Finite Nuclear Size Effect

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Though it is pedagogically beneficial to assume a point particle description of the nucleus when studying the hydrogen atom, how will those results change once this assumption is changed? This paper undergoes a first order perturbation theory approach of a finite sized nucleus with a uniform distribution of charge. The energy correction factors for low energy levels and their corresponding angular momenta are computed to determine the significance of a point-particle assumption of the nucleus that is so often employed. Correlations between quantum numbers and energy correction factors are made, and the strength of the largest correction factor is evaluated.

I. INTRODUCTION

The method of attacking complicated, real physics problems by simplifying their parts is a modus operandi employed by all physicists. When studying the hydrogen atom in an undergraduate quantum mechanics class, many assumptions are made about the system in order to provide a simple, approachable potential that produces an analytic solution. The point-particle assumption of the nucleus is addressed this paper. Though the potential conveniently provides an analytic solution, it diverges as r approaches 0. As a more realistic assumption, the nucleus will instead be described with a finite size and a uniform distribution of charge. This will produce an energy potential that will require a different approach. After producing the potential from the assumption of a uniformly distributed charge over a finite sized nucleus, the Hamiltonian is all but trivial to form.

Applying first order perturbation theory to evaluate the size of the energy corrections implies that the original radial wavefunctions need to be reproduced. Though the method of calculating the energy correction terms is straight forward, it does leave behind exponentials. This expression will be expanded using a Taylor series that can be truncated, as the high order terms diverge quickly. Once this is done, an array of energy correction terms is evaluated and analyzed.

II. FORMING THE POTENTIAL

When assuming the nucleus (proton) of the Hydrogen atom is a point particle, all of its charge is concentrated on a point located at r = 0, leading to the potential

$$V(r) = -\frac{e^2}{r} \qquad (1)$$

The graph of this potential can be seen by the solid line in Figure 1. Though the potential diverges at $r =$ 0, it does provide an analytic solution to the following Hamiltonian:

$$H = \frac{p^2}{2m} - \frac{e^2}{r} \qquad (2)$$

Note, the Hamiltonian is formed by the addition the kinetic energy term.

Writing out a more accurate Hamiltonian in the conventional form, we can break it down into convenient pieces

$$H_{real} = \frac{p^2}{2m} + V_{real}(r)$$

$$= \frac{p^2}{2m} - \frac{e^2}{r} + \left[\frac{e^2}{r} + V_{real}(r)\right] \qquad (3)$$

$$= H + H_{pert}$$

Now we can form our real Hamiltonian, H_{real}, from our analytic H and a new perturbation Hamiltonian, H_{pert}. To find $V(r)$, let's not assume the nucleus is a point particle, but instead let's make the less sophomoric, yet still incomplete assumption that the nucleus has a uniform distribution of charge over a finite radius, given by

$$\rho = \frac{Q}{\frac{4}{3}\pi R_n^3} \qquad (4)$$

This finite nuclear size assumption leads to a new potential

$$V_{real}(r) = \int_0^{R_n} \frac{Q(r)}{r^2}\, dr$$

$$= -\frac{q}{r} + \frac{1}{2}\frac{r^2 R_n^3}{q} - \frac{1}{2}\frac{q}{R_n} \qquad (5)$$

$$= -\frac{3}{2}\frac{q}{R_n} + \frac{1}{2}\frac{q}{R_n}\left(\frac{r}{R_n}\right)^2$$

This potential curve can be seen in Figure 1, represented by the dashed line.

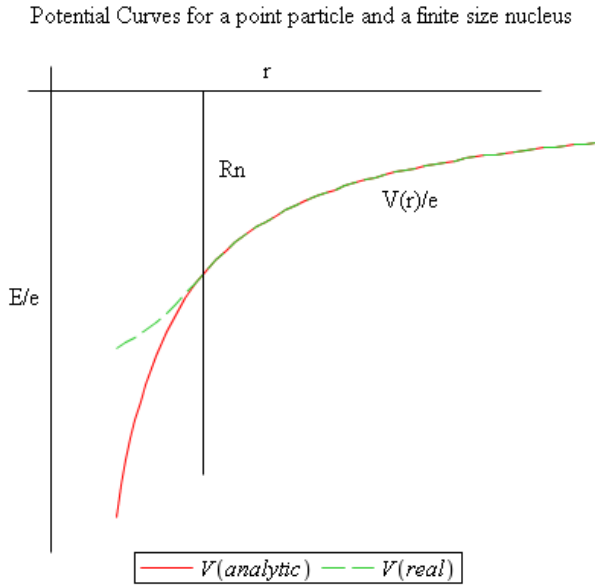Figure 1: The analytic potential curve can be seen by the solid line, falling to -∞ as $r \to 0$. The finite nuclear size potential can be seen as the dashed line. Note how the two potentials separate at $r = R_n$.

Notice how the analytic potential and the real potential curves separate only at $r = R_n$, due to the finite size of the nucleus. As you can see, this potential is finite when $r = 0$, however, this potential does not present analytic solutions, and instead will be used to help with consequent perturbation theory calculations.

III. THE PERTURBATION HAMILTONIAN

To form H_{pert}, one simply needs to subtract the theoretical potential, $V(r)$, from finite nuclear size potential, $V_{real}(r)$

$$H_{pert} = V_{real}(r) - V(r)$$

$$= -\frac{3}{2}\frac{q}{R_n} + \frac{1}{2}\frac{q}{R_n}\left(\frac{r}{R_n}\right)^2 + \frac{q^2}{r}$$

$$= \frac{e^2}{a_0}\left[-\frac{3}{2}\frac{a_0}{R_n} + \frac{1}{2}\frac{a_0}{R_n}\left(\frac{r/a_0}{R_n/a_0}\right)^2 + \frac{a_0}{r}\right]$$ (6)

$$= \frac{e^2}{a_0}\left[-\frac{3}{2}\frac{1}{K} + \frac{1}{2}\frac{1}{K}\left(\frac{x}{K}\right)^2 + \frac{1}{x}\right]$$

where $r \leq R_n$, $K = R_n/a_0$, $x = r/a_0$, and e is elementary charge. Now we've conveniently written the perturbation Hamiltonian as a dimensionless polynomial with a factor out front that is approximately $2 \cdot 13.6 eV$.

IV. ENERGY CORRECTIONS

Since the potential is radially symmetric, the angular wavefunctions are trivial and only the radial wavefunctions need to be produced. The exact work can be found in the appendix, but the method is straightforward. After accessing a library with working Laguerre polynomials, these are differentiated appropriately to produce the associated Laguerre polynomials. Next, each associated Laguerre polynomial is multiplied by a factor of

$$e^{-\frac{r}{n}}\left(\frac{2r}{n}\right)^l$$ (7)

where n and l are the familiar principal quantum number and angular quantum number, respectively. This constructs the normalized hydrogenic radial wavefunctions. Checks are done to be sure they are normalized and integrating properly. With the radial functions constructed, the perturbation Hamiltonian may be introduced.

Using 1st order perturbation theory, we can calculate the energy correction due to this finite nuclear size consideration by

$$\Delta E(n, l) = \langle \Psi_{100}|H_{pert}|\Psi_{100}\rangle$$

$$= e^{2/a_0} \int_0^K R_{nl}(r)^2 \left[-\frac{3}{2}K + \frac{1}{2K}\left(\frac{x}{K}\right)^2\right]$$ (8)

which is simply the expectation value of the perturbation Hamiltonian while the system is in the unperturbed state. Since the result involves exponentials, it's much more enlightening to take a Taylor series expansion and to truncate the higher order terms.

V. RESULTS

Only the first five energy levels were computed, with corresponding angular momenta. The truncated Taylor series expansions can be seen in the appendix for consultation. The correction factors reported are the first term in these expansions, as the series diverges rapidly. The correction factors for these energy levels are represented in Figure 2.

a much smaller correction factor. Again, with a higher probability of being farther from the nucleus, the finite size of the nucleus still approaches a point-particle like effect.

How significant is the largest correction term? The correction factor for the $n = 1$ energy orbital is $2/5$, but the dimensional factors need to be considered as well:

$$\Delta E(n,l) = \frac{e^2}{a_0} \left(\frac{2}{5}\right) K^2$$

$$= 2 \cdot 13.6 \cdot \left(\frac{2}{5}\right) \left(\frac{1.27 \cdot 10^{-13} cm}{0.5 \cdot 10^{-8} cm}\right)^2 \tag{9}$$

$$\simeq 7.02 \cdot 10^{-9} eV$$

Though this may not seem like a substantial correction term, experiments that aim to be highly accurate would certainly need to consider it. As for higher energy terms, especially high orbital angular momentum terms, it's significance decreases rapidly.

This procedure has shown that though the concept of finite nuclear size does have an impact on the energy spectrum of the hydrogen atom, for pedagogical reasons it's still very beneficial to study the point-like particle assumption of the nucleus. The energy correction factors become decrease rapidly in significance as the principal quantum number, n, or the angular quantum number, l, is increased. This massages one's ego for having intuitive understandings for quantum mechanical depictions, and provides insight for other hydrogenic systems.

	K^2	K^4	K^6	K^8	K^{10}
$n=4$	$\frac{2}{625}$	$\frac{8}{109375}$	$\frac{4}{17578125}$	$\frac{16}{101513671875}$	$\frac{4}{164959716796875}$
$n=3$	$\frac{1}{160}$	$\frac{1}{7168}$	$\frac{1}{2580480}$	$\frac{1}{5449973760}$	
$n=2$	$\frac{2}{135}$	$\frac{8}{25515}$	$\frac{4}{6200145}$		
$n=1$	$\frac{1}{20}$	$\frac{1}{1120}$			
$n=0$	$\frac{2}{5}$				
	$l=0$	$l=1$	$l=2$	$l=3$	$l=4$

Figure 2: Each bar represents an energy orbital corresponding to unique n and l quantum numbers. Atop each bar is the energy correction factor for that orbital. Each l value contributes an additional $K^{2(l+1)}$ factor to the correction term.

Each correction factor has a e^2/a_0 coefficient that is approximately $27.2 \, eV$, and a corresponding dimensionless K factor ($K = \frac{R_n}{a_0} = 2.54 \cdot 10^{-8}$) as depicted in the figure.

VI. CONCLUSION

Though this is only a first order correction, many correlations can be recognized to help understand the behavior of finite nuclear size corrections. Noting the rapid decline of the scaling factor, this uniform distribution of charge assumption gives the largest energy correction to the lowest energy orbital, $n = 1$. This much should be intuitive, considering that on average an electron is closer to the nucleus in this lower energy orbital, and therefor experiences this distribution of charge to a larger degree than a more distant electron in the $n = 4$ orbitals. Likewise, each increasing orbital angular momenta has

VII. REFERENCES

An interview with Dr. Robert Gilmore, who graciously saved a poor soul (me) from the dearth of knowledge found in Drexel's library.