Thus

(257) $$\boxed{\Delta W_{ba} = \frac{\omega_{ab}^3}{3\pi}\,|\vec{d}_{ab}|^2}$$

Einstein A coefficient of spontaneous emission

where

(258) $$\vec{d}_{ab} = e\,\langle b|\hat{\vec{r}}\,|a\rangle$$

is the transition dipole matrix element

III.4 Lamb shift according to Bethe

With the help of microwave and Laser spectroscopy W.E. Lamb and W.E. Retherford found in 1947 that there is an energy splitting between the $2S_{1/2}$ and $2P_{1/2}$ state of Hydrogen despite the fact that these states are precisely degenerate in relativistic quantum mechanics (Dirac theory). This splitting is called Lamb shift and is a direct consequence of the quantization of the elm.

field. (Lamb & Retherford Phys. Rev. 72 241 (1947)) The following calculation is due to Hans Bethe (H. A. Bethe Phys. Rev. 72, 339 (1947)) which allegedly was done on a train ride.

starting point: non-relativistic interaction operator

(259) $$\hat{H}_I = \int d^3r \; \hat{\psi}^+(\vec{r}) \left[-\frac{e}{m} \hat{\vec{p}} \cdot \hat{\vec{A}} + \frac{e^2 \hat{\vec{A}}^2}{2m} \right] \hat{\psi}(\vec{r})$$

- calculate energy shift in 2nd order perturbation

(260) $$|\alpha\rangle = |a, 0\rangle \qquad E_\alpha^{(0)} = E_a^{(0)}$$

atom photon

(261) $$\Delta E_\alpha = \langle \alpha | \hat{H}_I | \alpha \rangle + \sum_{\beta \neq \alpha} \frac{\langle \alpha | \hat{H}_I | \beta \rangle \langle \beta | \hat{H}_I | \alpha \rangle}{E_\alpha^{(0)} - E_\beta^{(0)}}$$

the $\hat{\vec{A}}^2$ term yields a constant (and divergent) energy shift, which is however the same for all atomic states and thus will be ignored. This amounts to

$$\hat{\vec{A}}^2 \longrightarrow :\hat{\vec{A}}^2:$$

$$\Rightarrow \quad \langle\alpha|\hat{H}_I|\alpha\rangle = 0$$

def.: $\quad :\hat{\phi}_1\hat{\phi}_2: \equiv \hat{\phi}_1\hat{\phi}_2 - \langle 0|\hat{\phi}_1\hat{\phi}_2|0\rangle$

(262) normal ordering

example: boson field

$$:\hat{a}\hat{a}^\dagger: = \hat{a}\hat{a}^\dagger - \langle 0|\hat{a}\hat{a}^\dagger|0\rangle$$

$$= \hat{a}^\dagger\hat{a} + 1 - 1 = \hat{a}^\dagger\hat{a}$$

In the following we ignore the $:\hat{\vec{A}}^2:$ term.

$$|\beta\rangle = |b\rangle\,|1(\vec{k},\lambda)\rangle$$

all possible atomic states — single photon state in mode $\vec{k},\lambda$

(263) $E_\beta^{(0)} = E_b^{(0)} + \omega_{\vec{k}}$

You will show in the problem course that

$$\langle\beta|\hat{H}_I|\alpha\rangle = \frac{1}{\sqrt{L^3}}\, e^{i(E_\beta - E_\alpha)t}\, f_{\beta\alpha}$$

(270)

$$f_{\beta\alpha} = \frac{e}{m}\frac{1}{\sqrt{2\omega_{\vec{k}}}}\,\vec{e}^{\,*}_{\vec{k}\lambda}\cdot\underbrace{\langle b|\hat{\vec{p}}|a\rangle}_{\equiv\vec{p}_{ba}}$$

$\Rightarrow$ energy shift

(271) $$\Delta E_a = \sum_b \sum_{\vec{k},\lambda} \frac{1}{L^3} \frac{|f_{\beta\alpha}|^2}{E_a^{(0)} - E_b^{(0)} - \omega_{\vec{k}}}$$

Note that the sum also contains $b = a$.

$L \to \infty$ (notation: $E_a^{(0)} = E_a \quad E_b^{(0)} = E_b$)

$$\Delta E_a = \sum_{b,\lambda} \int \frac{d^3k}{2\omega_k (2\pi)^3} \frac{e^2}{m^2} \frac{|\vec{e}^{\,*}_{k\lambda} \cdot \vec{p}_{ba}|^2}{E_a - E_b - \omega_{\vec{k}}}$$

$$= \frac{1}{2\pi} \sum_b \int_0^\infty \frac{d\omega}{E_a - E_b - \omega} \underbrace{\left[\frac{e^2}{4\pi} \frac{\omega}{2\pi m^2} \sum_\lambda \int d\Omega_{\vec{k}} \, |\vec{e}^{\,*}_{k\lambda} \cdot \vec{p}_{ba}|^2 \right]}_{\equiv \Delta \tilde{W}_{ba}(\omega)}$$

divergent

$\curvearrowright \omega \to \omega - i\varepsilon$

It holds:

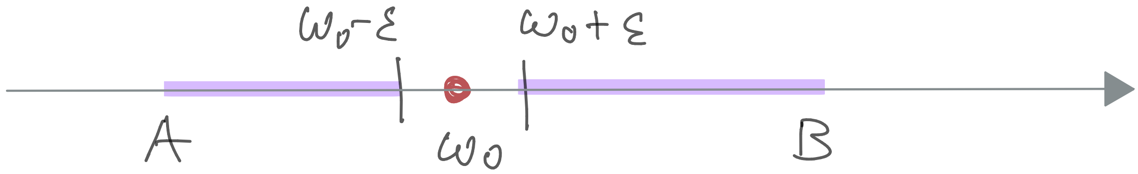
(272) $$\frac{1}{E_a - E_b - \omega + i\varepsilon} = P \frac{1}{E_a - E_b - \omega} - i\pi \delta(E_a - E_b - \omega)$$

principle part

principle part:

$$\int_A^B d\omega \, P \frac{1}{\omega_0-\omega} \equiv \lim_{\varepsilon\to 0}\left[\int_A^{\omega_0-\varepsilon} d\omega \frac{1}{\omega_0-\omega} + \int_{\omega_0+\varepsilon}^{B} d\omega \frac{1}{\omega_0-\omega}\right]$$

(273)



With this we find: $\omega_{ab} \equiv E_a - E_b$

$$\Delta E_a = \frac{1}{2\pi}\sum_b P\int_0^\infty d\omega \frac{\Delta\tilde{W}_{ba}(\omega)}{E_a-E_b-\omega} - \frac{i}{2}\sum_{\substack{b\\E_a>E_b}} \Delta\tilde{W}_{ba}(\omega_{ab})$$

(274)

remarks

- the second imaginary term corresponds to spontaneous emission and will be ignored here
- the first term is divergent ! ☹

Lets first calculate $\Delta\tilde{W}_{ba}(\omega)$!

$$\Delta\tilde{W}_{ba}(\omega) = \frac{e^2}{4\pi}\frac{\omega}{2\pi m^2}\sum_\lambda \int d\Omega_{\vec{k}} \left|\vec{e}^{\,*}_{\vec{k}\lambda}\cdot\vec{P}_{ba}\right|^2$$

Without loss of generality $\vec{p}_{ba} = p_{ba} \vec{e}_z$

$$\vec{e}^{\,*}_{b\lambda} \cdot \vec{p}_{ba} = p_{ba} \cos\vartheta_{\vec{k}}$$ for linear polarization

$$\sum_\lambda \int d\Omega_{\vec{k}} \, |\vec{e}^{\,*}_{k\lambda} \cdot \vec{p}_{ba}|^2 = 2 \cdot 2\pi \int_0^\pi d\vartheta_k \sin\vartheta_k \cos^2\vartheta_k \cdot p_{ba}^2$$

$$= 4\pi \int_{-1}^{1} d\xi \, \xi^2 \, p_{ba}^2 = \underline{\underline{\frac{8\pi}{3} p_{ba}^2}}$$

$$\Rightarrow \quad \Delta\tilde{W}_{ba}(\omega) = \frac{e^2}{4\pi} \frac{4\omega}{3m^2} |\vec{p}_{ba}|^2 \tag{275}$$

$$\boxed{\Delta E_a = \frac{e^2}{4\pi} \frac{2}{3\pi} \frac{1}{m^2} \sum_b P \int_0^\infty d\omega \underbrace{\frac{\omega}{E_a - E_b - \omega}}_{\text{UV divergent!}} |\vec{p}_{ba}|^2} \tag{276}$$

Divergencies of this type a common feature in QFTh. To remove it or at least to make it less severe we use an idea of Kramers:

Mass renormalization

Kramers noted that also the unbounded electron interacts with the quantized elm. field in the vacuum state. Thus the only observable quantity is the energy difference between the shift of the bound and the unbound electron with the same average kinetic energy as in state $|a\rangle$:

$$\Delta E_a^{free} = \frac{e^2}{4\pi} \frac{2}{3\pi} \frac{1}{m^2} \sum_b P \int_0^\infty d\omega \frac{\omega \left|\vec{P}_{ba}^{free}\right|^2}{\frac{P_a^2}{2m} - \frac{P_b^2}{2m} - \omega} \tag{277}$$

Here $$\vec{P}_{ba}^{free} = \int d^3r \frac{1}{L^3} e^{-i\underbrace{(\vec{P}_b + \vec{b})}_{\text{final state momentum should include photon}}\vec{r}} (-i\vec{\nabla}) e^{i\vec{P}_a\vec{r}}$$

$$= \vec{P}_a \underbrace{\delta(\vec{P}_a - \vec{P}_b - \vec{b})}_{\text{momentum conservation}}$$

Thus

$$\frac{P_a^2}{2m} - \frac{P_b^2}{2m} - \omega = \frac{P_a^2}{2m} + \frac{(\vec{P}_a - \vec{b})^2}{2m} - \omega$$

$$= \frac{\vec{P}_a \cdot \vec{b}}{m} - \omega\left(1 + \frac{\omega}{2m}\right) \underset{\text{for non-relativistic particle}}{\approx} -\omega\left(1 + \frac{\omega}{2m}\right)$$

$$\Rightarrow \Delta E_a^{free} \simeq -\frac{e^2}{4\pi}\frac{2}{3\pi}\frac{1}{m^2} P\int_0^\infty d\omega \frac{1}{1+\frac{\omega}{2m}} \sum_b |\vec{p}_{ba}|^2$$

Using $\sum_b |\vec{p}_{ba}|^2 = \sum_b \langle a|\hat{\vec{p}}|b\rangle\langle b|\hat{\vec{p}}|a\rangle$

$$= \sum_b \langle a|\hat{\vec{p}}^2|a\rangle$$

$$\Delta E_a^{free} = -\frac{C}{2}\langle a|\hat{\vec{p}}^2|a\rangle \tag{278}$$

can thus be interpreted as a renormalization of the electron mass

$$\frac{\langle\hat{\vec{p}}^2\rangle}{2m^*} = \frac{\langle\hat{\vec{p}}^2\rangle}{2m} - \frac{C}{2}\langle\hat{\vec{p}}^2\rangle \tag{279}$$

$$\boxed{\frac{1}{m^*} = \frac{1}{m} - C}$$

Since the coupling to the elm. field cannot be switched off only m^* is physically observable. The "bare" mass m is not!

We thus find for the observable energy shift

$$\Delta E_a^{obs} = \Delta E_a - \Delta E_a^{free}$$

$$\Delta E_a^{obs} = \frac{e^2}{4\pi}\frac{2}{3\pi}\frac{1}{m^2} P\int_0^\infty d\omega \sum_b \left[\frac{\omega |\vec{p}_{ab}|^2}{-E_a - E_b - \omega} + \frac{|\vec{p}_{ab}|^2}{1+\frac{\omega}{2m}}\right]$$

This expression is still uv-divergent but if we introduce a uv-cutoff

(281) $$\omega_{max} = E_{max} \ll m$$

$$\boxed{\Delta E_a^{obs} = \frac{e^2}{4\pi}\frac{2}{3\pi}\frac{1}{m^2} P\int_0^{\omega_{max}} d\omega \sum_b \frac{(E_a - E_b)|\vec{p}_{ab}|^2}{E_a - E_b - \omega}}$$

(282)

we find only a logarithmic divergency with ω_{max}!

$\boxed{\omega_0 > 0}$

$$P\int_0^{\omega_{max}} d\omega \frac{1}{\omega_0 - \omega} = \int_0^{\omega_0 - \varepsilon} d\omega \frac{1}{\omega_0 - \omega} + \int_{\omega_0+\varepsilon}^{\omega_{max}} d\omega \frac{1}{\omega_0 - \omega}$$

$$= -\ln(\omega_0 - \omega)\Big|_0^{\omega_0 - \varepsilon} - \ln(\omega_0 - \omega)\Big|_{\omega_0+\varepsilon}^{\omega_{max}}$$

$$= -\ln\frac{\varepsilon}{\omega_0} - \ln\frac{\omega_{max} - \omega_0}{\varepsilon} \underset{(\omega_{max} \gg \omega_0)}{\simeq} -\ln\frac{\omega_{max}}{\omega_0}$$

$\boxed{\omega_0 < 0}$

$$P\int_0^{\omega_{max}} d\omega \frac{1}{\omega_0 - \omega} = -\ln\frac{\omega_{max}}{|\omega_0|}$$

$$\Delta E_a^{obs} \simeq -\frac{e^2}{4\pi}\frac{2}{3\pi}\frac{1}{m^2}\sum_b (E_a-E_b)\ln\left(\frac{E_{max}}{|E_a-E_b|}\right)|\vec{p}_{ba}|^2$$

Since the logarithm has a large argument and thus only slowly changes with E_b it can be taken out of the sum

$$\Delta E_a^{obs} \simeq -\frac{e^2}{4\pi}\frac{2}{3\pi}\frac{1}{m^2}\ln\frac{E_{max}}{\langle |E_a-E_b|\rangle}\underbrace{\sum_b (E_a-E_b)|\vec{p}_{ba}|^2}_{\text{this can be calculated explicitely!}} \tag{283}$$

$$\sum_b (E_a-E_b)|\vec{p}_{ba}|^2 = \sum_b \langle a|\hat{H}_{atom}\hat{p}^j - \hat{p}^j\hat{H}_{atom}|b\rangle \cdot \langle b|\hat{p}^j|a\rangle$$

$$= \frac{1}{2}\langle a|\left[[\hat{H}_{at},\hat{p}^j],\hat{p}^j\right]|a\rangle \tag{284}$$

Consider Coulomb-like potential $V(\vec{r}) = -\dfrac{Ze^2}{4\pi r}$

$$\left[[\hat{H}_{at},\hat{p}^j],\hat{p}^j\right] = \left[i\frac{\partial}{\partial x_j}V, -i\frac{\partial}{\partial x_j}\right] = -\vec{\nabla}^2 V$$
$$= -Ze^2\delta^{(3)}(\vec{r}) \tag{285}$$

This gives with

$$\alpha = \frac{e^2}{4\pi} \simeq \frac{1}{137} \quad \text{fine structure constant}$$

$$\boxed{\Delta E_a^{obs} = Z\alpha^2\left(\frac{4}{3m^2}\right)\left|\phi_a(\vec{r}=0)\right|^2 \ln\frac{E_{max}}{\langle|E_a-E_b|\rangle}}$$

(286)

Lamb shift a'la Bethe

remarks:

- $\Delta E_a \neq 0$ only for states with $\phi_a(\vec{r}=0)\neq 0$
  $\longrightarrow$ S-states
  (for p-states higher order contributions needed, which are however much smaller)
- $E_{max} > \langle|E_a-E_b|\rangle \Rightarrow \Delta E_a^{obs} > 0$
- $\langle|E_a-E_b|\rangle$ difficult to calculate
  $\langle|E_{2s}-E_b|\rangle \simeq 226.3\,eV$, $E_{max} \overset{!}{=} m$
  $$\ln\frac{m}{\langle|E_{2s}-E_b|\rangle} \simeq 7.72$$
- Hydrogen $Z=1$ $\quad |\phi_{2s}(0)|^2 = \frac{1}{\pi}\frac{1}{(2a_0)^3}$

$$\Delta E_{S_{1/2}-P_{1/2}} \simeq m\alpha^5\,\frac{7.72}{6\pi} \simeq 1051\ \text{MHz}$$

Exp: 1057845(9) kHz (1986)

Theory: 1057857(14) kHz (1984)

QED extremely successful!