LAMB SHIFT & VACUUM POLARIZATION CORRECTIONS TO THE ENERGY LEVELS OF HYDROGEN ATOM

Student, Aws Abdo

The hydrogen atom is the only system with exact solutions of the non-relativistic Schrödinger equation and relativistic Dirac equation. Therefore any discrepancy between analytic and experiment is a very evident of new physics.

This is the first effect demonstrating the influence of physical vacuum. Zero point vacuum fluctuations (which comes form the uncertainty principle, where we have a non zero value for the energy of the ground state,like the ground state energy of ($\hbar\omega/2$) for the harmonic oscillator) create additional field acting on the electron, historically this was the first discovery of quantum electrodynamics.

If we have fluctuating fields of given frequency $\overrightarrow{E_\omega}$ and $\overrightarrow{B_\omega}$then there time average $\langle\overrightarrow{E_\omega}\rangle_t = \langle\overrightarrow{B_\omega}\rangle_t = 0$, but fluctuations are present, $\langle\overrightarrow{E^2_\omega}\rangle_t \neq 0$,$\langle\overrightarrow{B^2_\omega}\rangle_t \neq 0$. Their energy is

$$E_\omega = \frac{\hbar\omega}{2} \tag{1}$$

But

$$\begin{aligned} E_\omega &= \frac{\langle\overrightarrow{E^2_\omega}\rangle_t + \langle\overrightarrow{B^2_\omega}\rangle_t}{8\pi}V, \qquad (2) \\ &= \frac{\langle\overrightarrow{E^2_\omega}\rangle_t}{4\pi}V \qquad (3) \end{aligned}$$

Where $\langle\overrightarrow{E^2_\omega}\rangle_t = \langle\overrightarrow{B^2_\omega}\rangle_t$ since we have a set of plane waves.

From (1) & (3) we get :

$$\langle\overrightarrow{E^2_\omega}\rangle_t = \frac{2\pi}{V}\hbar\omega \tag{4}$$

Consider an electron in a nonrelativistic atom, $v/c \ll 1$. Then magnetic effects are weak. The equation of motion for the electron acquires an additional displacement,

$$\overrightarrow{r} \to \overrightarrow{r} + \overrightarrow{\xi}$$

This additional displacement ξ comes from the zero point fluctuations which create an additional field that can be felt by the electron, so we can count for the presence of this new field by introducing ξ and we have ,

$$m\overrightarrow{\xi} = e\overrightarrow{E} \tag{5}$$

Only the field components with the wavelength $\gg \xi$ can contribute, otherwise their actions cancel(since for $\lambda \sim \xi$ the fluctuations of the field will be very small and they will cancel each other), so we have $\kappa\xi \ll 1$, and the field $\overrightarrow{E}$ can be considered uniform over the length $\sim \xi$. For the frequency ω we have,

$$\begin{aligned} -m\omega^2\overrightarrow{\xi_\omega} &= e\overrightarrow{E_\omega}, \qquad (6)\\ \langle\overrightarrow{\xi_\omega}\rangle_t &= 0 \qquad (7) \end{aligned}$$

Mean square fluctuations of the displacement is

$$\begin{aligned} \langle\overrightarrow{\xi^2_\omega}\rangle_t &= \frac{e^2}{m^2\omega^4}\langle\overrightarrow{E^2_\omega}\rangle_t, \qquad (8)\\ &= \frac{2\pi}{V}\frac{\hbar e^2}{m^2\omega^3} \qquad (9) \end{aligned}$$

Full mean square fluctuation is the result of noncoherent action of all components of the field,

$$\langle\overrightarrow{\xi^2_\omega}\rangle_t = \int d\omega\langle\overrightarrow{\xi^2_\omega}\rangle_t\rho(\omega) \tag{10}$$

Where $\rho(\omega)$ is the density of states for the field

$$\begin{aligned} \rho(\omega)d\omega &= \frac{Vd^3\kappa}{(2\pi)^2} * 2, \qquad (11)\\ &= \frac{V\omega^2 d\omega}{\pi^2 c^3} \qquad (12) \end{aligned}$$

$$\langle\overrightarrow{\xi^2_\omega}\rangle_t = \frac{2\hbar e^2}{\pi m^2 c^3}\int\frac{d\omega}{\omega} \tag{13}$$

This result is formally divergent, but there are physical factors that cut off the integral. At large frequencies there occurs the relativistic growth of the electrons mass; for small frequencies the perturbation does not work if $\hbar\omega \ll$ distance to the first excited state.

The divergence is only logarithmic so that it is sufficient to estimate those limits approximately, so we have

$$\hbar\omega_{max} \sim mc^2$$

$$\hbar\omega_{min} \sim \triangle E_{hydrogen} \sim (Z\alpha)^2 mc^2$$

Where Z is the nuclear charge, and $\alpha = e^2/\hbar c = 1/137$.

With these approximations the integral evaluates to :

$$\begin{aligned} \langle \overrightarrow{\xi_\omega^2} \rangle_t &= \frac{2\hbar e^2}{\pi m^2 c^3} Ln\left(\frac{\omega_{max}}{\omega_{min}}\right), && (14) \\ &= \frac{2\hbar e^2}{\pi m^2 c^3} Ln\left(\frac{f}{(Z\alpha)^2}\right) && (15) \end{aligned}$$

Where f is a numerical factor ~ 1

This amplitude of chaotic motion is small,

$$\langle \overrightarrow{\xi_\omega^2} \rangle_t \sim \frac{\hbar e^2}{m^2 c^3} \sim \frac{e^2}{\hbar c}\left(\frac{\hbar}{mc}\right)^2 = \alpha\lambda_c^2 \qquad (16)$$

Where λ_c is compton wave length of the electron $\sim 4 * 10^{-10} cm$, this is much smaller than the size of the Bohr orbit

$$\langle \overrightarrow{\xi_\omega^2} \rangle_t \sim \alpha a^2 \frac{\lambda_c^2}{a^2} \sim \alpha^3 a^2 \ll a^2$$

Since $\hbar\omega \le mc^2$, $\hbar\kappa \le mc$,$\lambda \sim 1/\kappa > \hbar/mc > \lambda_c$ Then the assumption $\kappa\xi \ll 1$ is fulfilled ,

$$\kappa\xi \sim \kappa a \alpha^{(3/2)} \le \frac{mc}{\hbar} a \alpha^{(3/2)} \sim \frac{a}{\lambda_c} \alpha^{(3/2)} \sim \sqrt{\alpha} \ll 1$$

Everything is self-consistent.

Now the potential acting on the electron fluctuates ;

$$U(\overrightarrow{r}) \to U(\overrightarrow{r} + \overrightarrow{\xi}) \sim U(\overrightarrow{r}) + \overrightarrow{\xi}.\nabla U(\overrightarrow{r}) + \frac{1}{2}\xi_\alpha\xi_\beta \frac{\partial^2 U}{\partial x_\alpha \partial x_\beta}, \qquad (17)$$

This should be averaged over $\overrightarrow{\xi}$,

$$\langle \overrightarrow{\xi} \rangle_t = o$$

$$\langle \xi_\alpha \xi_\beta \rangle_t = \frac{1}{3}\langle \overrightarrow{\xi^2} \rangle_t \delta_{\alpha\beta}$$

$$\langle U(\overrightarrow{r} + \overrightarrow{\xi}) \rangle_t = U(\overrightarrow{r}) + \frac{1}{6}\langle \overrightarrow{\xi^2} \rangle_t \nabla^2 U.$$

This is a small perturbation that shifts the atomic levels.

In the first order of perturbation theory the shift of the level ψ_{nl} :

$$\triangle E_{nl}^{(1)} = \frac{1}{6}\langle \overrightarrow{\xi^2} \rangle_t \langle nl/\nabla^2 U/nl \rangle, \tag{18}$$

$$= \frac{\alpha^3}{3\pi} a^2 Ln\left(\frac{f}{(Z\alpha)^2}\right)\langle \nabla^2 U \rangle_{nl} \tag{19}$$

In the coulomb field,

$$U = -\frac{Ze^2}{r}, \nabla^2 U = 4\pi Z e^2 \delta(\overrightarrow{r}), \langle \nabla^2 U \rangle_{nl} = 4\pi Z e^2 |\psi_{nl}(0)|^2$$

Only S - levels are shifted up (other states have $|\psi_{nl}(0)|^2 \to 0$)

For hydrogen - like atoms

$$|\psi_{n0}(0)|^2 = \frac{Z^3}{\pi a^3 n^3}$$

We notice that this shift is decreasing fast with increasing n.

For the ground state ($n = 1$) → we have only one significant shift.

$$\triangle E_n \sim \frac{\alpha^3 a^2}{3\pi} Ln\left(\frac{f}{(Z\alpha)^2}\right)\frac{4\pi Z^4 e^2}{\pi a^3 n^3} = \frac{4}{3\pi}\frac{Z^4 e^2}{a n^3}\alpha^3 Ln\left(\frac{f}{(Z\alpha)^2}\right)$$

In hydrogen $Z = 1$,

$$\triangle E_n = \frac{4}{3\pi}\alpha^3 Ln\left(\frac{f}{\alpha^2}\right)\frac{e^2}{an^2}\frac{1}{n} \sim E_n \frac{\alpha^3}{n} Ln\left(\frac{f}{\alpha^2}\right) \sim mc^2\alpha^5 \tag{20}$$

the shift in the energy is equal to $4 * 10^{-6}$ eV.

VACUUM POLARIZATION

Is vacuum really empty ?

In an attempt to avoid the negative energy solutions and the negative probability density that arise form the solution of the Klein-Gordon equation, Dirac devised a relativistic wave equation that is linear in both $\partial/\partial t$ and ∇, although he succeeded in avoiding the negative probability density, negative-energy solutions still occurred. That means that an atomic electron can have both negative and positive energies. But according to the quantum theory of radiation, an excited atomic state can lose its energy by spontaneously emitting a photon even in the absence of any external field. This is why all excited states have finite lifetimes. but if the electron is allowed to have negative energies then what we call the ground state is not really the lowest-energy state since there exists a continuum of negative-energy states from $-mc^2$ to $-\infty$, and then what would happen is that the electron in the ground state can emit spontaneously a photon and fall into a negative-energy state, and since there is *no lower bound state*, the electron will keep emitting photons and keep falling indefinitely to lower negative-energy states.

To over come this catastrophe, Dirac proposed that *all the negative energy states are completely filled under normal conditions*, so now the catastrophic transitions are prevented because of the exclusion principle, and what we usually called the *vacuum* is nothing but an infinite sea of negative-energy electrons.

It may happen that a negative energy electron absorbs a photon of energy $\hbar\omega > 2mc^2$ and make a transition to a positive energy state, as a result a "hole" is created in the Dirac sea, and this will give us two important results,

First, the energy of the Dirac sea is the energy of the vacuum minus the energy of the vacated state, which will give us a positive quantity, so the absence of a negative-energy electron will appear as a presence of a positive-energy particle.

Second, the total charge of the dirac sea is now the charge of the vacuum minus the charge of the electron i.e,

$$Q = Q_{vacuum} - (-e) = Q_{vacuum} + |e|$$

and the observed charge of the hole is

$$Q_{obs} = Q - Q_{vacuum} = |e|$$

This means that a hole in the Dirac sea looks like a positive energy particle of charge $|e|$. First Dirac thought the a proton is a good candidate for this particle, then it was shown by H.Weyl that according to the symmetry properties of the Dirac equation that the mass of this particle should be equal to the mass of the electron. Finally it was accepted that the positron is the right candidate.

So what is vacuum polarization ?

Now that we accept the idea that vacuum is nothing but a homogeneous sea of negative-energy electrons, lets consider what will happen when a nucleus of charge $Z|e|$ is placed in the Dirac sea. The presence of this positively charged nucleus will disturb the homogeneity of the Dirac sea because the charge distribution of the negative-energy electrons is different from that of the free-field case. In the electron-positron language this is due to the fact that a virtual electron-positron pair created in the Coulomb field behaves in such a way that the electron tends to be attracted to the nucleus while the positron tends to escape form it. This is shown in fig(1).

Fig(1)

As a result, the net charge observed at large but finite distance is smaller than the bare charge of the nucleus. In fact what we call the observed charge of the nucleus is the original bare charge of the nucleus partially cancelled by the virtual electrons surrounding the nucleus. In other words,because of the virtual electron-positron pairs the vacuum behaves like a polarizable medium.

Photon self-energy; vacuum polarization.

Fig(2)

Fig(2) represents the vacuum polarization of the photon. Here the photon propagator is modified because the covariant photon can virtually disintegrate into an electron-positron pair for a certain fraction of time, this diagram is actually known as the *photon self-energy diagram.*

This diagram is equal to,

$$\begin{aligned} &= (-ie)(-1)\int \frac{d^4k}{(2\pi)^4} tr\left[\gamma^\mu \frac{i}{\not k - m}\gamma^\nu \frac{i}{\not k + \not q - m}\right] && (21)\\ &= i\Pi_2^{\mu\nu}(q) && (22)\end{aligned}$$

Where $\Pi^{\mu\nu}$ is the *polarization tensor* which characterizes the proportionality between the induced current and the external potential.

We can define $i\Pi^{\mu\nu}(q)$ to be the sum of all 1-particle irreducible insertions into the propagator,

$$= i\Pi^{\mu\nu}(q) \qquad (23)$$

so that $\Pi_2^{\mu\nu}(q)$ is the second-order (in e) contribution to $\Pi^{\mu\nu}(q)$.

The only tensors that can appear in $\Pi^{\mu\nu}(q)$ are $g^{\mu\nu}$ and $q^\mu q^\nu$. However, the Ward identity [1] tells us that $q_\mu \Pi^{\mu\nu}(q) = 0$. This implies that $\Pi^{\mu\nu}$ is pro-

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[1] The Ward identity states that if $M(k) = \epsilon_\mu(k) M^\mu(k)$ is the amplitude of some QED process involving an external photon with momentum k, then this amplitude vanishes if we replace ϵ_μ with k_μ:

$$k_\mu M^\mu(k) = 0$$

this is easily understood from the fact that the induced current is expected to satisfy the continuity equation portional to $(g^{\mu\nu} - q^{\mu}q^{\nu}/q^2)$.It is therefore convenient to write the polarization tensor $\Pi^{\mu\nu}$ in the following way:

$$\Pi^{\mu\nu}(q) = (q^2 g^{\mu\nu} - q^{\mu}q^{\nu})\Pi(q) \tag{24}$$

where $\Pi(q^2)$ is regular at $q^2 = 0$. Using this notation, the exact photon two-point function is

$$= \frac{-ig_{\mu\nu}}{q^2} + \frac{-ig_{\mu\rho}}{q^2}\left[i(q^2 g^{\rho\sigma} - q^{\rho}q^{\sigma})\Pi(q^2)\right]\frac{-ig_{\sigma\nu}}{q^2} + ...$$

this expression can be simplified to

$$= \frac{-i}{q^2(1-\Pi(q^2))}\left(g_{\mu\nu} - \frac{q_{\mu}q_{\nu}}{q^2}\right) + \frac{-i}{q^2}\left(\frac{q_{\mu}q_{\nu}}{q^2}\right) \tag{25}$$

For the purpose of calculating the S-matrix we can abbreviate

$$= \frac{-ig_{\mu\nu}}{q^2(1-\Pi(q^2))} \tag{26}$$

The residue of the $q^2 = 0$ pole is

$$\frac{1}{1-\Pi(0)} = Z_3$$

Since a factor of e lies at each end of the photon propagator, we can account for this shift by the replacement $e \longrightarrow \sqrt{Z_3}e$. This replacement is called *charge renormalization.* We should note that the observed electron charge is $\sqrt{Z_3}e$, i.e,

$$\text{Observed charge} = e = \sqrt{Z_3}.e_o = \sqrt{Z_3}.\text{bare charge}$$

To lowest order, $Z_3 = 1$ and $e = e_o$.

Computing Π_2

Going back to equation (20), we have

$$i\Pi_2^{\mu\nu}(q) = -(-ie)^2 \int \frac{d^4k}{(2\pi)^2} tr\left[\gamma^{\mu}\frac{i(\not{k}+m)}{k^2-m^2}\gamma^{\nu}\frac{i(\not{k}+\not{q}+m)}{(k+q)^2-m^2}\right]$$

$$= -4e^2 \int \frac{d^4k}{(2\pi)^2}\frac{k^{\mu}(k+q)^{\mu} + k^{\nu}(k+q)^{\mu} - g^{\mu\nu}(k.(k+q)-m^2)}{(k^2-m^2)\left((k+q)^2-m^2\right)} \tag{27}$$

After evaluating the above integral using Feynman trick we will actually find that the integral is divergent. To solve this problem, Dimensional Regulation[2]is applied, and we have the following result,

$$i\Pi_2^{\mu\nu}(q) = (q^2 g^{\mu\nu} - q^\mu q^\nu) i\Pi_2(q^2) \tag{28}$$

where

$$\Pi_2(q^2) = \frac{-8e^2}{(4\pi)^{d/2}} \int_0^1 dx x(1-x) \frac{\Gamma(2-\frac{d}{2})}{(m^2 - x(1-x)q^2)^{2-\frac{d}{2}}} \tag{29}$$

as $d \to 4$ we have

$$\Pi_2(q^2) = -\frac{2\alpha}{\pi} \int_0^1 dx x(1-x) \left(\frac{2}{\epsilon} - log\left(m^2 - x(1-x)q^2\right) - \gamma \right) \tag{30}$$

where $\gamma \sim 0.5772$ is the Euler-Mascheroni constant, and $\epsilon = (4-d)$.

We can now compute the shift in the electric charge,

$$e^2 - e_o^2 = \delta Z_3 = \Pi_2(0) \sim -\frac{2\alpha}{3\pi\epsilon} \tag{31}$$

We see that the bare charge is infinitely larger than the observed charge. But this difference is not observable. What can be observed is the q^2 dependence of the effective charge,

$$\widehat{\Pi}_2(q^2) = \Pi_2(q^2) - \Pi_2(0) = -\frac{2\alpha}{\pi} \int_0^1 dx x(1-x) log\left(\frac{m^2}{m^2 - x(1-x)q^2} \right) \tag{32}$$

Calculating the imaginary part of $\widehat{\Pi}_2$ for $q^2 > 4m^2$ we get,

$$\mathrm{Im}[\widehat{\Pi}_2] = \pm\frac{\alpha}{3}\sqrt{1 - \frac{4m^2}{q^2}} \left(1 + \frac{2m^2}{q^2}\right) \tag{33}$$

For the interaction between unlike charges, we have

$$V(x) = \int \frac{d^3q}{(2\pi)^3} e^{i\mathbf{q}\cdot\mathbf{x}} \frac{-e^2}{|\mathbf{q}|^2 \left[1 - \widehat{\Pi}_2(-|\mathbf{q}|^2)\right]} \tag{34}$$

For $|q^2| \ll m^2$, we can expand $\widehat{\Pi}$ and get,

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[2] The idea of dimensional regulation is simple: Compute the Feynman diagram as an analytic function of the dimensionality of space-time, d. For sufficiently small d, any loop-momentum integral will converge and therefore the Ward identity can be proved.The final expression for any observable quantity should have a well-defined limit as d → 4.

$$V(x) = -\frac{\alpha}{r} - \frac{4\alpha^2}{15m^2}\delta^{(3)}(\mathbf{x}) \tag{35}$$

Where the second term in equation (35) is the perturbation part due to vacuum polarization.

For hydrogen atom,

$$\triangle E = \int d^3x|\psi(\mathbf{x})|^2 \left(-\frac{4\alpha^2}{15m^2}\delta^{(3)}(\mathbf{x})\right) = -\frac{4\alpha^2}{15m^2}|\psi(0)|^2$$

The only nonzero wavefunctions at the origin are the s-wave states. For 2S state the energy shift is equal to $-1.123 * 10^{-7}$ eV.

There are also vacuum polarization effects due to virtual $\mu^+\mu^-$ pairs, $\pi^+\pi^-$ pairs, $\overline{p}p$ pairs, but these are much less important because $\Pi^{\mu\nu}(q^2)$ at small q^2 is inversely proportional to the square of the mass of the charged particle; for example, the vacuum polarization effect due to $\mu^+\mu^-$ pairs is $(205)^2$ times less than that due to e^+e^- pairs.

References

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