PERTURBATION THEORY FOR THE DIRAC EQUATION

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By reducing the Dirac equation to a Riccati equation we construct a perturbation theory for it for the case of a central electrostatic potential. This enables us to accelerate considerably the procedure of finding successive approximations in the perturbation parameter. We express all corrections to the wave function and the bound state energy in terms of the unperturbed wave function and the energy of the same state. As an example we calculate the first approximation to the wave function and the second approximation to the energy of the K electron when we take as perturbation the difference between the atomic potential and the Coulomb potential.

1. Zel'dovich[1] (see also[2]) has shown that one can formulate perturbation theory for the discrete spectrum of the Schrödinger equation in a central field in such a way that all corrections to the wave function and energy of a bound state can be expressed in terms not of the whole spectrum of eigenfunctions and eigenvalues of the unperturbed problem but only in terms of the wave function and eigenvalue of which we try to find the corrections.

In[2] a perturbation theory was constructed for the Riccati equation to which the radial Schrödinger equation was reduced. This makes it possible to evaluate in the n-th perturbation theory approximation the wave function of a bound state up to terms of order λ^{2^n} and the energy of this state to order $\lambda^{2^{n+1}}$, where λ is the perturbation parameter. The aim of the present paper is to obtain the same results for the Dirac equation.

It is well known (see, e.g.,[3]) that the relativistic wave function of the discrete spectrum in the case of a central electrostatic potential has the form

$$\Psi_{jlm} = r^{-1}\begin{pmatrix} iG(r)\Omega_{jlm}(\mathbf{r}/r) \\ -F(r)\Omega_{jl'm}(\mathbf{r}/r) \end{pmatrix} \tag{1}$$

where $l' = 2j - l$, Ω_{jlm} is a spherical spinor, and the radial wave functions G and F are determined by the system of two first-order equations:

$$\frac{dG}{dr} + \frac{\varkappa}{r}G - (E + m - V)F = 0,$$

$$\frac{dF}{dr} - \frac{\varkappa}{r}F + (E - m - V)G = 0. \tag{2}$$

Here and henceforth $\hbar = c = 1$, $\kappa = \mp(j + 1/2)$ when $j = l \pm 1/2$, E and m are the energy and mass of the electron, $V \equiv V(r)$ is the spherically symmetric potential. The functions G and F are finite as $r \to 0$ and $r \to \infty$.

The set (2) could be reduced to the Schrödinger equation and the results from a paper by one of the authors[2] could be used. However, this method is not very useful as it would mean that we had to do our calculations with a very complicated potential. We therefore proceed differently. In the set of coupled Eqs. (2) we put

$$F = G\Phi. \tag{3}$$

These equations then split up:

$$\Phi' - \frac{2\varkappa}{r}\Phi + B\Phi^2 + B - 2m = 0, \tag{4}$$

$$G' + \left(\frac{\varkappa}{r} - B\Phi\right)G = 0. \tag{5}$$

Here and henceforth a prime indicates differentiation with respect to r and $B = E + m - V$. For G we find at once

$$G = Cr^{-\varkappa}\exp\left(\int B\Phi dr\right), \tag{6}$$

where C is a constant (the integral in the exponent is an indefinite one) which is determined by the normalization condition for the wave function. The problem is thus reduced to finding the function Φ defined by the Riccati equation (4). The boundary conditions imposed upon Φ follow from the boundary conditions imposed upon G and F, and (3): Φ must be such that the product $G\Phi$ is finite as $r \to 0$ and $r \to \infty$.

Let

$$V(r) = V_0(r) + \lambda V_1(r), \tag{7}$$

where λV_1 is the perturbation while we know the solution for V_0 (i.e., the quantities F_0, G_0, Φ_0, and E_0) exactly. In accordance with (7) we put

$$E = E_0 + \lambda E_1(\lambda), \quad B = B_0 + \lambda B_1(\lambda), \quad \Phi = \Phi_0 + \lambda\Phi_1(\lambda);$$
$$B_0 = E_0 + m - V_0, \quad B_1 = E_1 - V_1. \tag{8}$$

Using the zeroth approximation equation

$$\Phi_0' - \frac{2\varkappa}{r}\Phi_0 + B_0\Phi_0^2 + B_0 - 2m = 0 \tag{9}$$

we then get from (4):

$$\Phi_1' + 2\left(B\Phi - \frac{\varkappa}{r}\right)\Phi_1 + B_1(1 + \Phi_0^2) - \lambda B\Phi_1^2 = 0. \tag{10}$$

If we discard in Eq. (10) terms $\sim\lambda$ we can integrate it and find $\Phi_1 = \varphi_1 + O(\lambda)$ and $E_1 = \epsilon_1 + O(\lambda)$. In accordance with this we get

$$E_1 = \varepsilon_1 + \lambda E_2(\lambda), \quad B_1 = \beta_1 + \lambda E_2(\lambda),$$
$$\Phi_1 = \varphi_1 + \lambda\Phi_2(\lambda), \quad \beta_1 = \varepsilon_1 - V_1. \tag{11}$$

The equations for φ_1 and Φ_2 have the form

$$\varphi_1' + 2(B_0\Phi_0 - \varkappa r^{-1})\varphi_1 + \beta_1(1 + \Phi_0^2) = 0, \tag{12}$$

$$\Phi_2' + 2(B\Phi - \varkappa r^{-1})\Phi_2 + 2B_1\varphi_1\Phi_0 + B\varphi_1^2 + E_2(1 + \Phi_0^2) - \lambda^2 B\Phi_2^2 = 0. \tag{13}$$

Using (6) we get from (12)

$$\varphi_1 = -\frac{1}{G_0^2}\int_a^r (\varepsilon_1 - V_1)(1+\Phi_0^2)G_0^2 dr. \tag{14}$$

Here

$$G_0 = C_0 r^{-\varkappa}\exp\left(\int B_0\Phi_0 dr\right), \tag{14a}$$

and C_0 is the zeroth approximation normalization constant.

In (14) occur two constants (a and ϵ_1) which we determine from the condition

$$G\Phi \to 0, \quad \text{as} \quad r\to 0 \text{ and } r\to\infty, \tag{15}$$

since

$$F\to 0,\ G\to 0, \quad \text{as} \quad r\to 0,\ r\to\infty.$$

The condition at the origin can be satisfied if we choose the lower limit of integration in (14) equal to zero. Then

$$\varphi_1 = -\frac{1}{G_0^2}\int_0^r (\varepsilon_1 - V_1)(1+\Phi_0^2)G_0^2 dr. \tag{16}$$

The condition at infinity will be satisfied if we require that

$$\int_0^\infty (\varepsilon_1 - V_1)(1+\Phi_0^2)G_0^2 dr = 0. \tag{17}$$

Hence, if we use the normalization condition for the zeroth approximation

$$\int_0^\infty (G_0^2 + F_0^2)dr = \int_0^\infty (1+\Phi_0^2)G_0^2 dr = 1, \tag{18}$$

we find

$$\varepsilon_1 = \int_0^\infty V_1(1+\Phi_0^2)G_0^2 dr = \int_0^\infty V_1(G_0^2+F_0^2)dr. \tag{19}$$

This is the usual expression for the correction to the energy in first approximation. The difference in and the advantage of the present method appear when higher-order corrections are evaluated. We obtain in the first approximation still a closed expression for the wave function. Using (6) and (8) we can write G in the form

$$G = C_0(1+\lambda C_1(\lambda))r^{-\varkappa}\exp\left\{\int B_0\Phi_0 dr + \lambda\int\left(B_1\Phi_0 + B_0\Phi_1 + \lambda B_1\Phi_1\right)dr\right\} = G_0(1+\lambda C_1(\lambda))\exp\left\{\lambda\int (B_1\Phi_0 + B_0\Phi_1 + \lambda B_1\Phi_1)dr\right\}. \tag{20}$$

Putting

$$C_1(\lambda) = c_1 + \lambda C_2(\lambda) \tag{21}$$

and using (11) we get in first approximation

$$G = G_0(1+\lambda c_1 + \lambda\int(\beta_1\Phi_0 + B_0\varphi_1)dr) = G_0 + \lambda g_1. \tag{22}$$

The constant c_1 is determined from the normalization condition

$$\int_0^\infty (G^2+F^2)dr = \int_0^\infty (1+\Phi^2)G^2 dr = 1, \tag{23}$$

whence we find up to terms of order $\sim\lambda$

$$c_1 = -\int_0^\infty G_0^2[\Phi_0\varphi_1 + (1+\Phi_0^2)\int(\beta_1\Phi_0 + B_0\varphi_1)dr]dr, \tag{24}$$

which together with (22), (16), (19), and (3) completely solves the problem of finding a closed expression for the first approximation to the wave function.

To obtain the next approximation we turn to (13). If we drop here terms $\sim\lambda^2$ this equation can easily be integrated and we get $\Phi_2 = \varphi_2(\lambda) + O(\lambda^2)$ and $E_2 = \epsilon_2(\lambda) + O(\lambda^2)$, where $\varphi_2(\lambda)$ and $\epsilon_2(\lambda)$ contain terms of zeroth and first order in λ. We thus put

$$E_2(\lambda) = \varepsilon_2(\lambda) + \lambda^2 E_3(\lambda), \qquad \Phi_2(\lambda) = \varphi_2(\lambda) + \lambda^2\Phi_3(\lambda). \tag{25}$$

Using the boundary conditions (5) for the function Φ and the normalization condition (23) we then get from (13):

$$\varphi_2 = -\frac{1}{G^2}\int_0^r [B\varphi_1^2 + 2\beta_1\varphi_1\Phi_0 + \varepsilon_2(1+\Phi^2)]G^2 dr, \tag{26}$$

$$\varepsilon_2 = -\int_0^\infty (B\varphi_1^2 + 2\beta_1\varphi_1\Phi_0)G^2 dr. \tag{27}$$

In (26) and (27) $G = G_0 + \lambda g_1$, $\Phi = \Phi_0 + \lambda\varphi_1$, $B = B_0 + \lambda\beta_1$ (see (22), (16), (8), and (11)) and when evaluating the integrals we must retain terms which are not higher than first order in λ.

Extending this procedure we find (we refer to paper [2] for details)

$$\Phi = \Phi_0 + \sum_{n=1}^\infty \lambda^{2^{n-1}}\varphi_n(\lambda), \qquad E = E_0 + \sum_{n=1}^\infty \lambda^{2^{n-1}}\varepsilon_n(\lambda),$$
$$G = G_0 + \sum_{n=1}^\infty \lambda^{2^{n-1}} g_n(\lambda), \tag{28}$$

where $\varphi_n(\lambda)$, $\epsilon_n(\lambda)$, and $g_n(\lambda)$ are polynomials of order $(2^{n-1} - 1)$ in powers of the perturbation parameter λ. We conclude from (28) that the n-th approximation of the perturbation theory constructed in this way allows us to evaluate the wave function up to terms of order $\sim\lambda^{2^n}$ and the energy up to terms $\lambda^{2^{n+1}}$ as the $(n+1)$-st approximation to the energy can be expressed in terms of the n-th (and lower) approximation to the wave function. Dalgarno and Stewart [4] have shown, using the usual perturbation theory, that the energy can be estimated to order $2s+1$ is the wave function is known up to s-th order.

We shall here not write down the general formulae which give the connection between consecutive approximations as these formulae are very complicated and in practice we hardly need know the wave function and energy with an accuracy better than the third order. This accuracy is just given by Eqs. (26) and (27).

2. As an example we consider a K electron and we calculate its wave function and energy up to first and second order in the perturbation, respectively, taking the difference between the atomic and the Coulomb potential as perturbation. This difference is small at distances of the order of the radius of the K-shell and comparable with the Coulomb potential at distances of the order of the radius of the atom. The ratio r/r_a, where r is a characteristic length occurring in the problem and r_a the radius of the atom, is a natural parameter for such a perturbation. For our example such a parameter will be $r_K/R_a \sim Z^{-2/3}$ where r_K is the radius of the K-shell and Z the atomic number of the element. The larger Z, the better this parameter.

The Coulomb potential $V_0 = -\alpha Z/r$ will determine the unperturbed solution which is well known (see, e.g., [3]):

$$G_0 = \sqrt{\frac{\eta(1+\gamma)}{\Gamma(1+2\gamma)}}\, e^{-\eta r}(2\eta r)^{\gamma}, \qquad \Phi_0 = -\frac{\alpha Z}{1+\gamma}, \tag{29}$$

Here

$$E_0 = m\gamma.$$

$$\gamma = \sqrt{1-\alpha^2 Z^2}, \qquad \eta = m\alpha Z, \qquad \alpha = e^2 = 1/137, \tag{30}$$

m is the electron mass and Γ the gamma function.

The potential produced by the electron cloud of the atom plays the role of the perturbation. We shall assume that the electron charge is distributed isotropically in space with a density $\rho(r)$. When the distribution is isotropic the potential is given by the formula

$$V_1(r) = 4\pi\alpha Z\left(\frac{1}{r}\int_0^r \rho(r')r'^2dr' + \int_r^\infty \rho(r')r'dr'\right). \tag{31}$$

We shall follow [5] and apply a Laplace transformation to the density ρ:

$$r\rho(r) = \frac{1}{4\pi}\int_0^\infty \chi(\mu)\mu^2 e^{-\mu r}d\mu. \tag{32}$$

We then get for (31)

$$V_1 = -\alpha Z S_\mu e^{-\mu r}/r, \tag{33}$$

where S_μ is the operator

$$S_\mu \equiv \int_0^\infty [\chi(\mu) - \delta(\mu)]\, d\mu, \tag{33a}$$

and $\delta(\mu)$ the delta function. When deriving (33) we used the equation

$$\int_0^\infty \chi(\mu)\, d\mu = 1, \tag{34}$$

which is a consequence of the normalization condition for ρ:

$$\int_0^\infty \rho(r)4\pi r^2 dr = 1. \tag{35}$$

We note still some relations which we need in the following. It follows from (32), (33a), and (34) that

$$S_\mu \mu^{n+2} = 4\pi\left\{\left(-\frac{\partial}{\partial r}\right)^n r\rho(r)\right\}_{r\to 0}, \qquad n \geqslant 0, \tag{36}$$

$$S_\mu \mu = \langle r^{-1}\rangle, \tag{37}$$

$$S_\mu 1 = 0; \tag{38}$$

$\langle r^{-1}\rangle$ is the average value of $1/r$ for the atom and is defined by

$$\langle r^{-1}\rangle = 4\pi\int_0^\infty \rho(r) r dr. \tag{37a}$$

If V_1 is defined by (33), Eqs. (19) and (16) give

$$\varepsilon_1 = -\frac{\alpha Z}{\gamma} S_\mu (1+\nu)^{-2\gamma}, \tag{39}$$

$$\varphi_1 = -\frac{\alpha Z}{1+\gamma} S_\mu (1+\nu)^{-2\gamma}\left[\frac{1}{\gamma} + 2\int_0^\nu e^{-x v}(1+v)^{2\gamma-1}dv\right]. \tag{40}$$

Here and henceforth

$$\nu = \mu/2\eta, \quad x = 2\eta r.$$

As the density of the electron cloud $\rho(r)$ decreases rapidly when $r > r_a$, we conclude from (32) that $\chi(\mu)$ is such that the main contribution to the integral which depends on μ comes from the region $\mu \sim 1/r_a$. However, a characteristic distance in the problem is $r \sim 1/\eta = r_K$ (see (29)). It is thus convenient for obtaining the correction to the wave function and the second correction to the energy to expand the exponent in (33) in a power series ($\mu r \sim r_K/r_a \ll 1$ for medium and large Z). We also expand (39) and (40) in power series in ν ($\nu \sim r_K/r_a$):

$$\varepsilon_1 = -\frac{\alpha Z\eta}{\gamma}\sum_{n=0}^{\infty}(-1)^n \frac{\Gamma(2\gamma+n)}{\Gamma(2\gamma)n!} S_\mu \nu^n$$
$$= 2\alpha Z\eta S_\mu\{\nu - 1/2(2\gamma+1)\nu^2 + O(\nu^3)\}, \tag{41}$$

$$\varphi_1 = -\frac{\alpha Z}{1+\gamma} S_\mu\left\{\frac{1}{\gamma} - \nu^2 x + O(\nu^3)\right\} = \frac{\alpha Z x}{1+\gamma} S_\mu \nu^2 (1 + O(\nu)). \tag{42}$$

We have used the property (38) of the operator S_μ in (41) and (42).

From (22) and (24) we get

$$c_1 = -1/2(1+\gamma)(1+2\gamma)(2-\gamma) S_\mu \nu^2 (1+O(\nu)), \tag{43}$$

$$G = G_0\{1 + S_\mu\nu^2[-1/2(1+\gamma)(1+2\gamma)(2-\gamma)$$
$$+ (1-\gamma)(3+2\gamma)(\eta r) + \gamma(\eta r)^2 + O(\nu)]\}, \tag{44}$$

$$F = F_0\{1 + S_\mu\nu^2[-1/2(1+\gamma)(1+2\gamma)(2-\gamma)$$
$$+ (1+\gamma)(1-2\gamma)(\eta r) + \gamma(\eta r)^2 + O(\nu)]\}, \tag{45}$$

$F_0 = G_0\Phi_0$, G_0 and Φ_0 are defined in (29).

Using (44) we can get from (27) the second and third corrections to the energy. If we restrict ourselves to only the second correction, we can put in (27) $B = B_0 = m(1+\gamma) + \alpha Z/r$, $G = G_0$. Then

$$\varepsilon_2 = -\alpha Z\eta(1+\gamma)(1+2\gamma) S_{\mu_1}\nu_1^2(1+O(\nu_1))$$
$$\times S_{\mu_2}\nu_2^2(1+O(\nu_2)), \qquad \nu_{1,2} = \mu_{1,2}/2\eta. \tag{46}$$

The quantities $S_\mu \cdot \mu/2\eta$ and $S_\mu(\mu/2\eta)^2$ which are defined in (36) and (37) occur in (41) to (46). If we give V_1 in (33) as a finite sum of Yukawa potentials (see in [6]):

$$V_1 = -\alpha Z\sum_{l=1}^{4} a_l \frac{e^{-\lambda_l r}}{r}, \qquad \lambda_l = \frac{m}{121} Z^{1/3} b_l, \tag{47}$$

where

$$a_1 = 0{,}10, \quad a_2 = 0{,}55, \quad a_3 = 0{,}35, \quad a_4 = -1,$$
$$b_1 = 6{,}0, \quad b_2 = 1{,}20, \quad b_3 = 0{,}30, \quad b_4 = 0, \tag{47a}$$

$$\sum_{l=1}^{4} a_l = 0, \tag{47b}$$

we get

$$S_\mu \nu = \frac{1}{2\eta}\left\langle\frac{1}{r}\right\rangle = \sum_{l=1}^{4} a_l \frac{\lambda_l}{2\eta} = 0{,}77 Z^{-2/3},$$

$$S_\mu \nu^2 = \frac{4\pi}{(2\eta)^2}[r\rho(r)]_{r\to 0} = \sum_{l=1}^{4} a_l\left(\frac{\lambda_l}{2\eta}\right)^2 = 1{,}42 Z^{-4/3}. \tag{48}$$

In conclusion we make the following remark. In [7] we looked for the correction to the relativistic photoeffect in the K-shell caused by screening. This correction was evaluated in the first approximation in the perturbation V_1 of (47) using the Coulomb Green function. We showed that if we restrict ourselves merely to terms of relative order in αZ not higher than first order (we used an expansion of the wave function and the Coulomb Green function in power series in αZ)) the contribution to the screening is only given by the correction to the wave function of the discrete spectrum. It is true that from corrections to the wave function of

the continuous spectrum there occur in the amplitude terms

$$\sim \alpha Z \sum_{l=1}^{4} a_l \ln \frac{\lambda_l}{2p}$$

where λl is the screening parameter and p the electron momentum but these terms vanish from the cross-section which indicates that they arise from the expansion of the phase factor. For the amplitude of the photoeffect, Q, we obtained in the first approximation in the screening the formula (logarithmic terms have been omitted)

$$Q = \left[1 - 3\sum_{l=1}^{4} a_l \left(\frac{\lambda_l}{2\eta}\right)^2\right] Q^c, \qquad (49)$$

where Q^c is the Coulomb amplitude of the photoeffect.

This result is obtained at once from (44), (45), and (1) if we bear in mind that the main contribution to the amplitude of the relativistic K-photoeffect is given by the region $r \sim 1/q$, where $q \sim m$ is the momentum transferred to the nucleus and if we drop in the corrections to G_0 and F_0 terms $\sim \alpha^2 Z^2$. In such an approximation we get

$$G = G_0[1 - 3S_\mu v^2(1 + O(v)) + O(\alpha^2 Z^2 S_\mu v^2)],$$
$$F = G(\Phi_0 + O(\alpha^2 Z^2 S_\mu v^2)),$$

$$\Psi = [1 - 3S_\mu v^2 + O(\alpha^2 Z^2 S_\mu v^2, S_\mu v^3)]\Psi_0 \approx \left[1 - 3\sum_{l=1}^{4} a_l \left(\frac{\lambda_l}{2\eta}\right)^2\right]\Psi_{0.} \qquad (50)$$

Here Ψ and Ψ_0 are the K-electron wave functions with and without account of screening. It is clear that the evaluation of the photoeffect amplitude with such functions leads to (49).

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24