Lectures 44 - 45 - 46

Interaction between charged particles and quantised radiation field

Hamiltonian for the system :

Recall ~~our~~ ~~lecture~~ that interaction of charges with Electromagnetic potential is given by principle of minimal coupling. Recall Eq. (258) ~~In~~ for a particle of mass m, mmtm. $\vec{p}$ and Vector potential $\vec{A}(\vec{x},t)$ is given by

$$H = -\frac{e}{mc}\vec{A}\cdot\vec{p} + \frac{ie\hbar}{2mc}\vec{\nabla}\cdot\vec{A} + \frac{e^2\vec{A}^2}{2mc^2} + e\phi + \frac{|\vec{p}|^2}{2m}$$

For an atomic e^- in a radiation field $m = \mu$: reduced mass. ; $\phi \equiv$ potential due to Nucleus

$\vec{A}$: ~~external~~ vector potential corresponding to the radiation field, with $\vec{\nabla}\cdot\vec{A} = 0$, dropping the ~~spin~~ interaction term due to spin

$$H = \frac{|\vec{p}|^2}{2m} + e\phi + \frac{e^2\vec{A}^2}{2\mu c^2} - \frac{e}{\mu c}\vec{A}\cdot\vec{p}$$

$$H = H_0 + \frac{e^2\vec{A}^2}{2\mu c^2} - \frac{e}{\mu c}\vec{A}\cdot\vec{p}$$

$$\Rightarrow \boxed{H_{int} = -\frac{e}{\mu c}\vec{A}\cdot\vec{p} + \frac{e^2\vec{A}^2}{2\mu c^2}} \quad - (322')$$

If one has N electrons each with charge e, ~~m~~ reduced mass μ ~~and~~ with momentum $\vec{P}_i$ and position given by $\vec{P}_i$, $\vec{x}_i$ $(i=1-N)$

the corresponding interaction ~~potential~~ Hamiltonian is given by

$$\mathcal{H}_{int} = -\frac{e}{\mu c}\sum_{i=1}^{N}\vec{A}(\vec{x}_i,t)\cdot\vec{P}_i + \frac{e^2}{\mu^2 c^2}\sum_{i=1}^{N}\vec{A}(\vec{x}_i,t)\cdot\vec{A}(\vec{x}_i,t)$$

$\vec{x}_i$: position of ith electron wrt. Nucleus at origin.

In Eq. 261 we had treated only the e^- quantum mechanically

$\Rightarrow$ $\vec{x}_i$, $\vec{P}_i$ were operators. Now $\vec{A}$ is also an operator.

From now on in this discussion I will used a $\hat{A}$ to indicate that the treatment involves treating both the e^- and the Radiation quantum mechanically.

$$\boxed{\hat{\mathcal{H}}_{int} = -\frac{e}{\mu c}\sum_{i=1}^{N}\hat{\vec{A}}_i\cdot\vec{P}_i + \frac{e^2}{\mu^2 c^2}\sum_{i=1}^{N}\hat{\vec{A}}_i\cdot\hat{A}_i} \quad (323)$$

$$\hat{\vec{A}}_i = \hat{A}(\vec{x}_i,t)$$

Space of states on which $\hat{H}$ ~~i~~ acts

This Hamiltonian operator acts on a space which is direct product of the state vectors of the atomic state and the occupation # states of radiation field.

Let $|i\rangle$: initial atomic state , $|f\rangle$: final atomic state

~~The~~ Initial state of this combined system is $|i, n_{\vec{k},\alpha}\rangle$

$|n_{\vec{k},\alpha}\rangle_g$: is a generic occupation # state ~~all possi~~ given by Eqn (322') and Eq. (315)

$|n_{\vec{k},\alpha}\rangle_g = |n_{\vec{k}_1 \alpha_1} \ldots \; n_{\vec{k}_i \alpha_i} \ldots \rangle$

consider the processes of absorption and emission of photons under the action of radiation field we discussed in letures 38 - 39 while calulating (for example) absorbtion cross-section.

The initial state of the system is radiation ~~is~~ and ~~an~~ ~~electron~~ an atom in a state $|i\rangle$. The radiation field ~~consists of~~ acts on ~~a~~ occupation # states. ~~It is made~~

~~The radiation field consists of all possible occupations~~

The state of the radiation field is characterised by the occupation no. states $|n_{\vec{k_i},\alpha_i}\rangle_g$ (g for generic)

I.e

$$\boxed{|n_{\vec{k_i}\alpha_i}\rangle_g = |n_{\vec{k_1},\alpha_1} \cdots n_{\vec{k_i}\alpha_i} \cdots\rangle}$$

where $\vec{k_i}$ run over all possible values corresponding to Eqs. (282) and ~~...~~ α takes values 1 or 2, depending on state of linear polarization of the field. If it is an unpolarized field occupation #s in both states would be equal.

As a ~~result~~ result of emission of a photon of ~~...~~ energy $\hbar\omega$, with polarization state α, the occupation number of the state $|n_{\vec{k}},\alpha\rangle$ will increase by one. For absorption from radiation field the occupation no. corresponding to state $|\vec{k},\alpha\rangle$ will decrease

~~@~~ by 1.

For absorption process the initial state of the atom + radiation field $|I\rangle$ is given by

(324) $\boxed{|I\rangle_{rad+atom} \equiv |i, n_{\vec{k},\alpha}\rangle \quad \text{where } |i\rangle \text{ initial atomic state}}$

The final state $|F\rangle$ will be

(325) $\boxed{|F\rangle_{rad+atom} \equiv |f, n_{\vec{k},\alpha} - 1\rangle \quad \text{where } |f\rangle: \text{final atomic state}}$

Please note that I have written only the occupation no. state corresponding to $\vec{k}$ ~~=~~ $|\vec{k}|c = \omega$ which corresponds to absorption of a photon of energy $\hbar\omega$ as all the other occupation no remain unchanged.

~~Any perturbation the~~

Look at now $\hat{H}_{int}$ given by Eq. (323) In ~~&~~ approximation of weak fields

$$\boxed{\hat{H}_{int} = -\frac{e}{\mu c} \sum_{i=1}^{N} \hat{A}_i \cdot \vec{p}_i)} \quad (326)$$

since one e^- 'jumps' at a time while discussing

interaction of radiation field with e^- ~~we~~ it is sufficient

to right now consider only for a single e^-: $\hat{H}^{(1)}_{int}$, the Hamiltonian corresponding to a single e^- is

$$\boxed{\hat{H}^{(1)}_{int} = -\frac{e}{\mu c} \hat{\vec{A}} \cdot \vec{p}} \quad (327)$$

$\hat{\vec{A}}$ has an explicit, ~~harmo~~ time dependence given by $e^{\pm i\omega t}$ for each Fourier component.

The action of this radiation field on the e^- is thus best analysed using methods of time-dependent perturbation theory, (cf. Eq. ~~?~~). Recall also Eqs. (264). Then the calculation of absorption rates involves computation of the ~~B~~ ~~R~~ interaction Hamiltonian between the initial & final states of the system

Transition Matrix elements:

~~$H^{int}_{FI} = \langle F | \hat{H}^{int} | I \rangle$~~

~~For~~ absorption the relevant matrix element is

$$H^{int}_{FI} \equiv \langle F | \hat{H}^{(1)}_{int} | I \rangle$$

Semi classical theory $\rightarrow$ $\boxed{W^{\dagger}_{fi}}$ $\boxed{H^{int}_{FI} = \langle f, n_{\vec{k},\alpha} - 1 | \hat{H}^{(1)}_{int} | i, n_{\vec{k}}\,\alpha \rangle}$ $\rightarrow$ (328)

Using $\hat{H}^{(1)}_{int}$ is equivalent to Neglecting spin interactions and dropping the quadratic terms as well as looking at the effect of transition of one electron at a time.

Use Eq. (298, 321) for expression of ~~quantise~~ quantised radiation field, given by

$$(328') \quad \hat{A}(\vec{x}, t) = \frac{1}{\sqrt{V}} \sum_{\vec{k}'} \sum_{\alpha'} c \sqrt{\frac{\hbar}{2\omega'}} \left[\hat{a}_{\vec{k}',\alpha'} \hat{\epsilon}_{\alpha'} e^{i\vec{k}'\cdot\vec{x} - i\omega' t} + \hat{a}^{\dagger}_{\vec{k}',\alpha'} \hat{\epsilon}^{*}_{\alpha'} e^{-i\vec{k}'\cdot\vec{x} + i\omega' t} \right]$$

It is clear, from Eq. (327), that Eq. (328) will ~~have nonzero~~ lead to ~~value~~ lead to a nonzero value only for the first term in the expansion.

$$H^{int}_{FI,\,absorp} = \frac{-e}{\mu c} \langle f, n_{\vec{k}\alpha} - 1 | \sum_{\vec{k}'\alpha'} \frac{1}{\sqrt{V}} \cdot c\sqrt{\frac{\hbar}{2\omega'}} \Big[\hat{\epsilon}_{\alpha'} \cdot \vec{p}\; \hat{a}_{\vec{k}'\alpha'}\, e^{i\vec{k}'\cdot\vec{x} - i\omega' t} + \hat{\epsilon}_{\alpha'} \cdot \vec{p}\; \hat{a}^{+}_{k'\alpha'}\, e^{-i\vec{k}'\cdot\vec{x} + i\omega' t} \Big] | i, n_{\vec{k},\alpha} \rangle \quad (329)$$

~~So only the since $a_{\vec{k}',\alpha'} | n_{\vec{k},\alpha}, \ldots n_{\vec{k}_1,\alpha_1} \rangle$~~

Action of $a_{\vec{k}',\alpha'}$ changes only the occupation number of the state corresponding to $\vec{k}', \alpha'$. Hence only the term corresponding to $\vec{k}' = \vec{k}$, $\alpha' = \alpha$ in the sum will yield a nonzero answer. and that too only the first term. ~~Recall Eq. ( ), $a_{\vec{k},\alpha} | n_{\vec{k},\alpha} \rangle = \sqrt{n}$~~

~~$\therefore H^{int}_{FI,\,abs.}$~~

Recall Eqs. ~~309~~, 312, 315, 315'

$$\boxed{\begin{aligned} & a_{\vec{k}_1\alpha_1} \,|\, n_{\vec{k}_1\alpha_1}, \ldots n_{\vec{k}_i\alpha_i} \ldots \rangle \\ (330) \quad & = \sqrt{n_{\vec{k}_1,\alpha_1}} \,|\, n_{\vec{k}_1,\alpha_1} - 1, \underbrace{n_{\vec{k}_2\alpha_2}, \ldots n_{\vec{k}_i\alpha_i}}_{\text{all other occupation nos unchanged}} \rangle \end{aligned}}$$

$|n_{\vec{k},\alpha}\rangle$ in Eq. 324 is a short hand for ~~P~~

$$|n_{\vec{k}',\alpha'}, n_{\vec{k}_1\alpha_1}, \ldots n_{\vec{k}_i\alpha_i} \ldots \rangle$$

So ~~action of a $a_{\vec{k}',\alpha'}$ on the state I will reduce the~~

Hence only for $\vec{k}' = \vec{k}$, $\alpha' = \alpha$ will there be a nonzero matrix element $H^{int}_{FI,abs}$ (from Eq. 329, 330)

$$\therefore \langle F | \hat{H}^{(1)}_{int} | I \rangle \equiv H^{int}_{FI\,abs}$$

$$\boxed{H^{int}_{FI,abs} = -\frac{e}{\mu c}\, c \sqrt{\frac{\hbar}{2\omega}} \frac{1}{\sqrt{V}} \sqrt{n_{\vec{k},\alpha}} \langle f | \epsilon_{\vec{\alpha}} \cdot \vec{P}\, e^{i\vec{k}\cdot\vec{x}} | i \rangle \cdot e^{-i\omega t}}$$

$$H^{int}_{FI,abs} = -\frac{e}{\mu \cancel{c}}\cancel{c}\sqrt{\frac{\hbar\, n_{\vec{k},\alpha}}{2\omega V}}\, \langle f|\hat{\epsilon}_\alpha\cdot p\, e^{i\vec{k}\cdot\vec{x}}|i\rangle\, e^{-i\omega t} \tag{331}$$

: When one takes into account all the e^-'s the net matrix element will be

$$H^{int, N}_{FI,abs} = -\frac{e}{\mu}\sqrt{\frac{\hbar\, n_{\vec{k},\alpha}}{2\omega V}}\left[\sum_i \langle f|\vec{\epsilon}_\alpha\cdot\vec{p}_i\, e^{i\vec{k}\cdot\vec{x}_i}|i\rangle\right]\cdot e^{-i\omega t} \tag{332}$$

Let us go back to the case of a single e^-; Eq. 331

Recall the result from the semi classical radiation theory for the same quantity. Which we had called W_{fi} then.

Recall Eq. (264.). The term in H_{int}. proportional to $e^{-i\omega t}$ caused absorption. The W^{+}_{mi} (or W^{+}_{fi}) obtained therein would be the same as Eq. (331) with

$$\boxed{A_0(\omega) \longrightarrow c\sqrt{\frac{\hbar n_{\vec{k},\alpha}}{2\omega V}}}$$

after one performs time dependent perturbation theory analysis while deriving Eq. (266).

~~In fact the time dependence $e^{-i\omega t}$~~

In Quantum theory of radiation absorption probability is then proportional to $n_{\vec{k},\alpha}$

In semi classical theory it was proportional to $|A_0|^2$

We in some sense recover the classical results even in the limit of small $n_{\vec{k},\alpha}$ (i.e. weak radiation).
(Recall the intensity $\propto |A_0(\omega)|^2$ Eq. 270)

Now let us consider the emission

In case of induced emission the term (in Eq. (265) for H^{int}) proportinal to $e^{i\omega t}$ is important. The relevant matrix element is W_{ni} (Semi classical theory of radiation)

Now let us consider the same using quantum theory of radiation. Neglecting the spin interaction and also the quadratic term in Eq. 322' the relevant matrix element of is between states $I \equiv |i, n_{\vec{k},\alpha}\rangle$ and $F \equiv |f, n_{\vec{k},\alpha}+1\rangle$
Using Eq (322') the matrix element is then

$$-\frac{e}{\mu c}\langle f, n_{\vec{k},\alpha}+1 | \hat{A}\cdot\vec{P} | i, n_{\vec{k},\alpha}\rangle$$

Look at $\hat{\vec{A}}\cdot\vec{P}$ from Eq. (329)

$$= -\frac{e}{\mu c}\langle f, n_{\vec{k},\alpha}+1 | \sum_{k',\alpha'} c\sqrt{\frac{\hbar}{2w'V}}\Big[\hat{\epsilon}_{\alpha'}\cdot\vec{P}\, e^{i\vec{k'}\cdot\vec{x}-iw't}\,\hat{a}_{\vec{k'},\alpha'} + \hat{\epsilon}^{*}_{\alpha'}\cdot\vec{P}\, e^{-i\vec{k'}\cdot\vec{x}+iw't}\,\hat{a}^{+}_{\vec{k'}\alpha'}\Big] | i, n_{\vec{k},\alpha}\rangle$$

Now only the second term ~~and that too for~~ with $\hat{a}^{+}_{\vec{k'},\alpha'}$ and that too for $\vec{k'}=\vec{k}$ and $\alpha'=\alpha$ will contribute a nonzero matrix element.

$\therefore$ The matrix element is $\propto -\frac{e}{\mu c}\cdot\langle f|\hat{\epsilon}^{*}_{\alpha}\cdot\vec{P}\, e^{-i\vec{k}\cdot\vec{x}+iwt}|i\rangle$

This is the counterpart of W_{fi} ~~of~~ from Eq. (265).

$$\therefore H^{int}_{FI,emiss} = \langle f, n_{\vec{k},\alpha}+1 | \left(-\frac{e}{\mu c}\vec{A}\cdot\vec{P}\right) | i\, n_{\vec{k},\alpha}\rangle$$

$$\boxed{H^{int}_{FI,emiss} = -\frac{e}{\mu c}\cdot\sqrt{\frac{(n_{\vec{k},\alpha}+1)\hbar}{2wV}}\cdot c\cdot\langle f|\hat{\epsilon}^{*}_{\alpha}\cdot\vec{P}\, e^{-i\vec{k}\cdot\vec{x}+iwt}|i\rangle} \quad (333)$$

This should be compared to W_{fi} from Eq. 265

Now there are two important observations to make.

i) The $H^{int}_{FI,\,emission}$ ~~is~~ looks like W_{fi} with the replacement ~~A_0^{emiss}~~

$$\boxed{A_0^{emission}(\omega) = c\sqrt{\frac{(n_{\vec{k},\alpha}+1)\hbar}{2\omega V}}}$$

If $n_{\vec{k},\alpha}$ is large so that $\sqrt{n_{\vec{k},\alpha}} \doteq \sqrt{n_{\vec{k},\alpha}+1}$ then the result of the semi classical theory for stimulated emission is equivalent to the result from quantum theory.

Thus Eq. 333, for large $\sqrt{n_{\vec{k},\alpha}+1}$ in fact represents matrix element for stimulated emission.

~~If $n_{\vec{k},\alpha} = 0$~~

ii) Even with $n_{\vec{k},\alpha} = 0$ Eq. 333 gives a nonzero transition probability. This means there is a transition without radiation. This is the spontoneous emission.

iii) In Quantum theory the same matrix element (given by Eq. 333) describes both the process of spontaneous and induced emission, with $n_{\vec{k},\alpha} = 0$ and $n_{\vec{k},\alpha} \neq 0$.

~~iii~~ (iv) Thus in semi classical theory of radiation when there is emission or absorption, the state of radiation is not changed. In Quantum theory the occupation number corresponding to $\omega = |\vec{k}| c$ with polarization $\hat{\epsilon}_\alpha$, i.e. $n_{\vec{k},\alpha}$ changes by ± 1. Thus there is back reaction on radiation. In the limit of large $n_{\vec{k},\alpha}$, change is insignificant. But when $n_{\vec{k},\alpha} = 0$ this describes spontaneous emission.