Physica 142A (1987) 467–487
North-Holland, Amsterdam

A NEW APPROACH TO BOUND-STATE QUANTUM ELECTRODYNAMICS

I. THEORY

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Received 18 July 1986

A fully covariant two-body equation is applied to the theory of hydrogen, muonium, and positronium spectra. Both particles are treated fully relativistically and complete spin algebras for both particles are taken into account. The major part of the 16×16 wave equation is exactly soluble including recoil of both particles to all orders. The terms of order α^5, α^6 are treated perturbatively (although the equation is in principle numerically solvable to all orders). Self-energy (loop) effects are partly considered by an (effective) anomalous magnetic moment, but in a dynamical way using a Pauli coupling from the beginning. The theory simplifies and improves the bound-state QED problems in a number of ways.

1. Introduction

Relativistic dynamics of two (or more) interacting fermions is the basic problem of the tests of quantum electrodymanics in low energy bound state problems (hydrogen, muonium, positronium-fine and hyperfine structures and spectra) as well as for composite models of hadrons and leptons. The QED bound state theory is a very old but fundamental problem and has been reviewed periodically many times[1,2]).

Although the Bethe–Salpeter formalism[3]) provides an approach to the bound-state problems from first principles of field theory, it has been recognized quite early by Salpeter[4]) and by many other authors later, that one needs an appropriate 3-dimensional exactly soluble wave equation as a starting point. This equation is generally a one-body equation of the Schrödinger–Coulomb

0378-4371/87/$03.50

type with relativistic kinematics, or more recently of the Dirac–Coulomb type which takes into account some aspects of the behavior of the second particle[5]). The recoil and radiative corrections are then performed at various stages, and spin magnetic moment structure of the particles are introduced gradually.

As the accuracy of the tests of QED in bound state problems is steadily improving, the relativistic treatment of recoil and other radiative processes become very crucial even for these low energy processes. There are at the present time still important differences between theory and experiment in many of such tests[6]).

In the present work we have studied a genuinely 2-body, 16-component spinor equation obtained from the Maxwell–Dirac Lagrangian which treats fully the spin and recoil properties of both of the particles. We have introduced the anomalous magnetic moment in a dynamic way, in the Lagrangian instead of adding it simply as a correction to the normal magnetic moment in the nonrelativistic approximation. The major part of the interaction in the 2-body Hamiltonian is exactly soluble, thus taking into account the recoil corrections to all order. The remaining spin–orbit, spin–spin and anomalous magnetic moment interactions, although in principle soluble also to all orders (for example numerically), are treated here, in order to compare it with the other work, as a perturbation to the exactly soluble part.

We show that we obtain agreement with QED up to order α^5 for hydrogen and muonium spectra. At order α^5 there is in principle a small difference with the currently quoted results which become rather important in the case of positronium.

In the case of positronium, the advantages of the fully relativistic treatment shows itself clearly by the fact that l is not a good quantum number. There is a mixing of the $j = l \pm 1$ levels at the α^5-order in the anomalous magnetic moment terms.

But we must await the inclusion of all other radiative terms of order α^5 for positronium in order to be able to make a fuller comparision with experiments.

2. Review of the basic equations

The starting point is the coupled Maxwell–Dirac action for two fermion fields $\psi_1(x)$ and $\psi_2(x)$ interacting via the electromagnetic field A_μ,

$$W = \sum_{j=1}^{2} \int \mathrm{d}^4x \, \{ \bar{\psi}_j (\overset{(j)}{\gamma}{}^{\mu} \, \mathrm{i}\, \partial_\mu - m_j) \psi_j - e_j \bar{\psi}_j \overset{(j)}{\gamma}{}^{\mu} \psi_j A_\mu - a_j \bar{\psi}_j \overset{(j)}{\sigma}{}^{\mu\nu} \psi_j F_{\mu\nu} - \tfrac{1}{4} F_{\mu\nu} F^{\mu\nu} \} \,, \qquad (1)$$

where we have also introduced a Pauli-coupling representing the anomalous magnetic moments. From this action we obtain a relativistic 2-body wave equation in the following way[7,8]). We define a 16-component composite field

$$\Phi(x_1, x_2) = \psi_1(x_1)\psi_2(x_2) ,$$

eliminate in (1) A_μ and $F_{\mu\nu}$ using the equations of motion and rewrite W in terms of $\bar{\Phi}$ and Φ. The (new) variational principle of W with respect to Φ then gives the following equation:

$$[(\overset{(1)}{\gamma}{}^\mu \mathrm{i}\,\partial_\mu - m_1)\otimes \overset{(2)}{\gamma}{}^0 + \overset{(1)}{\gamma}{}^0 \otimes (\overset{(2)}{\gamma}{}^\mu \mathrm{i}\,\partial_\mu - m_2) + V]\Phi(x_1, x_2) = 0 , \qquad (2)$$

where V is a relativistic potential which we shall specify below. Eq. (2) can be written in a fully covariant way but we took a space like surface with normal $n^\mu = (1000)$. For massless exchanged particles, like in electrodynamics, V is a function of $r = |\boldsymbol{x}_1 - \boldsymbol{x}_2|$ only. Then the spinor equation (2) is exactly separable into center-of-mass and relative variables;

$$\{[a\overset{(1)}{\gamma}{}^\mu \otimes \overset{(2)}{\gamma}{}^0 + (1-a)\overset{(1)}{\gamma}{}^0 \otimes \overset{(2)}{\gamma}{}^\mu]P_\mu - (\overset{(1)}{\gamma}{}^\mu \otimes \overset{(2)}{\gamma}{}^0 - \overset{(1)}{\gamma}{}^0 \otimes \overset{(2)}{\gamma}{}^\mu)p_\mu$$
$$- [\overset{(1)}{I} \otimes \overset{(2)}{\gamma}{}^0 m_1 + \overset{(1)}{\gamma}{}^0 \otimes \overset{(2)}{I} m_2] + V\}\Phi(R_\mu, r_\mu) = 0 , \qquad (3)$$

where $r_\mu = x_{1\mu} - x_{2\mu}$ and $R_\mu = ax_{1\mu} + (1-a)x_{2\mu}$(e.g. $a = m_1/(m_1 + m_2)$). We see that actually the p_0-dependence drops out, hence Φ is a *one-time equation* and depends only on the 3-vector relative coordinate $\boldsymbol{r}$: $\Phi = \Phi(R_\mu, \boldsymbol{r})$.

The vector n^μ comes in necessarily via the normalization of the Dirac wave function on a space-like surface with normal n and via the directional δ-function in the Green's function $D(x-y)$.

We shall write in the tensor product $\otimes$ of spinors always particle 1 first and particle 2 second then we can omit the superscripts 1 and 2.

The mass operator P_0 for our system is

$$P_0 = \mathbb{M} = (\boldsymbol{\alpha}_1 \otimes I - I \otimes \boldsymbol{\alpha}_2)\cdot \boldsymbol{p} + (\beta_1 \otimes I m_1 + I \otimes \beta_2 m_2) + \beta_1 V \beta_2 . \qquad (4)$$

The 16-component equation (4) can be fully separated into radial and angular parts[9]) for potentials coming from the minimal and Pauli-couplings in eq. (1),

$$V_{\text{electric}} = e_1 e_2 \overset{(1)}{\gamma}{}^\mu \otimes \overset{(2)}{\gamma}{}_\mu \frac{1}{r}$$

and

$$V_{\text{magnetic}} = -2e_1a_2\left[i\gamma^0 \otimes \frac{\boldsymbol{\alpha}\cdot\boldsymbol{r}}{r^3} + \boldsymbol{\gamma}\otimes\frac{\boldsymbol{\sigma}\times\boldsymbol{r}}{r^3}\right]$$
$$+ 2a_1e_2\left[i\frac{\boldsymbol{\alpha}\cdot\boldsymbol{r}}{r^3}\otimes\gamma^0 + \frac{\boldsymbol{\sigma}\times\boldsymbol{r}}{r^3}\otimes\boldsymbol{\gamma}\right]$$
$$-4a_1a_2\left[\frac{3\boldsymbol{\sigma}\cdot\boldsymbol{r}\otimes\boldsymbol{\sigma}\cdot\boldsymbol{r}}{r^5} - \frac{3\boldsymbol{\alpha}\cdot\boldsymbol{r}\otimes\boldsymbol{\alpha}\cdot\boldsymbol{r}}{r^5} - \frac{\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2}{r^3} + \frac{\boldsymbol{\alpha}_1\cdot\boldsymbol{\alpha}_2}{r^3}\right.$$
$$\left.+\frac{8\pi}{3}\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\,\delta(\boldsymbol{r}) - \frac{4\pi}{3}\boldsymbol{\alpha}_1\cdot\boldsymbol{\alpha}_2\delta(\boldsymbol{r})\right].$$

We then obtain 16 radial equations which separate into two groups of eight[9]). The purpose of the present work is to study and solve these radial equations.

3. The first set of eight coupled equations

The first set of the 8 radial equations that follow from eq. (4) are[9])

$$\left(E + \frac{2\alpha}{r} + \frac{4a_1a_2}{r^3}\right)rz_1 + \Delta m\, ry_1 - 2\,\partial_r(ru_2) + \frac{2\sqrt{j(j+1)}}{r}ru_0 - \frac{\lambda}{r^2}rv_2 = 0\,, \tag{5a}$$

$$\left(E - \frac{2\alpha}{r}\right)rz_{00} + \Delta m\, ry_{00} - \frac{\tau}{r^2}rv_0 = 0\,, \tag{5b}$$

$$\left(E + \frac{2\alpha}{r} - \frac{4a_1a_2}{r^3}\right)ru_2 + Mrv_2 + 2\,\partial_r(rz_1) - \frac{\tau}{r^2}ry_1 = 0\,, \tag{5c}$$

$$Erv_2 + Mru_2 - \frac{2\sqrt{j(j+1)}}{r}ry_{00} - \frac{\lambda}{r^2}rz_1 = 0\,, \tag{5d}$$

$$Ery_1 + \Delta m\, rz_1 - \frac{\tau}{r^2}ru_2 = 0\,, \tag{5e}$$

$$\left(E + \frac{2\alpha}{r} + \frac{8a_1a_2}{r^3}\right)ru_0 + Mrv_0 + \frac{2\sqrt{j(j+1)}}{r}rz_1 + \frac{3\lambda}{r^2}ry_{00} = 0\,, \tag{5f}$$

$$\left(E + \frac{4\alpha}{r}\right)ry_{00} + \Delta m\, rz_{00} + 2\left(\frac{d}{dr} + \frac{1}{r}\right)(rv_0) - \frac{2\sqrt{j(j+1)}}{r}$$
$$\times rv_2 + \frac{3\lambda}{r^2}ru_0 = 0\,, \tag{5g}$$

$$Erv_0 + Mru_0 - 2\left(\frac{d}{dr} - \frac{1}{r}\right)(ry_{00}) - \frac{\tau}{r^2}rz_{00} = 0\,, \tag{5h}$$

Here $\alpha = -e_1e_2$ is the minimal electromagnetic coupling coefficient ($c = \hbar =$

1); The coefficients

$$\lambda = e_1 a_2 + e_2 a_1 ,$$
$$\tau = e_1 a_2 - e_2 a_1 , \tag{6}$$

measure the spin–orbit coupling due to anomalous magnetic moment, and $a_1 a_2$ is the corresponding spin–spin coupling where a is measured in units of $e/2m$. Total angular momentum is denoted by j, and

$$M = m_1 + m_2 , \quad \Delta m = m_1 - m_2 . \tag{7}$$

The indices on the wave functions components z_1, y_1, y_{00}, u_2, . . . etc. denote spin components ($S = 1$; $S_z = 1, 0, -1$ and $S = 0, S_z = 0$) . . . . Four of these 8 equations are algebraic.

We eliminate the functions ru_0, rv_2, ry_1 and rz_{00} using the four algebraic equations (5b, d, e and f) and obtain the following set of four first order differential equations:

$$V_1(ru_2) + 2\,\partial_+ rz_1 + \frac{2M\sqrt{j(j+1)}}{Er}\, ry_{00} = 0 , \tag{8a}$$

$$V_2 rz_1 - 2\,\partial_- ru_2 - \frac{2M\sqrt{j(j+1)}}{rV_5}\, rv_0 - \frac{2\lambda\sqrt{j(j+1)}}{r^3}\left(\frac{1}{E} + \frac{3}{V_5}\right) ry_{00} = 0 , \tag{8b}$$

$$V_3 ry_{00} + 2\,\bar{\partial}_+ rv_0 + \frac{2M\sqrt{j(j+1)}}{Er}\, ru_2 - \frac{2\lambda\sqrt{j(j+1)}}{r^3}\left(\frac{1}{E} + \frac{3}{V_5}\right) rz_1 = 0 , \tag{8c}$$

$$V_4 rv_0 - 2\,\bar{\partial}_- ry_{00} - \frac{2M\sqrt{j(j+1)}}{rV_5}\, rz_1 = 0 . \tag{8d}$$

Here we have used the following abbreviations:

$$V_1(r) \equiv E + \frac{2\alpha}{r} - \frac{M^2}{E} - \frac{4a_1a_2}{r^3} - \frac{\tau^2}{Er^4} , \tag{9a}$$

$$V_2(r) \equiv E + \frac{2\alpha}{r} - \frac{\Delta m^2}{E} - \frac{4j(j+1)/r^2}{V_5} + \frac{4a_1a_2}{r^3} - \frac{\lambda^2}{Er^4} , \tag{9b}$$

$$V_3(r) \equiv E + \frac{4\alpha}{r} - \frac{\Delta m^2}{E - 2\alpha/r} - \frac{4j(j+1)}{Er^2} - \frac{9\lambda^2}{r^4 V_5} , \tag{9c}$$

$$V_4(r) \equiv E - \frac{M^2}{V_5} - \frac{\tau^2}{r^4(E - 2\alpha/r)}\,, \tag{9d}$$

$$V_5(r) \equiv E + \frac{2\alpha}{r} + \frac{8a_1a_2}{r^3}\,, \tag{9e}$$

for potentials, and for derivatives we have set

$$\partial_\pm \equiv \partial_r \pm \frac{\lambda M + \tau\,\Delta m}{2Er^2}\,, \tag{10a}$$

$$\tilde{\partial}_\pm \equiv \partial_r \pm \frac{1}{r} \mp \left(\frac{3\lambda M/2r^2}{V_5} - \frac{\tau\,\Delta m/2r^2}{E - 2\alpha/r}\right). \tag{10b}$$

In the nest step we eliminate (ry_{00}) and (rz_1) between eqs. (8a, b, c and d). The result finally is the following set of *two coupled second order* equations:

$$\begin{aligned}
&\left\{\frac{V_1V_6}{4V_3} + \left[\frac{V_6}{V_3}\,\partial_+\,\frac{V_3}{V_6} + \frac{2\lambda Mj(j+1)}{Er^4V_3}\left(\frac{1}{E} + \frac{3}{V_5}\right)\right]\partial_-\right.\\
&\quad\left. - \frac{2\lambda Mj(j+1)V_6}{EV_3}\,\partial_+\,\frac{1}{r^4V_6}\left(\frac{1}{E} + \frac{3}{V_5}\right) - \frac{M^2j(j+1)}{E^2r^2V_3}\,V_2\right\}(ru_2)\\
&\quad + M\sqrt{j(j+1)}\left\{\frac{V_6}{V_3}\,\partial_+\,\frac{V_3}{V_6rV_5} + \frac{2\lambda Mj(j+1)}{Er^5V_3V_5}\left(\frac{1}{E} + \frac{3}{V_5}\right)\right.\\
&\quad\left. - \left[\frac{V_2}{rEV_3} + \frac{2\lambda V_6}{MV_3}\,\partial_+\,\frac{1}{V_6r^3}\left(\frac{1}{E} + \frac{3}{V_5}\right)\right]\tilde{\partial}_+\right\}(rv_0) = 0\,,
\end{aligned} \tag{11}$$

$$\begin{aligned}
&\left\{\frac{V_4V_6}{4V_2} + \left[\frac{V_6}{V_2}\,\tilde{\partial}_-\,\frac{V_2}{V_6} + \frac{2\lambda Mj(j+1)}{r^4V_2V_5}\left(\frac{1}{E} + \frac{3}{V_5}\right)\right]\tilde{\partial}_+\right.\\
&\quad\left. - \frac{2\lambda Mj(j+1)V_6}{V_2}\,\tilde{\partial}_-\,\frac{1}{V_6V_5r^4}\left(\frac{1}{E} + \frac{3}{V_5}\right) - \frac{M^2j(j+1)}{r^2V_2V_5^2}\,V_3\right\}(rv_0)\\
&\quad - M\sqrt{j(j+1)}\left\{ - \frac{V_6}{EV_2}\,\tilde{\partial}_-\,\frac{V_2}{rV_6} - \frac{2\lambda Mj(j+1)}{Er^5V_2V_5}\left(\frac{1}{E} + \frac{3}{V_5}\right)\right.\\
&\quad\left. + \left[\frac{V_3}{rV_5V_2} + \frac{2\lambda}{M}\,\frac{V_6}{V_2}\,\tilde{\partial}_-\,\frac{1}{r^3V_6}\left(\frac{1}{E} + \frac{3}{V_5}\right)\right]\partial_-\right\}(ru_2) = 0\,,
\end{aligned}$$

where we have introduced a further abbreviation V_6,

$$V_6 \equiv V_2V_3 - \frac{4\lambda^2j(j+1)}{r^6}\left(\frac{1}{E} + \frac{3}{V_5}\right)^2\,, \tag{12}$$

Two limiting cases of eqs. (11) are exactly soluble and have been treated elsewhere[10]). One is the free particle limit, the other case is when we keep the potentials up to order α^5 in a power series expansion. The exactly soluble part of eqs. (11) are

$$\begin{aligned}&\left[\frac{1}{4}\left(E-\frac{M^2}{E}\right)\left(E-\frac{\Delta m^2}{E}\right)+\frac{\alpha}{r}\left(E-\frac{M^2+\Delta m^2}{2E}\right)-\frac{j(j+1)-\alpha^2}{r^2}+\partial_r^2\right](ru_2)\\&\quad-\frac{2\sqrt{j(j+1)}}{r^2}\,rv_0(r)=0\,,\\&\left[\frac{1}{4}\left(E-\frac{M^2}{E}\right)\left(E-\frac{\Delta m^2}{E}\right)+\frac{\alpha}{r}\left(E-\frac{M^2+\Delta m^2}{2E}\right)-\frac{j(j+1)+2-\alpha^2}{r^2}+\partial_r^2\right](rv_0)\\&\quad-\frac{2\sqrt{j(j+1)}}{r^2}\,ru_2(r)=0\,,\end{aligned}\tag{13}$$

The spectrum and the solutions of (13), upon which we shall treat the remaining term as perturbations, are[10])

$$\begin{aligned}&\rho u_2(\rho)=A_0R_{n,l_-}(\rho)+A_2R_{n,l_+}(\rho)\,,\\&\rho v_0(\rho)=-\sqrt{\frac{j}{j+1}}\,A_0R_{n,l_-}(\rho)+\sqrt{\frac{j+1}{j}}\,A_2R_{n,l_+}(\rho)\,,\end{aligned}\tag{14}$$

and

$$E_\pm^2=\frac{M^2+\Delta m^2}{2}\pm\frac{M^2-\Delta m^2}{2}\left[1+\frac{\alpha^2}{(n_r+l)^2}\right]^{-1/2},\tag{15}$$

where

$$\begin{aligned}&l_-(l_-+1)+\alpha^2=j(j-1)\,,\\&l_+(l_++1)+\alpha^2=(j+1)(j+2)\,,\\&R_{n,l}=\mathrm{e}^{-\rho/2}\rho^{l+1}{}_1F_1(-n+l+1,2l+2;\rho)\,,\\&\rho\equiv\left[\frac{(M^2-E^2)(E^2-\Delta m^2)}{E^2}\right]^{1/2}r\,.\end{aligned}\tag{16}$$

The remaining terms in eqs. (11) are, to order α^5,

$$\begin{aligned}\Delta H_{11}=&\left\{\left[\frac{2\alpha}{r^2}-\frac{8j(j+1)}{Er^3}\right]\Big/\left(E-\frac{\Delta m^2}{E}\right)\right\}\partial_r-\frac{a_1a_2}{r^3}\,\frac{M^2-\Delta m^2}{E}\\&+\frac{\lambda M+\tau\,\Delta m}{Er^3}\,,\end{aligned}\tag{17a}$$

$$\Delta H_{12} = \sqrt{j(j+1)}\left[\frac{2}{r^2}\frac{E-M}{M} + \frac{4\alpha}{Er^3} - \frac{1}{r}\frac{\left(-\frac{2\alpha}{r^2} + \frac{8j(j+1)}{Er^3}\right)}{E-\Delta m^2/E} + \frac{2\alpha}{Er^3} + \frac{2\lambda M}{Er^3}\right], \tag{17b}$$

$$\Delta H_{21} = \sqrt{j(j+1)}\left[\frac{2}{r^2}\frac{E-M}{M} - \frac{1}{r}\frac{\left(-4\alpha/r^2 + \frac{2\alpha}{r^2}\frac{\Delta m^2}{E^2} + \frac{8j(j+1)}{Er^3}\right)}{E-\Delta m^2/E} + \frac{2\lambda M}{Er^3}\right], \tag{17c}$$

$$\Delta H_{22} = \frac{\frac{2\alpha}{r^2}\left(2 - \frac{\Delta m^2}{E^2}\right) - \frac{8j(j+1)}{Er^3}}{E-\Delta m^2/E}\left(\partial_r + \frac{1}{r}\right) + 2\frac{3\lambda M - \tau\,\Delta m}{Er^3} + \frac{2a_1a_2}{r^3}\frac{M^2-\Delta m^2}{E}\frac{M^2}{E^2}. \tag{17d}$$

Here all the E's refer to the unperturbed spectrum given in eq. (14). There are two methods of calculating the expectation values of ΔH_{ij}. One way is to calculate them directly between the basis states (15). The second way is to transform ΔH into a new basis of wave functions R_{n,l_-} and R_{n,l_+}. In this basis the unperturbed, exactly soluble part of the Hamiltonian is diagonal, so that the expectation values of the transformed ΔH can be calculated in diagonal form.

The transformation between the states with angular momentum $l_\pm$ and the states ρu_2 and ρv_0 is given by

$$\begin{pmatrix} R_{n,l_+}(\rho) \\ R_{n,l_-}(\rho) \end{pmatrix} = S\begin{pmatrix} \rho u_2(\rho) \\ \rho v_0(\rho) \end{pmatrix}, \tag{18}$$

where S is the following matrix:

$$S = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \tag{19}$$

and $\sin\theta$ and $\cos\theta$ are given by

$$\sin\theta = \sqrt{\frac{j}{2j+1}}, \quad \cos\theta = \sqrt{\frac{j+1}{2j+1}}. \tag{20}$$

Then the transformed Hamiltonian is

$$\tilde{H} = SHS^{-1} . \tag{21}$$

The transformed perturbations are obtained from the expressions given in eqs. (17a–d) by the transformation (21). The result is

$$\begin{aligned}\Delta\tilde{H}_{11} = {} & \frac{4j(j+1)}{2j+1}\,\frac{E-M}{Mr^2} + \frac{1}{Er^3}\Big[4\alpha(j+1) \\ & + \frac{j(\lambda M + \tau\,\Delta m) + 2(j+1)(3\lambda M - \tau\,\Delta m)}{2j+1} + \frac{4\lambda Mj(j+1)}{2j+1}\Big] \\ & + \frac{2\alpha(j+2)}{(E-\Delta m^2/E)r^3} - \frac{4j(j+1)(2j+5)}{(E^2-\Delta m^2)r^4} \\ & + a_1 a_2\,\frac{(M^2-\Delta m^2)(j+2)}{Mr^3(2j+1)} .\end{aligned} \tag{22}$$

$$\begin{aligned}\Delta\tilde{H}_{12} = \sqrt{j(j+1)}\Big[& -\frac{2}{r^2}\,\frac{(E-M)}{E} + \frac{4\alpha j}{Er^3} + \frac{2\alpha}{Er^2}\,\frac{(3-\Delta m^2/E^2)}{1-\Delta m^2/E^2}\,\partial_r \\ & - \frac{16j(j+1)}{(2j+1)E^2r^3(1-\Delta m^2/E^2)}\,\partial_r + \frac{\lambda M - \tau\,\Delta m}{Er^3} \\ & + \frac{3a_1a_2}{Er^3(2j+1)}\,(M^2-\Delta m^2)\Big] ,\end{aligned} \tag{23}$$

$$\Delta\tilde{H}_{21} = \Delta\tilde{H}_{12} , \tag{24}$$

$$\begin{aligned}\Delta\tilde{H}_{22} = {} & -\frac{4j(j+1)}{2j+1}\,\frac{E-M}{Mr^2} + \frac{\alpha}{Er^3}\Big[-4\alpha j \\ & + \frac{(j+1)(\lambda M + \tau\,\Delta m) + 2j(3\lambda M - \tau\,\Delta m) - 4\lambda j(j+1)M}{(2j+1)}\Big] \\ & - \frac{2\alpha(j-1)}{Er^3(1-\Delta m^2/E^2)} + \frac{4j(j+1)(2j-3)}{E^2r^4(1-\Delta m^2/E^2)} \\ & + \frac{a_1a_2(M^2-\Delta m^2)(j-1)}{Mr^3(2j+1)} .\end{aligned} \tag{25}$$

It is seen easily that $\Delta\tilde{H}_{22}$ can be obtained from $\Delta\tilde{H}_{11}$ by the following substitution:

$$j \to -(j+1) . \tag{26}$$

The matrix elements of $\Delta\tilde{H}_{12}$ and $\Delta\tilde{H}_{21}$ between the states R_{n,l_-} and R_{n,l_+} are

$$\langle n, l_+|\Delta\tilde{H}_{12}|n, l_-\rangle = \int_0^\infty \mathrm{d}r\, R^*_{n,l_+}(r)\,\Delta\tilde{H}_{12}R_{n,l_-}(r)\,, \tag{27}$$

$$\langle n, l_-|\Delta\tilde{H}_{21}|n,l_+\rangle = \langle n,l_+|\Delta\tilde{H}_{12}|n, l_-\rangle^*\,. \tag{28}$$

These can be calculated easily and the result is zero[11]). The expectation value of $\Delta\tilde{H}_{11}$ between the states $|n, l_+\rangle$ is

$$\begin{aligned}\langle\Delta\tilde{H}_{11}\rangle_{n,l_+} = {} & \frac{4j(j+1)}{2j+1}\,\frac{E_0 - M}{M}\left\langle\frac{1}{r^2}\right\rangle_{n,l_+} + \left\langle\frac{1}{r^3}\right\rangle_{n,l_+} A_j \\ & + \frac{2\alpha(j+2)}{(E_0 - \Delta m^2/E_0)}\left\langle\frac{1}{r^3}\right\rangle_{n,l_+} - \frac{4j(j+1)(2j+5)}{(E_0^2 - \Delta m^2)}\left\langle\frac{1}{r^4}\right\rangle_{n,l_+} \\ & + \frac{a_1a_2(M^2 - \Delta m^2)(j+2)}{(2j+1)M}\left\langle\frac{1}{r^3}\right\rangle_{n,l_+}\,,\end{aligned} \tag{29}$$

where

$$\begin{aligned}A_j = {} & 4\alpha(j+1) + \{j(\lambda M + \tau\,\Delta m) + 2(j+1)(3\lambda M - \tau\,\Delta m) \\ & + 4j(j+1)\lambda M\}/(2j+1)\,.\end{aligned}$$

We can use the expectation values of r^{-2}, r^{-3} and r^{-4} given by[12])

$$\langle r^{-2}\rangle_{n,l} = \frac{z^2}{n^3(l+\frac{1}{2})}\,. \tag{30}$$

$$\langle r^{-3}\rangle_{n,l} = \frac{z^3}{n^3(l+1)(l+\frac{1}{2})l}\,. \tag{31}$$

$$\langle r^{-4}\rangle_{n,l} = \frac{\frac{1}{2}z^4(3n^2 - l(l+1))}{n^5(l+\frac{3}{2})(l+1)(l+\frac{1}{2})l(l-\frac{1}{2})}\,. \tag{32}$$

Here l is given by eq. (16) [it is not an integer] and

$$z = \frac{\alpha}{4E}\,(2E^2 - (M^2 + \Delta m^2)) \cong \frac{\alpha}{4M}\,(M^2 - \Delta m^2) + \mathcal{O}(\alpha^2)\,. \tag{33}$$

We take also the *zeroth* order terms of the expression defining l, namely

$$l_\pm \cong l_\pm^{(0)} = (j \pm 1) + \mathcal{O}(\alpha^2)\,. \tag{34}$$

Then using eqs. (30)–(34), we calculate eq. (29). The result is

$$\langle \Delta \tilde{H}_{11} \rangle_{n,j+1} = \frac{2\alpha^4 (M^2 - \Delta m^2)^2/M^2}{4^3 n^3 (j+1)(j+\frac{3}{2})} + \frac{\alpha^4 (M^2-\Delta m^2)^3/M^4}{4^3 n^3 (j+\frac{1}{2})(j+\frac{3}{2})} \times \left(1 + \frac{(4j+3)\lambda M}{2(j+1)\alpha} - \frac{\tau \, \Delta m}{2(j+1)\alpha}\right) + \frac{a_1 a_2 \alpha^3 (M^2 - \Delta m^2)^4/M^4}{4^3 (2j+1)(j+1)(j+\frac{3}{2})} . \tag{35}$$

In the same way, we calculate the expectation value $\langle \Delta \tilde{H}_{22} \rangle_{n,j-1}$ which gives

$$\langle \Delta \tilde{H}_{22} \rangle_{n,j-1} = - \frac{2\alpha^4 (M^2 - \Delta m^2)^2/M^2}{4^2 n^3 j(j-\frac{1}{2})} - \frac{\alpha^4 (M^2-\Delta m^2)^3/M^4}{4^2 n^3 (j-\frac{1}{2})(j+\frac{1}{2})} \times \left(1 + \frac{(4j+1)\lambda M + \tau\,\Delta m}{2j\alpha}\right) + \frac{a_1 a_2 (M^2 - \Delta m^2)^4 \alpha^3/M^4}{2 \cdot 4^3 n^3 j(j-\frac{1}{2})(j+\frac{1}{2})} . \tag{36}$$

It is shown in appendix A, how to obtain the energy shifts of states $|n, j+1\rangle$ and $|n, j-1\rangle$ from $\langle \Delta \tilde{H}_{11} \rangle_{n,j+1}$ and $\langle \Delta \tilde{H}_{22} \rangle_{n,j-1}$, respectively. Using these procedures we obtain the following perturbative shifts to E^2:

$$\delta E_{11}^2 = - \frac{2\alpha^4 (M^2 - \Delta m^2)}{4^2 n^3 (j+1)(j+\frac{3}{2})} - \frac{\alpha^4 (M^2 - \Delta m^2)^2/M^2}{4^2 n^3 (j+\frac{1}{2})(j+\frac{3}{2})} \times \left(1 + \frac{(4j+3)\lambda M - \tau\,\Delta m}{2(j+1)\alpha}\right) - \frac{a_1 a_2 (M^2-\Delta m^2)^3 \alpha^3/M^2}{2\cdot 4^2 n^3 (j+\frac{1}{2})(j+1)(j+\frac{3}{2})} , \tag{37}$$

$$\delta E_{22}^2 = \frac{2\alpha^4 (M^2 - \Delta m^2)}{4^2 n^3 (j-\frac{1}{2})j} + \frac{\alpha^4 (M^2 - \Delta m^2)^2/M^2}{4^2 n^3 (j-\frac{1}{2})(j+\frac{1}{2})} \left(1 + \frac{(4j+1)\lambda M + \tau\,\Delta m}{2j\alpha}\right) - \frac{a_1 a_2 \alpha^3 (M^2 - \Delta m^2)^3/M^2}{2\cdot 4^3 n^3 (j-\frac{1}{2})j(j+\frac{1}{2})} . \tag{38}$$

Eqs. (15) and (37) give the expression of E^2 for the $|n, l_+ \simeq j+1\rangle$ state and (15) and (38) give E^2 for $|n, l_- \simeq j-1\rangle$ state.

Next we pass to ΔE by

$$E = E_0 + \frac{1}{2E_0} \delta E^2 + \dots , \tag{39}$$

or

$$\Delta E = \frac{1}{2E_0}\,\delta E^2 + \ldots \cong \frac{1}{2M}\,\delta E^2 + \mathscr{O}(\alpha^6)\,, \tag{40}$$

so that the final energy shifts are given by eqs. (37) and (38) divided by $1/2M$.

4. The second set of eight equations

The second set of the 8 radial equations is

$$\left(E + \frac{2\alpha}{r} - \frac{4a_1a_2}{r^3}\right)ru_1 + Mrv_1 + 2\frac{\mathrm{d}}{\mathrm{d}r}(rz_2) - \frac{2\sqrt{j(j+1)}}{r}\,rz_0 - \frac{\tau}{r^2}\,ry_2 = 0\,, \tag{41a}$$

$$\left(E + \frac{2\alpha}{r} + \frac{4a_1a_2}{r^3}\right)rz_2 + \Delta m\,ry_2 - 2\frac{\mathrm{d}}{\mathrm{d}r}(ru_1) - \frac{\lambda}{r^2}\,rv_1 = 0\,, \tag{41b}$$

$$\left(E + \frac{4\alpha}{r}\right)rv_{00} + Mru_{00} - 2\left(\frac{\mathrm{d}}{\mathrm{d}r} + \frac{1}{r}\right)(ry_0) + \frac{2\sqrt{j(j+1)}}{r}\,ry_2 + \frac{3\tau}{r^2}\,rz_0 = 0\,, \tag{41c}$$

$$Ery_0 + \Delta m\,rz_0 + 2\left(\frac{\mathrm{d}}{\mathrm{d}r} - \frac{1}{r}\right)(rv_{00}) - \frac{\lambda}{r^2}\,ru_{00} = 0\,, \tag{41d}$$

$$Ery_2 + \Delta m\,rz_2 + \frac{2\sqrt{j(j+1)}}{r}\,rv_{00} - \frac{\tau}{r^2}\,ru_1 = 0\,, \tag{41e}$$

$$Erv_1 + Mru_1 - \frac{\lambda}{r^2}\,rz_2 = 0\,, \tag{41f}$$

$$\left(E - \frac{2\alpha}{r}\right)ru_{00} + Mrv_{00} - \frac{\lambda}{r^2}\,ry_0 = 0\,, \tag{41g}$$

$$\left(E + \frac{2\alpha}{r} - \frac{8a_1a_2}{r^3}\right)rz_0 + \Delta m\,ry_0 - \frac{2\sqrt{j(j+1)}}{r}\,ru_1 + \frac{3\tau}{r^2}\,rv_{00} = 0\,. \tag{41h}$$

We solve (rv_1) from (41f) and substitute it into (41a, b) then solve (ru_{00}) from (41g) and insert it to (41c, d). We have two more algebraic equations. Next we solve (ry_2) and (rz_2) from (41b and e) and (ry_0) and (rz_0) from (41d and h). By inserting these into (41a and b) we have again two coupled second order equations:

$$\left\{\frac{1}{4}\,V_7V_8 + V_8\nabla_{(+)}\,\frac{1}{V_8}\,\nabla_{(-)} - \frac{\tau^2V_8}{4Er^4} - \frac{j(j+1)}{r^2}\,\frac{V_8(1+\Delta m^2/V_9)}{V_{11}}\right\}ru_1$$

$$+ \Delta m\sqrt{j(j+1)}\left\{V_8\nabla_{(+)}\,\frac{1}{ErV_8} + \frac{\tau V_8}{2\,\Delta m\,Er^3}\right.$$

$$-\frac{V_8}{rV_9}\left(\nabla_{(-)}-\frac{3\tau V_9}{2\,\Delta m\,r^2V_{11}}\right)\Bigg\}rv_{00}=0\,, \tag{42a}$$

$$\Bigg\{\frac{1}{4}\frac{V_9V_{10}}{V_{11}}+\frac{V_9}{V_{11}}\nabla_{(+)}\frac{V_{11}}{V_9}\nabla_{(-)}-\frac{9\tau^2V_9}{4r^4V_{11}}$$
$$-\frac{j(j+1)V_9\left(E+\frac{2\alpha}{r}-\frac{\lambda^2}{Er^4}\right)}{V_8V_{11}r^2}\Bigg\}rv_{00}$$

$$+\Delta m\sqrt{j(j+1)}\Bigg\{\frac{V_9}{V_{11}}\nabla_{(+)}\frac{1}{rV_9}+\frac{3\tau V_9}{2\,\Delta m\,r^3V_{11}^2}$$
$$-\frac{V_9}{ErV_8V_{11}}\left(\partial_r-\frac{\lambda M}{2Er^2}-\frac{\tau\left(E+\frac{2\alpha}{r}-\lambda^2/Er^4\right)}{2\,\Delta m\,r^2}\right)\Bigg\}ru_1=0\,, \tag{42b}$$

where

$$\nabla_{(\pm)}=\partial_r\pm\left(\frac{1}{r}-\frac{\lambda M}{2r^2(E-2\alpha/r)}+\frac{3\tau\,\Delta m}{2r^2V_{11}}\right). \tag{43}$$

and the following abbreviations have been used:

$$\begin{aligned}
V_7&=E+\frac{2\alpha}{r}-\frac{M^2}{E}-\frac{4a_1a_2}{r^3}\,,\\
V_8&=E+\frac{2\alpha}{r}+\frac{4a_1a_2}{r^3}-\frac{\lambda^2}{Er^4}-\frac{\Delta m^2}{E}\,,\\
V_9&=\left(E+\frac{2\alpha}{r}-\frac{8a_1a_2}{r^3}\right)\left(E-\frac{\lambda^2}{r^4(E-2\alpha/r)}\right)-\Delta m^2\,,\\
V_{10}&=E+\frac{4\alpha}{r}-\frac{M^2}{E-2\alpha/r}\,,\\
V_{11}&=E+\frac{2\alpha}{r}-\frac{8a_1a_2}{r^3}\,.
\end{aligned} \tag{44}$$

The free particle solutions of these equations are[9,10])

$$\rho u_1(\rho)=A\rho j_j(\rho)\,,\quad \rho v_{00}(\rho)=B\rho j_j(\rho)\,. \tag{45}$$

Again taking the potentials up to α^5, we have the main part of the equations

$$\left[\frac{1}{4}\left(E+\frac{2\alpha}{r}-\frac{M^2}{E}\right)\left(E+\frac{2\alpha}{r}-\frac{\Delta m^2}{E}\right)+\partial_r^2-\frac{j(j+1)}{r^2}\right.$$
$$\left.+\frac{\frac{\mathrm{d}}{\mathrm{d}r}\left(E+\frac{2\alpha}{r}-\frac{\Delta m^2}{E}\right)}{\left(E+\frac{2\alpha}{r}-\frac{\Delta m^2}{E}\right)}\partial_r+\frac{\lambda M+\tau\,\Delta m}{Er^3}-\frac{a_1a_2}{Er^3}(M^2-\Delta m^2)\right](ru_1)$$
$$+\sqrt{j(j+1)}\,\frac{\Delta m}{E}\left[\frac{\frac{\mathrm{d}}{\mathrm{d}r}\left(1+\frac{2\alpha}{r}-\frac{\Delta m^2}{E^2}\right)}{r\left(1+\frac{2\alpha}{r}-\frac{\Delta m^2}{E^2}\right)}+\frac{2\tau E}{\Delta m r^3}\right](rv_{00})=0\,. \tag{46a}$$

$$\left[\frac{1}{4}\left(E-\frac{\Delta m^2}{E}+\frac{\Delta m^2}{E^2}\frac{2\alpha}{r}-\frac{\Delta m^2\,4\alpha^2}{E^3r^2}\right)\left(E+\frac{4\alpha}{r}-\frac{M^2}{E}-\frac{M^2}{E}\frac{2\alpha}{r}\right.\right.$$
$$\left.\left.-\frac{M^2}{E}\frac{4\alpha^2}{E^2r^2}\right)+\partial_r^2-\frac{j(j+1)}{r^2}\right](rv_{00})$$
$$+\sqrt{j(j+1)}\,\frac{\Delta m}{E}\left[\frac{1}{\left(1+\frac{2\alpha}{Er}\right)}\,\frac{\frac{\mathrm{d}}{\mathrm{d}r}\left(1+\frac{2\alpha}{r}-\frac{\Delta m^2}{E}\right)}{r\left(1+\frac{2\alpha}{Er}-\frac{\Delta m^2}{E}\right)}+\frac{2\tau E}{\Delta m\, r^3}\right](ru_1)=0\,. \tag{46b}$$

The exactly soluble part of these equations are, in this case, the following two uncoupled equations:

$$\left[\frac{1}{4}\left(E-\frac{M^2}{E}\right)\left(E-\frac{\Delta m^2}{E}\right)+\frac{\alpha}{r}\left(E-\frac{M^2+\Delta m^2}{2E}\right)\right.$$
$$\left.-\frac{j(j+1)-\alpha^2}{r^2}+\partial_r^2\right](ru_1)=0\,, \tag{47a}$$

$$\left[\frac{1}{4}\left(E-\frac{M^2}{E}\right)\left(E-\frac{\Delta m^2}{E}\right)+\frac{\alpha}{2r}\left(2E-\frac{M^2+\Delta m^2}{E}\right)\right.$$
$$\left.-\frac{j(j+1)-\alpha^2\delta_E}{r^2}+\partial_r^2\right](rv_{00})=0\,. \tag{47b}$$

Note the appearance of the factor δ_E in the second equation by

$$\delta_E=\frac{\Delta m^2-M^2}{E^2}+\frac{M^2\,\Delta m^2}{E^4}\,. \tag{48}$$

The solutions of (47a and b) can be written down immediately in terms of the hydrogenic wave functions

$$\rho u_1(\rho) = A\,\mathrm{e}^{-\rho/2}\rho^{l+1}\,{}_1F_1(-n+l+1, 2l+2, \rho)\,, \tag{49a}$$

$$\rho v_{00}(\rho) = B\,\mathrm{e}^{-\rho/2}\rho^{l+1}\,{}_1F_1(-n+l+1, 2l+2, \rho)\,. \tag{49b}$$

The spectrum is given by

$$E^2 = \frac{M^2+\Delta m^2}{2} \pm \frac{M^2-\Delta m^2}{2}\left(1+\frac{\alpha^2}{(n_r+l)^2}\right)^{-1/2}. \tag{50}$$

For eq. (47a) the angular momentum l is given by

$$l(l+1) = j(j+1) - \alpha^2\,, \tag{51}$$

but for (47b) we have

$$l(l+1) = j(j+1) - \alpha^2\delta_E\,. \tag{52}$$

We see from eq. (48) that $\delta_E = +1$ for $E = \Delta m$, and $\delta_E = -1$ for $E = M$. Hence for the same physical l-values as in eq. (51) (that is for $\delta_E = +1$) the solutions of eq. (47b) lie near the "negative" continuum, thus belong to the (−) sign in eq. (50). Since these values are unphysical energies, the solutions must be correctly interpreted. This can be done if we change the sign of the mass of one of the constituents, say, $m_2 \to -m_2$. This means a change of $\Delta m \leftrightarrow M$, which brings the spectrum back near the "positive" continuum at $E^2 = (m_1 + m_2)^2$. The remaining terms of equations (47a), (47b) are invariant under $\Delta m \leftrightarrow M$.

The difficulties with the Møller (and Breit) potential of the form $(1 - \boldsymbol{\alpha}_1 \cdot \boldsymbol{\alpha}_2)/r$ have been continuously discussed in the last thirty years by many authors. In the light of the above results, an answer to this problem is to consider from the beginning two equations of the type (4), one as it stands and the other with one of the masses of opposite sign, say $m_2 \to -m_2$, and to take only the positive or physical solutions from both sets.

This procedure is in fact used in the one-particle Dirac–Coulomb problem: When the first order equations are reduced to second order equations, one component of the wave function gives the correct physical spectrum, the other does not. However, the change $m \to -m$ maps the second equation into first, hence the second spectrum can be mapped again into the physical spectrum. In this case the ± signs in front of the Dirac spectrum $E = \pm m[1 + \alpha^2/n^2]^{-1/2}$ are trivially adjusted. In our two-body case, the ± signs occur in the middle, see eq. (50), hence the adjustment is more crucial. The change of the sign of the mass in the Dirac equation has been called "mass conjugation" and is another way of treating the negative energy solutions or the antiparticles in the first quantized Dirac theory[13]).

The perturbations are given by

$$\Delta H_{11} = \frac{\frac{\mathrm{d}}{\mathrm{d}r}\left(1 + \frac{2\alpha}{Er} - \frac{\Delta m^2}{E^2}\right)}{\left(1 + \frac{2\alpha}{Er} - \frac{\Delta m^2}{E^2}\right)} \frac{\mathrm{d}}{\mathrm{d}r} + \frac{\lambda M + \tau \Delta m}{Er^3} - \frac{a_1 a_2}{Er^3} (M^2 - \Delta m^2) , \tag{53a}$$

$$\Delta H_{12} = \frac{\Delta m \sqrt{j(j+1)}}{E} \left[\frac{-\frac{\mathrm{d}}{\mathrm{d}r}\left(1 + \frac{2\alpha}{Er} - \frac{\Delta m^2}{E^2}\right)}{r\left(1 + \frac{2\alpha}{Er} - \frac{\Delta m^2}{E^2}\right)} + \frac{2\tau E}{\Delta m\, r^3} \right] , \tag{53b}$$

$$\Delta H_{21} = \frac{\Delta m \sqrt{j(j+1)}}{E} \left[\frac{-\frac{\mathrm{d}}{\mathrm{d}r}\left(1 + \frac{2\alpha}{Er} - \frac{\Delta m^2}{E^2}\right)}{r\left(1 + \frac{2\alpha}{Er}\right)\left(1 + \frac{2\alpha}{Er} - \frac{\Delta m^2}{E^2}\right)} + \frac{2\tau E}{\Delta m\, r^3} \right] , \tag{53c}$$

$$\Delta H_{22} = 0 . \tag{53d}$$

In appendix B we discuss the relation between the expectation values of these 2 × 2 matrices and the expectation values of the diagonal system. This relation is

$$\langle \Delta H \rangle_{n,l} = \frac{1}{2} [\langle \Delta H_{11} \rangle_{n,l} + \langle \Delta H_{22} \rangle_{n,l}] \pm \left[\frac{(\langle \Delta H_{11} \rangle_{n,l} + \langle \Delta H_{22} \rangle_{n,l})^2}{4} + \langle \Delta H_{12} \rangle_{n,l} \langle \Delta H_{21} \rangle_{n,l} \right]^{1/2} . \tag{54}$$

Up to order α^5 the perturbations are simply

$$\Delta H_{22} = 0 ,$$

$$\Delta H_{12} = \Delta H_{21} = \frac{2\sqrt{j(j+1)}}{r^3} \frac{\Delta m}{E} \left(\frac{\alpha}{E - \Delta m^2/E} + \frac{\tau E}{\Delta m} \right) , \tag{55}$$

$$\Delta H_{11} = \frac{-\dfrac{2\alpha}{Er^2}\dfrac{\mathrm{d}}{\mathrm{d}r}}{1-\Delta m^2/E^2} + \frac{\lambda M + \tau\,\Delta m}{Er^3} - \frac{a_1 a_2}{Er^3}\,(M^2 - \Delta m^2)\,,$$

and we obtain the energy shifts

$$\delta E^2_{\pm} = -\frac{\alpha^4 (M^2 - \Delta m^2)}{4^2 n^3 j(j+\frac{1}{2})(j+1)}\,\Delta^{(j)}_{\pm}\,, \tag{56}$$

where

$$\begin{aligned}\Delta^{(j)}_{\pm} &= 1 + \frac{\lambda M + \tau\,\Delta m}{2\alpha}\left(1 - \frac{\Delta m^2}{M^2}\right) - \frac{a_1 a_2}{2M^2\alpha}(M^2 - \Delta m^2)^2 \\ &\quad \pm \left[\left(1 + \frac{\lambda M + \tau\,\Delta m}{2\alpha}\left(1 - \frac{\Delta m^2}{M^2}\right) - \frac{a_1 a_2}{2M^2\alpha}\,(M^2 - \Delta m^2)^2\right)^2 \right. \\ &\quad \left. + 4j(j+1)\left(\frac{\Delta m}{M} + \frac{\tau M}{\alpha}\left(1 - \frac{\Delta m^2}{M^2}\right)\right)^2\right]^{1/2}.\end{aligned} \tag{57}$$

or

$$\left.\begin{aligned}\Delta^{(j)}_{+} &= 2\left(1 + \frac{\lambda M}{2\alpha} - \frac{a_1 a_2}{2\alpha}\,M^2\right) \\ \Delta^{(j)}_{-} &= 0\end{aligned}\right\}\quad \text{for } \Delta m = 0\,.$$

Inserting the values of λ and τ and with

$$\begin{aligned}\lambda &= e_1 a_2 + e_2 a_1 = \frac{1}{2}\,e_1 e_2\left(\frac{g_1}{m_1} + \frac{g_2}{m_2}\right), \\ \tau &= e_1 a_2 - e_2 a_1 = \frac{1}{2}\,e_1 e_2\left(\frac{g_2}{m_2} - \frac{g_1}{m_1}\right),\end{aligned} \tag{58}$$

we have

$$\begin{aligned}\Delta^{j}_{(\pm)} &= A \pm \sqrt{A^2 + B}\,, \\ A &= 1 + \frac{2}{M^2}(m_1^2 g_2 + m_2^2 g_1 - m_1 m_2 g_1 g_2)\,, \\ B &= \frac{4j(j+1)}{M^2}\,(m_1 - m_2 + 2(m_1 g_2 - m_2 g_1))^2\,.\end{aligned} \tag{59}$$

which gives for the energy shift

$$\Delta E_{\pm} = -\left(\frac{m_1 m_2}{m_1 + m_2}\right) \frac{\alpha^4}{8n^3 j(j+\frac{1}{2})(j+1)} \Delta^j_{(\pm)} . \tag{60}$$

For positronium ($\Delta m = 0$), the results are

$$\Delta E_+ = -\frac{2m_e \alpha^4 (1 + g - g^2)}{16n^3 j(j+\frac{1}{2})(j+1)} ,$$
$$\Delta E_- = 0 . \tag{60a}$$

The applications of the recoil energies (15) and the spin perturbations (37)–(39) for the $l = j \pm 1$ levels, and (56)–(57) for $l = j$ levels, together with the Lamb-shift and annihilation corrections are given explicitly in a separate part II[14]) of this paper for hydrogen, muonium and positronium.

Acknowledgements

This work was supported in part by the Alexander v. Humbolt Foundation, a NATO Research Grant, NSF International SDC Programs, and by the Scientific and Technical Research Council of Turkey.

Appendix A

Calculation of perturbations for energy-dependent squared hamiltonians

We have two problems. The first one is the calculation of δE^2 from $\Delta H(E)$. The second is the calculation of $\langle \Delta H \rangle$ when ΔH is not a diagonal matrix. Note that here ΔH is not energy, but energy squared (E^2). We shall write the counterpart of the equation $(H - E)|\psi\rangle = 0$ from now on as $H(E)|\psi\rangle = 0$. Suppose $H(E)$ has two parts

$$H = H^{(0)}(E^2) + \lambda\, \Delta H(E^2) , \tag{A.1}$$

where $H^0(E^2)$ is exactly soluble

$$H^{(0)}(E_0^2)|\overset{0}{\psi}\rangle = 0 . \tag{A.2}$$

In the equation

$$(H^{(0)}(E^2) + \lambda\, \Delta H(E^2))|\psi\rangle = 0 . \tag{A.3}$$

we expand as usual

$$|\psi\rangle = |\overset{0}{\psi}\rangle + \lambda|\delta\psi\rangle \ . \tag{A.4}$$

Hence eq. (A.3) gives, using (A.2) to lowest order in λ:

$$\langle \overset{0}{\psi}|H^0(E^2)|\overset{0}{\psi}\rangle + \langle \overset{0}{\psi}|\Delta H(E^2)|\overset{0}{\psi}\rangle + \langle \delta\psi|H^{(0)}(E^2)|\overset{0}{\psi}\rangle + \langle \overset{0}{\psi}|H^{(0)}(E^2)|\delta\psi\rangle$$
$$= 0 \ . \tag{A.5}$$

$$E^2 = E_0^2 + \lambda\, \delta E^2 \ . \tag{A.6}$$

we get

$$\langle \psi^0|H^{(0)}(E^2 + \lambda\delta E^2)|\overset{0}{\psi}\rangle + \lambda\langle \overset{0}{\psi}|\Delta H(E^2 + \lambda\delta E^2)|\psi_0\rangle$$
$$+ \lambda\langle \delta\psi|H^{(0)}(E^2 + \lambda\delta E^2)|\overset{0}{\psi}\rangle + \lambda\langle \overset{0}{\psi}|H^{(0)}(E^2 + \lambda\delta E^2)|\delta\psi\rangle = 0 \ , \tag{A.7}$$

or

$$\langle \overset{0}{\psi}|H^{(0)}(E_0^2 + \lambda\delta E^2) + \lambda\Delta H(E_0^2)|\psi_0\rangle + \lambda\langle \delta\psi|H^{(0)}(E_0^2)|\psi_0\rangle$$
$$+ \lambda\langle \overset{0}{\psi}|H^{(0)}(E_0^2)|\delta\psi\rangle = 0 \ . \tag{A.8}$$

From (A.2)

$$\langle \delta\psi|H^{(0)}(E_0^2)|\overset{0}{\psi}\rangle = 0 \ . \tag{A.9}$$

Hence

$$(\overset{0}{\psi}|H^{(0)}(E_0^2 + \delta E^2)|\overset{0}{\psi}\rangle + \lambda\langle \overset{0}{\psi}|\Delta H(E_0^2)|\overset{0}{\psi}\rangle = 0 \ . \tag{A.10}$$

In our case

$$\langle H^{(0)}(E_0^2\rangle_0 = -\frac{1}{4}\,\frac{(E_0^2 - \Delta m^2)(M^2 - E_0^2)}{E_0^2}$$
$$+ \frac{\alpha^2}{4n^2}\,\frac{(2E_0^2 - M^2 - \Delta m^2)^2}{4E_0^2} = 0 \ , \tag{A.11}$$

so that

$$\langle H^{(0)}(E_0^2 + \lambda\delta E^2)\rangle_0 = \frac{1}{4}\,\lambda\delta E^2\,\frac{M^2 - \Delta m^2}{M^2}\,. \tag{A.12}$$

Inserting this into (A.10) we have

$$\frac{1}{4}\,\lambda\delta E^2\,\frac{M^2 - \Delta m^2}{M^2} + \langle \Delta H(E_0^2)\rangle_0 = 0\,, \tag{A.13}$$

so finally

$$\lambda\delta E^2 = -\frac{4M^2}{(M^2 - \Delta m^2)}\,\langle \Delta H(E_0^2)\rangle_0\,. \tag{A.14}$$

Appendix B

Matrix perturbation theory

Consider a matrix differential eigenvalue problem

$$\begin{pmatrix} H_{11}(E) & H_{12}(E) \\ H_{21}(E) & H_{22}(E) \end{pmatrix}\begin{pmatrix} \varphi \\ \chi \end{pmatrix} = 0\,. \tag{B.1}$$

It can be converted into an algebraic eigenvalue equation by expanding ψ and χ into a set of eigenfunctions

$$\varphi = \sum_n C_n R_n(r)\,, \quad \chi = \sum_n D_n R_n(r)\,. \tag{B.2}$$

Inserting these into (B.1) and taking the scalar products we get a set of algebraic equations in terms of expectation values

$$\begin{pmatrix} \langle H_{11}\rangle_n & \langle H_{12}\rangle_n \\ \langle H_{21}\rangle_n & \langle H_{22}\rangle_n \end{pmatrix}\begin{pmatrix} C_n \\ D_n \end{pmatrix} = 0\,. \tag{B.3}$$

Eq. (B.3) has nontrivial solutions only if the determinant is zero,

$$\langle H_{11}\rangle_n \langle H_{22}\rangle_n - \langle H_{12}\rangle_n \langle H_{21}\rangle_n = 0\,. \tag{B.4}$$

Again if H consists of two parts, an exactly soluble part H^0 and a perturbation part ΔH. In our case

$$\begin{pmatrix} \langle H^0\rangle_n + \langle \Delta H_{11}\rangle_n & \langle \Delta H_{12}\rangle_n \\ \langle \Delta H_{21}\rangle_n & \langle H^0\rangle_n + \langle \Delta H_{22}\rangle_n \end{pmatrix}\begin{pmatrix} C_n \\ D_n \end{pmatrix} = 0\,. \tag{B.5}$$

Inserting (B.5) into (B.4) we have

$$\langle H^{(0)}\rangle_n + \tfrac{1}{2}\,(\langle \Delta H_{11}\rangle_n + \langle \Delta H_{22}\rangle_n) \pm [\tfrac{1}{4}\,(\langle \Delta H_{11}\rangle + \langle \Delta H_{22}\rangle)^2 + \langle \Delta H_{12}\rangle\langle \Delta H_{21}\rangle]^{1/2} = 0\,,$$

or

$$\langle H^{(0)}\rangle + \langle \Delta H\rangle = 0\,, \tag{B.6}$$

hence

$$\langle \Delta H\rangle = \tfrac{1}{2}\,(\langle \Delta H_{11}\rangle + \langle \Delta H_{22}\rangle) \pm [\tfrac{1}{4}\,(\langle \Delta H_{11}\rangle + \langle \Delta H_{22}\rangle)^2 + \langle \Delta H_{12}\rangle\langle \Delta H_{21}\rangle]^{1/2}\,. \tag{B.7}$$

References

1) B.E. Lautrup et al., Phys. Rep. **3** (1972) 193.
T. Kinoshita, Proc. XIX Conf. High Energy Physics, Tokyo (1978).
2) M.A. Stroscio, Phys. Rep. **22** (1975) 215.
A. Rich, Rev. Mod. Phys. **53** (1981) 127.
V.W. Hughes, in Exotic Atoms 79, K. Crowe et al., eds. (Plenum, New York, 1980).
3) J. Schwinger, Proc. Nat. Acad. Sci. **37** (1951) 452, 455.
E. Salpeter and H. Bethe, Phys. Rev. **84** (1951) 1232.
4) E.E. Salpeter, Phys. Rev. **87** (1952) 328.
5) G.P. Lepage, Phys. Rev. A **16** (1977) 863.
G.T. Bodwin, D.R. Yennie and M.A. Gregoria, Rev. Mod. Phys. **57** (1985) 723; and references to earlier three-dimensional formalisms therein.
6) For the latest numbers see, for example, D.R. Yennie, in: AIP Conference Proceedings, No. 123, R.E. Mischke, ed. (Am. Inst. of Physics, New York, 1984) p. 468.
T. Kinoshita and J. Sapirstein, Proc. Ninth Int. Conf. Atomic Physics, Seattle, WA (Plenum, New York, 1984).
7) A.O. Barut, in Lecture Notes in Physics, Vol. 180 (Springer, Berlin, 1983) p. 332.
8) A.O. Barut and S. Komy, Fortschritte der Physik **33** (1985) 309.
9) A.O. Barut and N. Ünal, Fortschritte der Physik **33** (1985) 319.
10) A.O. Barut and N. Ünal, J. Math. Phys. **27** (1986) 3055.
11) W. Magnus, F. Oberhettinger and R.P. Soni, Formulas and Theorem for the Special Functions of Mathematical Physics (Springer, Berlin 1966) p. 280.
12) H. Bethe and E. Salpeter, Quantum Mechanics of One- and Two-Electron Atoms (Plenum, New York, 1977) p. 17.
13) A.O. Barut, Phys. Rev. Lett. **20** (1968) 893.
14) A.O. Barut and N. Ünal, Physica **142A** (1987) 488, part II, see following paper, this volume.