Hydrogen Had a Little Lamb-Shift

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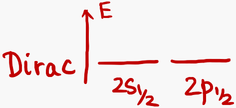
A little History

- Energy eigenvalues of Hydrogen atom from Dirac Equation-

$$E_{nj} = mc^2 \left[1 + \left(\frac{Z\alpha}{n + \frac{1}{2} + \sqrt{\left(j + \frac{1}{2}\right)^2 - (Z\alpha)^2}} \right)^2 \right]^{-\frac{1}{2}} \tag{1}$$

- Eigenvalues independent of orbital angular momentum number ℓ.
- $^{2}2s_{\frac{1}{2}}$ and $^{2}2p_{\frac{1}{2}}$ have same energy according to the energy eigenvalues.
- Spectroscopic notation $\quad {}^{2s+1}\ell_j$

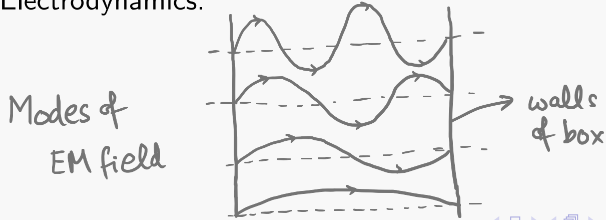


A little History (contd.)

- Lamb and Retherford carried out experiments to stimulate transitions between $^2 2s_{\frac{1}{2}}$ and $^2 2p_{\frac{1}{2}}$ states.
- A transition of $\approx$ 1000 MHz was found between the two levels. This shift is famously known as the Lamb-Shift.
- First evidence of quantum vacuum fluctuations!

Vacuum pushing on Hydrogen

- There is a lot going on in empty space!
- Quantized EM Field $\rightarrow$ each mode is a QHO (virtual photons).
- The quantized modes are fluctuating even in their ground states.
- The ideas eventually lead to development of Quantum Electrodynamics.



Hans Bethe's Calculation

The Hamiltonian of a free particle in an electromagnetic field can be written as

$$H = \frac{(\vec{p} - e\vec{A})^2}{2m} = \frac{\vec{p}^2}{2m} + \frac{e^2\vec{A}^2}{2m} - \frac{e}{m}(\vec{p}\cdot\vec{A}) \tag{2}$$

Hans Bethe trated the $\vec{p}\cdot\vec{A}$ as a perturbation and calculated the energy shift using second-order perturbation theory.

The calculation also involves fairly advanced concepts like 'renormalisation' to deal with infinities.

Welton's method deals with the shift on a more intuitive basis.

Welton's derivation

Analysis of orbit fluctuations-

Fluctuations in the orbit $\delta\vec{r}$ cause a shift in energy. The difference in potential energy is given by-

$$\Delta V = V(\vec{r}+\delta\vec{r}) - V(\vec{r}) = \delta\vec{r}\cdot\nabla V(\vec{r}) + \frac{1}{2}(\delta\vec{r}\cdot\nabla)^2 V(\vec{r}) + \dots$$

$$\approx \delta x\frac{\partial V}{\partial x} + \delta y\frac{\partial V}{\partial y} + \delta z\frac{\partial V}{\partial z} + \frac{1}{2}\left(\delta x^2\frac{\partial^2 V}{\partial x^2} + \delta y^2\frac{\partial^2 V}{\partial y^2} + \delta z^2\frac{\partial^2 V}{\partial z^2}\right)$$

If we treat this difference in potential energy as a perturbation, then by first-order perturbation theory-

$$\Delta E = \langle \Delta V \rangle = \langle \psi | \Delta V | \psi \rangle$$

Welton's derivation (contd.)

Assuming isotropic fluctuations-

$$\langle \delta \vec{r} \rangle = \langle \delta x \rangle \hat{e_x} + \langle \delta y \rangle \hat{e_y} + \langle \delta z \rangle \hat{e_z} = 0$$

$$\langle \delta x^2 \rangle = \langle \delta y^2 \rangle = \langle \delta z^2 \rangle = \frac{1}{3} \langle \delta r^2 \rangle$$

Using the above assumptions, the shift in energy for a Coulomb potential would be-

Help Box:
$\nabla^2 \frac{1}{r} = -4\pi \delta^3(\vec{r})$

$$\implies \Delta E = \langle \Delta V \rangle = \frac{1}{6} \left\langle \delta r^2 \right\rangle \left\langle \nabla^2 V_{\text{Coul}} \right\rangle$$

$$\boxed{\Delta E = \frac{e^2}{6\epsilon_0} \left\langle \delta r^2 \right\rangle \langle \psi | \delta^3(\vec{r}) | \psi \rangle = \frac{e^2}{6\epsilon_0} \left\langle \delta r^2 \right\rangle |\psi(0)|^2} \tag{3}$$

$\Delta E \sim$ mean square fluctation in position (δr^2)

Welton's derivation (contd.)

Calculation of the average fluctuation $\langle \delta r^2 \rangle$

The classical equation of motion for the e^- displacement is

$$m\frac{\mathrm{d}^2(\delta r)}{\mathrm{d}t^2} = -eE$$

where E is the vacuum electric field fluctuation. Separate into contributions from different modes ω.

So to each mode of the quantized EM field, we associate a fluctuation δr_ω-

$$\implies m\frac{\mathrm{d}^2(\delta r_\omega)}{\mathrm{d}t^2} = -eE_\omega \sim -eE_0 \sin(\omega t)$$

$\ddot{\varphi} \sim -\sin(\omega t) \implies \varphi \sim \sin(\omega t)$

Welton's derivation (contd.)

$$\delta r_\omega = \frac{eE_0}{m\omega^2}\sin(\omega t) = \frac{e}{m\omega^2}E_\omega$$
$$\implies \left\langle (\delta r_\omega)^2 \right\rangle = \frac{e^2}{(m^2\omega^4)}\left\langle (E_\omega)^2 \right\rangle \quad (4)$$

should be related to energy

Fluctuation for mode ω ~ avg. amplitude of E field

- The standard expression for number of modes per unit volume (density of modes) is $g(\omega)\mathrm{d}\omega = (\omega^2/\pi^2 c^3)\mathrm{d}\omega$. ← mode density.
- The vacuum energy of each mode (QHO) is $\hbar\omega/2$. ← mode energy

Therefore, the energy density should be given as

$$U(\omega)\mathrm{d}\omega = \frac{\hbar\omega}{2}\frac{\omega^2}{\pi^2 c^3}\mathrm{d}\omega = \frac{\hbar\omega^3}{2\pi^2 c^3}\mathrm{d}\omega$$

Energy density of quantized modes = Energy density of EM field

$$U(\omega)\mathrm{d}\omega \equiv \epsilon_0 \left\langle (E_\omega)^2 \right\rangle \mathrm{d}\omega$$

$$\implies \left\langle (E_\omega)^2 \right\rangle = \frac{\hbar\omega^3}{2\pi^2 c^3 \epsilon_0}$$

Now we can use eqn (4) to calculate the mean squared fluctuation of the orbit for ω^{th} mode -

$$\boxed{\left\langle (\delta r_\omega)^2 \right\rangle = \frac{e^2}{m^2\omega^4}\left(\frac{\hbar\omega^3}{2\pi^2 c^3 \epsilon_0}\right) = \frac{\hbar e^2}{2\pi^2 m^2 c^3 \epsilon_0}\frac{1}{\omega}} \qquad (5)$$

mean fluctuation due to ω^{th} mode

ADD THEM ALL UP!

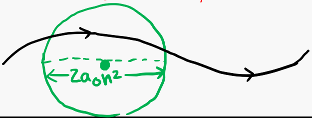
Welton's derivation (contd.)

Now we sum up the fluctuation contriburions from all the modes-

$$\langle \delta r^2 \rangle = \int \mathrm{d}\omega \, \langle (\delta r_\omega)^2 \rangle = \frac{\hbar e^2}{2\pi^2 m^2 c^3 \epsilon_0} \int_0^\infty \frac{\mathrm{d}\omega}{\omega} \qquad (6)$$

To get a finite result, we introduce a lower and higher cutoffs in the limits of the integral.

- On the higher side, the energy of the mode shouldn't be higher than $m_e c^2$ or that $\omega_{\text{high}} = mc^2/\hbar$.
- On the lower side, the mode frequency shouldn't be so low that its wavelength is smaller than the diameter of orbit, i.e. $\omega_{\text{low}} = \pi c / n^2 a_0$.



Welton's derivation (contd.)

Using the appropriate limits in equation (6)-

$$\langle \delta r^2 \rangle = \frac{\hbar e^2}{2\pi^2 m^2 c^3 \epsilon_0} \int_{\pi c / n^2 a_0}^{mc^2/\hbar} \frac{\mathrm{d}\omega}{\omega} = \frac{\hbar e^2}{2\pi^2 m^2 c^3 \epsilon_0} \ln\left(\frac{mc^2}{\hbar}\frac{n^2 a_0}{\pi c}\right)$$

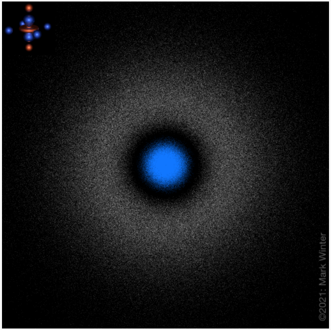
$$\langle \delta r^2 \rangle = \frac{\hbar e^2}{2\pi^2 m^2 c^3 \epsilon_0} \ln\left(\frac{n^2}{\pi\alpha}\right) \qquad \text{where } \alpha \approx 1/137$$

Finally substituting this into equation (3), we get the expression of the energy shift as-

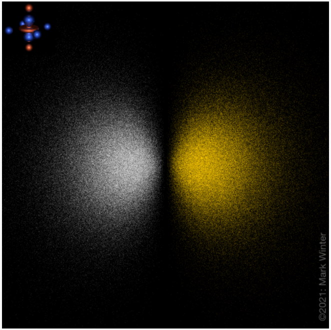
$$\boxed{\Delta E = \frac{\hbar e^4}{12\pi^2 m^2 c^3 \epsilon_0^2} \ln\left(\frac{n^2}{\pi\alpha}\right) |\psi(0)|^2} \tag{7}$$

First-order energy correction to state ψ

For the ${}^2 2p_{\frac{1}{2}}$ orbital, the wavefunction has a node at $r = 0$, so $\Delta E_{2p} = 0$.
But for the ${}^2 2s_{\frac{1}{2}}$ orbital, there is a finite value of the wavefunction at the origin, which causes the change in energy of the level.



(a) $2s_{\frac{1}{2}}$ orbital density plot



(b) $2p_{\frac{1}{2}}$ orbital density plot

Figure: Electron density plots from `https://winter.group.shef.ac.uk/orbitron/`

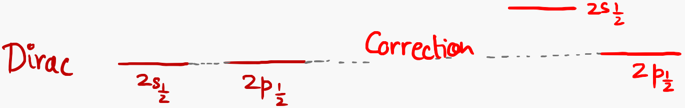
Calculation of energy shift (contd.)

Proceeding with the calculation of $^22s_{\frac{1}{2}}$ energy shift-

$$\psi_{2s}(0) = \frac{1}{\sqrt{8\pi a_0^3}} \implies |\psi_{2s}(0)|^2 = \frac{1}{8\pi a_0^3}$$

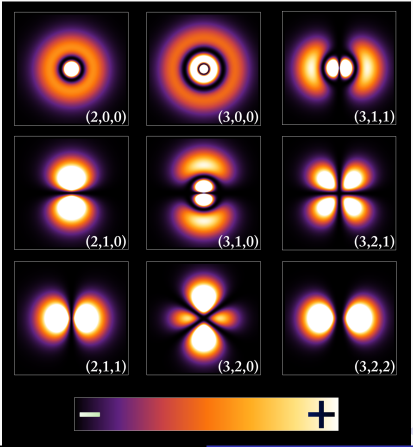
$$\Delta E_{2s} = \frac{\hbar e^4}{12\pi^2 m^2 c^3 \epsilon_0^2} \frac{1}{8\pi a_0^3} \ln\left(\frac{n^2}{\pi\alpha}\right) = \boxed{\alpha^5 m_e c^2 \frac{1}{6\pi} \ln\left(\frac{4}{\pi\alpha}\right)} \quad (8)$$

which corresponds to a shift of $\approx$ 700.17 MHz, within an order of magnitude and close enough to the measured value of 1057 MHz.



Interpretation of the Lamb Shift

The only reason why the Lamb Shift appears is because the probability density has a peak at the centre. If it didn't have a peak — say, if it went to zero near the center — then there would be no Lamb shift. This difference can be observed as a faint microwave signal from interstellar hydrogen.



References

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That's all Folks!