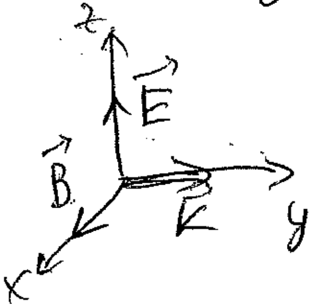
Lecture #9



## Interaction of radiation with matter

Consider a plane (electromagnetic) wave, with wave vector $\vec{k}$ (say, $\vec{k} \parallel Oy$)

and angular frequency $\omega = ck$




Introduce vector potential $\vec{A}$ =>

$$\vec{A}(\vec{r},t) = \left(A_0 e^{i(ky-\omega t)} + A_0^* e^{-i(ky-\omega t)}\right)\vec{e}_z$$

$\vec{e}_z$ — unit vector $\parallel Oz$

Then, $\vec{E} = -\frac{\partial}{\partial t}\vec{A}(\vec{r},t) =$

$$= i\omega\left(A_0 e^{i(ky-\omega t)} - A_0^* e^{-i(ky-\omega t)}\right)\vec{e}_z$$

$$\vec{B} = \vec{\nabla}\times\vec{A}(\vec{r},t) = ik\left(A_0 e^{i(ky-\omega t)} - A_0^* e^{-i(ky-\omega t)}\right)\vec{e}_x$$

$$\begin{vmatrix} \vec{e}_x & \vec{e}_y & \vec{e}_z \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ 0 & 0 & A \end{vmatrix}$$

<u>Set</u> $i\omega A_0 = \frac{E_0}{2}$, $ikA_0 = \frac{B_0}{2}$ =>

imaginary

$$\frac{E_0}{B_0} = \frac{\omega}{k} = c \Rightarrow \vec{E}(\vec{r},t) = E_0\vec{e}_z\cos(ky-\omega t)$$

$$\vec{B}(\vec{r},t) = B_0\vec{e}_x\cos(ky-\omega t)$$

(Here we assumed the Coulomb gauge $\varphi = 0$, $\vec{\nabla}\cdot\vec{A} = 0$

a.k.a. radiation / transverse

How do we describe interaction between matter & E&M field? $\Rightarrow$ full treatment $\Downarrow$ need relativistic QM!

For now $\Rightarrow$ simplified version:

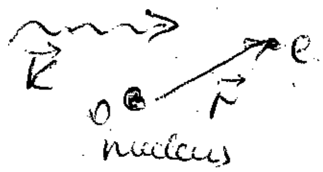
$$\underset{\substack{\uparrow \\ \text{total Hamiltonian} \\ \text{for the combined matter-field system}}}{H} = H_{\text{matter}} + H_{EM}\,, \quad \underset{\substack{\uparrow \\ \text{space}}}{\mathcal{E}} = \mathcal{E}_{\text{matter}} \otimes \mathcal{E}_{EM}$$

$$H_{EM} = \sum_{\lambda} \hbar\omega_{\lambda}\, \underbrace{a_{\lambda}^{+} a_{\lambda}}_{\uparrow \text{ number operator}} \iff \text{Adv. QM!}$$

$$H_{\text{matter}} = \sum_{\substack{i \\ \uparrow \\ \text{particles}}} \frac{1}{2m_i}\left[p_i - \frac{q_i}{c}\vec{A}(\vec{r}_i, t)\right]^2 +$$

$$+ \sum_{i<j} \frac{q_i q_j}{|\vec{r}_i - \vec{r}_j|} - \sum_i \vec{\mu}_i \cdot \vec{B}(\vec{r}_i, t)$$

Consider the simplest case $\Rightarrow$ H like atom with a single electron $\Rightarrow q = -|e|$, $\vec{\mu} = \frac{e}{mc}\vec{S}$ and assume that nucleus is very heavy




$$H_{\text{matter}} = \frac{1}{2m}\left[\vec{p} + \frac{e}{c}\vec{A}(\vec{r}, t)\right]^2 - \frac{Ze^2}{|\vec{r}|} + \frac{e}{mc}\vec{S} \cdot \vec{B}_{(\vec{r}, t)}$$

$$H = \underbrace{\frac{\vec{p}^2}{2m} - \frac{Ze^2}{|\vec{r}|} + \sum_\lambda \hbar\omega_\lambda a_\lambda^\dagger a_\lambda}_{H_0''} +$$

$$+ \underbrace{\frac{e}{mc}\vec{p}\cdot\vec{A}(\vec{r},t)}_{1} + \underbrace{\frac{e}{mc}\vec{S}\cdot\vec{B}(\vec{r},t)}_{2} + \underbrace{\frac{e^2}{2mc^2}\vec{A}(\vec{r},t)^2}_{3}$$

perturbation $V(\vec{r},t)$ (interaction Hamiltonian)

if $\vec{A}=0 \Rightarrow 0 \Leftarrow$

Estimate relative orders of magnitude $\Rightarrow$

$V_{1} = \frac{e}{mc}\vec{p}\cdot\vec{A} \sim \frac{e}{mc} p A_0$ ← momentum of the electron

$V_{2} = \frac{e}{mc}\vec{S}\cdot\vec{B} \sim \frac{e}{mc}\hbar(kA_0)$ ← wave vector of the EM wave

$\Delta p \Delta x \sim \hbar$

$\sim a_0$ for an atom

$$\frac{V_{2}}{V_{1}} \sim \frac{\hbar k}{p} = \frac{\hbar}{p}\cdot\frac{2\pi}{\lambda} \sim \frac{a_0}{2\lambda} << 1$$

$\lambda$ ← wavelength of light

$a_0 = 0.5 Å$

$\lambda \sim 500$ nm ← visible light

So, $V_{1}$ dominates!

$V_{3} \sim \vec{A}^2$ and in most cases can be neglected (unless dealing with amplified laser sources!)

Consider $V_{①} = \frac{e}{mc} \vec{P} \cdot \vec{A}(\vec{r},t) = \frac{e}{mc} P_z \cdot$
$\cdot \left[ A_0 e^{i(ky-\omega t)} + A_0^* e^{-i(ky-\omega t)} \right]$

(Recall $V = \underbrace{V_0 e^{i\omega t}}_{\text{emission}} + \underbrace{V_0^+ e^{-i\omega t}}_{\text{absorption}}$)

Example

Transition rate in the case of absorption $\Rightarrow$

$$\underbrace{P_{i\to f}}_{\text{discrete}} = \frac{2\pi}{\hbar} \left(\frac{e}{mc}\right)^2 |A_0|^2 \left| \langle f | e^{iky} P_z | i \rangle \right|^2,$$

$$E_f = E_i + \hbar\omega$$

Approximations:

the region of interaction between EM wave and an atom is confined to $\sim a_0$ $\Rightarrow$

$$ky \sim \frac{2\pi}{\lambda} \cdot a_0 \ll 1 \Rightarrow$$

$$e^{iky} \simeq 1 + iky - \frac{1}{2} k^2 y^2 + \ldots$$

If consider $e^{iky} \simeq 1 \rightarrow$ electric dipole approximation

$\Rightarrow$

$$V_{①} \approx \underbrace{V_{DE}}_{\text{electric dipole}} = \frac{e}{mc} P_z \underbrace{\left(A_0 e^{-i\omega t} + A_0^* e^{i\omega t}\right)}_{\Uparrow} =$$

$$A_0 = \frac{E_0}{2i\omega}$$
$\uparrow$ p. 1

$$= -\frac{eE_0}{mc\omega} P_z \sin\omega t$$

So, what is $\langle f | V_{DE} | i \rangle$ ? $\Rightarrow$

$$\left\langle f \left| -\frac{eE_0}{mc\omega} P_z \sin\omega t \right| i \right\rangle = -\frac{eE_0}{m\omega} \sin\omega t \langle f | P_z | i \rangle =$$

$$= \underline{-ie\frac{\omega_{fi}}{\omega} E_0 \sin\omega t \langle f | z | i \rangle}$$ ← looks familiar!

$\uparrow$

$$\underbrace{\left\langle \frac{dz}{dt} \right\rangle}_{\frac{P_z}{m}} = \frac{i}{\hbar} \langle \overbrace{[H_0, z]}^{= -i\hbar\frac{P_z}{m}} \rangle$$ ← time evolution of expectation values (Phys 657)

$\uparrow$ consider only $H_{0,\text{matter}}$

$$\langle f | [z, H_0] | i \rangle = \underline{\frac{i\hbar}{m} \langle f | P_z | i \rangle} =$$

$$= \langle f | z \underbrace{H_0 | i}_{E_i |i\rangle} \rangle - \langle \underbrace{f | H_0}_{E_f \langle f|} z | i \rangle =$$

$$= -(E_f - E_i) \langle f | z | i \rangle = \underline{-\hbar\omega_{fi} \langle f | z | i \rangle}$$

$$\underline{\langle f | P_z | i \rangle = im\omega_{fi} \langle f | z | i \rangle}$$

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Consider $\langle f | z | i \rangle \Rightarrow$ if it's not $\neq 0$

transition $|i\rangle \Rightarrow |f\rangle$ is allowed in electric dipole approximation

$|i\rangle \Rightarrow R_{n_i l_i}(r)\, Y_{l_i}^{m_i}(\theta, \varphi)$

$|f\rangle \Rightarrow R_{n_f l_f}(r)\, Y_{l_f}^{m_f}(\theta, \varphi)$

$$\langle f | z | i \rangle = \sqrt{\frac{4\pi}{3}} \int_0^\infty R^*_{n_f l_f}(r)\, R_{n_i l_i}(r)\, r^3 dr \,\cdot$$

$z = r\cos\theta =$
$= r \cdot \sqrt{\frac{4\pi}{3}}\, Y_1^0$

$$\cdot \int Y_{l_f}^{m_f *}(\theta,\varphi)\, Y_1^0(\theta)\, Y_{l_i}^{m_i}(\theta,\varphi)\, d\Omega$$

Recall Phys 652 $\Rightarrow$ addition of angular momenta + parity of $Y_l^m$

$$\boxed{\begin{aligned} l_f &= l_i \pm 1 \\ m_f &= m_i \end{aligned}}$$

$\leftarrow$ selection rules for $z$-polariz.

$\Delta m = m_f - m_i = \pm 1 \leftarrow$ for $x, y$-polariz.

**HW:** How is $V_{DE}$ on p. 5 related to our "usual" $V = -e\vec{E}\cdot\vec{r}$ potential for interaction with electric fi[eld]