Διπολική προσέγγ. → κανόνες επιλογής

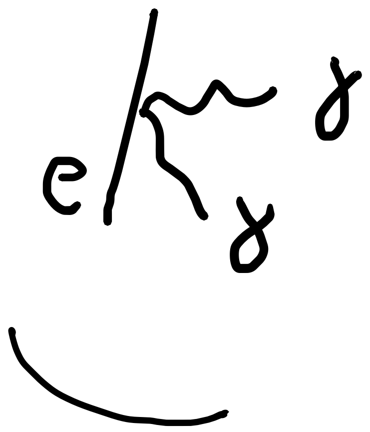
$H = H_0 + V \rightarrow$ διατ.

$\downarrow$

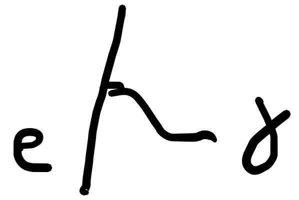
αδιατάρ.

$$H_0 = \frac{\vec{p}^{\,2}}{2m} \quad , \quad \vec{p} \rightarrow \vec{p} - \frac{e}{c}\vec{A} \quad \leftarrow \text{CGS} \qquad \text{SI } (\vec{p} \rightarrow \vec{p} - e\vec{A})$$

$$H = \underbrace{\frac{1}{2m}\left(p^2\right.}_{H_0} - \frac{2e}{c}\vec{A}\cdot\vec{p} + \underbrace{\left.\frac{e^2}{c^2}\vec{A}^{\,2}\right)}_{\rightarrow\, O(e^2)}$$



$$= H_0 - \frac{e}{mc}\vec{A}\cdot\vec{p} = H_0 + V$$



$\rightarrow \vec{k}\vec{r} \ll 1$

$e^{i\vec{k}\vec{r}} \sim 1$

Από τον ΗΜ $\vec{\nabla}\cdot\vec{A} = 0$, $\phi = 0$

$$\vec{E} = -\frac{1}{c}\frac{\partial \vec{A}}{\partial t}$$

$$k = \frac{\omega}{c}$$

$$\vec{B} = \vec{\nabla}\times\vec{A}$$

Για επίπεδα κύματα

$$\rightarrow \vec{A}(\vec{r},t) = \vec{A}_0(\omega)\, e^{i(\vec{k}\cdot\vec{r}-\omega t)} + \vec{A}_0^{+}(\omega)\, e^{-i(\vec{k}\cdot\vec{r}-\omega t)}$$

$$= \vec{A}_0(\vec{k},\vec{r})\, e^{-i\omega t} + \vec{A}_0^{+}(\vec{k},\vec{r})\, e^{i\omega t}$$

$$V(t) = -\frac{e}{mc}\vec{A}\cdot\vec{P} = -\frac{e}{mc}\left\{\vec{A}_0(\vec{k},\vec{r})\cdot\vec{P}\, e^{-i\omega t} + h.c\right\} = V_0\, e^{-i\omega t} + V_0^{+} e^{i\omega t}$$

Αρμονική διαταρ.

$$V(t) = V_0 e^{-i\omega t} + V_0^\dagger e^{i\omega t}$$

απορρόφηση
absorption

Διεγερμένη εκπομπή
St. emission

$$|i\rangle \longrightarrow |f\rangle \qquad w_{fi} \sim |\langle f|V_0|i\rangle|^2 \qquad |\langle f|V_0^\dagger|i\rangle|^2$$

$$\vec{A}_0 = ?$$

$$u_{EM} = \frac{1}{8\pi}(E^2+B^2) \sim |\vec{A}_0|^2$$

$\hookrightarrow n_\gamma \hbar\omega$

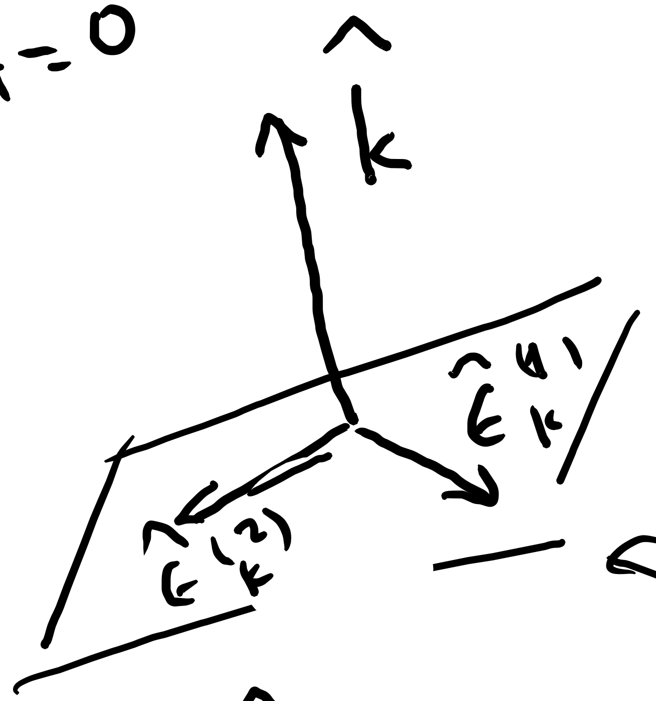
Μπορούμε να γράψουμε

$$\vec A(\vec r,t) = \vec A_0(\vec k,\vec r)\, e^{-i\omega t} + h.c$$

$$= A_0(\vec k,\vec r)\,\hat\varepsilon_{\vec k}\, e^{-i\omega t} + A_0^*(\vec k,\vec r)\,\hat\varepsilon^*_{\vec k}\, e^{i\omega t}$$

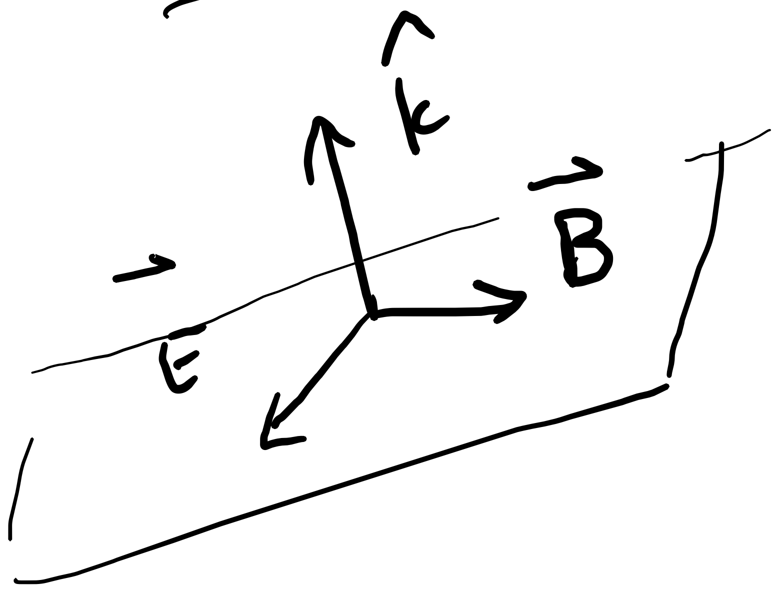
διάνυσμα πόλωσης

$\vec\nabla\cdot\vec A=0$



$\hat\epsilon_k^{(\lambda)}$

$\vec A \rightarrow \vec E = -\dfrac{\partial \vec A}{c\,\partial t}$



$$V(t) = -\frac{e}{mc}\vec{A}_0(\vec{k},\vec{r})\cdot\vec{p}\,e^{-i\omega t} + h.c.$$

$$A_0(\vec{k},\vec{r})\,\hat{\varepsilon}_k$$

$$= -\frac{e}{mc}A_0(\vec{k},\vec{r})\hat{\varepsilon}_k\cdot\vec{p}\,e^{-i\omega t} + h.c. = V_0 e^{-i\omega t} + h.c.$$

$$e^{i\vec{k}\cdot\vec{r}} = 1 + i\,\cancel{\vec{k}\cdot\vec{r}} + \ldots$$

διπολική προσέγγιση.

$$V_0 = -\frac{e}{mc}A_0(\vec{k},\vec{r})\,\hat{\varepsilon}_k\cdot\vec{p}$$

$k = ?$ ← ενέργεια των φωτονίων.

$k\cdot r \sim 10^{-3}$

$r = ?$ ← ατομικές ακτίνες

$k\cdot r \ll 1$

Στη διπολική προσέγγιση

$$V_0 \sim \hat{\epsilon}_{\vec{k}} \cdot \vec{p}$$

$$\langle f | V_0 | i \rangle \sim \hat{\epsilon}_{\vec{k}} \cdot \langle f | \vec{p} | i \rangle$$

$$\vec{p} = m \frac{d\vec{r}}{dt} = \frac{im}{\hbar} [H, \vec{r}] \quad , \quad p_x = \frac{im}{\hbar} [H, x]$$

$$m \hat{\epsilon}_{\vec{k}} \cdot \langle f | [H, \vec{r}] | i \rangle = m \hat{\epsilon}_{\vec{k}} \cdot \langle f | H\vec{r} - \vec{r} H | i \rangle$$

$$= \frac{im (E_f - E_i)}{\hbar} \hat{\epsilon}_k \cdot \langle f | \vec{r} | i \rangle$$

$$\langle f | V_d | i \rangle = -ie \frac{A_0 \omega}{c} \hat{\epsilon}_{\vec{k}} \cdot \langle f | \vec{r} | i \rangle$$

$$\vec{E} = -\frac{1}{c}\frac{\partial \vec{A}}{\partial t} \quad \mu\epsilon \quad \vec{A} = A_0 \hat{\epsilon}_{\vec{k}} e^{-i\omega t} + h.c$$

$$\rightarrow \langle f | V_0 | i \rangle = -e\vec{E} \cdot \langle f | \vec{r} | i \rangle = -\vec{E} \cdot \vec{d}$$

γι' αυτό λέγεται διπολική προσέγγ.

$$\vec{d} = e\vec{r} \qquad U = -\vec{E} \cdot \vec{d}$$

Κανόνες επιλογής για τη διπολική προσέγγιση

$$|2p\rangle \longrightarrow \underbrace{|1s\rangle + \gamma}_{|\ell' m'\rangle}$$

$\underbrace{|2p\rangle}_{|\ell m\rangle}$

γ: spin = 1

κανόνες επιλογής διπ. προσ. →

$$\Delta \ell = \ell' - \ell = \pm 1$$

$$\Delta m = m' - m = 0, \pm 1$$

Θυμόμαστε

$$\vec{L} = \vec{r} \times \vec{p}$$

$$L^2 |\ell m\rangle = \hbar^2 \ell(\ell+1) |\ell m\rangle \qquad \langle \ell' m' | \ell m\rangle = \delta_{\ell\ell'} \delta_{mm'}$$

$$L_3 |\ell m\rangle = \hbar m |\ell m\rangle$$

$$Y_{\ell m}(\hat{r}) = \langle \hat{r} | \ell m\rangle \quad , \hat{r} = (\vartheta, \varphi)$$

$$Y_{\ell m}^* = (-1)^m Y_{\ell, -m}$$

$$Y_{1,1} = -\frac{1}{2}\sqrt{\frac{3}{2\pi}}\sin\vartheta e^{i\varphi}$$ ((Condon, Shortley, Rose) (CSR)

(ϑ, φ)

$\cos\vartheta = \hat{r}\cdot\hat{z}$

$$Y_{1,\pm 1}(\hat{r}) = \mp\sqrt{\frac{3}{8\pi}}\,\hat{r}\cdot(\hat{x} \pm i\hat{y})$$

$$Y_{1,0} = \sqrt{\frac{3}{4\pi}}\,\hat{r}\cdot\hat{z}$$

$$Y_{00} = \frac{1}{\sqrt{4\pi}}$$

$l = 1$

$m = 0, \pm 1$

$$\hat{r} = \ldots Y_{1,1} + \ldots Y_{1,-1} + \ldots Y_{10}$$

$$\hat{x} = \sin\vartheta\cos\varphi\,\hat{r} + \cos\vartheta\cos\varphi\,\hat{\vartheta} - \sin\varphi\,\hat{\varphi}$$

$$\hat{y} = \ldots$$

$$\hat{z} = \ldots$$

$$\sum_m \langle \hat{r} | lm \rangle \langle lm | \hat{r}' \rangle = \sum_m Y^*_{lm}(\hat{r}')\, Y_{lm}(\hat{r})$$

$$= \frac{2l+1}{4\pi} P_l(\hat{r}' \cdot \hat{r})$$

i.e. $$P_l(\hat{r}' \cdot \hat{r}) = \frac{4\pi}{2l+1} \sum_{m=-l}^{l} Y^*_{lm}(\hat{r}')\, Y_{lm}(\hat{r})$$

Διατήρηση στροφορμής

$$\frac{i}{\hbar}\frac{d\vec{L}}{dt} = [\vec{L}, H] = 0$$

$$[L^2, H] = [L_z, H] = 0$$

$$\langle l'm|\,[H, L^2]\,|lm\rangle = \langle l'm|\,HL^2 - L^2H\,|lm\rangle$$

$$= \hbar^2\left[l(l+1) - l'(l'+1)\right]\langle l'm|H|lm\rangle$$

$$[L^2, H] = 0 \Rightarrow l = l'$$

$$\langle l m' | [H, L_3] | l m \rangle = 0$$

$$\Rightarrow (m - m')\hbar \langle l m' | H | l m \rangle = 0$$

$$\Rightarrow \underline{m = m'}$$

n'

$$\boxed{\langle l' m' | H | l m \rangle = \delta_{ll'} \delta_{mm'}}$$

Ομοτιμία (Parity)

$|\vec r\rangle$

$$\underset{\text{τελ.}}{\hat{\vec r}}\,|\vec r\rangle = \underset{\text{ιδιοτ.}}{\vec r}\,|\vec r\rangle$$

$$P|\vec r\rangle = |-\vec r\rangle$$

$$(\theta,\varphi) \xrightarrow{P} (\pi-\theta,\ \pi+\varphi)$$

$$P|lm\rangle = (-1)^l\,|lm\rangle$$

$$P\,Y_{lm} = (-1)^l\,Y_{lm}$$

$$P^\dagger = P = P^{-1}$$

$$P^2 = \underline{1}$$

loxin $\quad P\vec{r}P = -\vec{r}$

$\vec{r}|\vec{r}\rangle = \vec{r}|\vec{r}\rangle$

$$\underbrace{\langle\vec{r}|P\vec{r}P|\psi\rangle} = \langle-\vec{r}|\,\vec{r}\,|\underbrace{P\psi}\rangle = -\vec{r}\,\langle-\vec{r}\underbrace{|}P|\psi\rangle$$

$$= -\vec{r}\,\langle\vec{r}|\psi\rangle$$

$$= \underbrace{-\langle\vec{r}|\,\underset{\uparrow\ \mathrm{T(r)}}{\vec{r}}\,|\psi\rangle}$$

$\rightarrow \boxed{P\vec{r}P = -\vec{r}}$

Στη διπολ. προσεγγ.

$$\vec{d}_{fi} = \langle f | \vec{r} | i \rangle$$

$$= -\langle f | P \vec{r} P | i \rangle = -P_f P_i \langle f | \vec{r} | i \rangle$$

$$\Rightarrow \boxed{P_f P_i = -1}$$