Leading-order relativistic corrections to the Zeeman splitting of hyperfine structure levels in two-fermion bound-state systems

Andrei G. Terekidi\textsuperscript{a}, Jurij W. Darewych\textsuperscript{b}, Marko Horbatsch\textsuperscript{c}

Department of Physics and Astronomy, York University, Toronto, Ontario, M3J 1P3, Canada
\textsuperscript{a}terekidi@yorku.ca, \textsuperscript{b}darewych@yorku.ca, \textsuperscript{c}marko@yorku.ca

Abstract

The relativistic calculations of the Zeeman splitting of hyperfine levels in two-fermion systems (hydrogen, anti-hydrogen, muonium, muonic hydrogen) are presented. Our approach is based on the variational equation for bound states derived from quantum electrodynamics [1]. Relativistic corrections to the \( g \)-factor are obtained up to \( O (\alpha^2) \). Calculations are provided for all quantum states and for arbitrary fermionic mass ratio. The results will be useful for comparison with high-precision measurements.

1. Introduction

In a recent paper [2] we have presented a self-consistent variational method for calculating the non-relativistic Landé \( g \) factor of the two-fermion bound-state system. In the lowest-order approximation the linearly dependent part of the energy splitting for a two-fermion system placed in a weak static magnetic field \( B \) can be written as [2-4]

\[
\Delta E_{J,m,J,S,\ell,s_1,s_2}^{\text{ext}} = (\mu_{B1} g_1 + \mu_{B2} g_2) B m_J,
\]

(1)

where \( J, m_J, S, \ell, s_1, s_2 \) are quantum numbers, which characterize the system: \( s_1 \) and \( s_2 \) are the spins of the first and second particle respectively, \( S = s_1 + s_2, s_1 + s_2 - 1,..., |s_1 - s_2| \) is the total spin of the particles, \( \ell \) and \( J \) represent the orbital and total angular momentum quantum numbers, where \( J = \ell + S, \ell + S - 1,..., |\ell - S| \). The projection of the total angular momentum on the \( B \) field direction is labeled by \( m_J = -J, -J + 1,..., J - 1, J \). The “Bohr magnetons” for the two particles are defined as \( \mu_{B1} = Q_1 \hbar / 2m_1c, \) and \( \mu_{B2} = -Q_2 \hbar / 2m_2c, \) where \( Q_1 = Z_1e \) and \( Q_2 = Z_2e \) represent the magnitude of the charges (\( e > 0 \)). In our notation, \( m_1 \) and \( m_2 \) correspond to the masses of the light and heavy particle respectively. The description of the interacting system by the set of quantum numbers \( J, m_J, S, \ell, s_1, s_2 \) is not conserved. In this case we designate the states by an additional quantum number \( q \), which takes on the values of 0 or 1 for quasisinglet (\( sg_q \)) and quasitriplet (\( tr_q \)) states respectively.

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In our calculations we assume that the energy-level splitting (1) is smaller than the hyperfine structure (HFS) splitting, \( \Delta E^{ext} << \Delta E^{HFS} \), i.e., we treat the interaction with an external magnetic field as a perturbation.

The \( g \)-factors in (1) can be written more generally as \( g_i = g_{iNR} + \Delta g_i^{REL} \), where \( g_{iNR} \) are the nonrelativistic Landé factors obtained in [2], and \( \Delta g_i^{REL} \) are the relativistic correction. In the next section we calculate \( \Delta g_i^{REL} \) to order \( O \left( (Z_1 Z_2 \alpha)^2 \right) \) for all quantum states and arbitrary masses of particles. In most expressions we use natural units, i.e., \( \hbar = c = 1 \), \( \alpha = e^2 / 4 \pi \). The coupling constant is defined as \( \alpha' = Z_1 Z_2 \alpha \).

### 2. Relativistic corrections to \( g \)-factors of two-fermion systems

The relativistic wave equations for two-fermion systems in the absence of external fields were derived in [1] and [6] on the basis of a modified (reformulated) QED Lagrangian [8]-[10]. In this approach a simple Fock-space trial state taken in the rest frame is

\[
\psi_{\text{trial}} = \sum_{s_1 s_2} \int d^3 p F_{s_1 s_2}(p) b^\dagger_{s_1 s_2} D^\dagger_{p s_2} |0\rangle.
\]

This form is sufficient to obtain the HFS levels correct to fourth order in the coupling constant \( \alpha' \). Here \( b^\dagger_{s_1 s_2} \) and \( D^\dagger_{q_{s_2}} \) are creation operators for a free fermion of mass \( m_1 \) and an (anti) fermion of mass \( m_2 \) respectively, and \( |0\rangle \) is the trial vacuum state such that \( b_{s_1 s_2} |0\rangle = D_{q_{s_2}} |0\rangle = 0 \). The \( F_{s_1 s_2} \) are four-component adjustable functions. The trial state is taken to be an eigenstate of total linear momentum \( \mathbf{p} = 0 \), total angular momentum squared \( \mathbf{J}^2 \), its projection \( \mathbf{J}_3 \), parity \( \mathbf{P} \), and the Hamiltonian \( \mathbf{H} \), which corresponds to the hyperfine interaction [6]. The adjustable functions \( F_{s_1 s_2}(p) \) can be specified for two categories:

1. The spin-mixed (quasi-singlet and quasi-triplet) states

   In this case we have \( \ell = J \), and the general solution under the condition of well-defined eigenvalues of \( \mathbf{P}, \mathbf{J}^2, \mathbf{J}_3 \), and \( \mathbf{P} \) can be expressed as [1], [6]

\[
F_{s_1 s_2}(p) = C_{j_{m_1 s_2}}^{(S_1)} j_{f_1}(p) Y_{j_{m_1 s_2}}(\mathbf{p}) + C_{j_{m_2 s_2}}^{(S_2)} j_{f_2}(p) Y_{j_{m_2 s_2}}(\mathbf{p}),
\]

where \( C_{j_{m_1 s_2}}^{(S_1)} = \langle \ell m_1 S m_S | J j_{m_1 s_2} \rangle \) are the Clebsch-Gordan (CG) coefficients with total spin \( S \), where \( S = 0 \) (with index \( S_1 \) ) for the singlet states and \( S = 1 \) (with index \( S_2 \) ) for the triplet states respectively. Note that \( m_1 = 1 \) if \( m_S = 1 \), \( m_1 = 0 \) if \( m_S = 0 \), and \( m_2 = -1 \) if \( m_S = 1 \). Here \( j_{f_1}(S_1)(p) \) and \( j_{f_2}(S_2)(p) \) are radial functions to be determined. They represent the contributions of spin-singlet and spin-triplet states (the total spin \( S = 0, 1 \) is not conserved in general).

2. The \( \ell \)-mixed triplet states

   These states occur for \( \ell = J \pm 1 \). Their radial decomposition can be written as

\[
F_{s_1 s_2}(p) = C_{j_{m_1 s_2}}^{(\ell_1)} j_{f_1}(p) Y_{\ell_1 m_1 s_2}^{\ell_1}(\mathbf{p}) + C_{j_{m_2 s_2}}^{(\ell_2)} j_{f_2}(p) Y_{\ell_2 m_2 s_2}^{\ell_2}(\mathbf{p}).
\]

Again, the \( C_{j_{m_1 s_2}}^{(\ell_1)} = \langle \ell_1 m_1 S m_S | J j_{m_1 s_2} \rangle \) are CG coefficients. For these states the system is characterized by \( J, m_j, \) and \( \mathbf{P} = (-1)^\ell \). The orbital angular momentum \( \ell = \ell_1,2 \) is not a good quantum number. Mixing of this type occurs only for states with principal quantum number \( n \geq 3 \).
From the variational principle \( \delta \langle \psi_{\text{trial}} | \hat{H} - E | \psi_{\text{trial}} \rangle = 0 \), where \( \hat{H} \) is the QED Hamiltonian is invoked to obtain a momentum-space wave equation \([1]\), we get a system of coupled radial equations expressed in matrix form as

\[
(\omega_p + \Omega_p - E) F(p) = \frac{m_1 m_2}{(2\pi)^3} \int \frac{d^3q}{\sqrt{\omega_q \Omega_q \Omega_p \Omega_p}} K(p, q) F(q),
\]

where \( \omega_p^2 = p^2 + m_1^2 \) and \( \Omega_p^2 = p^2 + m_2^2 \), and \( q = |q| \). Here \( F(p) \) is the two-component matrix of radial functions \( F^\dagger(p) = \begin{bmatrix} f_f^{(S_1)}(p) & f_f^{(S_2)}(p) \end{bmatrix} \), \( f_f(p) = f_f(p) f_f(p) \) for spin-mixed and \( \ell \)-mixed states respectively. The kernel of this equation is the \( 2 \times 2 \) matrix \( K_{ij} = \mathcal{K}_{ij} \), which has the following form

\[
\mathcal{K}_{ij} = -i \sum_{s_1 s_2 \sigma_1 \sigma_2} C_{s_1 s_2 \sigma_1 \sigma_2}^{i j} \int d^3q d\hat{p} \ Y_{\ell_1}^{m_{s_1 s_2} \sigma_1 \sigma_2}(\hat{p}) Y_{\ell_j}^{m_{s_1 s_2} \sigma_1 \sigma_2}(\hat{q}) \tilde{\mathcal{M}}_{s_1 s_2 \sigma_1 \sigma_2}(p_1, p_2, q_1, q_2). \]

(5)

Here the \( C_{s_1 s_2 \sigma_1 \sigma_2}^{i j} \) are related to the CG coefficients by: \( C_{s_1 s_2 \sigma_1 \sigma_2}^{i j} = C_{j_{s_1 s_2} \sigma_1 \sigma_2}^{j_{s_1 s_2} \sigma_1 \sigma_2} C_{j_{s_1 s_2} \sigma_1 \sigma_2}^{j_{s_1 s_2} \sigma_1 \sigma_2} \) and \( C_{j_{s_1 s_2} \sigma_1 \sigma_2}^{i j} = C_{j_{s_1 s_2} \sigma_1 \sigma_2}^{j_{s_1 s_2} \sigma_1 \sigma_2} C_{j_{s_1 s_2} \sigma_1 \sigma_2}^{j_{s_1 s_2} \sigma_1 \sigma_2} \) for the spin- and \( \ell \)-mixed states respectively. For the spin-mixed states we should take \( \ell_i \equiv \ell_j \equiv \ell \). The inter-particle interaction is represented by the generalized invariant matrix \( \tilde{\mathcal{M}} = \sum_{n=1}^\infty \mathcal{M}^{(n)} \), obtained as part of the derivation. It includes reducible and irreducible effects in all orders of the coupling constant \( \alpha' \), and the sum contains all relevant Feynman diagrams. A discussion of the derivation and structure of the \( \tilde{\mathcal{M}} \)-matrix to one-loop level is provided in \([1]\). This equation allows one to obtain, in principle, all relativistic and QED corrections to the \( g \)-factor.

The lowest-order QED corrections appear within the term \( \mathcal{M}^{(2)} \) and can be formally included in the intrinsic factor \( g_{\alpha j} \), however we shall not do so in this work. In this paper we restrict our consideration to the first term \( \mathcal{M}^{(1)} \) of the expansion, i.e., only tree level diagrams are included. The term \( \mathcal{M}^{(1)} \) contains only relativistic corrections and it can be broken into two parts, namely \( \mathcal{M}^{(1)} = \mathcal{M}^{\text{tree}} + \mathcal{M}^{\text{ext}} \), where \( \mathcal{M}^{\text{tree}} \) is the usual invariant matrix element, corresponding to the one-photon exchange Feynman diagram \([1]\). The element \( \mathcal{M}^{\text{ext}} \) represents the interaction with a given external classical field \( A^{\mu}_{\text{ext}} \).

\[
\mathcal{M}^{\text{ext}} = (2\pi)^{3/2} \left( \frac{\sqrt{m_2 \Omega_p \Omega_q Q_1}}{m_2} A^{\mu}_{\text{ext}}(p_1 - q_1) \overline{\pi}(p_1, s_1) \gamma^\mu u(q_1, \sigma_1) \delta_{s_2 \sigma_2} + \frac{\sqrt{m_1 \Omega_p \Omega_q Q_2}}{m_1} A^{\mu}_{\text{ext}}(q_2 - p_2) \overline{\pi}(p_2, \sigma_2) \gamma^\mu V(q_2, s_2) \delta_{s_1 \sigma_1} \right). \]

(6)

The non-relativistic limit of this matrix element was considered in \([2]\). Using the relativistic expansion of the expression \( \overline{\pi}(p_1, s_1) \gamma^\mu u(q_1, \sigma_1) \) up to order \( 1/c^3 \) we obtain the lowest-order relativistic correction to \( \mathcal{M}^{\text{ext}} \). The solution of equation (4) including only the first two terms with the \( \mathcal{M}^{\text{tree}} \) and \( \mathcal{M}^{(1)\text{ext}} \) matrices was discussed in \([2]\). This solution describes the Zeeman splitting of the HFS energy levels in the non-relativistic limit. In order to obtain the Landé factors to order \( O(\alpha'^2) \) we solve the radial equation (4) with the additional term \( \mathcal{M}^{(2)\text{ext}} \) in the kernel (5), which is evaluated perturbatively using hydrogen-like radial functions in momentum space \([4]\).
The calculations are straightforward, and yield the relativistic corrections to the \( g \)-factor for both particles of the system. We obtain for the triplet states

\[
\Delta g_i^{\text{REL}} = -\frac{\mu_i^2}{2} \left( \mu_j + \frac{\mu_i}{\mu'} - \frac{1}{2J+1} \right) \left( \frac{\alpha'}{n} \right)^2,
\]

where \( \mu' = J \), when \( l = J - 1 \), and \( \mu' = J + 1 \), when \( l = J + 1 \). For the spin-mixed states we have \((l = J)\)

\[
\Delta g_i^{\text{REL}} = -\frac{\mu_i^2}{2} \left( \mu_j + \mu_i \frac{1 + \xi}{4J(J+1)} \right) \left( \frac{\alpha'}{n} \right)^2.
\]

The mass factors \( \mu_i \) are defined as \( \mu_i = m_i / (m_1 + m_2) \), where \( i = 1, 2 \) is the index designating the particle. The index \( j \) is defined as \( j = 1 \) when \( i = 2 \), and \( j = 2 \) when \( i = 1 \). The parameter \( \xi \) is defined as \( \xi = (4(\mu_1 - \mu_2)^2 J(J+J+1)^{-1/2} \). The upper and lower sign in (8) corresponds to \( sg \) and \( tr \) states respectively. Our result (7)-(8) is applicable to a system of two equal masses (positronium). However, up to the order we consider here, due to a symmetry of the system like positronium (\( \mu_{Be^{-}}g_{e^{-}} = -\mu_{Be^{+}}g_{e^{+}} \)), the total effect of the energy splitting (1) is zero.

There are several works based on the Breit equation (e.g. [11]-[15]), where the relativistic corrections to the \( g \)-factor of two-fermion bound states were considered. Some of the calculations were obtained only for small mass ratio [11]; in others the orbital motion of the heavy particle was ignored [12]. These calculations did not take into account the mixed nature of the quantum states. We emphasize, that only mixed states diagonalize the Hamiltonian of HFS [2], [6]. Our result (7)-(8) is new and overcomes the above-mentioned shortcomings. For the relatively simple case of the ground state \( 1S_{1/2} \) (\( J = 1 \), \( \mathcal{P} = -1 \)) our results agree with the previous result of Hegstrom [13] and Grotch [14], namely \( \Delta g_i^{\text{REL}} = -\mu_i^2 \alpha^2 / 3 \). Note that their definition of \( g_e \) based upon \( \Delta E_e = \mu B g_e B m_e \), Eq. (12) of [13], differs by a factor of 2 from our definition (1).

We provide our result (7), (8) in numerical form for the lighter particle in atomic hydrogen, muonium, and muonic hydrogen, for which \( \alpha' = \alpha \). We consider only states with principal quantum number \( n = 1, 2 \). We used the following values for the mass ratios: \( m_e/m_p = 5.4461702 \times 10^{-4} \) and \( m_p/m_\mu = 8.8802433 \). The fine-structure constant is taken as \( \alpha = 7.2973523 \times 10^{-3} \).

Table. The relativistic correction \( \Delta g_i^{\text{REL}} \) to the Landé factor for \( n = 1, 2 \) states in hydrogen, muonium and muonic hydrogen.

| \( n \)     | \( 1S_{1/2}(J=1) \) | \( 2S_{1/2}(J=1) \) | \( 2P_{1/2}(J=1) \) | \( 2P_{3/2}(J=1) \) | \( 2P_{3/2}(J=2) \) |
|-----------|----------------------|----------------------|----------------------|----------------------|----------------------|
| \( pe^- \) | -0.0000177           | -0.0000044           | -0.0001331           | -0.0001331           | -0.0000053           |
| \( \mu^+e^- \) | -0.0000176          | -0.0000044           | -0.0001313           | -0.0001313           | -0.0000053           |
| \( p^+\mu^- \) | -0.0000143         | -0.0000036           | -0.0000999           | -0.0000998           | -0.0000040           |

For the systems considered in the Table the relativistic corrections for the heavier particle \( \Delta g_2^{\text{REL}} \) are negligible in comparison with \( \Delta g_1^{\text{REL}} \) due to the small mass factor \( \mu_1 \). For a realistic comparison of the \( g \)-factor with experiment one would also need to calculate the
QED corrections up to second order in $\alpha$, that is the higher order matrix element $\mathcal{M}^{(2)}$ would have to be included.

In our calculations we assumed that the trial state is an eigenstate of the total linear momentum operator $\hat{P}$. However this is only an approximation, because one can show that the operator $\hat{P}$ does not commute with the HFS Hamiltonian. To fix this problem we need to modify the trial state, or use an appropriate unitary transformation for the HFS Hamiltonian. The latter approach was discussed in the literature [11], [12], [15]. An analysis shows, that in our case the unitary transformation leads to the appearance of additional terms in the invariant $\mathcal{M}$-matrix. This is a technically difficult problem which we postpone for the future.

We note that, in contrast to the Breit approach, the anomalous magnetic moment is not introduced from another calculation. As discussed below equation (5) all QED effects are contained in the $\mathcal{M}$-matrix. The anomalous magnetic moment will appear naturally in our calculations if we include the next term $\mathcal{M}^{(2)}$ of the expansion of $\mathcal{M}$-matrix. The present work will be of practical importance when these measurements will be extended to all $n = 2$ (or higher-$n$) levels.

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