RELATIVISTIC RADIAL EQUATIONS FOR TWO SPIN-1/2 PARTICLES WITH A STATIC INTERACTION: PART TWO*

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The relativistic radial equations for two spin-1/2 particles with a static interaction, which were derived previously, turn out to exclude the lowest value $n_r = 0$ of the radial quantum number. New equations valid for all $n_r = 0, 1, 2, \ldots$ are obtained. They are equivalent to the former for $n_r > 0$ as far as the spectrum of energy levels is concerned, but the former are necessary to supplement new equations in describing the complete set of energy wave functions. Energy levels for Coulomb bound states with $j = 0$, previously found in an implicit way in the weak-potential approximation, are now calculated numerically for hydrogen and positronium. In Appendix, the relativistic radial equations are derived in the case of a more general interaction including nonstatic Breit-like terms.

In a recent paper [1] we considered the relativistic equation

$$[E - c(\vec{\alpha}^{(1)} \cdot \vec{p} + \beta^{(1)} m^{(1)} c) - c(-\vec{\alpha}^{(2)} \cdot \vec{p} + \beta^{(2)} m^{(2)} c) - V(\vec{r})]\psi(\vec{r}) = 0 \tag{1}$$

for a system of two spin$-1/2$ particles interacting via a static central potential $V(\vec{r}) = V(r)$. Making use of the separation method of angular coordinates described before [2] we reduced equation (1) to the radial equation

$$\left\{\varepsilon + i(\alpha_3^{(1)} - \alpha_3^{(2)})\left[\frac{d}{dr} + \frac{1 + \frac{1}{2}(\alpha_1^{(1)}\alpha_1^{(2)} + \alpha_2^{(1)}\alpha_2^{(2)})}{r}\right]\right.$$

$$\left. - i(\alpha_1^{(1)} - \alpha_1^{(2)}) \frac{\alpha_2^{(1)}\alpha_2^{(2)}\sqrt{j(j+1)}}{r} - \beta^{(1)}\kappa^{(1)} - \beta^{(2)}\kappa^{(2)} - v(r)\right\} \psi(r) = 0, \tag{2}$$

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where

$$\varepsilon = \frac{E}{\hbar c}, \quad \kappa^{(i)} = \frac{m^{(i)}c^2}{\hbar c}, \quad v(r) = \frac{V(r)}{\hbar c} \tag{3}$$

and $j(j+1)\hbar^2$ is the eigenvalue of $\vec{J}^2$ corresponding to the wave function $\psi(\vec{r})$ and

$$\vec{J} = \vec{r}\times\vec{p} + \frac{\hbar}{2}(\vec{\sigma}^{(1)}+\vec{\sigma}^{(2)}). \tag{4}$$

By choosing a special representation of the Dirac matrices appearing in (2) we were able to write this radial equation in the form of a system of eight equations listed in Table I in Ref. [1]. Now, if we slightly change this representation by replacing $\beta^{(1)} \to -\beta^{(1)}$, we get a new system of eight equations differing from the former only by the substitution $\kappa^{(1)} \to -\kappa^{(1)}$. In particular for $j = 0$ we have now the equations

$$\begin{aligned} &\frac{d}{dr}f_2 + \tfrac{1}{2}\left[\varepsilon - v - \frac{(\kappa^{(1)}-\kappa^{(2)})^2}{\varepsilon - v}\right]f_3 = 0, \\ &-\left(\frac{d}{dr}+\frac{2}{r}\right)f_3 + \tfrac{1}{2}\left[\varepsilon - v - \frac{(\kappa^{(1)}+\kappa^{(2)})^2}{\varepsilon - v}\right]f_2 = 0 \end{aligned} \tag{5}$$

in place of the equations (27) in Ref. [1].

In the case of weak potential when $1/(\varepsilon - v) \simeq \left(1+\frac{v}{\varepsilon}\right)\Big/\varepsilon$, equations (5) take approximately the form

$$\begin{aligned} &\frac{d}{dr}f_2 + \left(\frac{1}{a_2} - k_2 v\right)f_3 = 0, \\ &\left(\frac{d}{dr}+\frac{2}{r}\right)f_3 + \left(\frac{1}{a_1} + k_1 v\right)f_2 = 0 \end{aligned} \tag{6}$$

which replaces formula (30) in Ref. [1]. Here

$$\begin{aligned} &\frac{1}{a_1} = \frac{\varepsilon}{2}\left[\left(\frac{\kappa^{(1)}+\kappa^{(2)}}{\varepsilon}\right)^2 - 1\right], \quad \frac{1}{a_2} = \frac{\varepsilon}{2}\left[1 - \left(\frac{\kappa^{(1)}-\kappa^{(2)}}{\varepsilon}\right)^2\right], \\ &k_1 = \tfrac{1}{2}\left[1 + \left(\frac{\kappa^{(1)}+\kappa^{(2)}}{\varepsilon}\right)^2\right], \quad k_2 = \tfrac{1}{2}\left[1 + \left(\frac{\kappa^{(1)}-\kappa^{(2)}}{\varepsilon}\right)^2\right] \end{aligned} \tag{7}$$

are the same as in Ref. [1].

In the case of bound states in the Coulomb potential $v = -\alpha/r$, the polynomial method applied to equations (6) leads to the energy levels $\varepsilon = \varepsilon_{n_r j=0}$ given by the algebraic equation

$$\frac{n_r+\gamma}{\alpha} = \frac{\sqrt{a_1 a_2}}{2}\left(\frac{k_1}{a_2} - \frac{k_2}{a_1}\right), \quad n_r = 0, 1, 2, \ldots, \tag{8}$$

where

$$\gamma = \sqrt{1-k_1k_2\alpha^2}\,. \tag{9}$$

Formulae (8) and (9) are the same as in Ref. [1] except for the fact that in Ref. [1] the lowest value $n_r = 0$ is excluded because it leads to contradictory equations for polynomial coefficients (this point has been overlooked in Ref. [1]). The values of $\varepsilon_{n_r j=0}$, numerically

TABLE I

Coulomb energy levels $E_{n_r j} - (m^{(1)}+m^{(2)})c^2$ with $j = 0$ (in eV) for hydrogen and positronium given by Balmer formula, Sommerfeld formula and equation (8) as well as (for positronium) by more exact equations (5). Here we use the values: $1/\alpha = 137.035982$, $m_p = 938.2796$ MeV, $m_e = 0.5110034$ MeV and $\hbar c = 1.9732858 \times 10^{-5}$ eV · cm. Digits in parentheses are influenced by experimental error of physical constants but differences between columns calculated with the use of these digits are not affected

Hydrogen

n_r	Balmer	Sommerfeld	Eq. (8)
0	−13.598(409)	−13.598(590)	−13.598(590)
1	− 3.3996(022)	− 3.3996(588)	− 3.3996(588)
2	− 1.5109(343)	− 1.5109(544)	− 1.5109(544)
3	− 0.84990(057)	− 0.84990(976)	− 0.84990(975)

Positronium

n_r	Balmer	Sommerfeld	Eq. (8)	Eq. (5)
0	−6.8029(075)	−6.8029(981)	−6.8030(207)	−6.8028(4)
1	−1.7007(269)	−1.7007(551)	−1.7007(453)	−1.7007(2)
2	−0.75587(861)	−0.75588(867)	−0.75588(448)	−0.75587(8)
3	−0.42518(172)	−0.42518(632)	−0.42518(428)	−0.42518(1)

calculated from equation (8) for hydrogen and positronium, are listed in Table I and compared there with the values following from Balmer and Sommerfeld formulae (*both* with reduced mass).

In the case of positronium, the values of $\varepsilon_{n_r j=0}$ have been obtained also by numerically solving our equations (5) without making use of weak-potential approximation. The results are given in the last column of Table I. For a relevant comparison of these results with the data (and with the previous perturbative calculations based on the Pauli approximation with Breit terms included and annihilation and radiation corrections added, cf. e.g. [3]), the values of $\varepsilon_{n_r j}$ for $j \neq 0$ are needed. They might be obtained by numerically solving the system of eight equations listed in Table I in Ref. [1] (where now $\kappa^{(1)} \to -\kappa^{(1)}$), in the case of $v = -\alpha/r$. These equations, however, do not contain Breit terms (i.e., the leading magnetic and retardation terms) which might be here treated in practical calcula-

tions as a perturbation. A more consequent and elegant procedure would be, of course, to solve numerically a system of relativistic radial equations already containing Breit terms. Such a system, in fact, is derived in Appendix and presented in Table II. It consists of eight equations like the previous system and is reduced to it if Breit terms are neglected. We hope to turn back to the task of solving these equations later on.

TABLE II

The radial equation (A3) written in our representation of Dirac matrices

$$\frac{d}{dr}f_2+\tfrac{1}{2}(\kappa^{(1)}-\kappa^{(2)})f_4+\tfrac{1}{2}(\varepsilon-v-\tfrac{1}{2}v')f_3+\tfrac{1}{4}v'f_1 = 0,$$

$$-\left(\frac{d}{dr}+\frac{2}{r}\right)f_3+\tfrac{1}{2}(\kappa^{(1)}+\kappa^{(2)})f_1+\tfrac{1}{2}(\varepsilon-v-\tfrac{1}{2}v')f_2+\tfrac{1}{4}v'f_4+\frac{i\sqrt{j(j+1)}}{r}g_4 = 0,$$

$$\tfrac{1}{2}(\kappa^{(1)}-\kappa^{(2)})f_3+\tfrac{1}{2}(\varepsilon-v+\tfrac{1}{2}v')f_4+\tfrac{1}{4}v'f_2+\frac{i\sqrt{j(j+1)}}{r}g_2 = 0,$$

$$\tfrac{1}{2}(\kappa^{(1)}+\kappa^{(2)})f_2+\tfrac{1}{2}(\varepsilon-v+\tfrac{3}{2}v')f_1+\tfrac{1}{4}v'f_3 = 0,$$

$$\left(\frac{d}{dr}+\frac{1}{r}\right)g_2+\tfrac{1}{2}(\kappa^{(1)}-\kappa^{(2)})g_4+\tfrac{1}{2}(\varepsilon-v-v')g_3-\tfrac{1}{4}v'(f_2+f_4) = 0,$$

$$-\left(\frac{d}{dr}+\frac{1}{r}\right)g_3+\tfrac{1}{2}(\kappa^{(1)}+\kappa^{(2)})g_1+\tfrac{1}{2}(\varepsilon-v-v')g_2-\tfrac{1}{4}v'(f_3-f_1)-\frac{i\sqrt{j(j+1)}}{r}f_4 = 0,$$

$$\tfrac{1}{2}(\kappa^{(1)}-\kappa^{(2)})g_3+\tfrac{1}{2}(\varepsilon-v+v')g_4-\tfrac{1}{4}v'(f_1-f_3)-\frac{i\sqrt{j(j+1)}}{r}f_2 = 0,$$

$$\tfrac{1}{2}(\kappa^{(1)}+\kappa^{(2)})g_2+\tfrac{1}{2}(\varepsilon-v+v')g_1-\tfrac{1}{4}v'(f_2+f_4) = 0.$$

In the one-body limit when $\varepsilon = \varepsilon^{(1)}+\kappa^{(2)}$ and $\kappa^{(1)}/\kappa^{(2)} \to 0$, equation (8) gives the Sommerfeld formula with $j^{(1)} = 1/2$:

$$\varepsilon^{(1)} = \frac{\kappa^{(1)}}{\sqrt{1+\left(\dfrac{\alpha}{n_r+\gamma^{(1)}}\right)^2}}, \qquad n_r = 0, 1, 2, \ldots, \tag{10}$$

where

$$\gamma^{(1)} = \sqrt{1-\alpha^2}\,. \tag{11}$$

Formula (10) is the same as in Ref. [1] but there $n_r \neq 0$. In the present paper this formula corresponds to the eigenvalue $k^{(1)} = 1$ of the operator (cf. [4])

$$K^{(1)} = \beta^{(1)}[\vec{\sigma}^{(1)} \cdot (\vec{r}\times\vec{p})/\hbar+1], \tag{12}$$

while in Ref. [1] it relates to $k^{(1)} = -1$. So, in the one-body limit, we have actually to do with two special cases (with $j^{(1)} = 1/2$) of the Sommerfeld formula:

$$\varepsilon^{(1)} = \frac{\kappa^{(1)}}{\sqrt{1+\left(\dfrac{\alpha}{n_r+\gamma^{(1)}}\right)^2}}, \qquad n_r = \begin{cases} 0, 1, 2, \ldots, \\ \text{or} \\ 1, 2, 3, \ldots \end{cases} \tag{13}$$

where

$$\gamma^{(1)} = \sqrt{(j^{(1)}+\tfrac{1}{2})^2-\alpha^2}\,, \quad j^{(1)} = \tfrac{1}{2}\,,\ \tfrac{3}{2}\,,\ \tfrac{5}{2}\,,\ \ldots \tag{14}$$

and

$$k^{(1)} = \begin{cases} 1, 2, 3, \ldots \\ \text{or} \\ -1, -2, -3, \ldots \end{cases}, \quad l = \begin{cases} k^{(1)}-1 = j^{(1)}-\tfrac{1}{2} = 0, 1, 2, \ldots \\ \text{or} \\ -k^{(1)} = j^{(1)}+\tfrac{1}{2} = 1, 2, 3, \ldots \end{cases}, \tag{15}$$

$l(l+1)\hbar^2$ being the eigenvalue of the operator $(\vec{r}\times\vec{p})^2$ corresponding to the "large" components of the wave function $\psi(\vec{r})$ (cf. [4]). The principal quantum number is

$$n = n_r+j^{(1)}+\tfrac{1}{2} = \begin{cases} 1, 2, 3, \ldots \\ \text{or} \\ 2, 3, 4, \ldots \end{cases}. \tag{16}$$

In the nonrelativistic limit when $\varepsilon = \kappa^{(1)}+\kappa^{(2)}+\Delta\varepsilon$ and $\Delta\varepsilon/(\kappa^{(1)}+\kappa^{(2)}) \to 0$, equation (8) leads to the Balmer formula

$$\Delta\varepsilon = -\frac{\alpha^2\kappa}{2n^2}\,, \quad n = n_r+1 = 1, 2, 3, \ldots \tag{17}$$

which is the same as in Ref. [1] but there $n = n_r+1 \neq 1$. In equation (17)

$$\frac{1}{\kappa} = \frac{1}{\kappa^{(1)}} + \frac{1}{\kappa^{(2)}}\,. \tag{18}$$

In the general case (where not necessarily $j = 0$) the principal quantum number is

$$n = \begin{cases} n_r+l+1 = 1, 2, 3, \ldots \\ \text{or} \\ n_r+l = 2, 3, 4, \ldots \end{cases}, \tag{19}$$

where $n_r \geqslant 0$ or $n_r \geqslant 1$, respectively.

APPENDIX

Consider the relativistic equation (1), where now the interaction energy $V(\vec{r})$ is no longer a static central potential $V(r)$ but has a more general form

$$V(\vec{r}) = V(r)-\tfrac{1}{2}(\vec{\alpha}^{(1)}\cdot\vec{\alpha}^{(2)}+\alpha_r^{(1)}\alpha_r^{(2)})V'(r), \tag{A1}$$

where $V(r)$ and $V'(r)$ are some static central potentials and

$$\alpha_r^{(i)} = \frac{\vec{r}}{r}\cdot\alpha^{(i)}. \tag{A2}$$

The electromagnetic interaction equal to the Coulomb potential plus Breit terms is just of the form (A1), where $V(r) = V'(r) = \mp e^2/r$.

Applying our separation method of angular coordinates we get in this case the following radial equation:

$$\left\{\varepsilon+i(\alpha_3^{(1)}-\alpha_3^{(2)})\left[\frac{d}{dr}+\frac{1+\frac{1}{2}(\alpha_1^{(1)}\alpha_1^{(2)}+\alpha_2^{(1)}\alpha_2^{(2)})}{r}\right]\right.$$

$$-i(\alpha_1^{(1)}-\alpha_1^{(2)})\frac{\alpha_2^{(1)}\alpha_2^{(2)}\sqrt{j(j+1)}}{r}-\beta^{(1)}\kappa^{(1)}-\beta^{(2)}\kappa^{(2)}$$

$$\left.-v(r)+\tfrac{1}{2}(\alpha_1^{(1)}\alpha_1^{(2)}+\alpha_2^{(1)}\alpha_2^{(2)}+2\alpha_3^{(1)}\alpha_3^{(2)})v'(r)\right\}\psi(r)=0, \tag{A3}$$

where

$$v'(r)=\frac{V'(r)}{\hbar c}. \tag{A4}$$

In particular, for the interaction equal to the Coulomb potential plus Breit terms $v(r) = v'(r) = \mp\alpha/r$.

If we choose the representation of the Dirac matrices appearing in (A3) in such a way as in Ref. [1] but with the change $\beta^{(1)} \to -\beta^{(1)}$, we obtain from the radial equation (A3) the system of eight equations listed in Table II. Obviously, it reduces to the previous system given in Table I in Ref. [1] (where now $\kappa^{(1)} \to -\kappa^{(1)}$) if we put $v'(r) = 0$.

For $j = 0$ we can separate from the system of eight equations in Table II a closed subsystem of four equations for f's. If we eliminate from this subsystem f_1 and f_4, we get the following two equations:

$$\left[\frac{d}{dr}-\tfrac{1}{4}v'\left(\frac{\kappa^{(1)}-\kappa^{(2)}}{\varepsilon-v+\frac{1}{2}v'}+\frac{\kappa^{(1)}+\kappa^{(2)}}{\varepsilon-v+\frac{3}{2}v'}\right)\right]f_2$$

$$+\tfrac{1}{2}\left[\varepsilon-v-\tfrac{1}{2}v'-\frac{(\kappa^{(1)}-\kappa^{(2)})^2}{\varepsilon-v+\frac{1}{2}v}-\frac{v'^2}{\varepsilon-v+\frac{3}{2}v}\right]f_3=0,$$

$$\left[-\left(\frac{d}{dr}+\frac{2}{r}\right)-\tfrac{1}{4}v'\left(\frac{\kappa^{(1)}-\kappa^{(2)}}{\varepsilon-v+\frac{1}{2}v'}+\frac{\kappa^{(1)}+\kappa^{(2)}}{\varepsilon-v+\frac{3}{2}v'}\right)\right]f_3$$

$$+\tfrac{1}{2}\left[\varepsilon-v-\tfrac{3}{2}v'-\frac{(\kappa^{(1)}+\kappa^{(2)})^2}{\varepsilon-v+\frac{3}{2}v'}-\frac{v'^2}{\varepsilon-v+\frac{1}{2}v'}\right]f_2=0. \tag{A5}$$

Obviously, they reduce to the previous equations (5) if $v'(r) = 0$.

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