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Quasi-Stationary States of Hydrogen

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Abstract

We consider the hydrogen atom within the context of a theory of relativistic quantum mechanics that allows for a probabilistic interpretation of the wave function. We find the radial equation that determines the energy levels of bound states, represented by quasi-stationary states. We compute the order of magnitude of the shifts from the usual spectrum obtained from the Dirac equation, and we find that the leading terms for these corrections are of the order of $\alpha^6 \log \alpha$ for s-states and α^6 for other states. They are small compared to the Lamb shift, which is of the order of $\alpha^5 \log \alpha$.

1. *Introduction*

The energy spectrum of the hydrogen atom obtained from the Dirac equation is in excellent agreement with experimental results, especially when corrected for effects of the nuclear spin and the radiation field. Nevertheless, we have been unable to find a consistent interpretation of the corresponding wave functions along the lines of the probability amplitudes of non-relativistic quantum mechanics.

On the other hand, we have developed a probabilistic interpretation of relativistic quantum mechanics, which leads to the notion of quasi-stationary states to describe bound states (Marx, 1970, Walter & Marx, 1971). It is related to the use of causal Green functions and the specification of initial and final conditions (Marx, 1969).

In Section 2 we find the corresponding radial equation and reduce it to a Fredholm integral equation. Since the solution of either equation appears to be difficult and we already have the corresponding solutions of the Dirac equation, we use the latter to estimate the shift in the levels due to this different approach; in Section 3 we find that they are of the order of $\alpha^6 \log \alpha$ for s-states and of the order of α^6 for the others. This gives a small correction to the Lamb shift, which is of the order of $\alpha^5 \log \alpha$, and comes from the consideration of a dynamical radiation field. We collect some of the mathematical derivations and formulas in an Appendix.

We use natural units and the time-favoring metric. Other details on notations can be found in Marx (1969, 1970) and Walter & Marx (1971).

2. *Eigenvalue Problem for Quasi-Stationary States*

We start our discussion of the energy spectrum of the hydrogen atom from the Dirac equation

$$(-i\gamma\cdot D + m)\psi(x) = 0 \tag{2.1}$$

where

$$D_\mu = \partial_\mu - ieA_\mu \tag{2.2}$$

$$A_0(x) = e/r, \qquad \mathbf{A}(x) = 0 \tag{2.3}$$

We rewrite this equation in terms of the probability amplitude $g(x)$, which is related to $\psi(x)$ by a free-field Foldy–Wouthuysen transformation (Foldy & Wouthuysen, 1950; Bjorken & Drell, 1964; Marx, 1969)

$$g(x) = [(\tilde{E} + m)/(2\tilde{E})]^{1/2}\,[1 - i\boldsymbol{\gamma}\cdot\boldsymbol{\nabla}/(\tilde{E} + m)]\,\psi(x) \tag{2.4}$$

where $\tilde{E}$ is the integral operator

$$\tilde{E} = (\mathbf{p}^2 + m^2)^{1/2}, \qquad \mathbf{p} = -i\boldsymbol{\nabla} \tag{2.5}$$

and equation (2.1) becomes

$$i\dot{g}(x) = H' g(x) \tag{2.6}$$

where

$$H' = \begin{pmatrix} H_{++} & -H_{+-} \\ H_{-+} & H_{--} \end{pmatrix} \tag{2.7}$$

$$H_{\pm\pm} = \pm\tilde{E} - e^2\left(\frac{\tilde{E}+m}{2\tilde{E}}\right)^{1/2}\left(\frac{1}{r} + \frac{\boldsymbol{\sigma}\cdot\mathbf{p}}{\tilde{E}+m}\frac{1}{r}\frac{\boldsymbol{\sigma}\cdot\mathbf{p}}{\tilde{E}+m}\right)\left(\frac{\tilde{E}+m}{2\tilde{E}}\right)^{1/2} \tag{2.8}$$

$$H_{+-} = H_{-+} = e^2\left(\frac{\tilde{E}+m}{2\tilde{E}}\right)^{1/2}\left(\frac{1}{r}\frac{\boldsymbol{\sigma}\cdot\mathbf{p}}{\tilde{E}+m} - \frac{\boldsymbol{\sigma}\cdot\mathbf{p}}{\tilde{E}+m}\frac{1}{r}\right)\left(\frac{\tilde{E}+m}{2\tilde{E}}\right)^{1/2} \tag{2.9}$$

In order to have a conserved charge instead of a conserved 'probability', we modify the Dirac equation by replacing H' in equation (2.6) by

$$H = \begin{pmatrix} H_{++} & H_{+-} \\ H_{-+} & H_{--} \end{pmatrix} \tag{2.10}$$

We obtain the energy spectrum of the bound states from the eigenvalue equation

$$H_{++}q^{(+)}(\mathbf{x}) = Eq^{(+)}(\mathbf{x}) \tag{2.11}$$

This equation is much more difficult to solve than the usual ones found in quantum mechanics due to the presence of the operator $\tilde{E}$ in H_{++}. It is still

possible, though, to separate the angular and radial parts of the equation, since the angular momentum operator†

$$\mathbf{J} = \mathbf{x} \wedge \mathbf{p} + \tfrac{1}{2}\boldsymbol{\sigma} \tag{2.12}$$

commutes with H_{++}. We consequently can write (Rose, 1961; Bjorken & Drell, 1964; Akhiezer & Berestetskii, 1965)

$$q^{(+)}(\mathbf{x}) = a(r)\,\mathscr{Y}^m_{j=l\pm 1/2}(\theta, \phi) \tag{2.13}$$

where‡

$$\mathscr{Y}^m_{j=l\pm 1/2}(\theta, \phi) = \begin{pmatrix} [(j \pm m)^{1/2}/(2j)^{1/2}]\; Y_l^{m-1/2}(\theta, \phi) \\ \pm[(j \mp m)^{1/2}/(2j)^{1/2}]\; Y_l^{m+1/2}(\theta, \phi) \end{pmatrix} \tag{2.14}$$

We use equation (A.4) to show that a function of $\tilde{E}$ gives

$$\Phi(\tilde{E})\,[a(r)\,\mathscr{Y}^m_{j=l\pm 1/2}(\theta, \phi)] = \mathscr{Y}^m_{j=l\pm 1/2}(\theta, \phi)\,\Phi(\tilde{E}_l)\,a(r) \tag{2.15}$$

where the operator $\Phi(\tilde{E}_l)$ is defined in equation (A.5), and we recall that

$$\boldsymbol{\sigma}\cdot\mathbf{p}a(r)\,\mathscr{Y}_\kappa{}^m(\theta, \phi) = \mathscr{Y}_{-\kappa}{}^m(\theta, \phi)\,i[d/dr + (1+\kappa)/r]\,a(r) \tag{2.16}$$

where

$$\kappa = \mp(j + \tfrac{1}{2}) \qquad \text{for } j = l \pm \tfrac{1}{2} \tag{2.17}$$

We note that κ determines both j and l, since we can rewrite equation (2.17) as

$$j = \begin{cases} l - \tfrac{1}{2} = \kappa - \tfrac{1}{2} & \text{for } \kappa > 0 \\ l + \tfrac{1}{2} = -\kappa - \tfrac{1}{2} & \text{for } \kappa < 0 \end{cases} \tag{2.18}$$

We substitute equation (2.13) into equation (2.11) and use equations (2.15) and (2.16) to obtain the radial equation for a given value of κ (independent of m),

$$H_\kappa\, a(r) = Ea(r) \tag{2.19}$$

where

$$\begin{aligned} H_\kappa = \tilde{E}_l &- e^2[(\tilde{E}_l + m)/(2\tilde{E}_l)]^{1/2}\, r^{-1}[(\tilde{E}_l + m)/(2\tilde{E}_l)]^{1/2} \\ &+ e^2[2\tilde{E}_l(\tilde{E}_l + m)]^{-1/2}\,[-r^{-1}\,d^2/dr^2 - r^{-2}\,d/dr \\ &+ (1+\kappa)^2 r^{-3}]\,[2\tilde{E}_l(\tilde{E}_l + m)]^{-1/2} \end{aligned} \tag{2.20}$$

The complicated properties of the operator $\tilde{E}_l$ do not allow us to solve this equation by an expansion in powers of r. We can change its form somewhat by replacing $a(r)$ and H_κ by $\Phi(\tilde{E}_l)a(r)$ and $\Phi(\tilde{E}_l)\,H_\kappa[\Phi(\tilde{E}_l)]^{-1}$ respectively, or by using $(H_\kappa)^2$ to find E^2, but we have not been able to find the eigenvalues and eigenfunctions in this way.

† We note that $\mathbf{x}$ is the correct choice for the position operator *in the Foldy-Wouthuysen representation*, and similarly the angular momentum operator is given by equation (2.12). These matters are discussed in more detail in Schröder (1964) and Marx (1968).

‡ We use the sign convention of Rose (1961) and Akhiezer & Berestetskii (1965), while the signs in $\mathscr{Y}^m_{j=l-1/2}$ are reversed by Bjorken & Drell (1964). We also think that no confusion should arise from the use of the letter m for both the mass of the electron and the magnetic quantum number.

We can rewrite equation (2.19) in still another form, in terms of a spherical Hankel transform of $a(r)$,

$$\tilde{a}(K) = (2/\pi)^{1/2} \int_0^\infty r^2\, dr j_l(Kr)\, a(r) \tag{2.21}$$

it becomes

$$\int_0^\infty K^2\, dK H_\kappa(K', K)\, \tilde{a}(K) = E\tilde{a}(K') \tag{2.22}$$

where

$$H_\kappa(K', K) = (2/\pi) \int_0^\infty r^2\, dr j_l(K' r)\, H_\kappa j_l(Kr) \tag{2.23}$$

We can calculate the integral in equation (2.23) with the help of equations† (A.7), (A.9), (A.10), (E'-8.11.9), (E-2.8.18), (E-2.8.33), (E-2.8.36), (E-3.2.45) and (E-3.3.2); we find

$$H_\kappa(K', K) = (k_0/K^2)\, \delta(K - K') + H_{I\kappa}(K', K) \tag{2.24}$$

where

$$\begin{aligned} H_{I\kappa}(K', K) = -\frac{e^2}{2\pi} \Bigg\{ & \left[\frac{(k_0 + m)(k_0' + m)}{k_0 k_0'}\right]^{1/2} \frac{1}{KK'}\, Q_l\left(\frac{K^2 + K'^2}{2KK'}\right) \\ & + \left[\frac{1}{(k_0 + m)(k_0' + m) k_0 k_0'}\right]^{1/2} \left[\frac{K^2 + K'^2}{2KK'}\, Q_l\left(\frac{K^2 + K'^2}{2KK'}\right)\right. \\ & \left. + \left(1 - \frac{(1+\kappa)^2}{l(l+1)}\right) \frac{|K^2 - K'^2|}{2KK'}\, Q_l^1\left(\frac{K^2 + K'^2}{2KK'}\right)\right] \Bigg\} \end{aligned} \tag{2.25}$$

where

$$k_0 = (K^2 + m^2)^{1/2}, \qquad k_0' = (K'^2 + m^2)^{1/2} \tag{2.26}$$

and Q_l and Q_l^1 are Legendre and associated Legendre functions of the second kind. The function $H_\kappa(K', K)$ is symmetric in K and K', which is expected from the Hermitian nature of H_{++}. We substitute equation (2.24) into equation (2.22) to obtain

$$\tilde{a}(K') = (E - k_0')^{-1} \int_0^\infty K^2\, dK H_{I\kappa}(K', K)\, \tilde{a}(K) \tag{2.27}$$

which is a homogeneous Fredholm equation of the second kind (Morse & Feshbach, 1953). It has nontrivial solutions only for certain values of the parameter E, which are the energy levels of the quasi-stationary states.

† The letter E preceding an equation number indicates that it belongs to Erdélyi (1953), while E' refers to Erdélyi (1954).

3. *Lowest Order Approximation to the Level Shifts*

Since the eigenvalue problem discussed in the previous section does not appear to have a simple solution, we now take advantage of our knowledge of the solutions of the Dirac equation for the hydrogen atom in the case of stationary states to compute the small shifts to the levels of the quasi-stationary states. In particular, we compute the order of magnitude of these shifts for the $2s_{1/2}$ and $2p_{1/2}$ levels, and find that they are small compared to the Lamb shift.

The energy spectrum for the hydrogen atom obtained from stationary states is given by

$$E_{n\kappa} = m[1 + \alpha^2(n' + \gamma)^{-2}]^{-1/2} \tag{3.1}$$

where α is the fine-structure constant and

$$n' = n - |\kappa| \tag{3.2}$$

$$\gamma = (\kappa^2 - \alpha^2)^{1/2} \tag{3.3}$$

We see that the value of the energy depends only on $|\kappa|$, that is, it depends on j but not on l, bringing about the degeneracy that is lifted by the Lamb shift. The wave functions for these states are

$$\psi_{n\kappa m}(\mathbf{x}) = \begin{pmatrix} g(r)\,\mathscr{Y}_{\kappa}^{\,m}(\theta,\phi) \\ if(r)\,\mathscr{Y}_{-\kappa}^{\,m}(\theta,\phi) \end{pmatrix} \tag{3.4}$$

where† f and g can be expressed in terms of confluent hypergeometric functions by

$$f(r) = -N(1 - W)^{1/2}(2\lambda r)^{\gamma-1}\exp[-\lambda r](F_1 + F_2) \tag{3.5}$$

$$g(r) = N(1 + W)^{1/2}(2\lambda r)^{\gamma-1}\exp[-\lambda r](-F_1 + F_2) \tag{3.6}$$

where

$$N = (\lambda/m)^2\{2\Gamma(2\gamma + n' + 1)/[n'!\alpha(\alpha m/\lambda - \kappa)]\}^{1/2}/\Gamma(2\gamma + 1) \tag{3.7}$$

$$W = E_0/m \tag{3.8}$$

$$\lambda = \alpha E_0/(n' + \gamma) \tag{3.9}$$

$$F_1(2\lambda r) = n'F(-n' + 1, 2\gamma + 1, 2\lambda r) \tag{3.10}$$

$$F_2(2\lambda r) = (\alpha m/\lambda - \kappa)F(-n', 2\gamma + 1, 2\lambda r) \tag{3.11}$$

the hypergeometric functions in equations (3.10) and (3.11) are polynomials in r. We then determine $q_0^{(+)}(\mathbf{x})$ and $q_0^{(-)}(\mathbf{x})$, where the subindex indicates that they correspond to stationary states, by means of equation (2.4), to be

$$q_0^{(+)}(\mathbf{x}) = [(\tilde{E} + m)/(2\tilde{E})]^{1/2}[g\mathscr{Y}_{\kappa}^{\,m} + i(\tilde{E} + m)^{-1}\,\boldsymbol{\sigma}\cdot\mathbf{p}f\mathscr{Y}_{-\kappa}^{\,m}] \tag{3.12}$$

$$q_0^{(-)}(\mathbf{x}) = [(\tilde{E} + m)/(2\tilde{E})]^{1/2}[if\mathscr{Y}_{-\kappa}^{\,m} - (\tilde{E} + m)^{-1}\,\boldsymbol{\sigma}\cdot\mathbf{p}g\mathscr{Y}_{\kappa}^{\,m}] \tag{3.13}$$

† We have dropped the indices n and κ from f and g, and we designate the corresponding $E_{n\kappa}$ simply by E_0, the 'unperturbed' energy level.

We use equations (2.15), (2.16) and

$$df/dr = (\kappa - 1)f/r - (E_0 - m + \alpha/r)\,g \tag{3.14}$$

$$dg/dr = (E_0 + m + \alpha/r)f - (\kappa + 1)\,g/r \tag{3.15}$$

to reduce them to the form

$$q_0^{(+)}(\mathbf{x}) = \mathscr{Y}_\kappa{}^m[(\tilde{E}_l + m)/(2\tilde{E}_l)]^{1/2}\,[1 + (\tilde{E}_l + m)^{-1}\,(E_0 - m + \alpha/r)]\,g \tag{3.16}$$

$$q_0^{(-)}(\mathbf{x}) = i\mathscr{Y}_{-\kappa}{}^m[(\tilde{E}_{\bar{l}} + m)/(2\tilde{E}_{\bar{l}})]^{1/2}\,[1 - (\tilde{E}_{\bar{l}} + m)^{-1}\,(E_0 + m + \alpha/r)]f \tag{3.17}$$

where $\bar{l}$ is given by equation (A.12). These functions satisfy

$$H_{++}q_0^{(+)} - H_{+-}q_0^{(-)} = E_0 q_0^{(+)} \tag{3.18}$$

which we obtain from equation (2.6). We assume that these eigenfunctions and eigenvalues do not differ much from those for quasi-stationary states, and we write

$$q^{(+)}(\mathbf{x}) = q_0^{(+)}(\mathbf{x}) + \delta q^{(+)}(\mathbf{x}) \tag{3.19}$$

$$E = E_0 + \delta E \tag{3.20}$$

We multiply both sides of equation (2.11) by $q_0^{(+)\dagger}$ and integrate to obtain

$$\int d^3x(q_0^{(+)\dagger} H_{+-}q_0^{(-)} + q_0^{(-)\dagger} H_{+-}^{\dagger}\delta q^{(+)}) = (\delta E)\int d^3x(q_0^{(+)\dagger} q_0^{(+)} + q_0^{(-)\dagger}\delta q^{(+)}) \tag{3.21}$$

where we have used equation (3.18) and the Hermitian property of H_{++}. We neglect small terms to obtain the lowest order correction for the energy level,

$$\delta E \approx \int d^3x q_0^{(+)\dagger} H_{+-}q_0^{(-)} \tag{3.22}$$

since the normalization of ψ implies that $q_0^{(+)}$ is normalized to lowest order, We substitute $q_0^{(+)}$ and $q_0^{(-)}$ from equations (3.16) and (3.17), we use equations (2.15), (2.16), (A.11), (3.14) and (3.15), we integrate over the angles and use integration by parts to obtain

$$\begin{aligned}\delta E \approx \tfrac{1}{4}\alpha \int_0^\infty r^2\,dr\,\{&g(\tilde{E}_l + E_0 + \alpha/r)\,\tilde{E}_l^{-1}\,r^{-1} \\ &\times \tilde{E}_l^{-1}(\tilde{E}_l + m)^{-1}\,[(\tilde{E}_l - E_0 - \alpha/r)\,(E_0 - m + \alpha/r)\,g - \alpha f/r^2] \\ &- [f(E_0 + m + \alpha/r)\,(\tilde{E}_{\bar{l}} + E_0 + \alpha/r) - \alpha g/r^2] \\ &\times (\tilde{E}_{\bar{l}} + m)^{-1}\,\tilde{E}_{\bar{l}}^{-1}\,r^{-1}\,\tilde{E}_{\bar{l}}^{-1}(\tilde{E}_{\bar{l}} - E_0 - \alpha/r)f\}\end{aligned} \tag{3.23}$$

We now change the variable of integration to

$$\rho = \alpha m r \tag{3.24}$$

and substitute f and g from equations (3.5) and (3.6) to find

$$\begin{aligned}\delta E \approx{}& \tfrac{1}{4}\alpha^{-1} N^2 m \int_0^\infty \rho^2 d\rho (2\lambda'\rho)^{\gamma-1} \exp[-\lambda'\rho] \\ &\times \{(1+W)^{1/2}(-F_1+F_2)(\mathscr{E}_l + W + \alpha^2/\rho)\mathscr{E}_l^{-1}\rho^{-1}\mathscr{E}_l^{-1} \\ &\times (\mathscr{E}_l+1)^{-1}[(\mathscr{E}_l - W - \alpha^2/\rho)(W-1-\alpha^2/\rho)(1+W)^{1/2} \\ &\times (-F_1+F_2) + (\alpha^3/\rho^2)(1-W)^{1/2}(F_1+F_2)] - [(1-W)^{1/2} \\ &\times (F_1+F_2)(W+1+\alpha^2/\rho)(\mathscr{E}_{\bar{l}} + W + \alpha^2/\rho) \\ &+ (\alpha^3/\rho^2)(1+W)^{1/2}(-F_1+F_2)](\mathscr{E}_{\bar{l}}+1)^{-1}\mathscr{E}_{\bar{l}}^{-1}\rho^{-1}\mathscr{E}_{\bar{l}}^{-1} \\ &\times (\mathscr{E}_{\bar{l}} - W - \alpha^2/\rho)(1-W)^{1/2}(F_1+F_2)\}(2\lambda'\rho)^{\gamma-1}\exp[-\lambda'\rho] \quad (3.25)\end{aligned}$$

where the argument of F_1 and F_2 has been changed to $2\lambda'\rho$, we use the operator $\mathscr{E}_l$ which is defined in equation (A.13) and we have set

$$\lambda' = \lambda/(\alpha m) = W/(n'+\gamma) \quad (3.26)$$

We can now try a straightforward expansion in powers of α, keeping only the lowest order terms. In particular, we expand the operator $\mathscr{E}_l$, using equation (A.7), and find

$$\mathscr{E}_l = 1 + \tfrac{1}{2}\alpha^2[-\rho^{-1}(d^2/d\rho^2)\rho + l(l+1)\rho^{-2}] + \cdots \quad (3.27)$$

which leads to a correct results in some cases, and to apparent divergences in others.† The resulting expression for the energy shift is

$$\begin{aligned}\delta E \approx{}& 4^{|\kappa|-2} n^{-2|\kappa|-4} n'![(n+|\kappa|)!(n-\kappa)]^{-1} m\alpha^6 \\ &\times \int_0^\infty d\rho \rho^{|\kappa|-3}\exp[-\rho/n]\{(-\Lambda_1+\Lambda_2)[(-\rho^2 d^2/d\rho^2 \\ &+ l^2 + l + \rho^2/n^2 - 2\rho)(2n^2-\rho)(-\Lambda_1+\Lambda_2) + 2n\rho(\Lambda_1+\Lambda_2)] \\ &- (\Lambda_1+\Lambda_2)(-\rho^2 d^2/d\rho^2 + \bar{l}^2 + \bar{l} + \rho^2/n^2 - 2\rho)\rho \\ &\times (\Lambda_1+\Lambda_2)\}\rho^{|\kappa|-1}\exp[-\rho/n] \quad (3.28)\end{aligned}$$

where we have expressed the confluent hypergeometric functions in terms of Laguerre polynomials‡

$$\Lambda_1 = (n+|\kappa|)L_{n'-1}^{2|\kappa|}(2\rho/n) \quad (3.29)$$

$$\Lambda_2 = (n-\kappa)L_{n'}^{2|\kappa|}(2\rho/n) \quad (3.30)$$

† We can obtain logarithmic divergences, as seen below, or linear divergences as in the calculation of the norm of $q_0^{(-)}$ shown in the Appendix.

‡ We have chosen the normalization of the Laguerre polynomials of Erdélyi (1953), not that of Morse & Feshbach (1953).

It is possible to carry out the integration† in equation (3.28), but the general result is of little interest. We first study the behavior of the integrand near the origin. For s-states, we have

$$\kappa = -1, \qquad l = 0, \qquad \bar{l} = 1 \tag{3.31}$$

and the integrand of equation (3.28) goes as ρ^{-1} for small ρ, whence the integral diverges logarithmically, and we have to go back to equation (3.25). For $p_{1/2}$-states, we have

$$\kappa = 1, \qquad l = 1, \qquad \bar{l} = 0 \tag{3.32}$$

and a cancellation of the constant terms in $-\Lambda_1 + \Lambda_2$ avoids this divergence problem. A similar conclusion is reached for all other states, due to the higher values of $|\kappa|$.

We conclude from the analysis above that the leading term in the expansion of δE for s-states has the form $\alpha^6 \log\alpha$, and we make a rough estimate of the integral in order to obtain the coefficient. We expand as before, but we keep only the lowest powers in ρ together with one of the factors $\mathscr{E}_0$ or $\mathscr{E}_1$ in the denominator, in order to obtain a convergent integral. The result for the $2s_{1/2}$ level is

$$\delta E \approx -2^{-4} m\alpha^6 \int_0^\infty \rho\, d\rho \exp[-\tfrac{1}{2}\rho]\,(2\mathscr{E}_0^{-1} + \mathscr{E}_1^{-1})\,\rho^{-2} \exp[-\tfrac{1}{2}\rho] \tag{3.33}$$

We use equation (A.13) and do the integrations over ρ and ρ' with the help of equation (E'-8.6.6) to obtain

$$\begin{aligned}\delta E \approx -\tfrac{1}{2} m\alpha^6 \int_0^\infty dK (1 + \alpha^2 K^2)^{-1/2} K \\ \times (1 + 4K^2)^{-1} \{P_{1/2}^{-1/2}[(1 + 4K^2)^{-1/2}]\, P_{-1/2}^{-1/2}[(1 + 4K^2)^{-1/2}] \\ + P_{1/2}^{-3/2}[(1 + 4K^2)^{-1/2}]\, P_{-1/2}^{-3/2}[(1 + 4K^2)^{-1/2}]\}\end{aligned} \tag{3.34}$$

where P_ν^μ are associated Legendre functions. There are no problems of convergence at $K = 0$, as we can see from equations (E-3.9.8), and we start the integral at $K = 1$ to obtain the coefficient of $\log\alpha$ from the behavior of the integrand at large K. We have

$$P_{1/2}^{-1/2}(0) = (2/\pi)^{1/2} \tag{3.35}$$

$$P_{-1/2}^{-1/2}(0) = (\pi/2)^{1/2} \tag{3.36}$$

$$P_{1/2}^{-3/2}(0) = (\pi/8)^{1/2} \tag{3.37}$$

$$P_{-1/2}^{-3/2}(0) = (2/\pi)^{1/2} \tag{3.38}$$

† We can use the equations on pp. 784 and 785 of Morse & Feshbach (1953), with some minor changes due to the different normalization.

from equation (E-3.4.20), where we can use equation (E-1.2.6) to find the value of the indeterminate expression obtained in the cases of equations (3.36) and (3.37). The integral we obtain is that in equation (A.20), and our final result is

$$\delta E \approx -(3/16)\, m\alpha^6 \log \alpha \tag{3.39}$$

On the other hand, we can find the shift of the $2p_{1/2}$ level from equation (3.24), and we obtain

$$\delta E \approx (1/192)\, m\alpha^6 \tag{3.40}$$

which is much smaller and of the opposite sign than the one for the $2s_{1/2}$ level.

These results imply a small correction to the Lamb shift, which is of the order of $\alpha^5 \log \alpha$ and is due mainly to the properties of a dynamical electromagnetic field.

4. *Concluding Remarks*

We have obtained a radial equation for the eigenvalue problem that gives the energy levels for the quasi-stationary states of the hydrogen atom. Instead of trying to solve it, we have estimated the magnitude of the shifts of the levels from the usually considered energy spectrum, obtained for stationary states from the Dirac equation; we find that these shifts are small, as expected. In particular, the shift for the $2s_{1/2}$ level is of the order of $\alpha^6 \log \alpha$ and that of the $2p_{1/2}$ is of the order of α^6 with a small coefficient, and this is small even compared to the Lamb shift. It falls within the order of magnitude of a large number of corrections to the Lamb shift, which are still largely open to question, especially within the context of a new theory.

The bulk of the Lamb shift should be obtained when we consider the much more complicated problem of the interaction of two charged particles and a dynamical electromagnetic field.

Appendix

In this Appendix we collect a number of useful mathematical† relations and derivations, mainly for the operators $\tilde{E}$ and $\tilde{E}_l$.

We define an operator that is a function of $\tilde{E}$ by the relation (Margenau & Murphy, 1964)

$$\Phi(\tilde{E}) f(\mathbf{x}) = (2\pi)^{-3} \int d^3k \exp[i\mathbf{k}\cdot\mathbf{x}]\, \Phi(k_0) \times \int d^3x' \exp[-i\mathbf{k}\cdot\mathbf{x}'] f(\mathbf{x}') \tag{A.1}$$

where

$$k_0 = (\mathbf{k}^2 + m^2)^{1/2} = (K^2 + m^2)^{1/2} \tag{A.2}$$

† We assume that the mathematical conditions that are necessary for the existence of integrals and that allow interchange of orders of integrations are satisfied. We do not claim more mathematical rigor than is usual for a paper in physics.

We use spherical coordinates r, θ, ϕ for $\mathbf{x}$ and K, $\bar{\theta}$, $\bar{\phi}$ for $\mathbf{k}$ to expand

$$\exp[i\mathbf{k}\cdot\mathbf{x}] = 4\pi \sum_{l=0}^{\infty} i^l j_l(Kr) \sum_{m=-l}^{l} Y_l^{m*}(\bar{\theta},\bar{\phi})\, Y_l^m(\theta,\phi) \tag{A.3}$$

and substitute it into equation (A.1); the orthonormality of the spherical harmonics readily gives, for a function of the form $a(r)\, Y_l^m(\theta,\phi)$,

$$\Phi(\tilde{E})\, a(r)\, Y_l^m(\theta,\phi) = Y_l^m(\theta,\phi)\, \Phi(\tilde{E}_l)\, a(r) \tag{A.4}$$

where $\tilde{E}_l$ is defined by

$$\Phi(\tilde{E}_l)\, a(r) = (2/\pi) \int_0^{\infty} K^2\, dK j_l(Kr)\, \Phi(k_0) \int_0^{\infty} r'^2\, dr'\, j_l(Kr')\, a(r') \tag{A.5}$$

We can use this equation to show that, for

$$\Phi(\tilde{E}) = \tilde{E}^2 - m^2 = -\nabla^2 \tag{A.6}$$

we have

$$\Phi(\tilde{E}_l) = -r^{-1}(d^2/dr^2)\, r + l(l+1)/r^2 \tag{A.7}$$

If we set $\Phi(\tilde{E}_l) = 1$ in equation (A.5), we find that

$$\delta(r - r') = r'^2(2/\pi) \int_0^{\infty} K^2\, dK j_l(Kr)\, j_l(Kr') \tag{A.8}$$

We find the formula for integration by parts,

$$\int_0^{\infty} r^2\, dr a(r)\, \Phi(\tilde{E}_l)\, b(r) = \int_0^{\infty} r^2\, dr b(r)\, \Phi(\tilde{E}_l)\, a(r) \tag{A.9}$$

by rearranging the order of integrations.

If we designate by a bar on top of a function its spherical Hankel transform (2.21), we can use equation (A.8) to show that

$$\overline{\Phi(\tilde{E}_l)\, a}(K) = \Phi(k_0)\, \bar{a}(K) \tag{A.10}$$

Since $\Phi(\tilde{E}_l)$ commutes with $\boldsymbol{\sigma}\cdot\mathbf{p}$, equation (2.16) implies that†

$$[d/dr + (1+\kappa)/r]\, \Phi(\tilde{E}_l) = \Phi(\tilde{E}_{\bar{l}})\, [d/dr + (1+\kappa)/r] \tag{A.11}$$

where l is determined by κ through equation (2.18), and

$$\bar{l}(\kappa) = l(-\kappa) \tag{A.12}$$

† We point out that equation (A.11), as well as others, can be derived directly from the properties of the spherical Bessel functions.

When we change the variable of integration to $\rho = \alpha mr$, we have to replace the operator $\tilde{E}_l$ by $\mathscr{E}_l$, defined by

$$\Phi(\mathscr{E}_l)\, a(\rho) = (2/\pi) \int_0^\infty K^2\, dK j_l(K\rho) \times \Phi[(1 + \alpha^2 K^2)^{1/2}] \int_0^\infty \rho'^2\, d\rho'\, j_l(K\rho')\, a(\rho') \qquad \text{(A.13)}$$

As a simple example of an expansion in α that appears to lead to a divergent integral, we compute

$$\|q_0^{(-)}\| = \int d^3 x q_0^{(-)\dagger}(\mathbf{x}) q_0^{(-)}(\mathbf{x}) \qquad \text{(A.14)}$$

for the $1s_{1/2}$ level. We use equations (3.17) and (3.5), and proceed as in Section 3 to obtain

$$\|q_0^{(-)}\| = [\tfrac{1}{4}(1 - W)/\Gamma(2\gamma + 1)] \int_0^\infty \rho^2\, d\rho \times [\mathscr{E}_1^{-1/2}(\mathscr{E}_1 + 1)^{-1/2}(\mathscr{E}_1 - W - \alpha^2/\rho)\, \rho^{\gamma-1} e^{-\rho}]^2 \qquad \text{(A.15)}$$

If we use equation (3.27) to expand $\mathscr{E}_1$, we obtain an integrand that goes as ρ^{-2} at the origin, and the integral would diverge linearly. This is clearly wrong, since

$$\|q_0^{(+)}\| + \|q_0^{(-)}\| = 1 \qquad \text{(A.16)}$$

When we proceed without this expansion, we use†

$$\int_0^\infty r^2\, dr a(r)\, b(r) = \int_0^\infty K^2\, dK \bar{a}(K)\, \bar{b}(K) \qquad \text{(A.17)}$$

for these spherical Hankel transforms to obtain

$$\|q_0^{(-)}\| = [\tfrac{1}{4}(1 - W)/\Gamma(2\gamma + 1)] \int_0^\infty K^2\, dK [\phi(K)]^2 \qquad \text{(A.18)}$$

where equations (A.10) and (E′-8.6.6) give

$$\phi(K) = (1 + \alpha^2 K^2)^{-1/4} [(1 + \alpha^2 K^2)^{1/2} + 1]^{-1/2} K^{-1/2} \times (1 + K^2)^{-\gamma/2 - 3/4}\, \Gamma(\gamma + 2) \{(\gamma + 2)[(1 + \alpha^2 K^2)^{1/2} - W] \times P_{\gamma+1/2}^{-3/2}[(1 + K^2)^{-1/2}] - \alpha^2 (1 + K^2)^{1/2} P_{\gamma-1/2}^{-3/2}[(1 + K^2)^{-1/2}]\} \qquad \text{(A.19)}$$

We note that $\phi(K)$ goes as K^{-3} for large K, and the integral in equation (A.18) converges; on the other hand, it is clear that an expansion in α would give an integrand that goes as K^{-1} to lowest order, which makes the integral diverge linearly.

† We obtain equation (A.17) with the help of equations (2.21) and (A.8).

A similar expansion for the level shift of an s-state leads to a logarithmically divergent integral. We also note that an estimate of the Lamb shift† requires the introduction of cutoffs to obtain an $\alpha^5 \log \alpha$ term, which makes us wonder whether formal expansions in the coupling constant might not be responsible for at least some of the difficulties with divergences in quantum electrodynamics.

A simple example of such an integral that can be done exactly is

$$\int_1^\infty \frac{dx}{x(1+\alpha^2 x^2)^{1/2}} = \log \frac{1+(1+\alpha^2)^{1/2}}{\alpha} = -\log \alpha + \log 2 + \tfrac{1}{4}\alpha^2 + \cdots \quad \text{(A.20)}$$

We find that the coefficient of $\log \alpha$ does not depend on the exact form of the integrand. For instance,

$$\int_1^\infty \frac{dx}{x(1+\nu\alpha^2 x^2)} = -\tfrac{1}{2} \log \frac{\nu\alpha^2}{1+\nu\alpha^2} = -\log \alpha - \tfrac{1}{2} \log \nu + \tfrac{1}{2}\nu\alpha^2 + \cdots \quad \text{(A.21)}$$

which for $\nu = 1$ is obtained when we have two such convergence factors in the denominator, and for $\nu = \frac{1}{2}$ corresponds to the expansion of the square root in equation (A.20).

Since

$$\log \alpha \approx -4{\cdot}92 \quad \text{(A.22)}$$

we do not expect to get a good approximation of an integral unless we also compute the term independent of α, but we do not know of a general method to find it.

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† See Bjorken & Drell (1964), p. 60.