Lecture 17 — 11/6

Announce:

Next week (11/13 + 15), I'll be gone ⇒

11/13, class will be at 9 o'clock (instead of 3)

11/15: class will be taught by Abigail

Program:

- spontaneous emission etc
- Selection rules etc.

d) Bound-to-continuum transitions

(Bound-to-bound in ch 2)

Assume rotating frame, RWA

$$H = \hbar \sum_k \underbrace{(\omega_k - \nu)}_{-\delta_k} |k\rangle\langle k| - \hbar \sum_k \left(\frac{\Omega_k}{2} |k\rangle\langle 0| + |0\rangle\langle k| \frac{\Omega_k^*}{2} \right)$$

$|k\rangle$: continuum states

$|0\rangle$: bound state

$$\dot{c}_0 = i \sum_k \frac{\Omega_k^*}{2} c_k$$
$$\dot{c}_k = i\delta_k c_k + i \frac{\Omega_k}{2} c_0$$
$$+ \ c_0(0) = 1$$

Why do we go back to the Schr. Eq. formalism instead of density mx? Here, the modes of the q. vacuum are considered part of the system (rather than 'environment').

$$\boxed{\dot{c}_0 = - \sum_k \left| \frac{\Omega_k}{2} \right|^2 \int_0^t dt' c_0(t') e^{-i\delta_k (t'-t)}}$$

strongest contribution from $t' \approx t$

$\Rightarrow c_0(t') \approx c_0(t)$

$$\lim_{\epsilon \to 0+} \int_0^t dt' e^{-i(\delta_k + i\epsilon)(t'-t)} = \lim_{\epsilon \to 0+} i \frac{1 - e^{(i\delta_k - \epsilon)t}}{\delta_k + i\epsilon}$$

$$\xrightarrow{t \to \infty} \lim_{\epsilon \to 0+} \frac{i}{\delta_k + i\epsilon} = \pi \delta(\delta_k) + i \mathcal{P} \frac{1}{\delta_k}$$

$$\Rightarrow \dot{c}_0 = - c_0 \left(\frac{\gamma}{2} - i\Delta \right)$$

$$\Rightarrow \boxed{c_0(t) = e^{-\frac{\gamma}{2}t} e^{i\Delta t}}$$

$$\gamma = 2\pi \sum_k \left| \frac{\Omega_k}{2} \right|^2 \delta(\nu - ck)$$

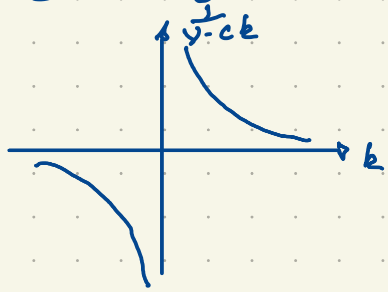
$$\Delta = \sum_k \left| \frac{\Omega_k}{2} \right|^2 \mathcal{P} \frac{1}{\nu - ck}$$

γ: "decay" (into continuum)

non-zero only above ionization threshold

Δ: shift : - present below the ionization threshold

- mostly cancels above —"—



$\Rightarrow$ shift always present for bound-to-bound transitions, especially if excited state close to ionization threshold.

Wigner-Weisskopf:

e) Spontaneous emission: (same thing other way round...)

start in (excited) state: $|e,0\rangle$ (excited of atom, no photon)

end in (g.s) $|g,1_k\rangle$ (g.s + one photon in mode k)

"continuum"

Hamiltonian of TLS + all modes of vacuum field:

$$H = \hbar\omega |e\rangle\langle e| + \sum_k \hbar c k \left(a_k^\dagger a_k + \tfrac{1}{2}\right) - \hbar \sum_k \left(g_k |e\rangle\langle g| a_k + g_k^* |g\rangle\langle e| a_k^\dagger \right)$$

relevant state space : $|\xi\rangle = |e,0\rangle + \sum_k |g,1_k\rangle$

$$H_{eff} = |\xi\rangle\langle\xi| \, H \, |\xi\rangle\langle\xi|$$ (projection into relevant space)

$$H_{eff} = \hbar\omega |e,0\rangle\langle e,0| + \hbar c \sum_k k \, |g,1_k\rangle\langle g,1_k| - \hbar\left(\sum_k g_k |e,0\rangle\langle g,1_k| + h.c.\right)$$

going to rotating frame $\Rightarrow$

same H as above (*) if

$|e,0\rangle \longrightarrow$ "$|0\rangle$" in (*)

$|g,1_k\rangle \longrightarrow$ "$|k\rangle$" in (*)

} like bound-to-continuum

$\rightarrow$ shift $\Rightarrow$ "Lamb shift"

- decay (for polarization α)

$$\gamma = 2\pi \sum_{k,\alpha} |g_{k\alpha}|^2 \delta(ck-\omega) \rightarrow$$

$$= 2\pi \sum_{\alpha} \frac{V}{(2\pi)^3} \int k^2 dk \int d\varphi \int d\vartheta \sin\vartheta \; |g_{k\alpha}|^2 \delta(ck-\omega)$$

NB: projection on allowed α ($\perp \hat{k}$), independent of φ

$$\sum_{\alpha} |g_{k\alpha}|^2 = |g_k|^2 \sin^2\vartheta \quad (\text{b/o } e^{i\underline{k}\cdot\underline{r}})$$

$$= 2\pi \frac{V}{(2\pi)^3} 2\pi \int dk\, k^2 \int d\vartheta \sin^3\vartheta \; \delta(ck-\omega)$$

$$= \frac{8\pi}{3} \frac{\cancel{V}}{(2\pi)^3} \left(\frac{\omega}{c}\right)^2 \frac{1}{c} \underbrace{|g_{k=\frac{\omega}{c}}|^2}_{\frac{|\wp|^2 \omega}{\hbar\, 2\epsilon_0 \cancel{V}}}$$

$$\boxed{\gamma = \frac{\omega^3 |\wp|^2}{3\epsilon_0 \pi \hbar c^3}}$$

spontaneous emission ($\hat{=}$ Einstein-A coeff.)

$\Rightarrow$ $\gamma \propto \omega^3$: strong for high frequencies

$\gamma \propto |\wp|^2$: strong if strongly allowed

$\wp = \langle f | e\hat{r} | i \rangle$

f) Higher-order radiation processes

full interaction term:

$$\langle H \rangle_{ba} = -\frac{e}{mc} \langle b | \vec{p} \cdot \vec{A}(\vec{r}) | a \rangle \quad \left(\begin{array}{l} \vec{B} = -ikA\hat{y} \\ \vec{E} = ikA\hat{z} \end{array} \right)$$

$$\langle H \rangle_{ba} \propto \vec{p} \cdot \hat{z}\, e^{ikx} \quad (\text{propagation dir } \hat{x}, \text{ polarization } \hat{z})$$

dipole approx: $e^{ikx} \approx 1$

now: use $e^{ikx} = 1 + ikx - \frac{1}{2}(kx)^2 \ldots$

$$\langle H \rangle = \underbrace{H(E1)}_{\substack{\text{electric}\\ \text{dipol}}} + \underbrace{H(B1)}_{\substack{\text{mgn.}\\ \text{dipole}}} + \underbrace{H(E2)}_{\substack{\text{el.}\\ \text{quadrupole}}} + \ldots$$

$$H(B1) = \underline{B} \cdot \langle b | \underbrace{\mu_0 \vec{L}}_{\text{even}} | a \rangle$$ magnetic dipole transition

$$H(E2) = \frac{ie\omega}{2c} E \langle b | \underbrace{xz}_{\text{even}} | a \rangle$$ electric quadrupole transition

$\vdots$

in atomic units: $\left.\begin{aligned} \mu_0 &= \frac{\alpha}{2} \\ \frac{1}{c} &= \alpha \end{aligned}\right\}$ Both (B1, E2) are $\sim \alpha$ weaker than E1 !

$\Rightarrow$ "forbidden"

rate $\left(\propto |H(E2)|^2, |H(B1)|^2 \right)$ is α^2 weaker!

g) Selection rules - Wigner-Eckart theorem

E1 transition:

$\langle b, j_b, m_b | \hat{\vec{r}} | a, j_a, m_a \rangle$ — allowed?

Wigner-Eckart theorem:

T: spherical tensor, e.g. $T_{\ell m} \propto Y_{\ell m}$

$$\boxed{\langle j, m | T_{kq} | j', m' \rangle = \langle j, m, k, q | j', m' \rangle \langle j \| T_k \| j' \rangle}$$

$\Rightarrow$ all (m, m') pairs differ only by ratios of Clebsch-Gordan coefficients (where $\langle j, m, k, q \mid j', m' \rangle$ are Clebsch-Gordan coefficients).

$\Rightarrow$ only <u>one</u> $\langle j' m \| T_{kq} \| j' m' \rangle$ needs to be fully calculated.

Proof idea: spherical symmetry of problem, all (m, m') elements are related by rotation.

<u>Example</u>: E1 for $L (= k) = 1$:

$\vec{r}$ can be expressed (in polar coordinates) via Y_{1m}:

$$Y_{10} = \sqrt{\frac{3}{4\pi}} \cos\vartheta \,, \quad Y_{1\pm1} = \sqrt{\frac{3}{8\pi}} \sin\vartheta \, e^{\pm i\varphi}$$

$$\Rightarrow \left.\begin{aligned} r_0 &= r\cos\vartheta = \sqrt{\frac{4\pi}{3}}\, r\, Y_{10} \\ r_\pm &= \sqrt{\frac{4\pi}{3}}\, r\, Y_{1\pm1} \end{aligned}\right\} \text{define } r_m \equiv r\, T_{1m}(\vartheta, \varphi)$$

$$\Rightarrow \langle b, j_b, m_b | r_m | a, j_a, m_a \rangle = \underbrace{\langle b, j_b | r | a, j_a \rangle}_{\text{radial } (r)} \cdot \underbrace{\langle j_b, m_b | T_{1m} | j_a, m_a \rangle}_{\text{spherical } (\vartheta, \varphi)}$$

parity selection rules

(just calculate - simple integrals ...)

$$\Rightarrow \begin{cases} j_b - j_a = \pm 1, 0 \,, & \text{but } j_a = j_b = 0 \text{ forbidden} \\ m_b - m_a = \pm 1, 0 \end{cases}$$

NB: if $\vec{L}, \vec{S}$ good q. numbers (instead of $\vec{J}$):

$\Delta L = \pm 1, 0 \,, \quad \Delta m_L = \pm 1, 0 \qquad 0 \not\leftrightarrow 0$

$\Delta S = 0 \qquad \Delta m_S = 0$

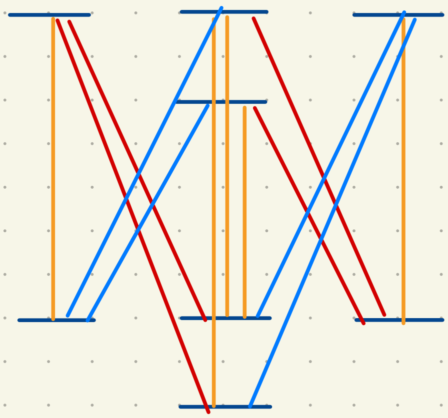
$(\Delta \ell \neq 0$ for single e^- ! $)$

Example:

X: $\updownarrow$ $\hat{z}$

X: $\circlearrowright$ $\hat{e}_{+}$

X: $\circlearrowleft$ $\hat{e}_{-}$



$j'=1$

$j'=0$

$j=1$

$j=0$

$m_{j^{(\prime)}} = \quad -1 \qquad 0 \qquad +1$

•, •, •, allowed

Complicated calculation only for

- $\langle j'=1 | T | j=0 \rangle$
- $\langle j'=1 | T | j=1 \rangle$
- $\langle j'=0 | T | j=1 \rangle$

Rest is just Clebsch-Gordan

Higher order (M1, E2, ...) transitions:

similar logic $\Rightarrow$

$\Delta j = \pm 2, \pm 1, 0 \quad , \Delta m_j = \pm 2, \pm 1, 0$