

Atomic Two-Body \((Z\alpha)^6\) Predictions

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For muonic hydrogen, positronium, and ordinary hydrogen, we show that the existence of a relativistic two-body wave equation whose energy levels are physically accurate to order \((Z\alpha)^4\) (where \(Z\alpha\) is the binding coupling constant) implies a previously unknown two-body Sommerfeld energy formula which can be used to predict energy terms to order \((Z\alpha)^6\) using simple algebra. Two such terms are verified to be physically correct by earlier \((Z\alpha)^6\) calculations for positronium. For muonic hydrogen and ordinary hydrogen, these terms are predictions.

I. INTRODUCTION

Although the Dirac equation for a single fermion in a static Coulomb field was solved analytically in 1928 [1], including the derivation of the single-particle Sommerfeld formula expressing the energy levels to any order in the binding coupling constant never been found for atomic two-particle systems such as muonic hydrogen, positronium, and ordinary hydrogen. For these atomic systems, energy levels have always been calculated using first-order perturbation theory to obtain energy levels to order \((Z\alpha)^4\), and second-order perturbation theory to find energy levels to order \((Z\alpha)^6\).

In this note we demonstrate a possible first step towards an analytic solution to the atomic two-body bound-state problem. It is shown that a two-body relativistic wave equation which predicts physically accurate energy levels to order \((Z\alpha)^4\) also leads to a new, two-body, Sommerfeld energy-level formula which, by simple algebra, predicts two energy-level terms in order \((Z\alpha)^6\) which have already been found to be physically correct in positronium by various authors. These terms constitute predictions for ordinary hydrogen and muonic hydrogen.

We start with the new predictions. Afterwards we will state the two-body relativistic wave equation and show how it leads to the two-body Sommerfeld formula.

II. PREDICTIONS

The simple condition that the two-body relativistic wavefunction exists leads directly to what we believe is the first known two-body Sommerfeld energy formula:

\[
E = \sqrt{m^2 + M^2 + \frac{2mmM}{(Z\alpha)^2} + \frac{2mM}{(Z\alpha)^2 + (N + \Delta \epsilon)^2}} \tag{1}
\]

Here \(m\) and \(M\) are the masses of the bound particles and \(N\) is the Bohr quantum number. The quantity

\[
\Delta \epsilon = (Z\alpha)^2 \epsilon_2 + (Z\alpha)^4 \epsilon_4 + (Z\alpha)^6 \epsilon_6 + \cdots \tag{2}
\]

is a function of the total system spin \(F\), and of mixtures of \(L\) and \(S\). The leading coefficient \(c_2\) is evaluated below.

With the usual definition \(\mu = mM/(m+M)\), and using the abbreviation \(x = \mu/(m+M)\), the expansion of (1) in powers of \((Z\alpha)^2\) gives

\[
E = m + M + C_2 (Z\alpha)^2 \mu + C_4 (Z\alpha)^4 \mu + C_6 (Z\alpha)^6 \mu + \cdots \tag{3}
\]

in which

\[
C_2 = -\frac{1}{2N^2} \tag{4}
\]

\[
C_4 = \frac{3 - x}{8N^4} + \frac{\epsilon_2}{N^3} \tag{5}
\]

\[
C_6 = -\frac{5 - 3x + x^2}{16N^6} - \frac{(3 - x)\epsilon_2}{2N^5} - \frac{3\epsilon_2^2}{2N^4} + \frac{\epsilon_4}{N^3} \tag{6}
\]

Equation (5) shows that the leading coefficient \(\epsilon_2\) in (2) can be read off from an ordinary first-order-perturbation calculation of the energy. This will be done in Sec. III, in which \(\epsilon_2\) is shown as eqn. (14). Therefore \(\epsilon_2\) is known.

Equation (6) contains four \((Z\alpha)^6\) energy terms, three of which can be predicted since \(\epsilon_2\) is known. We shall see that two of these simple predictions agree with far more complicated perturbation calculations in the case of positronium, whose \((Z\alpha)^6\) terms have already been worked out by various authors. We will discuss why.

We now review the predictions and report on their verification for positronium.

A. Prediction for \((Z\alpha)^6/N^6\)

Equation (6) predicts that the \((Z\alpha)^6/N^6\) energy term due to the binding interaction \(Z\alpha\) of atomic two-body bound states is

\[
-\frac{5 - 3x + x^2}{16} \frac{(Z\alpha)^6}{N^6} \mu \tag{7}
\]

for every \(N\), and every angular quantum number, including those of \(L = 0\).

B. Verification for Positronium

For positronium, in which \(m = M\), \(\mu = m/2\), and \(x = 1/4\), it is easy to see that for every angular state
of positronium, equation (7) predicts that the $(Z\alpha)^6/N^6$ term of the energy will always be

$$-\frac{69}{512} \frac{(Z\alpha)^6}{N^6} m$$

Precisely this value was found for all P-states by Khriplovich et al. [2], for both S-states by Czarnecki et al. [3], and then in all $L \geq 2$ states in Zatorski’s recent calculations [4].

To contrast the methods, the predictions (7) and (8) come from the simple algebraic expansion of the two-body Sommerfeld formula (1). The calculations of (8) in standard perturbation theory by Zatorski are the sum of five terms. Three terms are from second-order perturbation theory (eqns. (159), (160) and (162) of ref. [4]). Two terms are first-order (eqns. (91) and (122) of ref. [4]). One contains the expectation value of $p^6$.

Equation (7) is a prediction of the results of future calculations on ordinary hydrogen and muonic hydrogen.

C. Prediction for $(Z\alpha)^6/N^4$

Equation (6) with the coefficient $\epsilon_2$ given in eqn. (14) below predicts that the $(Z\alpha)^6/N^4$ energy term of atomic two-body bound states is

$$\frac{3}{2} \epsilon_2 \frac{(Z\alpha)^6}{N^4} \mu$$

D. Verification for Positronium

As an example, for $L = F + 1$, the coefficient $\epsilon_2$ in eqn. (14) below is

$$\epsilon_2(\text{Positronium}, L = F + 1) = -\frac{1}{2} \left[ \frac{1}{L} + \frac{1}{(2L + 1)(2L - 1)} \right]$$

In eqn. (211) of Zatorski [4] the calculated coefficient of the $(Z\alpha)^6 m/N^4$ term for $L = F + 1$ is

$$-\frac{3 - 6L - 21L^2 + 24L^3 + 48L^4}{16L^2(2L - 1)^2(2L + 1)^2}$$

Bearing in mind that $\mu = m/2$, this is exactly the predicted term (9) above. This verifies the prediction of the two-body Sommerfeld formula for the positronium $L = F + 1$ state. Our prediction is also found to hold for the other three positronium states (eqns. (207), (215) and (219) of ref. [4]). (For the $1^3S_0$ and $3^1S_1$ states of positronium, the coefficients of the $(Z\alpha)^6 m/N^4$ term contain other contributions (see ref. [3]) and no prediction can be made.)

To contrast the methods, our prediction comes from simple algebra using the $(Z\alpha)^4$ first-order perturbation result for $\epsilon_2$. In ref. [4], six second-order perturbation results had to be added together (eqns. (153), (158), (164), (171), (174) and (177)).

Equation (9) is a prediction of the results of future calculations on ordinary hydrogen and muonic hydrogen.

E. Prediction for $(Z\alpha)^6/N^5$

Equation (6) predicts that the $(Z\alpha)^6/N^5$ energy contribution due to the two-body wave equation is

$$-\frac{(3 - x)\epsilon_2}{2} \frac{(Z\alpha)^6}{N^5} \mu$$

The $1/N^5$ terms of Zatorski [4] do not agree with this prediction. This leads to a review of what an analytic solution of the relativistic two-body problem would provide.

We recall that different theoretical starting points (for example the one-photon-exchange Bethe-Salpeter equation, and the conventional Breit equation) can lead to the same $(Z\alpha)^4$ energy levels but different $(Z\alpha)^6$ levels. In Hamiltonian language, with $H_0$ the Coulomb Schrödinger Hamiltonian, one can have $H_0 + V_1$ and $H_0 + V_2$ such that $\langle V_1 \rangle = \langle V_2 \rangle$ to order $(Z\alpha)^4$, while $\langle V_1 - V_2 \rangle \neq 0$ to order $(Z\alpha)^6$. However, it is easy to show that in this case $\langle V_1 \rangle (E_{(E_0 - H_0)} V_1) = \langle V_2 \rangle (E_{(E_0 - H_0)} V_2)$ to order $(Z\alpha)^6$. This means that the differences in the theories can be corrected using only first-order perturbation theory to order $(Z\alpha)^6$. Thus if any theory, physically correct to order $(Z\alpha)^4$, is able to calculate its energy levels to order $(Z\alpha)^6$ easily, the physically correct levels to order $(Z\alpha)^6$ can be calculated as first-order corrections only. That is one of the motivations for the present work.

Examination of Zatorski’s $(Z\alpha)^6$ results (ref. [4], Appendix A) shows that $1/N^6$ and $1/N^5$ appear in the second-order perturbation terms, while $1/N^3$ and $1/N^3$ dominate in the first-order expectation values. It is not surprising therefore that our $(Z\alpha)^6$ predictions for the $1/N^6$ and $1/N^4$ terms are physically correct, while the $1/N^5$ and $1/N^3$ predictions would need first-order corrections.

III. TWO-BODY WAVE EQUATION

The relativistic atomic two-body wave equation from which these results are obtained was derived in ref. [5] from the Bethe-Salpeter equation for two spin-1/2 point particles bound by a single-photon-exchange kernel in the Coulomb gauge. The derivation used a simple quasi-potential approximation [6, 7] with its associated Blankenbecler-Sugar correction series [8].

The bound-state energy $E$ is parametrised by a quantity $\beta$ as follows:

$$E = \sqrt{m^2 - \beta^2} + \sqrt{M^2 - \beta^2}$$

The particles’ individual bound-state energies also occur:

$$t = \sqrt{m^2 - \beta^2}, \quad T = \sqrt{M^2 - \beta^2}$$

The Pauli matrices $\sigma$ and the Dirac matrices $\gamma_1, \gamma_0$ refer to the particle of mass $m$, while $\Sigma, \Gamma$ and $\Gamma^0$ refer to the
particle of mass $M$. The operator $p$ is $-i\nabla$, where $\nabla$ refers to the relative position coordinate $r$. Also $r = |r|$ and $r \equiv r/r$. The only constant of the motion is $F = L + r/r + \Sigma/2$.

The relativistic bound-state wave equation in the centre-of-mass system is

$$[p^2 + \beta^2]\psi(r) = -\frac{1}{2E} \left[ m - \gamma \cdot p + \gamma^0 t \right] [M + \Gamma \cdot p + \Gamma^0 T] \times$$

$$\times \left\{ -\gamma^0 r o \frac{Z \alpha}{r} + \frac{\gamma}{2} \frac{\Gamma + \frac{\gamma}{2} \frac{\Gamma}{r} \frac{\Sigma}{2} Z \alpha}{r} + \frac{1}{2E} \left( \frac{Z \alpha}{r} \right)^2 - \frac{g - 2}{4M} \gamma \cdot \frac{\Sigma}{2} \frac{Z \alpha}{r^2} \right\} \psi(r)$$

The eigenvalue is $\beta^2$, not $E$. The constant $\beta^2$ is substituted into the square roots in equation (10) to obtain the energy $E$. There are no non-local operators of the form $\sqrt{p^2 + m^2}$. No terms $p^4$, $p^6$ appear in perturbation theory.

The first and second terms in the curly brackets are the standard binding potential and Breit interaction. The third term is $1/2E$ times the square of the binding potential. This term is a consequence of the Blankenbecler-Sugar correction formalism. It ensures that the relativistic energies are correct to first order [9].

The final term in the curly brackets, which was not included in ref. [5], contains an anomalous magnetic moment for the particle of mass $M$. It is derived by adding a term $(g - 2)(\mathbf{k} \times \Sigma)/4M$ to the Dirac matrix $\Gamma$ in the vertex function of the particle of mass $M$ in the originating Bethe-Salpeter equation (see e.g. Carlson [10], eqn. (5)). The term is included so that the particle of mass $M$ may represent a point proton.

The wave equation (12) has two singularities: one at $r = 0$ as usual, and another at roughly $M$ well inside the proton. For positronium, with $Z = M$ and $g = 2$, we find the standard energy levels, without the annihilation term (Bethe and Salpeter [11], Sec. 23).

The hyperfine splittings are also correct to order $m/M$ (Bethe & Salpeter [11], Sec. 22, or White [12], Sec. 18.3). (Note that in the literature the factor $Z$ is not included in the magnetic moment of the proton, so $Z$ appears cubed. Here for consistency we carry $Z$, which is one, to the fourth power.) For muonic hydrogen, using $\Delta \epsilon = (Z \alpha)^4 \epsilon_2$ in the Sommerfeld formula (1), we find that the energy difference between the standard hyperfine levels (first-order in $m/M$), and the Sommerfeld formula, is at most 0.005 meV.

It only remains to obtain the two-body Sommerfeld energy-level formula (1).

IV. DERIVATION OF THE TWO-BODY SOMMERFELD FORMULA

Following conventional treatments of the Coulomb Schrödinger equation and the Coulomb Dirac equation, we substitute

$$\psi(r) = e^{-\beta r} r^j \sum_j a_j r^j$$

into the wave equation (12). Here the coefficients $a_j$ are 16-dimensional vectors. The expansion is expected to be valid for $r \gg Z \alpha/2E$. One obtains a four-term recurrence relation for the coefficients $a_j$.

When the dominant terms acting on the large component of the wave function in the wave equation (12) are examined, we see that they are the same as in the Coulomb Schrödinger equation. That means that if the series (17) does not terminate for some $j = n$, the wavefunction will diverge as $e^{r/\beta}$ for large $r$. So that the
wavefunction (17) will exist, we assume that the series terminates at \( j = n \). Then it is easy to find that with \( a_j = 0 \) for \( j > n \), the recurrence relation gives this equation for \( a_n \):

\[
2\beta(\epsilon + 1 + n)a_n = -\frac{Z\alpha}{2E}m\tilde{M}\left[ -\gamma^0\Gamma^0 + \frac{\gamma \cdot \Gamma + \gamma \cdot \hat{r} \cdot \Gamma \cdot \hat{r}}{2} \right] a_n
\]

(18)

containing the projection operators

\[
\tilde{m} = m - i\beta\gamma \cdot \hat{r} + \gamma^0 t, \quad \tilde{M} = M + i\beta\Gamma \cdot \hat{r} + \Gamma^0 T.
\]

(19)

To solve equation (18), we note that \( a_n \) has the form

\[
a_n = \tilde{m} \tilde{M} b.
\]

Substituting that back into (18) puts \( \tilde{m} \tilde{M} \) on each side of the Coulomb and Breit terms. Multiplying them out gives a scalar multiple of \( \tilde{m} \tilde{M} \) again. One thus finds

\[
2\beta(\epsilon + n + 1)a_n = -\frac{Z\alpha}{2E}[-4tT + 4\beta^2] a_n
\]

which is to say

\[
\frac{\beta E}{tT - \beta^2} = \frac{Z\alpha}{\epsilon + n + 1}
\]

(20)

In the case of the one-particle Dirac-Coulomb equation it is well known that

\[
n + \epsilon + 1 = N - \frac{(Z\alpha)^2}{(j + \frac{1}{2}) + \sqrt{(j + \frac{1}{2})^2 - (Z\alpha)^2}}
\]

(21)

This example suggests that in the two-body equation (20)

\[
n + \epsilon + 1 = N + \Delta\epsilon
\]

(22)

with \( \Delta\epsilon \) the expansion in powers of \((Z\alpha)^2\) shown in equation (2). With this assumption, using equations (10) and (11), equation (20) immediately gives the two-body Sommerfeld energy formula (1).

In conclusion, the surprising discovery of a Sommerfeld energy-level formula for two-body atoms, which predicts \((Z\alpha)^6\) energy terms two of which are verified to be physically correct for positronium, allows the hope that one day it may be possible to find an analytic solution to the atomic two-body bound-state problem analogous to the one-particle solution of 1928.

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