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1ST Order Perturbation Correction for the Atoms Energy Level

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ABSTRACT
The goal of this paper is to obtain an equation of the 1st order perturbation for the ground state. Dirac equations have been used to achieve the potential of the nucleus. It is considered that the equation obtained for the ground state is simpler and more accurate.
Keywords: Dirac, energy, perturbation, nucleus and potential.

INTRODUCTION
In quantum mechanics, perturbation theory is a set of approximation schemes directly related to mathematical perturbation for describing a complicated quantum system in terms of a simpler one (Aoyama et al., 2012). The idea is to start with a simple system for which a mathematical solution is known, and add an additional "perturbing" Hamiltonian representing a weak disturbance to the system. If the disturbance is not too large, the various physical quantities associated with the perturbed system (its energy levels and eigen states) can be expressed as "corrections" to those of the simple system (Frasca, 1998). These corrections, being small compared to the size of the quantities themselves, can be calculated using approximate methods such as asymptotic series. The complicated system can therefore be studied based on knowledge of the simpler one (Mostafazadeh, 1997). In effect, it is describing a complicated unsolved system using a simple, solved system. Perturbation theory is an important tool for describing real quantum systems, as it turns out to be very difficult to find exact solutions to the Schrödinger equation for Hamiltonians of even moderate complexity. The Hamiltonians to which we know exact solutions, such as the hydrogen atom, the quantum harmonic oscillator and the particle in a box, are too idealized to adequately describe most systems (Frasca, 2007). Using perturbation theory, we can use the known solutions of these simple Hamiltonians to generate solutions for a range of more complicated system.

An atom is the basic unit of matter. It is the smallest thing that can have a chemical property. There are many different types of atoms, each with its own name, atomic mass and size. These different atoms are called chemical elements. Atoms are very small, but the exact size depends on the element. Atoms range from 0.1 to 0.5 nanometers in width (Frederick, 2001). One nanometer is about 100,000 times smaller than the width of a human hair (James, 2005). This makes atoms impossible to see without special tools. Equations must be used to see the way they work and how they interact with other atoms. Atoms join together to make molecules: for example, two hydrogen atoms and one oxygen atom combine to make a water molecule. When atoms join together it is called a chemical reaction. Every atom is made up of three kinds of smaller particles, called protons which are positively charged, neutrons which have no charge and electrons which are negatively charged. The protons and neutrons are heavier, and stay in the middle of the atom. They

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are called the nucleus. They are surrounded by a cloud of electrons which are very light in weight and are attracted to the positive charge of the nucleus. This attraction is called electromagnetic force. The number of protons, neutrons and electrons an atom has tells us what element it is. Hydrogen, for example, has one proton, no neutrons and one electron; the element sulfur has 16 protons, 16 neutrons and 16 electrons. The number of protons is the atomic number. The number of protons and neutrons together is the atomic weight. Atoms move faster when they are in their gas form because they are free to move than they do in liquid form and solid matter. In solid materials, the atoms are tightly packed next to each other so they vibrate, but are not able to move there is no room as atoms in liquids do.

A quantum mechanical system or particle that is bound that is, confined spatially can only take on certain discrete values of energy. This contrasts with classical particles, which can have any energy. These discrete values are called energy levels. The term is commonly used for the energy levels of electrons in atoms which are bound by the electric field of the nucleus, but can also refer to energy levels of nuclei or vibrational or rotational energy levels in molecules. The energy spectrum of a system with such discrete energy levels is said to be quantized. In atomic physics, an electron shell, or a principal energy level, may be thought of as an orbit followed by electrons around an atom's nucleus. The closest shell to the nucleus is called the "1 shell" (also called "K shell"), followed by the "2 shell" or "L shell", then the "3 shell" or "M shell", and so on farther and farther from the nucleus. The shells correspond with the principal quantum numbers n = 1, 2, 3, 4 ... or are labeled alphabetically with letters used in the X-ray notation (K, L, M, ...). Each shell can contain only a fixed number of electrons: The first shell can hold up to two electrons, the second shell can hold up to eight (2 + 6) electrons, the third shell can hold up to 18 (2 + 6 + 10) and so on. The general formula is that the nth shell can in principle hold up to 2(n2) electrons (Rayleigh, 1999). Since electrons are electrically attracted to the nucleus, an atom's electrons will generally occupy outer shells only if the more inner shells have already been completely filled by other electrons. However, this is not a strict requirement: atoms may have two or even three incomplete outer shells. For an explanation of why electrons exist in these shells see electron configuration (Sakurai etal., 2011).

Materials and Methods

Solution of the Dirac equation exterior to the nucleus

The dependence of Ψ on the coordinate r, expressed through the radial functions $g(r)$ and$f(r)$, which the Dirac equation connects through the coupled equations

$$\left[\frac{d}{dr}+\frac{1+k}{r}\right]g(r)-\frac{1}{\hbar c}[E+mc^2-V(r)]f(r)=0 \qquad 1a$$

$$\left[\frac{d}{dr}+\frac{1-k}{r}\right]g(r)+\frac{1}{\hbar c}[E-mc^2-V(r)]g(r)=0 \qquad 1b$$

For values of the radial coordinate r greater than or equal to a value R which defines the nuclear radius, we assume that the central potential has the Coulomb form,

$$V(r)=-\frac{Ze^2}{r}, \qquad (r\geq R) \qquad 2$$

As is well known, introduction of the dimensionless coordinate variable ρ≡2qr, with

$$q\equiv\sqrt{\frac{((mc^2)^2-E^2)}{\hbar^2c^2}} \qquad 3$$

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and use of the sum and difference functions

$$u \pm (\rho) \equiv \rho^{\frac{3}{2}} \left(g \mp \sqrt{\frac{mc^2+E}{mc^2-E}} f \right) \quad 4$$

leads to uncoupled equations for

$$\left\{ \frac{d^2}{d\rho^2} - \frac{\left[\left(j+\frac{1}{2}\right)^2 - (\alpha Z)^2 - \frac{1}{4}\right]}{\rho^2} + \frac{\left[\alpha Z \frac{E}{\sqrt{(mc^2)^2 - E^2}} \pm \frac{1}{2}\right]}{\rho} - \frac{1}{4} \right\} u \pm \rho = 0 \quad 5$$

with $\alpha = \frac{e^2}{\hbar c}$. Equation (5) has the general form of Whittaker's equation

$$\left[\frac{d^2}{d\rho^2} - \frac{\gamma^2 - \frac{1}{4}}{\rho^2} + \frac{\beta}{\rho} - \frac{1}{4} \right] M(\rho) = 0 \quad 6$$

where

$$\gamma^2 = \left(j + \frac{1}{2}\right)^2 - (\alpha Z)^2, \qquad \beta = \beta_{\pm} = \alpha Z \frac{E}{\sqrt{(mc^2)^2 - E^2}} \pm \frac{1}{2} \quad 7$$

Subject to the condition that 2γ is not equal to zero or a positive or negative integer, the general solution of equation (6) is a linear combination of two particular solutions. Explicitly, the particular solutions corresponding to plus and minus γ can be expressed in terms of confluent hyper geometric functions ${}_1F_1$ through the relations

$$M_{\beta,\pm\gamma}(\rho) = \rho^{\pm\gamma+\frac{1}{2}} e^{-\frac{1}{2}} {}_1F_1\left(\pm\gamma - \beta + \frac{1}{2}, \quad \pm 2\gamma + 1, \rho\right) \quad 8$$

Where the function ${}_1F_1$ has the series representation,

$${}_1F_1(a, b; \rho) = 1 + \frac{a}{b}\rho + \frac{1}{2!}\frac{a(a+1)}{b(b+1)}\rho^2 + \cdots \quad 9$$

As a consequence of the divergence of the series in equation (9) at $\rho = \infty$ the functions $M_{\beta,\gamma}(\rho)$ and $M_{\beta,-\gamma}(\rho)$ are both divergent for larger unless the series forms of the solutions are terminated by a choice of the parameter β such that the first argument of ${}_1F_1$ is equal to a negative integer (James, 2003).

If the Coulomb potential is assumed to be valid at the origin, the divergence of the function $M_{\beta,-\gamma}(\rho)$ at ρ=0 requires the coefficient of this function in the general solution of equation (6) to be equated to zero. The condition on the parameter β required to terminate the series representation for the solution $M_{\beta,\gamma}(\rho)$ then leads to the familiar formula for the allowed energy eigenvalues of the electron given by

$$E = mc^2 \frac{\left(n' + \sqrt{\left(j+\frac{1}{2}\right)^2 - (\alpha Z)^2}\right)}{\sqrt{\left(n' + \sqrt{\left(j+\frac{1}{2}\right)^2 - (\alpha Z)^2}\right)^2 + (\alpha Z)^2}}, \qquad n' = 0, 1, 2, \ldots \quad 10$$

The relation 2γ= integer makes it impossible to terminate the series forms of both functions for the same value of β. As a result of this, a non-divergent solution of equation (5) can be obtained as a linear combination of $M_{\beta,\gamma}$ and $M_{\beta,-\gamma}$ only if the two functions are combined so that the divergences in the separate functions at ρ=∞ cancel exactly. For this purpose, it is possible to make use of the asymptotic forms of the confluent hyper geometric functions given by the equations

$$\lim_{\rho\to\infty} {}_1F_1\left(\gamma - \beta + \frac{1}{2}, 2\gamma + 1, \rho\right) = \frac{\Gamma(2\gamma+1)}{\Gamma\left(\frac{1}{2}+\gamma-\beta\right)} e^{\rho} \rho^{-\frac{1}{2}-\beta-\gamma} + \frac{\Gamma(2\gamma+1)}{\Gamma\left(\frac{1}{2}+\gamma+\beta\right)} (-\rho)^{-\frac{1}{2}+\beta-\gamma} \quad 11a$$

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$$\lim_{\rho\to\infty} {}_1F_1\left(-\gamma-\beta+\frac{1}{2},-2\gamma+1,\rho\right)=\frac{\Gamma(-2\gamma+1)}{\Gamma\left(\frac{1}{2}-\gamma-\beta\right)}e^{\rho}\rho^{-\frac{1}{2}-\beta+\gamma}+\frac{\Gamma(-2\gamma+1)}{\Gamma\left(\frac{1}{2}-\gamma+\beta\right)}(-\rho)^{-\frac{1}{2}+\beta+\gamma} \quad 11b$$

to determine the large ρ dependences of $M_{\beta,\gamma}$ and $M_{\beta,-\gamma}$ in the forms

$$\lim_{\rho\to\infty} M_{\beta,\gamma}(\rho)=\frac{\Gamma(2\gamma+1)}{\Gamma\left(\frac{1}{2}+\gamma-\beta\right)}e^{\frac{\rho}{2}}\rho^{-\beta} \quad 12a$$

$$\lim_{\rho\to\infty} M_{\beta,-\gamma}(\rho)=\frac{\Gamma(-2\gamma+1)}{\Gamma\left(\frac{1}{2}-\gamma-\beta\right)}e^{\frac{\rho}{2}}\rho^{-\beta} \quad 12b$$

These relations allow a′ bound state solution′ of Whittaker's equation that vanishes at infinity to be constructed from a linear combination of solutions that are respectively regular and irregular at the origin in the form

$$u_{\pm}(\rho)=N_{\pm}\left[M_{\beta_{\pm},+\gamma}(\rho)-\Delta\left(\beta_{\pm},\gamma\right)M_{\beta_{\pm},-\gamma}(\rho)\right]=N_{\pm}e^{-\frac{\rho}{2}}\left[\rho^{\gamma+\frac{1}{2}}{}_1F_1\left(\gamma-\beta_{\pm}+\frac{1}{2},2\gamma+1,\rho\right)-\Delta\left(\beta_{\pm},\gamma\right)\rho^{-\gamma+\frac{1}{2}}{}_1F_1\left(-\gamma-\beta_{\pm}+\frac{1}{2},-2\gamma+1,\rho\right)\right] \quad 13$$

with

$$\Delta\left(\beta_{\pm},\gamma\right)=\frac{\Gamma(2\gamma+1)}{\Gamma(-2\gamma+1)}\frac{\Gamma\left(\frac{1}{2}-\gamma-\beta_{\pm}\right)}{\Gamma\left(\frac{1}{2}+\gamma-\beta_{\pm}\right)} \quad 14$$

Under the condition that the coefficient of the singular function $M_{\beta,-\gamma}(\rho)$ was set to zero, the termination condition on the series form of the function $M_{\beta,\gamma}(\rho)$ produced the standard formula for the energy in equation (10), whereas, under the condition that the coefficient of the function $M_{\beta,\gamma}(\rho)$ was set to zero, the condition terminating the function $M_{\beta,-\gamma}(\rho)$ led instead to a formula for the energy expressible as

$$E=mc^2\frac{\left(n'-\sqrt{\left(j+\frac{1}{2}\right)^2-(\alpha Z)^2}\right)}{\sqrt{\left(n'-\sqrt{\left(j+\frac{1}{2}\right)^2-(\alpha Z)^2}\right)^2+(\alpha Z)^2}},\qquad n'=0,1,2,\ldots \quad 15$$

In the present analysis, the use of the solution in equation (13), in combination with equation (4) and the definition of u±(ρ), determines radial functions g and f corresponding to proper bound state solutions of the Dirac equation in the forms

$$g(r)=\frac{1}{2}\rho^{-\frac{3}{2}}[u_+(\rho)+u_-(\rho)] \quad 16$$

$$f(r)=-\frac{1}{2}\sqrt{\frac{mc^2-E}{mc^2+E}}\rho^{-\frac{3}{2}}[u_+(\rho)-u_-(\rho)] \quad 17$$

Here the coupling between the functions g and f demanded by the Dirac equation connects the coefficients in the separate solutions and through the equality

$$\frac{N_-}{N_+}=\frac{\gamma-\xi(E')}{k-\frac{\xi(E')}{E'}}\equiv-\eta_-(E') \quad 18$$

Where we use the notation

$$E'\equiv\frac{E}{mc^2},\quad \xi(E')\equiv\frac{\alpha ZE'}{\sqrt{1-E'^2}},\qquad \eta_{\pm}(E')=\frac{\gamma\pm\xi(E')}{k-\frac{\xi(E')}{E'}} \quad 19$$

Using equations (13), and (16)–(19), it can be shown that the functions g (r) and f(r) have the explicit forms

$$g(r)=\frac{1}{2}N_{\beta}e^{-\frac{\rho}{2}}\rho^{\gamma-1}[{}_1F_1(\gamma-\xi(E'),2\gamma+1,\rho)-\eta_-(E'){}_1F_1(\gamma+1-\xi(E'),2\gamma+1,\rho)-\Delta(\beta,\gamma)\rho^{-2\gamma}{}_1F_1(\gamma+1-\xi(E'),2\gamma+1,\rho)-\Delta(\beta,\gamma)\eta_+(E')\rho^{-2\gamma}{}_1F_1(-\gamma+1-\xi(E'),-2\gamma+1,\rho)] \quad 20a$$

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$$f(r)=\frac{1}{2}N_\beta\sqrt{\frac{1-E'}{1+E'}}\ e^{-\frac{\rho}{2}}\rho^{\gamma-1}[{}_1F_1(\gamma-\xi(E'),2\gamma+1,\rho)+\eta_-(E')\,{}_1F_1(\gamma+1-\xi(E'),2\gamma+1,\rho)-\Delta(\beta,\gamma)\rho^{-2\gamma}\,{}_1F_1(-\gamma-\xi(E'),2\gamma+1,\rho)+\Delta(\beta,\gamma)\eta_+(E')\,\rho^{-2\gamma}\,{}_1F_1(-\gamma+1-\xi(E'),-2\gamma+1,\rho)]$$ 20b

where N_β represents a normalization constant, and the energy parameter E must be derived from the continuity conditions at the value of r for which the Coulomb potential in equation(2) becomes invalid.

Solution of the Dirac equation inside the nucleus

The separate models correspond to functions V(r) of the forms

$$V(r)=-\frac{3}{2}\frac{Ze^2}{R}+\frac{Ze^2}{2R^3}\,r^2,\qquad (r<R)\quad \text{uniformly charged nucleus}$$ 21a

$$V(r)=-\frac{Ze^2}{R},\qquad (r<R)\quad \text{constant potential inside nucleus}$$ 21b

Which can be rescaled for $r<R$ in terms of dimensionless quantities as

$$\frac{V(r)}{mc^2}=-\left(b'-\xi r'^2\right)\quad \text{uniformly charged nucleus}$$ 22a

$$\frac{V(r)}{mc^2}=-\frac{\alpha Z}{R'}\quad \text{constant potential inside nucleus}$$ 22b

Where

$$r'=\left(\frac{mc}{\hbar}\right)r,\quad R'=\left(\frac{mc}{\hbar}\right)R,\quad b'=\frac{3}{2}\frac{\alpha Z}{R'},\qquad \xi=\frac{3}{2}\frac{\alpha Z}{R'^3}$$ 23

It is sufficient to construct a series solution of the radial equations (1) for r<R. For this purpose, it is useful to assume the forms

$$g(r')=Ar'^{v-1}\sum_{n=0}^{\infty}a_n r'^n,\qquad f(r')=Br'^{v-1}\sum_{n=0}^{\infty}b_n r'^n$$ 24

Substitution of equations (24) into equations (1) results in recursion relations for the coefficients an and bn that have non-trivial solutions only under either of the two conditions

$$v=-k,\quad b_0=0\quad k<0$$ 25a

$$v=+k,\quad a_0=0\quad k>0$$ 25b

The two choices result in the separate solutions

$$g(r')=Ar'^{|k|-1}\left(1+a_2r'^2+a_4r'^4+\cdots\right),\quad f(r')=Ar'^{|k|}\left(b_1+b_3r'^2+b_5r'^4+\cdots\right)\quad k<0$$ 26a

$$g(r')=Br'^{|k|}\left(a_1+a_3r'^2+a_5r'^4+\cdots\right),\quad f(r')=Br'^{|k|-1}\left(1+b_2r'^2+b_4r'^4+\cdots\right)\quad k>0$$ 26b

For V(r) in the form (22a), the coefficients of the leading terms have the forms

$$a_1=\frac{Q_+}{2|k|+1},\ a_2=-\frac{Q_+Q_-}{2(2|k|+1)},\ a_3=-\frac{1}{2|k|+3}\left(\frac{Q_+Q_-Q_+}{2(2|k|+1)}+\xi\right),\ a_4=\frac{(Q_+Q_-)^2}{8(2|k|+3)(2|k|+1)}+\frac{\xi}{4}\left[\frac{Q_+}{2|k|+3}+\frac{Q_-}{2|k|+1}\right],\quad a_5=-\frac{1}{2|k|+5}(Q_+b_4+\xi b_2)$$ 27

$$b_1=-\frac{Q_-}{2|k|+1},\ b_2=-\frac{Q_+Q_-}{2(2|k|+1)},\ b_3=-\frac{1}{2|k|+3}\left(\frac{Q_-Q_+Q_-}{2(2|k|+1)}+\xi\right),\ b_4=\frac{(Q_+Q_-)^2}{8(2|k|+3)(2|k|+1)}+\frac{\xi}{4}\left[\frac{Q_-}{2|k|+3}+\frac{Q_+}{2|k|+1}\right],\quad b_5=-\frac{1}{2|k|+5}(Q_-a_4+\xi a_2)$$ 28

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with

$$Q_{\pm} \equiv E' + b' \pm 1 \quad (29)$$

whereas, for V(r) in the form (22b),the corresponding coefficients have the above forms with $b' = \frac{\alpha Z}{R'}$ and $\xi = 0$ (James, 2003).

Results

The potential can be obtain by the use of integration

$$V(r) = -e\int_r^R R dr' - \frac{Ze^2}{R} \quad (30)$$

$$= \frac{Ze^2}{R^3}\int_r^R r' dr' - \frac{Ze^2}{R} \quad (31)$$

$$= -\frac{Ze^2 r^2}{2R}\Big|_r^R - \frac{Ze^2}{R^3} \quad (32)$$

$$= \frac{Ze^2 r^2}{2R^3} - \frac{Ze^2}{2R} \quad (33)$$

So we see that

$$V(r) = -\frac{Ze^2}{r} \qquad r > R \quad (34)$$

$$V(r) = \frac{Ze^2 r^2}{2R^3} - \frac{Ze^2}{2R} \qquad r \le R \quad (35)$$

$$H = H^0 + H' \quad (36)$$

$$H' = 0 \qquad r > R \quad (37)$$

$$H' = \frac{Ze^2 r^2}{2R^3} - \frac{Ze^2}{2R} + \frac{Ze}{r} \qquad r \le R \quad (38)$$

$$E' = \langle nlm|H'|nlm\rangle = \int_0^R R_{nl}^* \left(\frac{Ze^2 r^2}{2R^3} - \frac{Ze^2}{2R} + \frac{Ze}{r}\right) R_{nl} r^2 dr \quad (39)$$

∴ the 1st order perturbation correction for the ground state is

$$E_0^{[1]} = \langle 100|H'|100\rangle = \int_0^R Ze^{-\frac{2r}{a_0}} \left(\frac{Ze^2 r^2}{2R^3} - \frac{3Ze^2}{2R} + \frac{Ze}{r}\right) r^2 dr \quad (40)$$

$$E_0^{[1]} = \frac{Ze^2}{4\pi}\left(\frac{3{a_0}^3 - 3a_0R^2 + 3R^3 - 3a_0\, Ze^{-\frac{2r}{a_0}}(a_0+R)^2}{2R^3 a_0}\right) \quad (41)$$

DISCUSSION

Equation 41 is the expected equation that can be used to calculate the energy correction factor for the 1st order perturbation. Dependence correction of the energy level is on the form of the potential energy level is on have alternative forms. The nuclear size effect is small where Z=1 while if Z is having high values the effect becomes large which can be easily measured.

CONCLUSION

Potential function that has Separate dependence on the radial coordinate for r greater and less than a given value R have been achieved for the energy level. The method has advantage of allowing 1st order correction for the ground state and the method is considerably simpler and accurate than higher order perturbation.

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