Putting it all together: Second quantization

Eigenstates of the atomic Hamiltonian (as in chapter 2)

$$\hat{H}_A |i\rangle = \hbar\omega_i |i\rangle$$

Closure theorem: $\sum_i |i\rangle\langle i| = \mathbb{1}$

the identity operator.

Note that

$|a\rangle\langle b|$ is an operator

because it takes a ket to a new ket:

$$\big(|a\rangle\langle b|\big)|c\rangle = \langle b|c\rangle\, |a\rangle$$

and in particular,

$|j\rangle\langle j|$ is a projection operator:

If $|\psi\rangle = \sum_i c_i |i\rangle$ is a general state,

then $\big(|j\rangle\langle j|\big)|\psi\rangle = \sum_i c_i |j\rangle \underbrace{\langle j|i\rangle}_{=\delta_{ij}}$

$= c_j |j\rangle.$

projects the state $|\psi\rangle$ onto the basis vector $|j\rangle$.

From this, closure theorem follows:

$$\Big(\sum_j |j\rangle\langle j|\Big) \sum_i c_i |i\rangle = \sum_{ij} c_i |j\rangle\langle j|i\rangle$$

$$= \sum_j c_j |j\rangle = |\psi\rangle \quad \text{for any } |\psi\rangle.$$

Then we can write

$$\hat{H}_A = \left(\sum_i |i\rangle\langle i|\right)\hat{H}_A\left(\sum_j |j\rangle\langle j|\right)$$

$$= \sum_{ij} |i\rangle \underbrace{\langle i|\hat{H}_A|j\rangle}_{=\hbar\omega_j \delta_{ij}} \langle j|$$

$$\boxed{\hat{H}_A = \sum_j \hbar\omega_j |j\rangle\langle j|}$$

the Hamiltonian in <u>second-quantized</u> form.

- Now write the <u>dipole moment</u> in second quantized form:

$$\hat{\vec{D}} = \sum_{ij} |i\rangle\langle i|\hat{\vec{D}}|j\rangle\langle j|$$

$$= \sum_{ij} \vec{D}_{ij} |i\rangle\langle j|$$

<u>Note</u>: $\vec{D}_{ij} = 0$ if $i = j$ because of parity
(see chapter 2!)

Now the interaction Hamiltonian

$$\hat{H}_{ED} = e\hat{\vec{D}} \cdot \hat{\vec{E}}_T(\vec{R})$$ where $\vec{R}$ is position of nucleus
[We shifted the origin of coordinates]

$$= ie \sum_{\vec{k}} \sum_{\lambda} \sum_{ij} \sqrt{\frac{\hbar\omega_k}{2\varepsilon_0 V}}\, \vec{e}_{\vec{k}\lambda} \cdot \vec{D}_{ij} \cdot \left\{ \hat{a}_{\vec{k}\lambda} e^{i\vec{k}\cdot\vec{R}} - \hat{a}^{+}_{\vec{k}\lambda} e^{-i\vec{k}\cdot\vec{R}} \right\} \cdot |i\rangle\langle j|$$

Consider case of <u>two</u> atomic states again $\quad$ 8-3

Let $\omega_0 = \omega_2 - \omega_1$

<u>Define</u> $\hat{\pi}^+ = |2\rangle\langle 1| \qquad \hat{\pi} = |1\rangle\langle 2|$

then $\hat{\pi}^+|1\rangle = |2\rangle \qquad \hat{\pi}|1\rangle = 0$

$\hat{\pi}^+|2\rangle = 0 \qquad \hat{\pi}|2\rangle = |1\rangle$

$\left\{ \begin{array}{l} \hat{\pi}^+ \text{ shifts atom from lower to upper state.} \\ \hat{\pi} \quad \text{—— '' ——} \end{array} \right.$

<u>Also</u> note

$$\left.\begin{array}{l} \hat{\pi}^+\hat{\pi} = |2\rangle\langle 2| \\ \hat{\pi}\hat{\pi}^+ = |1\rangle\langle 1| \end{array}\right\} \Rightarrow \hat{\pi}^+\hat{\pi} + \hat{\pi}\hat{\pi}^+ = 1$$

$$\hat{\pi}\hat{\pi} = \hat{\pi}^+\hat{\pi}^+ = 0$$

= the atom must be in either $|1\rangle$ or $|2\rangle$

Now we only have <u>one</u> dipole matrix element
$\vec{D}_{12} = \vec{D}_{21}$ (assume real)

and

$$\hat{H}_{ED} = i \sum_{\vec{k}} \sum_{\lambda} \hbar g_{k\lambda} \left\{ \hat{a}_{k\lambda} e^{i\vec{k}\cdot\vec{R}} - \hat{a}^+_{k\lambda} e^{-i\vec{k}\cdot\vec{R}} \right\} (\hat{\pi}^+ + \hat{\pi})$$

$$\left\{ \text{where} \quad g_{k\lambda} = e\sqrt{\frac{\omega_k}{2\varepsilon_0 \hbar V}}\, \vec{e}_{k\lambda}\cdot\vec{D}_{12} \qquad [s^{-1}] \right\}$$

$$= i \sum_{\vec{k}} \sum_{\lambda} \hbar g_{k\lambda} \left\{ \hat{a}_{k\lambda} \hat{\pi}^+ e^{i\vec{k}\cdot\vec{R}} - \hat{a}^+_{k\lambda} \hat{\pi} e^{-i\vec{k}\cdot\vec{R}} \right\}$$

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because $\hat{a}\hat{\pi}$ and $\hat{a}^{+}\hat{\pi}^{+}$

are not "allowed" processes. (RWA!)

Skip part about time dependence & "pictures"

Consider states such as

$|n_{\vec{k}\lambda}, i\rangle$ $\begin{cases} n_{\vec{k}\lambda} \text{ photons in mode } \vec{k}\lambda \\ \text{atom is in state } i \ (=1,2) \end{cases}$

Absorption:

we start with $|n_{k\lambda}, 1\rangle = |i\rangle$

and end up in $|n_{k\lambda}-1, 2\rangle = |f\rangle$

The matrix element is:

$$\langle n_{k\lambda}-1, 2|\hat{H}_{ED}|n_{k\lambda}, 1\rangle = i\hbar g_{k\lambda}\, e^{i(\omega_0-\omega)t + i\vec{k}\cdot\vec{R}} \sqrt{n_{k\lambda}}$$

have to work a little harder to get this

Absorption rate $B_{12} \propto |\langle f|\hat{H}_{ED}|i\rangle|^2$

$\propto n_{k\lambda}$ prop. to # photons!

Careful calculation gives

$$B_{12} = \frac{\pi e^2 D_{12}^2}{3\varepsilon_0 \hbar^2}$$

• **Emission:**

$$\langle n_{k\lambda}+1, 1 | \hat{H}_{ED} | n_{k\lambda}, 2 \rangle = -i\hbar g_{k\lambda} e^{-i(\omega_0-\omega)t - i\vec{k}\cdot\vec{R}} \sqrt{n_{k\lambda}+1}$$

Emission rate $\propto g_{k\lambda}^2 (n_{k\lambda} + 1)$

B_{21} A_{21}

Spontaneous emission: even if no radiation is present.
A "vacuum" effect.

Stimulated emission: enhanced if there are already many photons in the mode.

Ultimately find $A_{21} = \dfrac{e^2 \omega_0^3 D_{12}^2}{3\pi \varepsilon_0 \hbar c^3} = 2\gamma_{sp}$

def.

Also observe that we may write

$$\boxed{\Omega^2 = 4 g_{k\lambda}^2 n_{k\lambda}}$$

for the Rabi frequency.

"Vacuum Rabi frequency" Def: $\Omega_{vac}^2 = 4 g_{k\lambda}^2$

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Irradiance operator

Measurement of the irradiance must correspond to some Hermitian operator.

Classically: Poynting vector

$$\vec{I}(\vec{r},t) = \varepsilon_0 c^2 \, \vec{E}(\vec{r},t) \times \vec{B}(\vec{r},t)$$

Q.M: $\vec{E}_T = \vec{E}_T^+ + \vec{E}_T^-$

$\vec{B} = \vec{B}^+ + \vec{B}^-$

$$\begin{cases} \vec{E}^- \text{ and } \vec{B}^- \text{ contain } \hat{a}^+ \\ E^+ \text{ and } B^+ \text{ contain } \hat{a} \end{cases}$$

the measured irradiance should be proportional to the number of photons $\hat{n}_{k\lambda} = \hat{a}^+_{k\lambda}\hat{a}_{k\lambda}$

→ discard $\hat{a}\hat{a}$ and $\hat{a}^+\hat{a}^+$ terms

$$\hat{\vec{I}}(\vec{r},t) = \varepsilon_0 c^2 \left\{ \hat{\vec{E}}_T^- \times \hat{\vec{B}}^+ - \hat{\vec{B}}^- \times \hat{\vec{E}}_T^+ \right\}$$

"normal ordered": all a^+ operators are to the left of $\hat{a}$.

Exercise: Prove that the magnitude is also

$$\boxed{\hat{I}(\vec{r},t) = 2\varepsilon_0 c \, \hat{E}_T^- \hat{E}_T^+}$$ irradiance operator.

Irradiance measurements.

Classically, the irradiance

$$I(\vec{r},t) = \frac{1}{2}\varepsilon_0 c \left|\vec{E}(\vec{r},t)\right|^2$$

For simplicity assume linearly polarized:

$$I(\vec{r},t) = \frac{1}{2}\varepsilon_0 c \, E(\vec{r},t)^2$$

Experiment: an atom in a phototube absorbs a photon.

The probability of this per unit time is given by Fermi's golden rule [sec. 2.4]

$$\text{Rate} = \frac{2\pi}{\hbar^2} \sum_f \left|\langle f|\hat{H}_{ED}|i\rangle\right|^2 \delta(\omega_f - \omega_i)$$

where $\hbar\omega_f$ and $\hbar\omega_i$ are eigenenergies of the states $|f\rangle$ and $|i\rangle$

[We convert energy to frequency to get the units right.]

$|i\rangle$ is the initial state of the combined (atom + light) system

$|f\rangle$ runs over all possible final states with the right energy & nonvanishing matrix element.

$|i\rangle = |n_{k\lambda}, 1\rangle$ n photons in the mode with $\omega = \omega_0$.

$|f\rangle = |n_{k\lambda}-1, 2\rangle$ is the only final state that gives a nonzero result.

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$$\text{Rate} \propto \left| \langle n_{k\lambda}-1, 2 | \hat{H}_{ED} | n_{k\lambda}, 1 \rangle \right|^2 =$$

$$= \left| \langle 2 | e\hat{D} | 1 \rangle \right|^2 \left| \langle n_{k\lambda}-1 | \hat{E}_T | n_{k\lambda} \rangle \right|^2$$

$$\propto \Big| \langle n_{k\lambda}-1 | \underbrace{\hat{E}_T^{(+)}(r,t)}_{\text{contains } \hat{a}} + \underbrace{\cancel{\hat{E}_T^{(-)}(r,t)}}_{\substack{\to 0 \\ \text{contains } \hat{a}^\dagger}} | n_{k\lambda} \rangle \Big|^2$$

$$= \left| \langle n_{k\lambda}-1 | \hat{E}_T^{(+)}(r,t) | n_{k\lambda} \rangle \right|^2$$

$$= \langle n_{k\lambda} | \hat{E}_T^{(-)}(r,t) \underbrace{\hat{E}_T^{(+)}(r,t) | n_{k\lambda} \rangle}_{|n_{k\lambda}-1\rangle\langle n_{k\lambda}-1| = 1 \text{ here}}$$

∴ What we measure is <u>not</u> $\left(\hat{E}(r,t)\right)^2$

<u>but</u>: $\hat{E}^{(-)}(r,t)\,\hat{E}^{(+)}(r,t)$

It is called the <u>normal ordered product</u>:
all operators $\hat{a}^\dagger$ appear to the left of all $\hat{a}$
⇒ yields zero for the vacuum state.

Turns out that the natural definition is with a factor 4:

$$\hat{I}(r,t) = 2\varepsilon_0 c\, \hat{E}^{(-)}(r,t)\, \hat{E}^{(+)}(r,t)$$

The poynting vector is

$$\hat{\vec{I}}(r,t) = \varepsilon_0 c^2 \left\{ \hat{\vec{E}}_T^{-} \times \hat{\vec{B}}^{+} - \hat{\vec{B}}^{-} \times \hat{\vec{E}}_T^{+} \right\}$$

The <u>coherences</u> will also be normal ordered:
see sec. 4.12