Finite Proton Size Contribution in the Energy Levels of Pionic Hydrogen Atom

M. El-Shabshiry1, M. Abdel Aziz2
1,2Physics Department, Faculty of Science, Ain-Shams University, Cairo, Egypt

Abstract: The energy level corrections for pionic hydrogen atom induced by Uehling potential are calculated. The density distribution of proton is used in this calculation to show the size effect of the proton on these corrections. The derivative expansion (DE) theory is applied to derive the approximate forms of the potentials. The results with these approximate potentials agree with those of point charge in the order of magnitude. The 2s-state gives the best agreement with the point charge.

Key words: Uehling potential, vacuum polarization, proton point charge, finite size proton, pionic hydrogen atom, energy level corrections.

I. Introduction

Electronic vacuum polarization plays an important role in calculating the energy levels of atoms. Although it is small in hydrogen atom it gives a dominant contribution to QED corrections for heavier orbital particles such as muons and pions. Borie [1] calculated the Lamb shift in case of muonic hydrogen. Karshenboim et.al. [2] used the Uehling potential to represent the role of free one loop vacuum polarization in calculating the pionic circular states. Carroll et.al. [3] investigated the muonic hydrogen 2p-2s transition by a precise non-perturbative numerical solution of the Dirac equation including the finite size Coulomb force and finite size vacuum polarization. Earlier perturbative calculations of Borie, Martynenko and Pachucki [4-9] are made for calculating the same transition. Comparison between experimental results presented by Pohl et.al. [10] is interpreted as requiring a modification of the proton charge radius from that obtained in electron scattering. Corrections to the energy levels of spin-0 particle bound in strong field are performed by Lee et.al. [11], they derived formulas for these corrections based on Klein-Gordon-Fock equation. Mohammadi [12] solved pionic atom with Klein-Gordon-Fock equation. Schlesser et. al. [13] investigated all pure quantum electrodynamics corrections to the np → 1s (n = 2-4) transition energies of pionic hydrogen larger than 1meV [13]. Recently, Hennebach et. al. [14] determined the hadronic shift in pionic hydrogen by X-ray spectroscopy of ground state transitions.

In this work the energy level corrections in pionic hydrogen atom are calculated using the vacuum polarization induced by the Uehling potential. The contribution of the finite size of the proton is introduced via its charge density. We apply the derivative expansion theory (DET) to obtain the approximate forms of the potentials.

II. Theory

The relativistic description of spin-0 particle is represented by Klein-Gordon-Fock equation as

\[(E_i - V(\vec{r}))^2 - \frac{p^2 c^2}{\hbar^2} - m^2 c^4 \] \[\Phi_i(\vec{r}) = 0 \] (1)

The solutions of this equation, \(\Phi_i\), are not orthogonal and their normalization is not trivial. Although exact solution of equation (1) with a non-Coulomb potential is possible [15-18], the perturbative theory with Coulomb potential has not been developed until now. We apply Lee et.al. [11], recent form for calculating the vacuum polarization corrections in the energy levels as

\[ \delta E_i = \frac{\langle \Phi_i^{(0)} | (E_i^{(0)} - V^{(0)}) | \delta V | \Phi_i^{(0)} \rangle}{\langle \Phi_i^{(0)} | (E_i^{(0)} - V^{(0)}) | \Phi_i^{(0)} \rangle} \] (2)

This equation is valid for any perturbation in case of electrostatic potential and especially for the Uehling correction. The Coulomb problem is considered as unperturbed case and we use the following eigenvalues and eigen-functions

\[ \Phi_{nl}^{(0)} = \frac{1}{r} R_{nl}(r) Y_{lm}(\theta, \phi). \] (3)
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\[ R_{nl}(r) = N(\beta r)^{s+1} \exp(-\frac{\beta r}{2}) F_1(-n + l + 2s + 2, \beta r) \]  

(4)

\[ E_l^{(0)} = \frac{\mu_\alpha e^2}{\sqrt{1 + \frac{(Z\alpha)^2}{\eta}}} \]  

(5)

Where \( Y_{ln}(\theta, \phi) \) stands for spherical harmonics, \( F_1(a, b; z) \) is the confluent hypergeometric function and \( \mu_\alpha \) is the pion reduced mass

\[ s = -\frac{1}{2} + \left( \frac{l + \frac{1}{2}}{2} - (Z\alpha)^2 \right)^{\frac{1}{2}}, \quad \eta = n - l + s \]  

and

\[ \beta = 2 \left( \frac{Z\alpha E_l^{(0)}}{c \hbar} \right). \]  

(6)

We take the Uehling potential for a point proton in the form

\[ \delta V = U_0(r) = -\frac{2Z\alpha^2}{3\pi} \int_1^{\infty} \left[ \frac{2x^2 + 1}{2x^4} \right] \sqrt{x^2 - 1} e^{-2m_e x} dx \]  

(7)

Where \( \alpha \) is the usual fine structure constant.

2.1 QED vacuum polarization

In momentum space, the propagator \( iD_{\rho\lambda}(q) \) is modified and becomes

\[ iD_{\rho\lambda}(q) = iD_{0\rho\lambda}(q) + iD_{0\gamma\lambda}(q) i\Pi^{\mu\nu}(q) iD_{0\nu\lambda}(q). \]  

(9)

Note that from gauge invariance \( q^\mu \Pi_{\mu\lambda}(q) = 0 \), which dictates the Lorentz invariant form

\[ \Pi^{\mu\nu} = (g^{\mu\nu} - \frac{q^\mu q^\nu}{q^2}) \Pi(q^2) \]  

(10)

So that

\[ iD_{\gamma\lambda}(q) = -i g_{\gamma\lambda} \frac{q^2 + i\epsilon}{(q^2 + i\epsilon)^2} \Pi(q^2). \]  

(11)

From the well known Feynman rules of QED with the usual charge renormalization, the propagator’s polarization insertion is found to be [19]

\[ \Pi(q^2) = \frac{2\alpha}{\pi} e^2 \int_0^\infty \frac{dz}{z} \ln (1 - z) \ln (1 - z - \frac{q^2}{m_e^2}) \]  

(12)

This integral can be evaluated, and for the case of stationary source, the momentum is space-like, \( q^2 = -q^2 \), and

\[ \Pi(-q^2) = -\frac{\alpha}{3\pi} \frac{e^2}{q^2} \left[ -\frac{5}{3} \frac{4m_e^2}{q^2} + (1 - \frac{2m_e^2}{q^2}) \sqrt{1 + \frac{4m_e^2}{q^2}} \ln \left( \frac{1 + \frac{4m_e^2}{q^2} + 1}{1 + \frac{4m_e^2}{q^2} - 1} \right) \right] \]  

(13)

The vacuum polarization potential is taken as the folding of a background spherically symmetric charge density of the source, \( \rho(r) \) over the new part of the propagator. This is most easily done in momentum space, where for a time independent source

\[ \delta V(\vec{r}) = \int \frac{d^3q}{(2\pi)^3} e^{i\vec{q}\cdot\vec{r}} \frac{\Pi(-q^2)}{|\vec{q}|^4} \rho(\vec{q}). \]  

(14)

The angular part is integrated, leaving

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\[
\rho(q) = \int d^3r \ e^{-iq \cdot r} \rho(r) = 4\pi \int_0^\infty \ dr \ r^2 \frac{\sin(qr)}{qr} \rho(r)
\]

This expression gives the “exact” effect of vacuum polarization in this theory (to \(O(\alpha^2)\)). To obtain the approximate potential, the DE coefficients has the form

\[
Z_1 = - \left. \frac{\partial \Pi(q^2)}{\partial q^2} \right|_{q^2=0}, \quad Z_2 = - \frac{1}{2} \left. \frac{\partial^2 \Pi(q^2)}{\partial q^2} \right|_{q^2=0}
\]

and

\[
\Pi(q^2) = -\frac{q^4}{15m_e^2} \frac{\alpha}{\pi}
\]

One can evaluate these coefficients using equations (17-a) and (17-b), giving

\[
Z_1 = 0,
\]

\[
Z_2 = \frac{\alpha}{15\pi m_e^2}
\]

The result \(Z_1 = 0\) is a manifestation of charge conservation, which implies that corrections to the charge density are total derivatives that vanish under spatial integration. This allows us to write an effective Lagrange equation is

\[
L_{\text{eff}} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} - \frac{\alpha}{30 \pi m_e^2} (\partial_{\mu} F^{\mu\nu})(\partial^\nu F_{\nu\nu}) - j^\mu A_\mu
\]

The fermion part of the Lagrangian has been dropped here, and an external source current \(j^\mu\) is included. The gauge fixing term can be dropped because we restrict ourselves to the time like part of the vector potential in the case where it is independent of time. The suitable form for the Euler-Lagrange equations is

\[
\frac{\partial L}{\partial A_\mu} - \partial_\lambda \left( \frac{\partial L}{\partial (\partial_\lambda A_\mu)} \right) + \partial^2 \left( \frac{\partial L}{\partial (\partial^2 A_\mu)} \right) = 0
\]

Considering the time-like part of the potential \(A_0\) and a source current \(j^\mu = \delta^{\mu 0} j_0\), we obtain a modified form of Maxwell’s equation

\[
\partial^2 A_0 = j_0 + \frac{\alpha}{15\pi m_e^2} \partial^4 A_0
\]

which for a time independent potential becomes

\[
\nabla^2 A_0 = -j_0 - \frac{\alpha}{15\pi m_e^2} \nabla^4 A_0
\]

Such that

\[
A_0(r) = \frac{1}{4\pi} \int d^3r' \frac{1}{|r' - r|} \left( j_0(r') + \frac{\alpha}{15\pi m_e^2} \nabla^4 A_0(r') \right)
\]

\[
= \frac{1}{4\pi} \int d^3r' \frac{1}{|r' - r|} j_0(r') + \frac{\alpha}{60\pi^2 m_e^2} \int d^3r' (\nabla^2 \frac{1}{|r' - r|}) \nabla^2 A_0(r')
\]

\[
= \frac{1}{4\pi} \int d^3r' \frac{1}{|r' - r|} j_0(r') - \frac{\alpha}{15\pi m_e^2} \nabla^2 A_0(r)
\]

For example, with a point proton-like source with charge \(-Ze\) we have
$A_\rho(\vec{r}) = -\frac{Ze^2}{4\pi|\vec{r}|} - \frac{\alpha}{15\pi m_e^2} \nabla^2 A_\rho(\vec{r})$

The second term is the familiar term which contributes to the Lamb shift in hydrogen [19].

To understand how useful the effective Lagrangian, is by considering the spherically symmetric charge density, $J_0 = \rho(r)$, solving (22) iteratively we have for the vacuum polarization contribution to the potential

$$\delta V(r) = \frac{4Z\alpha^2}{15m_e^2} \rho(r).$$

We made a comparison between the results obtained by using two densities. One in the Gaussian form

$$\rho(r) = \frac{1}{\pi^{1/2} a^2} e^{-r^2/(a^2)}, \quad \rho(q) = e^{-a^2q^2/4}$$

and the other in the exponential form

$$\rho(r) = \frac{\xi^3}{8\pi} e^{-\xi r}, \quad \rho(q) = \frac{1}{(1 + R^2 q^2)^{3/2}}, \quad R = \frac{1}{\xi}$$

where the parameter $a$ controls the shape of the potential and $< r_p^2 >$ is the mean square radius of the proton.

### III. Results and Discussion

In these calculations we use the relativistic units $\hbar = c = 1$, the pion mass $m_\pi = 139.577$ MeV, the electron mass $m_e = 0.5109989$ MeV and the fine structure constant $\alpha = 1/137.0359998$. Figure (1) shows spherically symmetric densities of the proton, $\rho(r)$ represent the exponential density for proton of radius $= 0.864$ fm and the Gaussian density for proton of radius $= 0.864$ fm. From the figure the exponential density is higher than the Gaussian density in the short range and they agree approximately for distances higher than $\approx 0.6$ fm. Figure (2) shows the Fourier transform of densities as in Figure (1). They have the same shape as that in Figure (1). Figures (3, 4, 5, and 6) show the square s, p, d, f- state wave-functions. From these figures the contribution of s- states at the origin is higher than the p-states which are higher than the d- states. Figure (7) shows the Uehling potential, $U_\rho(r)$ for proton charge distribution. It is clear that the large contribution exists around the centre of the nucleus; one expects that the states which have large density distribution near the centre of the nucleus give large values for the correction in energy levels. To display the effect of proton charge distribution on corrections in energy levels, the vacuum polarization function $\Pi(-q^2)$ (Figure (8)) is drawn against $q^2$. From the figure the higher values appear at low momentum and the Figure shows the decrease in the function with the increase in momentum. Figure (9) presents a comparison between the exact exponential vacuum polarization potential and the exact Gaussian. The two potentials coincide at the small distance until 0.01 fm. For larger range the Gaussian differs very small from the exponential. Figure (10) shows a comparison between the approximated exponential potential and the approximated Gaussian potential. The two potentials differ much around the centre and this difference decreases with increasing in $r$ and coincide for distances larger than 0.5 fm. Figure (11) shows a comparison between the exact Gaussian and its approximate form. From the figure they differ around the centre. This difference decreases with $r$ and they intersect at 0.45 fm. For further distances they differ again. Figure (12) the same as Figure (11) shows a comparison between the exponential potential and its approximated one. They differ around the centre. This difference decreases with $r$. They intersect at $r = 1$ fm and coincide for further. Table 1 shows the corrections in the energy levels for different potentials in meV. In general for any state the corrections decrease with the increase in the principle quantum number for all potentials. The last two columns have the same order of magnitude. The agreement between the results of the Uehling potential and the exact Gaussian potential is better than that between the exact exponential potential. Columns one, four and five agree better than the exact Gaussian and the exact exponential. The corrections obtained in case of exact exponential potential are the most far from the other potentials.
Figure (1): Two spherically symmetric charge densities of the proton. The exponential density for proton radius=0.90019 fm and the Gaussian density for radius=0.864 fm.

Figure (2): The Fourier transform of densities in Figure (1) in terms of momentum (q).

Figure (3): The square of the radial wave functions of the pion for different s-states against r.

Figure (4): The square of the radial wave functions of pion for different p-states.

Figure (5): The square of the radial wave functions of different d-states. $U_o (r)$

Figure (6): The square of the radial wave functions of different f-states.

Figure (7): The electronic Uehling potential for the point charge proton $U_o (r)$ (eq. (7)).

Figure (8): The variation of the Fourier transform of the Uehling potential with momentum (q).

Figure (9): Comparison between the two exact potentials (eq. (14)).

Figure (10): Comparison between the two approximated potentials (eq. (23)).
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Figure (11): Comparison between exact potential with Gaussian distribution (the red curve) and its approximated potential (the blue dashed curve).

Figure (12): Same as Figure (11) for the exact exponential potential (red curve) and its approximated potential (blue dashed curve).

Table 1. Values of the energy level corrections (δE) for pionic hydrogen atom in (meV)

<table>
<thead>
<tr>
<th>Energy state</th>
<th>Uehling potential (Point nucleus charge) Equation (7)</th>
<th>Exact potential with Gaussian density Equation (14)</th>
<th>Approximated potential with exponential density Equation (23)</th>
<th>Approximated potential with exponential density Equation (23)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1s</td>
<td>-3.42456 x10^7</td>
<td>-7.72768 x10^10</td>
<td>-9.30308 x10^10</td>
<td>-4.34451 x10^10</td>
</tr>
<tr>
<td>2s</td>
<td>-2.38373</td>
<td>-2.3261</td>
<td>-1.08002 x10^10</td>
<td>-2.99815</td>
</tr>
<tr>
<td>3s</td>
<td>-1.36168 x10^1</td>
<td>-9.93079 x10^-2</td>
<td>-6.98238 x10^1</td>
<td>-1.7224 x10^-1</td>
</tr>
<tr>
<td>4s</td>
<td>-1.28415 x10^-1</td>
<td>2.08535 x10^-2</td>
<td>-4.56396 x10^-3</td>
<td>-1.66268 x10^-3</td>
</tr>
<tr>
<td>5s</td>
<td>-1.5473 x10^-1</td>
<td>-7.64238 x10^-4</td>
<td>-2.69993 x10^-4</td>
<td>-1.03708 x10^-4</td>
</tr>
<tr>
<td>6s</td>
<td>-4.19229 x10^-1</td>
<td>-2.56641 x10^-4</td>
<td>-1.51748 x10^-4</td>
<td>-1.32877 x10^-4</td>
</tr>
<tr>
<td>7s</td>
<td>-1.43602 x10^-1</td>
<td>-8.97395 x10^-5</td>
<td>-9.6883 x10^-5</td>
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<tr>
<td>2p</td>
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<td>-6.07128</td>
<td>-1.68353 x10^1</td>
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<td>-1.22775</td>
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<td>-1.4107 x10^-1</td>
<td>-6.79247 x10^-1</td>
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<td>5p</td>
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<td>-7.48367 x10^-4</td>
<td>-8.72644 x10^-2</td>
<td>-3.65677 x10^-2</td>
</tr>
<tr>
<td>6p</td>
<td>-5.49892 x10^-6</td>
<td>-9.26226 x10^-6</td>
<td>-6.23266 x10^-2</td>
<td>-1.73816 x10^-2</td>
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<tr>
<td>7p</td>
<td>-7.16556 x10^-7</td>
<td>-2.86753 x10^-3</td>
<td>-4.27735 x10^-3</td>
<td>-1.78608 x10^-3</td>
</tr>
<tr>
<td>3d</td>
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<td>-2.18915</td>
<td>-8.16050 x10^-4</td>
</tr>
<tr>
<td>4d</td>
<td>-4.07397 x10^-1</td>
<td>-1.82879 x10^-1</td>
<td>-2.39907 x10^-2</td>
<td>-1.21025 x10^-2</td>
</tr>
<tr>
<td>5d</td>
<td>-8.36272 x10^-4</td>
<td>-3.61523 x10^-3</td>
<td>--</td>
<td>-2.63719 x10^-3</td>
</tr>
<tr>
<td>6d</td>
<td>-8.73938 x10^-4</td>
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<td>-5.12892 x10^-2</td>
<td>-3.90307 x10^-2</td>
</tr>
<tr>
<td>7d</td>
<td>-1.22703 x10^-7</td>
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<td>-2.22017 x10^-2</td>
<td>-3.58592 x10^-3</td>
</tr>
<tr>
<td>4f</td>
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<td>-2.43211 x10^-5</td>
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<td>-9.91793 x10^-3</td>
</tr>
<tr>
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</tr>
<tr>
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<td>8.65485 x10^-8</td>
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<td>-3.63974 x10^-1</td>
</tr>
<tr>
<td>7f</td>
<td>-4.76595 x10^-9</td>
<td>-4.73916 x10^-9</td>
<td>-1.24034 x10^-2</td>
<td>-1.02564 x10^-1</td>
</tr>
</tbody>
</table>

IV. Conclusion

Because the range of vacuum polarization potential is of the order of the Bohr radius of pion in pionic hydrogen, then there exists a large overlap of pion wave functions with the domain of Uehling potential. Therefore we cannot neglect the finite size of the proton in calculating the corrections in the energy levels. The derivative expansion (DE) theory gives approximated Gaussian and exponential potentials containing corresponding distributions of the proton charge density which show the proton size effect on the vacuum polarisation corrections for the energy levels of pionic hydrogen atom. No great difference exists between the two results. These corrections in the levels are higher than that calculated for hydrogen atom because the Bohr radius of pion is much smaller than that of electron which causes large overlap of pion wave function with the vacuum polarization potential which is clear from table (2).

Table 2. Vacuum polarization corrections for energy levels of the hydrogen atom calculated with Schrödinger wave function in (meV) [20]

<table>
<thead>
<tr>
<th>Hydrogen atom</th>
<th>Uehling potential (Point charge)</th>
<th>Approximated Gaussian potential</th>
<th>Approximated exponential potential</th>
</tr>
</thead>
<tbody>
<tr>
<td>1s</td>
<td>-8.39593 x10^-3</td>
<td>-8.91694 x10^-4</td>
<td>-8.91717 x10^-4</td>
</tr>
<tr>
<td>2s</td>
<td>-1.11397 x10^-4</td>
<td>-1.11461 x10^-4</td>
<td>-1.11396 x10^-4</td>
</tr>
<tr>
<td>3s</td>
<td>-3.29474 x10^-5</td>
<td>-3.30256 x10^-5</td>
<td>-3.30062 x10^-5</td>
</tr>
<tr>
<td>4s</td>
<td>-1.38997 x10^-4</td>
<td>-1.39326 x10^-4</td>
<td>-1.39245 x10^-4</td>
</tr>
<tr>
<td>2p</td>
<td>-3.16604 x10^-5</td>
<td>-3.18125 x10^-5</td>
<td>-3.18562 x10^-5</td>
</tr>
<tr>
<td>3p</td>
<td>-1.11180 x10^-6</td>
<td>-4.14815 x10^-6</td>
<td>-5.56170 x10^-6</td>
</tr>
<tr>
<td>3d</td>
<td>-9.73895 x10^-9</td>
<td>-4.87823 x10^-9</td>
<td>-3.13991 x10^-9</td>
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</tbody>
</table>

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