Quantum Electro-dynamic Corrections of $1s_{1/2}$ Energy Level in Hydrogen like Atoms

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Abstract: We have calculated the one loop QED corrections in $1s_{1/2}$ level for hydrogen like atoms for $Z=1$-$92$. The self energy (which now automatically contains the vertex correction) and the vacuum polarization corrections are calculated with finite size nucleus. The results are calculated using non relativistic and relativistic approaches. For light nuclei ($Z=1$-$20$) the two approaches give approximately the same results. For heavy nuclei ($Z=20$-$92$) the relativistic effect increases with increasing $Z$. The effect of finite size on the low energy part of self energy and the total energy shift is very small for light atoms and increases slowly until $Z=20$ and begins to decrease until $Z=20$ and then increases for higher $Z$. The volume of the nucleus gives a large difference for high $Z$ in the vacuum polarization and increases the vertex correction slowly with $Z$. The contribution of the shape of the density of light nuclei is very small.

Keywords: Self energy, vacuum polarization and vertex corrections; Po-int nucleus; Finite size nucleus; Hydrogen like atoms; $1s_{1/2}$ energy level.

I. Introduction

The vacuum fluctuations predicted by QED are clear in their influence on the energy of bound states in atoms. Since atomic transition energies are measured by spectroscopic methods very accurately, the calculation of level shifts gives a good test for the validity of the theory. This problem is very difficult. Besides we are dealing with bound states which can interact with the charge $Ze$ of the nucleus any number of times. Therefore one has to use the Dirac Coulomb wave functions. Mohr [1, 2] calculated the one photon self energy radiative $1s_{1/2}$ level shift of an electron in a Coulomb field for hydrogen like atoms. Soff and Mohr [3] examined vacuum polarization in a strong external field. Jentchura et al [4] evaluated the one-photon electron self energy for the k- and L-shell states of hydrogen like ions with nuclear charge numbers $Z=1$ to 5. El-Shabshiry et al [5] calculated the finite size effect of the nucleus on the energy levels of hydrogen atom.

In this work we have concerned with the evaluation of the finite size effect on the $1s_{1/2}$ bound state level shift associated with the self energy, vertex correction and vacuum polarization for hydrogen like atoms of $Z$ in the range 1-92.

II. One Photon Exchange QED Corrections

To evaluate QED corrections, one finds that light atoms $(Z\alpha) << 1$ allow for an approximate method of high accuracy. This method depends on the fact that the atomic binding energies are of the order of magnitude of $(Z\alpha)^2 m$ and hence electron states in light atoms can be treated non-relativistically. Thus one can split the evaluation of self energy into two steps 1) If the virtual emitted photon is of high energy $\omega \geq K \gg (Z\alpha)^2 m$, the effect of Coulomb potential can be neglected and one may use free states for calculation. 2) If the virtual emitted photon is of low energy $\omega \leq K \ll m$ then one can use ordinary quantum mechanical perturbation theory for the Schrodinger equation.
This procedure work successfully when one chooses the separating energy $K$ satisfies
\[ m \gg K \gg (Z\alpha)^2 m \]  
(1)
in light atoms there is no problem. Adding the energy shifts obtained in two regions gives results independent on $K$.

The High Energy Part of Self Energy (Vertex Correction):

To calculate this part we use the form factors $F_1(q^2)$, $F_2(q^2)$ for Free states.

\[ F_1(q^2) \approx \frac{\alpha q^2}{3\pi m^2} (\ln \frac{m}{\mu} - \frac{3}{8}), \quad F_2(0) \approx \frac{\alpha}{2\pi} \]

In first order perturbation theory this high energy shifts takes the form:

\[ \delta E_{\text{high}}^{\text{high}} = e \int d^3 x \psi^*_+ (x) \left[ \frac{\alpha}{3\pi m^2} (\ln \frac{m}{\mu} - \frac{3}{8} - \frac{1}{5}) \Delta A^0 (x) + \frac{\alpha}{2\pi} \frac{i}{2m} \bar{\gamma} \cdot \vec{E} \right] \psi_+ (x) \]

Where,

\[ A^0 (x) = -\frac{Ze}{|x|}, \]  
(2)
is the Coulomb potential of the nucleus. $K$ is the cut off parameter which play the role of $\Delta E$ which is the energy below which no photons are observed. Then, in equation (2) one must replace

\[ \ln \frac{m}{\mu} \rightarrow \ln \frac{m}{2K} + \frac{5}{6} \]  
(4)
The energy shift can be written as

\[ \delta E_{\nu} = \delta E_{\nu}^{(1)} + \delta E_{\nu}^{(2)} \]

Where

\[ \delta E_{\nu}^{(1)} = \frac{e \alpha}{3\pi m^2} \left( \ln \frac{m}{2K} + \frac{5}{6} - \frac{3}{8} - \frac{1}{5} \right) \langle \nu | \nabla^2 A^0 | \nu \rangle \]

and

\[ \delta E_{\nu}^{(2)} = \frac{e \alpha}{8\pi m^2} \left[ \langle \nu | \nabla^2 A^0 | \nu \rangle + 4 \langle \nu | \frac{1}{r} \frac{d A^0}{dr} \vec{S} \cdot \vec{L} | \nu \rangle \right] \]

The Contribution of Low energy Emitted Photons:
The unperturbed problem is described by the Schrodinger eq.

\[ \hat{H}_o \psi_{\nu} = \left( -\frac{\nabla^2}{2m} + eA^0 (x) \right) \psi_{\nu} = E \psi_{\nu} \]  
(8)
The perturbation operator

\[ \hat{H}' = 2 \frac{ie}{2m} \vec{A} \cdot \nabla, \]  
(9)where $\vec{A}$ is the potential of the transverse field. Since $\hat{H}'$ creates and annihilates photons, the energy shift in second order perturbation theory has the form
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\[ \delta E_{\text{low energy}}^{\text{low}} = \sum_{\nu k \lambda} \frac{\left| \langle \nu', k, \lambda | H' | \nu \rangle \right|^2}{E_{\nu'} - (E_{\nu'} + \omega)} \]  

(10)

\[ \nu' \text{ is the electron state, } \hat{J} \text{ is its momentum and } \hat{\lambda} \text{ is the polarization of the transverse field.} \]

\[ (\delta E_{\text{low}}^{\text{low}})_{\text{ren}} = \frac{e \alpha}{3 \pi n^2} \left[ \langle \nu | \nabla^2 A^0 | \nu \rangle + \ln \left( \frac{2K}{m} - 2 \ln(Z\alpha) \right) \right] \]

\[ + \frac{2 \alpha}{3 \pi} \sum_{\nu'} \left| \langle \nu' | \nu \rangle \right|^2 (E_{\nu'} - E_{\nu}) \ln \left( \frac{(Z\alpha)^2 (m/2)}{|E_{\nu'} - E_{\nu}|} \right) \]  

(11)

**The Total Energy Shift**

It is given by the following equation:

\[ \delta E_{\nu} = \frac{e \alpha}{3 \pi n^2} \left( \frac{5}{6} - \frac{1}{2} - 2 \ln(Z\alpha) \right) \langle \nu | \nabla^2 A^0 | \nu \rangle + \frac{e \alpha}{2 \pi n^2} \langle \nu | \frac{1}{r} \frac{dA^0}{dr} \hat{S} \cdot \hat{L} | \nu \rangle \]

\[ + \frac{2 \alpha}{3 \pi} \sum_{\nu'} \left| \langle \nu' | \nu \rangle \right|^2 (E_{\nu'} - E_{\nu}) \ln \left( \frac{(Z\alpha)^2 (m/2)}{|E_{\nu'} - E_{\nu}|} \right) \]

(12)

For point charge nucleus

\[ \delta E_{nj} = \frac{4m}{3 \pi^3} \alpha(Z\alpha)^4 \left[ L_{n\ell} + \left[ \frac{19}{30} - 2 \ln(Z\alpha) \right] \delta_{\ell0} \pm \frac{3}{4} \frac{1}{(2j+1)(2\ell+1)}(1-\delta_{\ell0}) \right] \]  

(13)

for states with \( j = \ell \pm \frac{1}{2} \). Where \( L_{n\ell} \) is the Bethe logarithm

\[ L_{n\ell} = \frac{n^3}{2m(Z\alpha)^4} \sum_{\nu'} \left| \langle \nu' | \nu \rangle \right|^2 (E_{\nu'} - E_{\nu}) \ln \left( \frac{(Z\alpha)^2 (m/2)}{|E_{\nu'} - E_{\nu}|} \right) \]

In this work we tried to find the finite size effect on the 1s_{1/2} level of hydrogen-like atoms for Z=1-92. We divide the range of energy emitted by the photon in self energy into:

a) High energy part in this case we calculate the finite size contributions to the vertex correction by taking free form factors and substituting about the separating energy (\( K = m \)) as Bethe. From equation (6)

\[ \delta E_{\nu e r}^{\text{high}} = \frac{e \alpha}{3 \pi n^2} \left( \ln \left( \frac{1}{2} \right) + \frac{5}{6} \right) \langle \nu | \nabla^2 A^0 | \nu \rangle \]  

(14)

b) Low energy part from eq. (11)

\[ \delta E_{\nu e f f}^{\text{low}} = \frac{e \alpha}{3 \pi n^2} \left[ \langle \nu | \nabla^2 A^0 | \nu \rangle \ln(2) - 2 \ln(Z\alpha) \right] + \frac{4 \alpha(Z\alpha)^4 m}{3 \pi} L_{n\ell} \]  

(15)

and the correction due to vacuum polarization from the formula

\[ \delta E_{\nu e c} = - \left( \frac{1}{5} \frac{e \alpha}{3 \pi n^2} \langle \nu | \nabla^2 A^0 | \nu \rangle \right) \]  

(16)
Substituting about
\[ \frac{e\alpha}{3\alpha^2} \left( \psi \right) \left( \nabla^2 A^\alpha \right) = \frac{4\pi Z\alpha^2}{3\alpha^2} \int \rho(r) |\psi_{n\ell}|^2 r^2 \, dr \]

in equations (14), (15) and (16) we obtain the corresponding formulas for finite size nucleus, where

\[ \rho(r) = \frac{\rho_o}{1 + e^{(r-R)/D}} \]

is the density of the nucleus, \( \Psi_{n\ell} \) is the \( 1s_{1/2} \) wave function of the electron which is taken one time non-relativistic and one time as Dirac wave function of electron in a Coulomb field, to show the relativistic effect.

**Table 1:** Represents the comparison between the corrections calculated for point and finite size nucleus.

<table>
<thead>
<tr>
<th>Z</th>
<th>( \delta E_{\text{point}} ) (eV)</th>
<th>( \delta E_{\text{Sch vac}} ) (eV)</th>
<th>( \delta E_{\text{Sch point}} ) (eV)</th>
<th>( \delta E_{\text{Sch self}} ) (eV)</th>
<th>( \delta E_{\text{point}} ) (eV)</th>
<th>( \delta E_{\text{Sch}} ) (eV)</th>
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</thead>
<tbody>
<tr>
<td>1</td>
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<td>6.291 x10^{-5}</td>
<td>6.332 x10^{-5}</td>
<td>6.067 x10^{-5}</td>
<td>6.097 x10^{-5}</td>
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<td>-1.309 x10^{-5}</td>
<td>1.007 x10^{-5}</td>
<td>9.178 x10^{-5}</td>
<td>9.127 x10^{-5}</td>
<td>9.525 x10^{-5}</td>
</tr>
<tr>
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<td>-6.459 x10^{-5}</td>
<td>5.096 x10^{-5}</td>
<td>4.528 x10^{-5}</td>
<td>4.049 x10^{-5}</td>
<td>4.047 x10^{-5}</td>
</tr>
<tr>
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<td>-4.747 x10^{-5}</td>
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<td>0.225</td>
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<td>1.611</td>
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<td>-4.085</td>
</tr>
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<td>-1.461</td>
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<td>-14.57</td>
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<td>2.022</td>
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<td>45.07</td>
<td>2.893</td>
<td>473.3</td>
<td>24.97</td>
</tr>
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</table>

**Table 2:** Represents the total energy shift. The second column for point charge, the third for non-relativistic finite size nucleus and the fourth for vacuum polarization and the vertex calculated with finite size + self energy for point charge nucleus.

<table>
<thead>
<tr>
<th>Z</th>
<th>( \delta E_{\text{point}} ) (eV)</th>
<th>( \delta E_{\text{finite Sch}} ) (eV)</th>
<th>( \delta E_{\text{Sch}} ) (eV)</th>
<th>( \delta E_{\text{vac}} ) (eV)</th>
<th>( \delta E_{\text{self}} ) (eV)</th>
</tr>
</thead>
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<tr>
<td>1</td>
<td>6.04015 x10^{-5}</td>
<td>6.06998 x10^{-5}</td>
<td>6.03998 x10^{-5}</td>
<td>6.03998 x10^{-5}</td>
<td>6.03998 x10^{-5}</td>
</tr>
<tr>
<td>2</td>
<td>9.0841 x10^{-5}</td>
<td>9.48588 x10^{-5}</td>
<td>9.08788 x10^{-5}</td>
<td>9.08788 x10^{-5}</td>
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<tr>
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<td>0.00473</td>
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<td>0.01265</td>
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<tr>
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<td>0.13513</td>
<td>0.13513</td>
</tr>
<tr>
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<td>0.259</td>
<td>0.5831</td>
<td>0.5831</td>
<td>0.5831</td>
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<tr>
<td>20</td>
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<td>1.73885</td>
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<td>7.2021</td>
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<tr>
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Table 3: Represents the comparison between the non-relativistic and relativistic total energy shift in the $1s_{1/2}$ level calculated for finite size nucleus.

<table>
<thead>
<tr>
<th>Z</th>
<th>$\delta E_{\text{Sch}}^{\text{finite}}$ (eV)</th>
<th>$\delta E_{\text{Dirac}}^{\text{finite}}$ (eV)</th>
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<td>0.01059</td>
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<tr>
<td>10</td>
<td>0.08428</td>
<td>0.08722</td>
</tr>
<tr>
<td>15</td>
<td>0.259</td>
<td>0.28054</td>
</tr>
<tr>
<td>20</td>
<td>0.53945</td>
<td>0.61988</td>
</tr>
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<td>0.1211</td>
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<tr>
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<td>23.737</td>
<td>27.075</td>
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</table>

III. Results and Discussion

In this paper the natural units are used $\hbar = c = 1$. The density of the nucleus is taken as Fermi distribution, the r.m.s radius of different nuclei is taken from Brown et al [6]. Figure (2) represents the Fermi charge density of the nucleus (Z=92). Figure (3) consists of a, b and c. It shows the variation of the QED corrections calculated non-relativistically for point and finite size nucleus with Z.
For light atoms (Z=1-20) the finite size effect is very small and then increases slowly for higher Z nuclei. The difference between the point charge and finite size results is very clear for higher Z nuclei. In figure (4) the effect of finite size on the total energy shift is very clear for heavy atoms.

Fig. (4) Represents the variation of the total energy shift calculated non-relativistically with and without finite size charge of the nucleus.

In figure (5) the low energy part of self energy is calculated for point charge nucleus and added to the vacuum polarization and vertex correction calculated for finite size nucleus, in this case the total energy shift gives reasonable agreement with the experimental data [7].

Fig. (5): Same as figure (4) with the low energy part of the self energy calculated for point charge nucleus.
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Figure (6) the relativistic and non-relativistic values of the total energy correction calculated for finite size nuclei.

![Graph showing the relativistic and non-relativistic values of the total energy correction](image)

\[ \delta E_{\text{vac}}^{\text{finite}} \] vs. \( Z \)

\[ \delta E_{\text{vac}}^{\text{finite}} \] vs. \( Z \)

(a) \hspace{5cm} (b)

**Fig. 6:** The relativistic effect for a) vacuum polarization (b) Vertex correction.

Figure (7) represents the relativistic and non-relativistic values of the total energy correction calculated for finite size nuclei.

![Graph showing the relativistic and non-relativistic values of the total energy correction](image)

\[ \delta E_{\text{total}}^{\text{finite}} \] vs. \( Z \)

**Fig. (7):** Represents the variation of the total energy shift of the 1s1/2 level for finite size nucleus with \( Z \), calculated in case of Dirac w. f. and in case of Schrödinger w.f.

The correction is constant for light nuclei it decreases smoothly with \( Z \) until \( Z=80 \) and increases fastly for higher \( Z \) nuclei. The difference between relativistic and non-relativistic values is small. From figure (8), the shape of the nucleus density has a very small contribution to the total correction for light atoms.

**Table 4:** Shows the non-relativistic and relativistic results of the total energy shifts in the 1s1/2 level for light hydrogen like atoms (Z= 1-15). The calculations are performed by using Fermi and Gaussian distributions for the light nucleus density.

<table>
<thead>
<tr>
<th>Z</th>
<th>( \delta E_{\text{finite}}^{\text{Sch}} ) (eV)</th>
<th>( \delta E_{\text{finite}}^{\text{G}} ) (eV)</th>
<th>( \delta E_{\text{finite}}^{\text{Dirac}} ) (eV)</th>
<th>( \delta E_{\text{finite}}^{\text{Dirac}} ) (eV)</th>
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</thead>
<tbody>
<tr>
<td>1</td>
<td>6.06998 x10^{-5}</td>
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<td>6.013 x10^{-5}</td>
</tr>
<tr>
<td>2</td>
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Fig. 8: The non-relativistic Total energy correction against $Z$ in case of Fermi and Gaussian density for light nucleus atoms.

Finally one can conclude that the effect of finite size of the nucleus on the shift in $1s_{1/2}$ level is very small for light atoms ($Z=1-20$). The size effect on the low energy part of self energy is higher than on the vacuum polarization and vertex corrections for heavy atoms (table 2). The difference between the corrections calculated relativistically and non-relativistically is small. To show the effect of the form density of the nucleus, we calculate the total energy correction in case of Gaussian and Fermi forms.

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References