IOSR Journal of Applied Physics (IOSR-JAP)
e-ISSN: 2278-4861. Volume 5, Issue 2 (Nov. - Dec. 2013), PP 37-40
www.iosrjournals.org

Vacuum polarization corrections in energy levels of hydrogen atom

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Abstract: *A numerical calculation of the one photon vacuum polarization corrections in 1s, 2s, 2p, 3s, 3p and 3d energy levels of hydrogen atom is presented using Schrödinger solutions taking the Uehling potential as a correction. The relativistic effect on 1s, 2s, $2p_{(1/2)}$ and $2p_{(3/2)}$ levels are calculated by using Dirac wave functions in the presence of Coulomb potential. The contribution of this correction decreases with the increase in principle quantum number n and orbital quantum number l.*
Keywords: *Vacuum polarization correction, hydrogen atom, Uehling potential*

I. Introduction

The calculation of corrections in energy levels in atoms needs many additional corrections including those due to quantum electro-dynamic (QED) effects. The largest QED effect in hydrogen is the self energy [1-2]. The second largest effect is the vacuum polarization [3-7] which is observed when a charged nucleus is placed in the Dirac Sea. This is because a virtual electron-positron pair is created in the Coulomb field of the nucleus. The electrons attract to the nucleus and the positrons escape from the nucleus. As a result the net charge observed at finite distances is smaller than the bare charge of the nucleus. The correction in this observed charge confined in the nucleus is called the vacuum polarization.

II. Vacuum Polarization

To find the influence of the creation of a virtual electron-positron pair on the propagation of the photon, one investigates how the unperturbed photon propagator

$$iD_{f\mu\nu}(q) = -\frac{4\pi i}{q^2 + i\epsilon} g_{\mu\nu} \tag{1}$$

Is modified by the correction of order e^2

$$i\acute{D}_{f\mu\nu}(q) = iD_{f\mu\nu}(q) + iD_{f\mu\lambda}(q)\frac{i\Pi^{\lambda\sigma}(q)}{4\pi} iD_{f\sigma\nu}(q) \tag{2}$$

Where the polarization tensor

$$i\frac{\Pi_{\lambda\sigma}}{4\pi} = -e^2 \int \frac{d^4k}{(2\pi)^4} Tr\left[\gamma_\lambda \frac{1}{k - m + i\epsilon}\gamma_\sigma \frac{1}{k - q - m + i\epsilon}\right] \tag{3}$$

By using the regularization method [8]

$$\Pi_{\mu\nu}(q) \to \overline{\Pi}_{\mu\nu}(q)$$

The gauge invariant polarization operator is obtained

$$\overline{\Pi}_{\mu\nu}(q^2) = -\frac{e^2}{3\pi}\ln\frac{\Lambda^2}{m^2} + \Pi^R(q^2) \tag{4}$$

Where

$$\Pi^R(q^2) = \frac{2e^2}{\pi}\int_0^1 d\beta\, \beta(1-\beta) ln\left[1 - \beta(1-\beta)\frac{q^2}{m^2}\right] \tag{5}$$

As it is known that the scattering cross section of two electrons or other charged particles will be influenced. The binding energy of an electron in an atom is affected. One can understand this effect if one considers the Coulomb potential of an external static source of a charge Ze

$$A_o(x) = -\frac{Ze}{|x|} \quad , \quad \vec{A}(x) = 0$$

The modified potential in momentum space

$$\acute{A}_o(q) = A_o(q) + \Pi^R(-q^2)A_o(q) \tag{6}$$

For low momentum transfer q

$$e\acute{A}_o(q) = -\frac{Z\alpha}{|x|} - Z\alpha^2\frac{4}{15m^2}\delta^3(\vec{x}) = eA_o(x) + e\Delta A_o(x)$$

$$e\Delta A_o(q) = -Z\alpha^2 \frac{4}{15m^2} \delta^3(\vec{x}) \tag{7}$$

The energy shift due to vacuum polarization in the first order perturbation theory is given by

$$\Delta E_{nl}^{VP} = < \psi_{nl}(r)|e\Delta A_o|\psi_{nl}(r) > \tag{8}$$

From equation 7

$$\Delta E_{nl}^{VP} = \frac{4m}{14\,\pi\,n^3} \alpha(Z\alpha)^4 \delta_{l0} \tag{9}$$

In this paper we calculated this correction using ψ_{1s}, ψ_{2s}, ψ_{2p}, ψ_{3s} and ψ_{3d} Schrodinger solutions of the hydrogen atom and the Uehling potential

$$e\Delta A_o\ \ (r) = -\frac{Z\alpha^2}{3\pi r}\int_1^\infty d\eta\ \frac{(2\eta^2+1)}{\eta^4}\sqrt{(\eta^2-1)}\ e^{-2m\eta r} \tag{10}$$

One may take the external electric field of the nucleus in the form of spherically symmetric potential [9]

$$V(r) = \begin{cases} -\frac{Ze^2}{|r|} & for \quad r > R \\ -\frac{Ze^2}{2R}\left(3 - \frac{r^2}{R^2}\right) & for \quad r < R \end{cases} \tag{11}$$

Where the nucleus radius R is given as

$$R = 1.2A^{1/3}$$

Where A is the mass number of the nucleus. To calculate the relativistic effect the energy shift has the form

$$\Delta E_{nl}^{VP} = \int d^3r|\phi_{nl}(r)|^2\, e\Delta A_o(r) \tag{12}$$

Where $\phi_{nl}(r)$ is the Dirac wave function for hydrogen in the presence of Coulomb field [1]. This can be written as

$$\Delta E_{nl}^{VP} = -\frac{Z\alpha^2}{2\pi}\int_1^\infty d\eta\ \frac{(2\eta^2+1)}{\eta^4}\sqrt{(\eta^2-1)}\, L_n(2\eta) \tag{13}$$

Where,

$$L_n(u) = \int dx\, |\phi_n(x)|^2 \frac{e^{-ux}}{x} = \int_0^\infty dx\ x\,[f_1^2(x) + f_1^2(x)]\, e^{-ux}$$

Where f_1 and f_2 are the radial wave functions as defined in [1].

III. Results and discussion

Figure 1 shows the spherically symmetric potential of the nucleus described by equation (11). Figure 2 shows the Uehling potential, equation (14), by introducing the spherically symmetric Coulomb potential which is shown in figure 1.

$$e\Delta A_o = \begin{cases} -\frac{Z\alpha^2}{6\pi R}\left(3-\frac{r^2}{R^2}\right)\int_1^\infty d\eta \frac{(2\eta^2+1)}{\eta^4}\sqrt{(\eta^2-1)}\ e^{-2m\eta r} & for \quad r \le R \\ -\frac{Z\alpha^2}{3\pi r}\int_1^\infty d\eta \frac{(2\eta^2+1)}{\eta^4}\sqrt{(\eta^2-1)}\ e^{-2m\eta r} & for \quad r > R \end{cases} \tag{14}$$

In this calculations we take $m = \hbar = c = 1$ and $R = 0.85$ Fm for the proton radius. From equation (8), ΔE_{nl}^{VP} is proportional to $|\psi_{nl}(r)|^2$ and since the Uelhing potential in figure 2 contributes large around the center of the nucleus, one expects that the states which have large density distribution near the center of the nucleus give large values for ΔE_{nl}^{VP}.

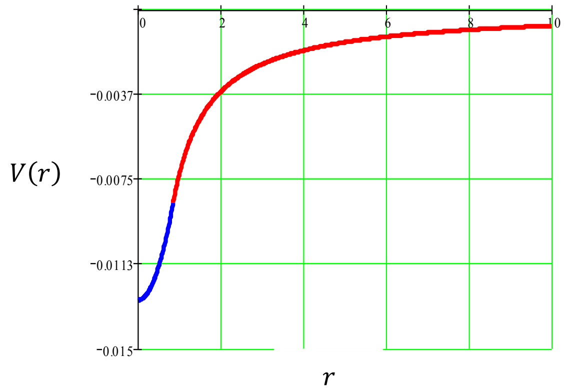

Figure 1. The Spherical symmetric potential of the nucleus as a function of r, equation (11).

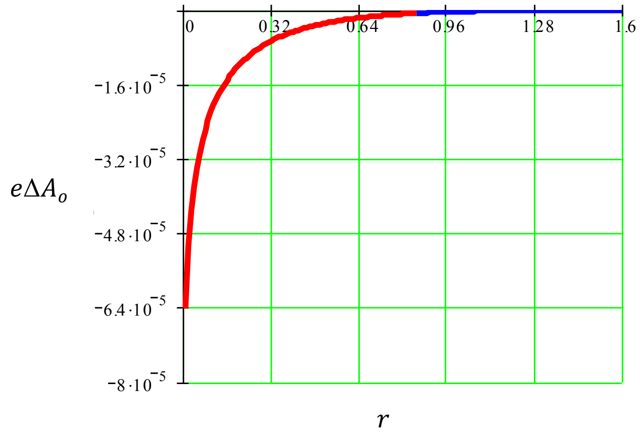

Figure 2 The Uehling potential as a function of r, equation (14).

From figures 3 and 4 the density distribution of the states decreases with the increase in the principle quantum number n at the center of the nucleus, this indicates that ΔE_{nl}^{VP} decrease with the increase in n as shown in table 1. From figure 4 the density distribution is very small at the center of the nucleus and we find

$$\left(\Delta E_{nl}^{VP}\right)_{2p} > \left(\Delta E_{nl}^{VP}\right)_{3p} > \left(\Delta E_{nl}^{VP}\right)_{3d}$$

in case of symmetric Coulomb potential as shown in table 2. Table 3 shows the relativistic values of ΔE_{nl}^{VP} calculated from equation (12). From this table it is clear that

$$(\Delta E_{nl}^{VP})_{1s} > (\Delta E_{nl}^{VP})_{2s} > (\Delta E_{nl}^{VP})_{2p_{1/2}} > (\Delta E_{nl}^{VP})_{2p_{3/2}}$$

From these results it is clear that the vacuum polarization appears largely at the center of the nucleus.

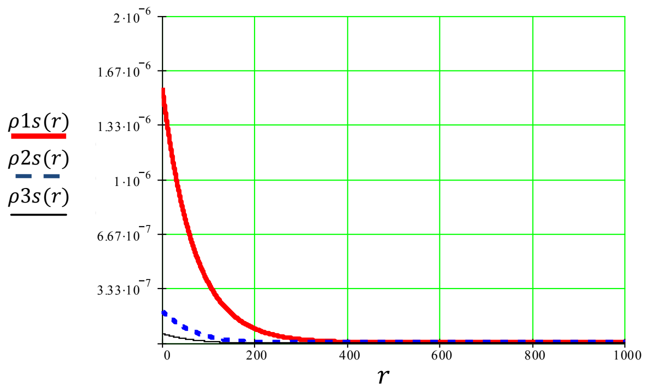

Figure 3 Density of 1s, 2s, 3s states in hydrogen atom.

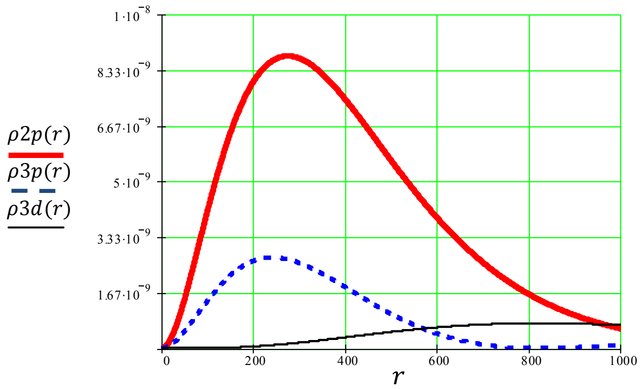

Figure 4. Density of 2p, 3p, 3d states in hydrogen atom.

From table 1, $\Delta E_{nl}^{VP}(eV)$ decreases with the increase in the principle quantum number n. The difference between the two columns decreases with the increase in principle quantum number. Table 2 shows that $\Delta E_{nl}^{VP}(eV)$ decreases with the increase in principle quantum number. The difference between the two columns decreases with the increase in principle quantum number. The correction of the same state calculated with Coulomb $1/r$ is larger than that calculated with symmetric potential. Table 3 shows Dirac corrections are larger than the Schrödinger corrections. The difference between $\Delta E_{nl}^{VP}(eV)$ in case of Dirac solutions and $\Delta E_{nl}^{VP}(eV)$ in case of Schrodinger solutions decreases with the increase in the principle quantum number. From table 3, we conclude that the relativistic effect in case of hydrogen atom is small, because $Z = 1$.

Table 1. Comparison between values of ΔE_{nl}^{VP} calculated with Schrödinger solutions One uses Uehling potential as a delta function and the second with an exact integral.

State	$\Delta E_{nl}^{VP}(eV)$		Difference
	$e\Delta A_0$ (equation 7)	$e\Delta A_0$ (equation 10)	
1s	-1.75×10^{-6}	-1.741×10^{-6}	-9×10^{-9}
2s	-2.196×10^{-7}	-2.176×10^{-7}	-2×10^{-9}
3s	-6.5066×10^{-8}	-6.448×10^{-8}	-5.86×10^{-10}

Table 2. Comparison between values of ΔE_{nl}^{VP} calculated with Schrödinger solution using Coulomb ($= 1/r$) and symmetric Coulomb potential equation 11.

State	ΔE_{nl}^{VP} (eV)		Difference
	Coulomb $V = 1/r$	Symmetric Coulomb equation 11	
1s	-1.741×10^{-6}	-1.18×10^{-6}	-5.61×10^{-7}
2s	-2.176×10^{-7}	-1.475×10^{-7}	-7.01×10^{-8}
3s	-6.448×10^{-8}	-4.371×10^{-8}	-2.077×10^{-8}
2p	-6.196×10^{-13}	-5.957×10^{-13}	-2.39×10^{-14}
3p	-2.179×10^{-13}	-2.092×10^{-13}	-8.7×10^{-15}
3d	-1.906×10^{-19}	-1.901×10^{-19}	-5×10^{-22}

Table 3. Comparison between values *of* ΔE_{nl}^{VP} for different states calculated with Uehling Potential using Schrödinger solutions and Dirac solutions taking Coulomb $1/r$.

State	ΔE_{nl}^{VP} (eV)		Difference
	Schrodinger Solutions	Dirac Solutions with Coulomb Potentials	
1s	-1.741×10^{-6}	-1.742×10^{-6}	-1×10^{-9}
2s	-2.176×10^{-7}	-2.177×10^{-7}	-1×10^{-10}
$2p_{(1/2)}$	-6.196×10^{-13}	-2.807×10^{-12}	-2.1874×10^{-12}
$2p_{(3/2)}$		-6.197×10^{-13}	-1×10^{-16}

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