More on the EM radiation

The EM radiation is represented by a classical $\vec{A}$ field.

$$\vec{A} = A_0 \vec{\epsilon}\, e^{i(\vec{k}_0\cdot\vec{r} - \omega_0 t)} + \underbrace{c.c.}$$

→ To make it hermitian so we can promote it to a QM operator

It interacts with the particle through

$$H = \frac{1}{2m}\left(\vec{p} + \frac{e}{c}\vec{A}\right)^2 - \vec{\mu}\cdot\vec{B}$$

$$= \underbrace{\frac{p^2}{2m}}_{H_0} + \underbrace{\frac{1}{2m}\left(\frac{2e}{c}\vec{p}\cdot\vec{A} + \cancel{\frac{e^2}{c^2}\vec{A}^2}\right) - \vec{\mu}\cdot(\vec{\nabla}\times\vec{A})}$$

usually ignored

* In coulomb gauge $\nabla\cdot\vec{A} = 0$, so $\vec{p}\cdot\vec{A} = \vec{A}\cdot\vec{p}$ and these terms are treated as perturbation

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☆ We are interested in the transition matrix element

$$\frac{-i}{\hbar}\int_0^t dt' \langle f | \frac{e}{mc}(\vec{p}\cdot\vec{A})_z | i \rangle$$

$$= \frac{A_0 e}{mc}\left(\frac{-i}{\hbar}\right)\int_0^t dt'\, e^{-\frac{i}{\hbar}(E_i - E_f)t'}\, \underbrace{e^{-i\omega_0 t'}}_{\text{for absorption}} \langle f | \vec{\epsilon}\cdot\vec{p}\, e^{i(\vec{k}_0\cdot\vec{r})} | i \rangle$$

$+\underbrace{c.c.}$ ⇒ corresponding to emittion

☆ When the wavelength is far longer then the atomic dimension

$$e^{i\frac{2\pi}{\lambda}\hat{k}_0\cdot\vec{r}} \simeq 1 + i\vec{k}_0\cdot\vec{r} + \cdots$$

☆ For the leading term "1", the matrix element is proportional to $\vec{\epsilon}\cdot\langle f | \vec{p} | i \rangle$.

Because $\vec{p} = m\dot{\vec{r}} = -\frac{m}{i\hbar}[H_0, \vec{r}]$ ← Same in Heisenberg and interaction pictures.

$$\Rightarrow \langle f | \vec{p} | i \rangle = \frac{im}{\hbar}\langle f | H_0\vec{r} - \vec{r}H_0 | i \rangle = im\underbrace{\left(\frac{E_f - E_i}{\hbar}\right)}_{\omega_{fi}}\langle f | \vec{r} | i \rangle$$

This is called electric dipole approximation.

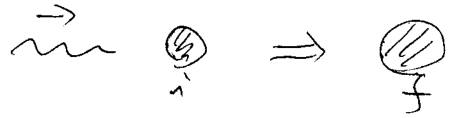
Since $\vec{r}$ is a sperical tensor of rank 1, by Wigner-Eckart theorem, we have the selection rule

$$\Delta \ell = \pm 1,\ 0$$

If the transition happens in H-like atom, $\Delta \ell = 0$ is forbidden by parity. This is called (E1) transition.

Absorption cross section

$$i + \gamma \to f$$



The transition rate is

$$W = \frac{2\pi}{\hbar}\,\delta(E_i + \hbar\omega_0 - E_f)\left|\frac{-iA_0 e}{\hbar m c}\right|^2 \left| i m \omega_{fi}\right|^2 \left| \vec{\epsilon}\cdot\langle f|\vec{r}|i\rangle\right|^2$$

Also, from the previous discussion, we know the flux of incident photon can be computed to be

$$j_\gamma = \frac{\omega_0 A_0^2}{2\pi\hbar c}\,\hat{k}_0$$

The absorption cross section is

$$\sigma_{abs} = \frac{W}{j_\gamma} = \frac{4\pi^2\hbar}{m^2\omega_0}\underbrace{\left(\frac{e^2}{\hbar c}\right)}_{=\alpha}\left|\vec{\epsilon}\cdot\langle f|\vec{p}|i\rangle\right|^2 \delta(E_i + \hbar\omega_0 - E_f)$$

$$= 4\pi^2 \alpha\, \omega_0 \left|\langle f|\vec{r}_\epsilon|i\rangle\right|^2 \delta(\omega_0 - \omega_{fi})$$

The total cross section is

$$\int \sigma_{abs}(\omega_0)\, d\omega_0 = \sum_n 4\pi^2 \alpha\, \omega_{fi} \left|\langle n|x|i\rangle\right|^2$$

In atomic physics, we define oscillation strength

$$f_{ni} \equiv \frac{2m\omega_{ni}}{\hbar}\left|\langle n|x|i\rangle\right|^2$$

Then, because $[X, H_0] = \frac{i\hbar}{m} P_x$, $[X, P_x] = i\hbar$

$$\Rightarrow \quad [X, [X, H_0]] = -\frac{\hbar^2}{m}$$

Sandwich the above eq by $\langle i|$ and $|i\rangle$, we have

$$-\frac{\hbar^2}{m} = \langle i | x[X, H_0] - [X, H_0]x | i\rangle$$
$$= \langle i | x^2 H_0 | i\rangle + \langle i | H_0 x^2 | i\rangle - 2\langle i | x H_0 x | i\rangle$$

Insert the identity

$$= \sum_m \Big\{ \langle i|x|m\rangle\langle m|x H_0|i\rangle + \langle i|H_0 x|m\rangle\langle m|x|i\rangle - 2\langle i|x|m\rangle\langle m|H_0 x|i\rangle \Big\}$$
$$= \sum_m 2(E_i - E_m)\langle i|x|m\rangle\langle m|x|i\rangle$$

namely,

$$1 = \sum_n \frac{2m(E_n - E_i)}{\hbar^2} |\langle n|x|i\rangle|^2 = \sum_n f_{ni}$$

This is the Thomas-Reiche-Kuhn sum rule

Therefore

$$\int \sigma_{abs}(\omega)\, d\omega = \sum_n 4\pi \alpha\, \omega_{ni} |\langle n|x|i\rangle|^2 = \frac{4\pi^2\hbar}{2m}\left(\frac{e^2}{\hbar c}\right) = \boxed{\frac{2\pi^2 e^2}{mc}}$$

$\Rightarrow$ no $\hbar$, in fact it is same as obtained in classical EM

Higher order Multipoles

Let's look at the next term in Taylor expansion,

$$e^{i\vec{k}_0\cdot\vec{r}}\, \vec{\epsilon}\cdot\vec{p} \simeq (1 + i\vec{k}_0\cdot\vec{r})\,\vec{\epsilon}\cdot\vec{p} = \underbrace{\vec{\epsilon}\cdot\vec{p}}_{\substack{E1 \\ \text{electric dipole} \\ \text{approximation}}} + \underbrace{i(\vec{k}_0\cdot\vec{r})(\vec{\epsilon}\cdot\vec{p})}_{E2 \text{ and } M1}$$

Only $\vec{r}$ and $\vec{p}$ are QM operators,

$\vec{\epsilon}$, and $\vec{k_0}$ are the given constant vectors.

We write the 2nd term as

$$i\, k_{0\alpha} \epsilon_\beta \ \hat{r}_\alpha \hat{p}_\beta \quad \Leftarrow \text{ a rank-2 Cartesian tensor}$$

$$= \underbrace{1}_{\substack{\text{scalar} \\ \times}} + \underbrace{3}_{\substack{\text{vector} \\ \Downarrow \\ M1}} + \underbrace{5}_{\substack{\text{spin-2} \\ \Downarrow \\ E2}}$$

To see it,

$$\hat{r}_\alpha \hat{p}_\beta = \underbrace{\frac{\hat{r}_\alpha \hat{p}_\beta - \hat{r}_\beta \hat{p}_\alpha}{2}}_{\text{anti-sym}} + \underbrace{\frac{\hat{r}_\alpha \hat{p}_\beta + \hat{r}_\beta \hat{p}_\alpha}{2}}_{\text{sym}} \quad \text{in } \alpha \leftrightarrow \beta$$

The anti-sym part can be viewed as the i-th component of $(\vec{r}\times\vec{p})$

$$(\hat{\vec{r}}\times\hat{\vec{p}})_i = \epsilon_{i\alpha\beta}\, \hat{r}_\alpha \hat{p}_\beta$$

similarly $\quad (\vec{k_0}\times\vec{\epsilon})_i = \epsilon_{i\alpha\beta}\, k_{0\alpha} \epsilon_\beta$

$$\Rightarrow \underbrace{\vec{\epsilon}\cdot\hat{\vec{p}}}_{\substack{\Downarrow \\ E1}} \underbrace{- \frac{i}{2}(\vec{\epsilon}\times\vec{k_0})\cdot(\underbrace{\hat{\vec{r}}\times\hat{\vec{p}}}_{= \vec{L}})}_{\substack{\Downarrow \\ M1}} + \frac{i}{2}\left((\vec{k_0}\cdot\hat{\vec{r}})(\vec{\epsilon}\cdot\hat{\vec{p}}) + (\vec{\epsilon}\cdot\hat{\vec{r}})(\vec{k_0}\cdot\hat{\vec{p}})\right)]$$

$\vec{L}$: orbital angular momentum

$\vec{j} = \rho\cdot\vec{V} = \frac{\rho\vec{P}}{m} \Rightarrow$ indeed, gives the magnetic dipole

☆ Comparing E1 & M1

$$\vec{\epsilon} \Longrightarrow -\frac{i}{2}(\vec{\epsilon}\times\vec{k_0})$$

$$\vec{P} \Longrightarrow \vec{L}$$

both $\vec{P}$ & $\vec{L}$ are spherical tensor of rank 1

☆ Say $\hat{k_0} = \hat{z}$,

$$\begin{cases} \vec{\epsilon_x}\times\hat{k_0} = -\hat{y} \\ \vec{\epsilon_y}\times\hat{k_0} = +\hat{x} \end{cases} \Rightarrow \begin{cases} \text{E1} \qquad \text{M1} \\ \epsilon_{1,2} \Rightarrow \mp\epsilon_{21}\, k_0 \end{cases}$$

☆ If we sum over photon polarization, the decay distribution must be identical to that for E1 radiation.

☆ The selection rule : $\Delta J = 0, \pm 1$, if no parity change

Since $\vec{L}$ is parity even, in the atomic transition (if no spin involved) $\Delta J = 0$

☆ Magnitude

$$\frac{\Gamma(M_1)}{\Gamma(E_1)} \sim (k_0 r)^2 \sim \left(\frac{a_0}{\lambda}\right)^2 << 1$$

☆ An important M1 transition :

Hydrogen hyperfine transition. $\Rightarrow \tau \simeq 10^7$ years !!

can only be observed in astrophysics.

For the symmetric part,

$$\frac{i}{2} \langle f | (\vec{k}\cdot\hat{r})(\vec{\epsilon}\cdot\hat{p}) + (\vec{\epsilon}\cdot\hat{r})(\vec{k}\cdot\hat{p}) | i \rangle$$

$$= \frac{i}{2} k_\alpha \epsilon_\beta \langle f | \hat{r}_\alpha \hat{p}_\beta + \hat{r}_\beta \hat{p}_\alpha | i \rangle$$

For atom, the Hamiltonian is always in the form

$$H_{atm} = \frac{p^2}{2m} + V(r), \qquad (V(r) \text{ could be very complecated!})$$

$$[H_{atm}, \hat{r}_\alpha \hat{r}_\beta] = \frac{1}{2m}[\hat{p}^2, \hat{r}_\alpha \hat{r}_\beta] = -\frac{i}{m}(\hat{p}_\alpha \hat{r}_\beta + \hat{r}_\alpha \hat{p}_\beta)$$

$$= \frac{-i}{m}(r_\beta p_\alpha - i\hbar \delta_{\alpha\beta} + r_\alpha p_\beta)$$

$k_\alpha \epsilon_\beta \delta_{\alpha\beta} = \vec{k}\cdot\vec{\epsilon} = 0$ in Coulomb gauge.

$$\Rightarrow \frac{i}{2} k_\alpha \epsilon_\beta \langle f | (im)[H_{atm}, \hat{r}_\alpha \hat{r}_\beta] | i \rangle$$

$$= -\frac{m}{2} k_\alpha \epsilon_\beta \langle f | H_{atm} \hat{r}_\alpha \hat{r}_\beta - \hat{r}_\alpha \hat{r}_\beta H_{atm} | i \rangle$$

$= -\frac{m}{2}(E_f - E_i)\, k_\alpha \epsilon_\beta \langle f | r_\alpha r_\beta | i \rangle$

① $\alpha \neq \beta \quad \because \vec{k} \cdot \vec{\epsilon} = 0$

$$\underbrace{r_\alpha r_\beta}_{=\,\cancel{\frac{r^2}{3}\delta_{\alpha\beta}} + \cancel{\frac{r_\alpha r_\beta - r_\beta r_\alpha}{2}} + \left(\frac{r_\beta r_\alpha + r_\alpha r_\beta}{2} - \frac{r^2}{3}\delta_{\alpha\beta}\right)}$$

② $k_\alpha \epsilon_\beta$ with the anti sym part $\Rightarrow 0$

$\Rightarrow$ The matrix element is proportional to

$$\langle f | Q_{\alpha\beta} | i \rangle, \quad Q_{\alpha\beta} = \frac{r_\alpha r_\beta + r_\beta r_\alpha}{2} - \frac{r^2}{3}\delta_{\alpha\beta}$$

This is the electric quadrupole moment operator.

By W-E theorem, the selection rule is

$$\Delta J = 0, \pm 1, \pm 2.$$

- Even higher order multipoles can be obtained from higher order Taylor expansion terms,
- The higher-order multipoles are tensor operators of rank $l = 2, 3 \ldots$ and have a form essentially identical to that in classical E&M.
- The angular momentum selection rule follow from the "triangular inequality" of the Wigner-Eckart theorem:

  if l is the multipole order,

$$|j_i - j_f| \le l \le j_i + j_f$$

- Magnetic and electric multipoles of the same order have opposite parity! ($\because$ $\vec{A}$ and $\vec{B}$ are vector and axial vector respectively).

The general result is

$$El : \text{parity change} = (-1)^l, \quad Ml : \text{parity change} = -(-1)^l$$

- e.g. $4^- \to 1^+$ is E3 but $4^+ \to 1^+$ is M3