Lamb shift

Introduction

Suppose there is a one-electron state 0. An interation of electrons with the electromaelegnetic field mixes this state with a set of states N, in which the electron occupies some state n, and additionally there is a photon, which can be described by its momentum and polarization. As a result, in the second order of the perturbation theory there appears an energy shift of the level |0>. This shift, as well as physical reasons producing it, is called the Lab shift.

A potential initiating this effect can be written in terms of the velocity of the electron and the vector potential

$$V = -e\,\vec{v}\cdot\vec{A} \tag{1}$$

Here the vector potential describes a photon with the given momentum and polarization

$$\vec{A} = \sqrt{\frac{4\pi}{2\omega}}\,\vec{\epsilon}\,\mathrm{Exp}\left[i\left(\vec{k}\cdot\vec{r}-\omega t\right)\right], \tag{2}$$

$\vec{k}$, $\vec{\epsilon}$ are the momentum and polarization, $\omega = k$ is the photon frequency. The normalization

factor $\sqrt{2\pi/\omega}$ is justified below.

In the dipole approximation, which we will use below, the vector − potential simplifies

$$\vec{A} \simeq \sqrt{\frac{4\pi}{2\omega}}\,\vec{\epsilon}\,\mathrm{Exp}[-i\omega t] \tag{3}$$

The matrix element, which mixes the states 0 and N reads

$$V_{N,0} = -e\sqrt{\frac{4\pi}{2\omega}}\,\vec{v}_{n,0}\cdot\vec{\epsilon} \tag{4}$$

For the energy shift one finds

$$\delta E_0 = \sum_N \frac{|V_{N,0}|^2}{E_0 - E_N} \tag{5}$$

$$= 4\pi e^2 \sum_{k,\epsilon} \sum_n \frac{1}{2\omega} \frac{|\vec{v}_{n,0} \cdot \vec{e}|^2}{E_0 - E_n - \omega} = 4\pi e^2 \sum_{\epsilon=1,2} \int \frac{d^3k}{(2\pi)^3} \sum_n \frac{1}{2\omega} \frac{|\vec{v}_{n,0} \cdot \vec{e}|^2}{E_0 - E_n - \omega} \tag{5}$$

Here it is taken into account that the summation over the photon intemediate states results in the integral over the photon momentum and sumation over its polarixation.

Normalization of the vector potential

Preliminary remarks

Suppose one needs to fulfill summation over a set of a continuum states of some particle. One can take some large volume, call it V, and assume that it is greater than the volume in which physical events considered take place. Then instead of summation over the continuum states one fulfilles summation over quasi-continuum set of states, for which periodical boundary conditions in the volume V are valid. After that one rewrites the summation as the integral using the following formulae

$$\sum_n \psi_{\vec{p}_n}(\vec{r})\, \psi^*_{\vec{p}_n}(\vec{r}\,') \underset{V\to\infty}{\to} V \int \frac{d^3p}{(2\pi)^3} \psi^{(V)}_{\vec{p}}(\vec{r})\, \psi^{(V)*}_{\vec{p}}(\vec{r}\,') \tag{6}$$

Here the superscript (V) indicates that the wave functions on the right-hand side are normalized in the volume V. Instead of this normalization it is convenient to introduce normalization for unit volume, in which the following obvious identity holds

$$\psi^{(V)}_{\vec{p}}(\vec{r}) = \frac{1}{\sqrt{V}} \psi^{(V=1)}_{\vec{p}}(\vec{r}) \tag{7}$$

Then the necessary summation reads

$$\sum_n \psi_{\vec{p}_n}(\vec{r})\,\psi^*_{\vec{p}_n}(\vec{r}\,') = \int \frac{d^3p}{(2\pi)^3}\,\psi_{\vec{p}}(\vec{r})\,\psi^*_{\vec{p}}(\vec{r}\,') \tag{8}$$

where the superscript (V=1) is suppressed.
Thus, to fulfil summation over the continuum set of states one can integrate over the momentum $d^3p/(2\pi)^3$, normalizing wave functions as "one particle per unit volume".

Photons

$$\langle 0 \,|\, \vec{A}^*_{\vec{k}}\,\vec{A}_{\vec{k}} \,|\, 0\rangle = \sum_m \langle 0 \,|\, \vec{A}^*_{\vec{k}} \,|\, m\rangle \langle m \,|\, \vec{A}_{\vec{k}} \,|\, 0\rangle = \langle 0 \,|\, \vec{A}^*_{\vec{k}} \,|\, 1\rangle \langle 1 \,|\, \vec{A}_{\vec{k}} \,|\, 0\rangle = |\langle 1 \,|\, \vec{A}_{\vec{k}} \,|\, 0\rangle|^2 \tag{9}$$

A photon represents a harmonic oscillator. Therefore the avaraged kinetic and potential energies equal half of the total energy. In the vacuum this total energy is half of the frequency. In this case

$$\bar{T} = \bar{U} = \frac{1}{2}\,E = \frac{1}{4}\,\omega \tag{10}$$

The kinetic energy of the oscillator can be written of from the energy of the electromagnetic field in a unit volume, which reads

$$\frac{d\varepsilon}{dV} = \frac{|\vec{E}_{\vec{k}}|^2 + |\vec{H}_{\vec{k}}|^2}{8\pi} \tag{11}$$

Here the energy is calculated "per unit volume", precisely as is necessary for the purposes of integration over the continuum states of the photon, see above. Since

$$\vec{E}_{\vec{k}} = -\frac{\partial}{\partial t}\,\vec{A}_{\vec{k}} \tag{12}$$

the first term in the energy represents the kinetic energy

$$T = |\vec{E}_{\vec{k}}|^2 = \omega^2\,\vec{A}^*_{\vec{k}}\,\vec{A}_{\vec{k}} \tag{13}$$

$$\bar{T} = \langle 0 \,|\, T \,|\, 0\rangle = \frac{\omega^2}{8\pi}\,\langle 0 \,|\, \vec{A}^*_{\vec{k}}\,\vec{A}_{\vec{k}} \,|\, 0\rangle \tag{13}$$

Combining this with the previous disscussion one finds

$$\bar{T} = \frac{\omega^2}{8\pi} \left| \langle 1 | \vec{A}_{\vec{k}} | 0 \rangle \right|^2 = \frac{1}{4}\omega \tag{14}$$

Thus considering creation (or annialation) of one photn one should have

$$\langle 1 | \vec{A}_{\vec{k}} | 0 \rangle = \sqrt{\frac{4\pi}{2\omega}} \tag{15}$$

Energy sfift

$$\delta E_0 = 4\pi e^2 \sum_{e=1,2} \int \frac{d^3k}{(2\pi)^3} \sum_n \frac{1}{2\omega} \frac{\left| \vec{v}_{n,0} \cdot \vec{e} \right|^2}{E_0 - E_n - \omega} = 4\pi e^2 \sum_n \int_0^\infty \frac{\omega^2 d\omega}{(2\pi)^3} \frac{1}{2\omega} \frac{1}{E_0 - E_n - \omega} \int \sum_{e=1,2} \left| \vec{v}_{n,0} \cdot \vec{e} \right|^2 d\Omega \tag{16}$$

Here dΩ represents integration over the spherical angle of the photon momentum

$$\int \sum_{i=1,2} \left| \vec{v}_{n,0} \cdot \vec{e}_i \right|^2 d\Omega = \int \left(\left| \vec{v}_{n,0} \right|^2 - \left| \vec{v}_{n,0} \cdot \vec{n} \right|^2 \right) d\Omega = \left| \vec{v}_{n,0} \right|^2 \int_{4\pi} (1 - \mathrm{Cos}[\theta]^2)\, d\Omega =$$
$$\left| \vec{v}_{n,0} \right|^2 2\pi \int_0^\pi (1 - \mathrm{Cos}[\theta]^2)\, \mathrm{Sin}[\theta]\, d\theta = \frac{2}{3} 4\pi \left| \vec{v}_{n,0} \right|^2, \tag{17}$$
$$\vec{n} = \frac{\vec{k}}{k}.$$

Thus, summation over the polarization and integration over the angles for a dipole transition gives a factor 2/3

$$\delta E_0 = \frac{4\pi e^2}{(2\pi)^3} \frac{1}{2} \frac{2}{3} 4\pi \sum_n \left| \vec{v}_{n,0} \right|^2 \int_0^\infty d\omega\, \omega^2 \frac{1}{\omega} \frac{1}{E_0 - E_n - \omega} \tag{18}$$

$$= \frac{2}{3\pi} e^2 \sum_n \left| \vec{v}_{n,0} \right|^2 \int_0^\infty d\omega \frac{\omega}{E_0 - E_n - \omega} \tag{18}$$

Renormalization

Repeating the argument for the vacuum one can write

$$(\delta E_0)_{vac} = \frac{2 e^2}{3\pi} \sum_n \left| \vec{v}_{n,0} \right|^2 \int_0^\infty d\omega \frac{\omega}{-\omega} \tag{19}$$

since in the vacuum the operator of velocity does not have nondiagonal matrix elements. For the energy difference one finds

$$(\delta E_0)_{ren} = \delta E_0 - (\delta E_0)_{vac} = \\ = \frac{2 e^2}{3\pi} \sum_n \left| \vec{v}_{n,0} \right|^2 \int_0^\infty d\omega \left(\frac{\omega}{E_0 - E_n - \omega} + 1 \right) = \frac{2 e^2}{3\pi} \sum_n \left| \vec{v}_{n,0} \right|^2 \int_0^\infty d\omega \frac{E_0 - E_n}{E_0 - E_n - \omega} \tag{20}$$

In the following discussion the subscript ren (for renormalized) is suppressed.
The physical picture considered can be only correct in the nonrelativistic approximation. Therefore the integration over ω should run only up to m (not to infinity, where different formulas need to be worked out).

$$\delta E_0 \Rightarrow \frac{2 e^2}{3\pi} \sum_n \left| \vec{v}_{n,0} \right|^2 \int_0^m d\omega \frac{E_0 - E_n}{E_0 - E_n - \omega} = -\frac{2 e^2}{3\pi} \sum_n (E_0 - E_n) \left| \vec{v}_{n,0} \right|^2 \operatorname{Log}\left[\frac{m}{E_0 - E_n} \right] \tag{21}$$

$$\vec{v}_{n,0} = \frac{1}{m} \vec{p}_{n,0} \equiv \frac{1}{m} \langle n | \vec{p} | 0 \rangle = \frac{i}{m} \langle n | i [H \vec{r}] | 0 \rangle = i \frac{E_0 - E_n}{m} \langle n | \vec{r} | 0 \rangle \equiv \frac{E_0 - E_n}{m} \vec{r}_{n,0} \tag{22}$$

$$\delta E_0 = -\frac{2 e^2}{3\pi} \sum_n (E_0 - E_n)^3 \left| \vec{r}_{n,0} \right|^2 \operatorname{Log}\left[\frac{m}{E_0 - E_n} \right] = \frac{2 e^2}{3\pi} \sum_n (E_n - E_0)^3 \left| \vec{r}_{n,0} \right|^2 \operatorname{Log}\left[\frac{m}{E_0 - E_n} \right] \tag{23}$$

This expression has a real and imaginary parts. The latter will be discussed when radiative widths are considered. For the real part, which is represents a proper energy, one finds

$$\mathrm{Re}[\delta E_0] = \frac{2e^2}{3\pi} \sum_n (E_n - E_0)^3 \left|\vec{r}_{n,0}\right|^2 \mathrm{Log}\left[\frac{m}{|E_n - E_0|}\right] \tag{24}$$

In absolute units

$$\mathrm{Re}[\delta E_0] = \frac{2}{3\pi c^3} \sum_n \omega_{n,0}^3 \left|\vec{d}_{n,0}\right|^2 \mathrm{Log}\left[\frac{m c^2}{|E_n - E_0|}\right] \tag{25}$$

where

$$\omega_{n,0} = \frac{E_n - E_0}{\hbar} \tag{26}$$

Large Log approximation

For atoms

$$E_n - E_0 \sim Z^2\, \mathrm{Ry} \tag{27}$$

$$\mathrm{Log}\left[\frac{m c^2}{|E_n - E_0|}\right] \simeq \mathrm{Log}\left[\frac{1}{(Z\alpha)^2}\right] \gg 1 \tag{28}$$

assuming that (Zα)•1.

$$\mathrm{Re}[\delta E_0] \simeq \frac{2e^2}{3\pi} \mathrm{Log}\left[\frac{1}{(Z\alpha)^2}\right] \sum_n (E_n - E_0)^3 \left|\vec{r}_{n,0}\right|^2 \tag{29}$$

Effective potential ~ $(e^2/m)\,\Delta U$

$$\mathrm{Re}[\delta E_0] = \frac{2e^2}{3\pi} \mathrm{Log}\left[\frac{1}{(Z\alpha)^2}\right] \sum_n (E_n - E_0)^3 \left|\vec{r}_{n,0}\right|^2 = \frac{2e^2}{3\pi} \mathrm{Log}\left[\frac{1}{(Z\alpha)^2}\right] \sum_n (E_n - E_0) \langle 0|\vec{v}|n\rangle \langle n|\vec{v}|0\rangle = \frac{2e^2}{3\pi m^2} \mathrm{Log}\left[\frac{1}{(Z\alpha)^2}\right] \sum_n (E_n - E_0) \langle 0|\vec{p}|n\rangle \langle n|\vec{p}|0\rangle \tag{30}$$

$$\frac{2e^2}{3\pi}\,\mathrm{Log}\left[\frac{1}{(Z\alpha)^2}\right]\times\frac{1}{2}\sum_n\left(\langle 0|\vec{p}|n\rangle\langle n|[H,\ \vec{p}]|0\rangle-\langle 0|[H,\ \vec{p}]|n\rangle\langle n|\vec{p}|0\rangle\right)=$$

$$\mathrm{Re}[\delta E_0]=\frac{e^2}{3\pi m^2}\,\mathrm{Log}\left[\frac{1}{(Z\alpha)^2}\right]S_0 \qquad (30)$$

$$S_0=\sum_n\left(\langle 0|\vec{p}|n\rangle\langle n|[H,\ \vec{p}]|0\rangle-\langle 0|[H,\ \vec{p}]|n\rangle\langle n|\vec{p}|0\rangle\right) \qquad (31)$$

$$\sum_n |n><n|=1$$

$$S_0=\langle 0|\vec{p}[H,\ \vec{p}]-[H,\ \vec{p}]\vec{p}|0\rangle=\langle 0|[\vec{p},\ [H,\ \vec{p}]]|0\rangle \qquad (32)$$

$$H=\frac{\vec{p}^{\,2}}{2m}+U(r) \qquad (33)$$

$$[H,\ \vec{p}]=i\vec{\nabla}U \qquad (34)$$

$$[\vec{p},\ [H,\ \vec{p}]]=i[\vec{p},\ \vec{\nabla}U]=\vec{\nabla}\cdot\vec{\nabla}U=\Delta U \qquad (34)$$

$$S_0=\Delta U \qquad (35)$$

$$\mathrm{Re}[\delta E_0]=\frac{e^2}{3\pi m^2}\,\mathrm{Log}\left[\frac{1}{(Z\alpha)^2}\right]\langle 0|\Delta U|0\rangle \qquad (36)$$

$$\delta U_{eff}(r)=\frac{1}{3\pi}\,\mathrm{Log}\left[\frac{1}{(Z\alpha)^2}\right]\frac{e^2}{m^2}\Delta U(r) \qquad (37)$$

$$U=-\frac{Ze^2}{r} \qquad (38)$$

$$\Delta\frac{1}{r}=-4\pi\delta(\vec{r}) \qquad (39)$$

$$\Delta U = 4\pi Z e^2 \delta(\vec{r}) \tag{40}$$

$$\delta E_0 = \frac{4 Z e^4}{3 m^2} \mathrm{Log}\left[\frac{1}{(Z\alpha)^2}\right] \varphi_0^2(0) \tag{41}$$

In the log approximation only the s-states exibit the Lamb shift. Other states are also influenced by the Lamb correction, but is does not have the large log factor.

$$\varphi_{ns_{1/2}}(0) = \sqrt{\frac{Z^3}{\pi a_0^3}} = \sqrt{\frac{Z^3 \alpha^3 m^3}{\pi}} \tag{42}$$

$$\delta E_{ns_{1/2}} \simeq \frac{4 Z e^4}{3 m^2} \frac{Z^3 \alpha^3 m^3}{\pi} \mathrm{Log}\left[\frac{1}{(Z\alpha)^2}\right] = \frac{4 Z^4 \alpha^5 m}{3\pi} \mathrm{Log}\left[\frac{1}{(Z\alpha)^2}\right] \tag{43}$$

$$\delta E_{np_{1/2}} \simeq \delta E_{np_{3/2}} \simeq 0 \tag{43}$$

Accurate relativistic calculations give

$$\delta E_{ns_{1/2}} = \frac{4 Z^4 \alpha^5 m c^2}{3\pi} \left(\mathrm{Log}\left[\frac{1}{(Z\alpha)^2}\right] + \frac{19}{30} + L_n\right) \tag{44}$$

n	1	2	3	∞
L_n	-2.984	-2.812	-2.768	-2.721

(44)

$$E_0 \sim Z^2 \alpha^2 m$$

$$\frac{\delta E_0}{E_0} \sim Z^2 \alpha^3 \mathrm{Log}\left[\frac{1}{(Z\alpha)^2}\right] \tag{45}$$

In Hydrogen (46)

$$\delta E_{2s_{1/2}} - E_{2p_{1/2}} \simeq 1050\ \mathrm{MHz} \tag{46}$$

Radiative decay of excited levels

For a quasistationary state 0 the energy has its real and imaginary parts

$$E_0 = \mathrm{Re}[E_0] - i\,\frac{\Gamma}{2} \tag{47}$$

Γ is called the width

$$\psi \sim \mathrm{Exp}[-i\,E\,t] = \mathrm{Exp}\left[-i\,\mathrm{Re}[E_0]\,t - \frac{\Gamma}{2}\,t\right],\quad \mathrm{Probability} \sim |\psi|^2 \sim \mathrm{Exp}[-i\,\Gamma\,t] \tag{48}$$

This means that probability of the decay *W* (of the excited state) per second equals the width

$$W = \Gamma \equiv \frac{\Gamma}{\hbar} \tag{49}$$

From the expression for the Lamb shift (see the Lamb shift)

$$\delta E_0 = \frac{2\,e^2}{3\,\pi} \sum_n (E_n - E_0)^3 \left|\vec{r}_{n,0}\right|^2 \mathrm{Log}\left[\frac{m}{E_0 - E_n}\right] \tag{50}$$

one finds

$$\mathrm{Im}[\delta E_0] = \frac{2\,e^2}{3\,\pi} \sum_n (E_n - E_0)^3 \left|\vec{r}_{n,0}\right|^2 \mathrm{Im}\left[\mathrm{Log}\left[\frac{m}{E_0 - E_n}\right]\right] = -\frac{2\,e^2}{3} \sum_{E_n<E_0} (E_0 - E_n)^3 \left|\vec{r}_{n,0}\right|^2 = -\frac{2}{3} \sum_{E_n<E_0} \omega_{0\,n}^3 \left|\vec{d}_{n,0}\right|^2 \tag{51}$$

This means that the radiative width of the state 0 equals

$$\frac{\Gamma}{2} = \frac{2}{3} \sum_{E_n<E_0} \omega_{0\,n}^3 \left|\vec{d}_{n,0}\right|^2 \tag{52}$$

Correspondingly, the probability of the radiative decay of the state 0 is

$$W = \sum_{E_n<E_0} W_{0\to n} = \frac{4}{3} \sum_{E_n<E_0} \omega_{0\,n}^3 \left| \vec{d}_{n,0} \right|^2 \tag{53}$$

Here

$$W_{0\to n} = \frac{4}{3}\, \omega_{0\,n}^3 \left| \vec{d}_{n,0} \right|^2 \equiv \frac{4\, \omega_{0\,n}^3}{3\, \hbar\, c^3} \left| \vec{d}_{n,0} \right|^2 \tag{54}$$

is the probability of the decay into some given state n, while W is the total probability of the radiative decay,

$$\vec{d}_{n,0} = e\, \vec{r}_{n,0} = e \int \psi_n^* (\vec{r})\, \vec{r}\, \psi_0 (\vec{r})\, d^3 r \equiv e \left\langle \psi_n^* \middle| \vec{r} \middle| \psi_0 \right\rangle \tag{55}$$

is the dipole matrix element and

$$\omega_{0\,n} = E_0 - E_n \equiv \frac{E_0 - E_n}{\hbar} \tag{56}$$

is the frequency of the transition. It is instructive to compare $W_{0\to n}$ with the classical expression. In the classical approximation the energy rate radiated by a dipole $\vec{d}$, which oscillates with the frequency ω is

$$P = \frac{4\, \omega^4}{3\, c^3} \left| \vec{d} \right|^2 \tag{57}$$

It follows from here that the probability of radiation of one quantum is

$$W = \frac{P}{\hbar\, \omega} = \frac{4\, \omega^3}{3\, \hbar\, c^3} \left| \vec{d} \right|^2 \tag{58}$$

Compare this calssical expression with the quantum one

$$W_{0\to n} = \frac{4\, \omega_{0\,n}^3}{3\, \hbar\, c^3} \left| \vec{d}_{n,0} \right|^2 \tag{59}$$

They mathch nicely.