670 (1992).
16. V. B. Berestetski, E. M. Lifshitz, and L. P. Pitaevski, Quantum Electrodynamics (Pergamon, New York, 1982).
17. G. Arfken and H. Weber Mathematical Methods for Physicists (Academic Press, 2001).
18. H. A. Bethe and E. E. Salpeter, Quantum Mechanics of One and Two-Electron Atoms (Springer-Verlag/Academic, New York, 1957).
19. M. A. Stroscio, Physics Reports C 22, 5, 215 (1975).
20. John H. Connell, Phys. Rev. D 43, 1393 (1991).
21. H. Hersbach, Phys. Rev. A 46, 3657 (1992).
22. J. W. Darewych and A. Duriryak Phys. Rev. A 66, 032102 (2002).
23. W. A. Barker, F. N. Glover, Phys. Rev. 99, 317 (1955).
24. Vernon W. Hughes, Gisbert zu Putlitz in Quantum Electrodynamics (World Scientific 1990), T. Kinoshita, edit.
25. F. M. Pipkin in Quantum Electrodynamics (World Scientific 1990), T. Kinoshita, edit.
26. H. Hellwig et al., IEEE Trans. Instrum. Meas. IM 19, 200 (1970); L. Essen et al., Nature 229, 110 (1971).
27. K. Pachucki, Phys. Rev. A 53, 2092 (1996).
28. D. Bakalov, E. Milotti, C. Rizzo, A. Vacchi and E. Zavattini, Physics Letters A 172, 277 (1993)
29. M. I. Eides, H. Grotch, V. A. Shelyuto, Phys. Report 342, 63 (2001).
30. J. R. Sapirstein, D. R. Yennie in *Quantum Electrodynamics* (World Scientific 1990), T. Kinoshita, edit.

31. M. Mizushima, *Quantum Mechanics of Atomic Spectra and Atomic Structure* (W. A. Benjamin, Inc., New York, 1970).