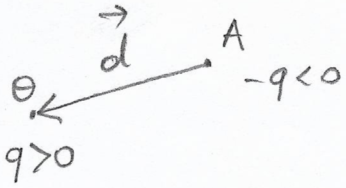
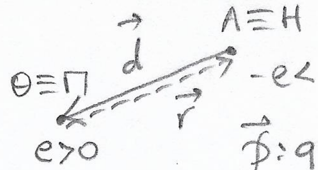
(ΗΛΕΚΤΡΙΚΗ) ΔΙΠΟΛΙΚΗ ΡΟΠΗ (electric) dipole moment

Ⓐ



$\vec d := \vec{A\Theta}$

$\vec{\wp} := q\cdot\vec d$



$\vec{\wp} := q\vec d = e(-\vec r)$

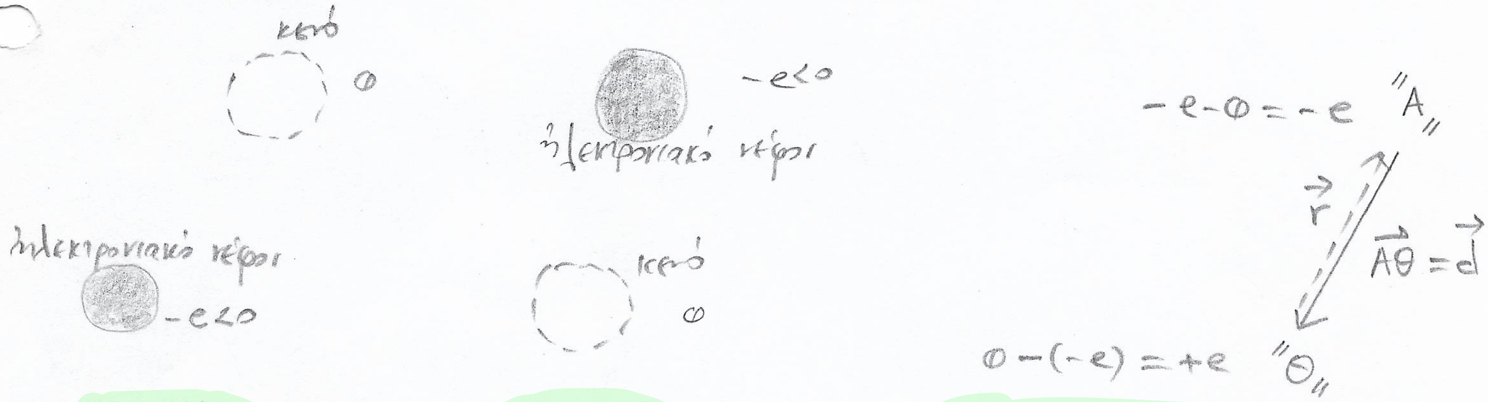
$\vec{\wp} = -e\vec r$

$[U] = N\cdot m = J$ $\qquad U = -\vec{\wp}\cdot\vec{\mathcal{E}}$ δυναμική ενέργεια (potential energy)

$[\vec\tau] = N\cdot m$ $\qquad \vec\tau = \vec{\wp}\times\vec{\mathcal{E}}$ (μηχανική) ροπή (torque)

ΗΛΕΚΤΡΙΚΗ ΔΙΠΟΛΙΚΗ ΡΟΠΗ ΜΕΤΑΒΑΣΕΩΣ

transition (electric) dipole moment



Αρχικώς $\qquad$ Τελικώς $\qquad$ Τελικώς − Αρχικώς

$\vec{\wp} = e\vec d = -e\vec r$

Τελεστής (ηλεκτρικής) διπολικής ροπής μετάβασης

$$\vec{\hat{d}} = \vec{\hat{p}} := \sum_{i=1}^{N} \sum_{j=1}^{N} \vec{d}_{ij} |\Phi_i\rangle\langle\Phi_j|$$

$$\vec{d}_{ij} = \vec{p}_{ij} = -e\langle\Phi_i|\vec{\hat{r}}|\Phi_j\rangle = \ldots = -e\int d^3r\, \Phi_i^*(\vec{r})\, \vec{r}\, \Phi_j(\vec{r})$$

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

$$\langle\Phi_i|\vec{\hat{r}}|\Phi_j\rangle = \sum_{|\vec{r}'\rangle}\sum_{|\vec{r}''\rangle} \langle\Phi_i|\vec{r}'\rangle\langle\vec{r}'|\vec{\hat{r}}|\vec{r}''\rangle\langle\vec{r}''|\Phi_j\rangle$$

$$= \sum_{|\vec{r}'\rangle}\sum_{|\vec{r}''\rangle} \Phi_i^*(\vec{r}')\, \vec{r}''\underbrace{\langle\vec{r}'|\vec{r}''\rangle}_{\delta_{\vec{r}'\vec{r}''}}\Phi_j(\vec{r}'')$$

$$= \sum_{|\vec{r}'\rangle} \Phi_i^*(\vec{r}')\, \vec{r}'\, \Phi_j(\vec{r}') = \sum_{|\vec{r}\rangle} \Phi_i^*(\vec{r})\, \vec{r}\, \Phi_j(\vec{r})$$

$$= \int d^3r\, \Phi_i^*(\vec{r})\, \vec{r}\, \Phi_j(\vec{r})$$

ΔΣ

$$\vec{\hat{p}} = \vec{d}_{11}|\Phi_1\rangle\langle\Phi_1| + \vec{d}_{12}|\Phi_1\rangle\langle\Phi_2| + \vec{d}_{21}|\Phi_2\rangle\langle\Phi_1| + \vec{d}_{22}|\Phi_2\rangle\langle\Phi_2|$$

$$\vec{d}_{11} = -e\int d^3r\, \Phi_1(\vec{r})^*\, \vec{r}\, \Phi_1(\vec{r}) = 0$$

$$\vec{d}_{12} = -e\int d^3r\, \Phi_1(\vec{r})^*\, \vec{r}\, \Phi_2(\vec{r}) \neq 0$$

$$\vec{d}_{21} = -e\int d^3r\, \Phi_2(\vec{r})^*\, \vec{r}\, \Phi_1(\vec{r}) \neq 0$$

$$\vec{d}_{22} = -e\int d^3r\, \Phi_2(\vec{r})^*\, \vec{r}\, \Phi_2(\vec{r}) = 0$$

$\vec{d}_{12} = \vec{d}_{21}$ για $\{\Phi_i(\vec{r})\}$ πραγματικές

$$\vec{\hat{p}} = \vec{d}_{12}\begin{pmatrix}0\\1\end{pmatrix}\begin{pmatrix}1 & 0\end{pmatrix} + \vec{d}_{21}\begin{pmatrix}1\\0\end{pmatrix}\begin{pmatrix}0 & 1\end{pmatrix} \Rightarrow \vec{\hat{p}} = \vec{d}_{12}\begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}$$

Γ

δυναμική ενέργεια

$$U_\mathcal{E} = -\vec{p}\cdot\vec{\mathcal{E}}$$

δυναμική ενέργεια m τρόπου

$$U_\mathcal{E}^m = -\vec{p}\cdot\vec{\mathcal{E}}_m^m$$

Τελεστής δυναμικής ενέργειας m τρόπου

$$\hat{U}_{\mathcal{E}m}^m = -\hat{\vec{p}}\cdot\hat{\vec{\mathcal{E}}}_m^m$$

$$\hat{U}_\mathcal{E}^m = -\sum_{i=1}^{N}\sum_{j=1}^{N}\vec{d}_{ij}\,|\Phi_i\rangle\langle\Phi_j|\cdot\hat{E}_x^m(z,t)\,\hat{x}$$

ΔΣ $\hat{U}_\mathcal{E}^m = -\vec{d}_{12}\begin{pmatrix}0&1\\1&0\end{pmatrix}\cdot\hat{E}_x^m(z,t)\,\hat{x} = -\begin{pmatrix}0&1\\1&0\end{pmatrix}\hat{E}_x^m(z,t)\;\vec{d}_{12}\cdot\hat{x}$

$$\vec{d}_{12}\cdot\hat{x} = -e\int d^3r\,\Phi_1^*(\vec{r})\,\vec{r}\,\Phi_2(\vec{r})\cdot\hat{x} =$$

$$= -e\int d^3r\,\Phi_1^*(\vec{r})\,x\,\Phi_2(\vec{r}) = -e\,x_{12} = p_{x12} := p$$

Άρα $\hat{U}_\mathcal{E}^m = e x_{12}\begin{pmatrix}0&1\\1&0\end{pmatrix}\hat{E}_x^m(z,t)$

$$\hat{E}_x^m(z,t) = \left(\frac{\hbar\omega_m}{\varepsilon_0 V}\right)^{1/2}\sin\left(\frac{m\pi z}{L}\right)\left(\hat{a}_m^\dagger + \hat{a}_m\right)$$

$$\hat{B}_y^m(z,t) = \left(\frac{\hbar\omega_m}{\varepsilon_0 V}\right)^{1/2}\frac{1}{c}\cos\left(\frac{m\pi z}{L}\right)i\left(\hat{a}_m^\dagger - \hat{a}_m\right)$$

$$\hat{S}_+ + \hat{S}_- = \begin{pmatrix}0&1\\0&0\end{pmatrix} + \begin{pmatrix}0&0\\1&0\end{pmatrix} = \begin{pmatrix}0&1\\1&0\end{pmatrix}$$

$\Rightarrow$

$$\hat{U}_\mathcal{E}^m = e x_{12}\left(\hat{S}_+ + \hat{S}_-\right)\left(\frac{\hbar\omega_m}{\varepsilon_0 V}\right)^{1/2}\sin\left(\frac{m\pi z}{L}\right)\left(\hat{a}_m^\dagger + \hat{a}_m\right)$$

$$\hat{U}_\mathcal{E}^m = \underbrace{e x_{12}\left(\frac{\hbar\omega_m}{\varepsilon_0 V}\right)^{1/2}\sin\left(\frac{m\pi z}{L}\right)}_{\hbar g^m}\left(\hat{S}_+ + \hat{S}_-\right)\left(\hat{a}_m^\dagger + \hat{a}_m\right)$$

$$\hbar g^m := e x_{12}\left(\frac{\hbar\omega_m}{\varepsilon_0 V}\right)^{1/2}\sin\left(\frac{m\pi z}{L}\right) \qquad (g_m)$$

$$\hat{U}_{\Sigma}^{m} = \hbar g^{m}(\hat{S}_{+}+\hat{S}_{-})(\hat{a}_{m}^{+}+\hat{a}_{m})$$

χαμιλτονιανή αλληλεπίδρασης ΔΣ – m τρόπου του ΗΜ πεδίου

(στην ατομική φυσική λέγεται συχνά $\hat{H}_{AF}$

AF = atom – field)

$$(g_m) \Rightarrow \hbar|g_m| = |\wp|\left(\frac{\hbar\omega_m}{\varepsilon_0 V}\right)^{1/2}\left|\sin\left(\frac{m\pi z}{L}\right)\right|$$

$$\Omega_R := 2\sqrt{n}\,g$$

$$\frac{\hbar\Omega_R}{2\sqrt{n}} = |\wp|\left(\frac{\hbar\omega_m}{\varepsilon_0 V}\right)^{1/2}\left|\sin\left(\frac{m\pi z}{L}\right)\right|$$

$$\Omega_R = \frac{|\wp|}{\hbar}\left(\frac{4\hbar\omega_m n}{\varepsilon_0 V}\right)^{1/2}\left|\sin\left(\frac{m\pi z}{L}\right)\right| := \frac{|\wp|E_{0m}}{\hbar}$$

πλάτος ηλεκτρικού πεδίου $\qquad E_{0m} = \left(\frac{4\hbar\omega_m n}{\varepsilon_0 V}\right)^{1/2}\cdot\underbrace{\left|\sin\left(\frac{m\pi z}{L}\right)\right|}$ χωρικά διαμορφωμένο

$$[E_{0m}] = \left(\frac{J}{\frac{F}{m}\cdot m^3}\right)^{1/2} = \frac{C\cdot V}{\frac{C}{V}\cdot m^2} = \frac{V}{m}$$

μονάδες ηλεκτρικού πεδίου

ΣΥΝΟΨΗ ΧΑΜΙΛΤΟΝΙΑΝΩΝ

$\hat{H}_{HM,m} = \hbar\omega_m\left(\hat{a}_m^{+}\hat{a}_m + \frac{1}{2}\right)$ m τρόπος HM πεδίου $\hbar\omega_m\left(\hat{N}_m + \frac{1}{2}\right)$

$\omega_m = \frac{m\pi c}{L}$, $m \in \mathbb{N}^*$

κι αγνοώνται τον όρο $\frac{\hbar\omega_m}{2}$

$\hat{H}_{HM,m} = \hbar\omega_m \hat{a}_m^{+}\hat{a}_m$ $\hbar\omega_m\hat{N}_m$

$\hat{H}_{\Delta\Sigma} = E_2\hat{S}_+\hat{S}_- + E_1\hat{S}_-\hat{S}_+$ $E_2 - E_1 = \hbar\Omega$ διστάθμικό σύστημα

θέτονται $E_1 = 0$

$\hat{H}_{\Delta\Sigma} = \hbar\Omega\hat{S}_+\hat{S}_-$

"πλάτος" $E_{0m} = \left|\left(\frac{4\hbar\omega_m\eta_m}{\varepsilon_0 V}\right)^{1/2}\sin\left(\frac{m\pi z}{L}\right)\right|$

$\hat{U}_{\varepsilon m} = \hbar g_m\left(\hat{S}_+ + \hat{S}_-\right)\left(\hat{a}_m^{+} + \hat{a}_m\right) = \hat{H}_{\text{αλληλ}\, HMm-\Delta\Sigma}$ αλληλεπίδραση m τρόπου HM πεδίου - ΔΣ

$\Omega_{Rm} = 2\sqrt{n_m}\, g_m$

$\Omega_{Rm} := \frac{|\wp| E_{0m}}{\hbar}$ συχνότητα Rabi

Άρα η συνολική Χαμιλτονιανή γράφεται

$\hat{H}_{Rm} = \hbar\omega_m\hat{a}_m^{+}\hat{a}_m + \hbar\Omega\hat{S}_+\hat{S}_- + \hbar g_m\left(\hat{S}_+ + \hat{S}_-\right)\left(\hat{a}_m^{+} + \hat{a}_m\right)$ ονομάζεται συχνά Χαμιλτονιανή Rabi

ΒΙΒΛΙΟ ΤΥΠΟΓΡΑΦΙΚΟ ΛΑΘΟΣ

~~ιδιο~~ καταστάσεων σελ. 155, 159

ΠΡΟΣΟΧΗ $|\uparrow, n_m\rangle$ κ $|\downarrow, n_m\rangle$ ιδιοκαταστάσεις της $\left(\hbar\omega_m\hat{a}_m^{+}\hat{a}_m + \hbar\Omega\hat{S}_+\hat{S}_-\right)$ $\hat{H}_{HMm} + \hat{H}_{\Delta\Sigma}$

και όχι της $\hat{H}_{HMm} + \hat{H}_{\Delta\Sigma} + \hat{H}_{\text{αλλ}\,\Delta\Sigma-HMm}$

Ας δούμε προσεκτικότερα τη Χαμιλτονιανή Αλληλεπίδρασης

ΔΣ – ενός τρόπου m του ΗΜ πεδίου

$$\hat{U}_{Em} = \hbar g_m (\hat{S}_+ + \hat{S}_-)(\hat{a}_m^{\dagger} + \hat{a}_m) =$$

$$= \hbar g_m \Big(\underbrace{\hat{S}_+ \hat{a}_m^{\dagger}}_{1ος} + \underbrace{\hat{S}_+ \hat{a}_m}_{2ος} + \underbrace{\hat{S}_- \hat{a}_m^{\dagger}}_{3ος} + \underbrace{\hat{S}_- \hat{a}_m}_{4ος} \Big)$$

1ος $\hat{S}_+ \hat{a}_m^{\dagger}$

$\rightsquigarrow$ f_i, ω_i $\quad \begin{pmatrix} \circ \\ \bullet \end{pmatrix}$ πριν $\quad \begin{pmatrix} \bullet \\ \circ \end{pmatrix}$ μετά $\rightsquigarrow$ $\rightsquigarrow$ $\quad \Delta E > 0$

$f_f < f_i$, $\omega_f < \omega_i$

άν έχω πολλούς τρόπους δεν είναι παράλογος μηχανισμός

2ος $\hat{S}_+ \hat{a}_m$

$\rightsquigarrow \begin{pmatrix} \circ \\ \bullet \end{pmatrix}$ πριν $\quad \begin{pmatrix} \bullet \\ \circ \end{pmatrix}$ μετά

Ίσως διατηρεί την ενέργεια

3ος $\hat{S}_- \hat{a}_m^{\dagger}$

$\begin{pmatrix} \bullet \\ \circ \end{pmatrix}$ πριν $\quad \begin{pmatrix} \circ \\ \bullet \end{pmatrix}$ μετά $\rightsquigarrow$

Ίσως διατηρεί την ενέργεια

4ος $\hat{S}_- \hat{a}_m$ $\rightsquigarrow$

$\rightsquigarrow$ f_i, ω_i $\quad \begin{pmatrix} \bullet \\ \circ \end{pmatrix}$ πριν $\quad \begin{pmatrix} \circ \\ \bullet \end{pmatrix}$ $\quad \Delta E < 0$

$\rightsquigarrow$ $f_f > f_i$, $\omega_f > \omega_i$

άν έχω πολλούς τρόπους δεν είναι παράλογος μηχανισμός

Αν αγνοήσουμε τον 1ο και τον 4ο όρο που ο καθένας μόνος του δε διατηρεί την ενέργεια

$$\Rightarrow \hat{U}_{Em} = \hbar g_m (\hat{S}_+ \hat{a}_m + \hat{S}_- \hat{a}_m^{\dagger})$$

$$\boxed{\hat{H}_{JCm} = \hbar \omega_m \hat{a}_m^{\dagger} \hat{a}_m + \hbar \Omega \hat{S}_+ \hat{S}_- + \hbar g_m (\hat{S}_+ \hat{a}_m + \hat{S}_- \hat{a}_m^{\dagger})}$$

Jaynes–Cummings Χαμιλτονιανή

$$\hat{H}_{\Delta\Sigma} = E_2 \hat{S}_+ \hat{S}_- + E_1 \hat{S}_- \hat{S}_+ \qquad E_2 - E_1 = \hbar\Omega$$

μπορούμε να θέσουμε

$$E_2 = \frac{\hbar\Omega}{2}$$

$\hbar\Omega$ μηδέν

$$E_1 = -\frac{\hbar\Omega}{2}$$

$$\hat{H}_{\Delta\Sigma} = \frac{\hbar\Omega}{2}\hat{S}_+\hat{S}_- - \frac{\hbar\Omega}{2}\hat{S}_-\hat{S}_+$$

$$\left.\begin{aligned} \hat{S}_+\hat{S}_- &= \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \\ \hat{S}_-\hat{S}_+ &= \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \end{aligned}\right\} \quad \begin{aligned} \hat{S}_+\hat{S}_- + \hat{S}_-\hat{S}_+ &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\ \hat{S}_+\hat{S}_- - \hat{S}_-\hat{S}_+ &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \hat{\sigma}_z \end{aligned}$$

Άρα $\hat{H}_{\Delta\Sigma} = \frac{\hbar\Omega}{2}\hat{\sigma}_z$ η μορφή του $\hat{H}_{\Delta\Sigma}$ στο άρθρο των Jaynes–Cummings

$\hat{a}^{+}|n\rangle = \sqrt{n+1}\,|n+1\rangle \qquad \hat{a}|n\rangle = \sqrt{n}\,|n-1\rangle$

ΑΣΚΗΣΗ

Να αποδειχτούν οι σχέσεις

α' $[\hat{a},\hat{a}] = 0$ β' $[\hat{a}^{+},\hat{a}^{+}] = 0$ γ' $[\hat{a},\hat{a}^{+}] = 1$ δ' $\hat{N}|n\rangle = n|n\rangle$

ε' $[\hat{N},\hat{a}] = -\hat{a}$ στ' $[\hat{N},\hat{a}^{+}] = \hat{a}^{+}$ ζ' $\hat{N}(\hat{a}|n\rangle) = (n-1)(\hat{a}|n\rangle)$

η' $\hat{N}(\hat{a}^{+}|n\rangle) = (n+1)(\hat{a}^{+}|n\rangle)$

α' $[\hat{a},\hat{a}] = \hat{a}\hat{a} - \hat{a}\hat{a} = 0$ β' $[\hat{a}^{+},\hat{a}^{+}] = \hat{a}^{+}\hat{a}^{+} - \hat{a}^{+}\hat{a}^{+} = 0$

γ' $$[\hat{a},\hat{a}^{+}]|n\rangle = \hat{a}\hat{a}^{+}|n\rangle - \hat{a}^{+}\hat{a}|n\rangle = \hat{a}\sqrt{n+1}\,|n+1\rangle - \hat{a}^{+}\sqrt{n}\,|n-1\rangle =$$
$$= \sqrt{n+1}\sqrt{n+1}\,|n\rangle - \sqrt{n}\sqrt{n}\,|n\rangle = (n+1)|n\rangle - n|n\rangle = 1.|n\rangle$$

$$\Rightarrow [\hat{a},\hat{a}^{+}] = 1$$

ε' $$[\hat{N},\hat{a}] = [\hat{a}^{+}\hat{a},\hat{a}] = \hat{a}^{+}\underbrace{[\hat{a},\hat{a}]}_{0} + \underbrace{[\hat{a}^{+},\hat{a}]}_{-1}\hat{a} = -\hat{a}$$

στ' $$[\hat{N},\hat{a}^{+}] = [\hat{a}^{+}\hat{a},\hat{a}^{+}] = \hat{a}^{+}\underbrace{[\hat{a},\hat{a}^{+}]}_{1} + \underbrace{[\hat{a}^{+},\hat{a}^{+}]}_{0}\hat{a} = \hat{a}^{+}$$

δ' $$\hat{N}|n\rangle = \hat{a}^{+}\hat{a}|n\rangle = \hat{a}^{+}\sqrt{n}\,|n-1\rangle = \sqrt{n}\sqrt{n}\,|n\rangle = n|n\rangle \Rightarrow \hat{N}|n\rangle = n|n\rangle$$

ζ' $$\hat{N}(\hat{a}|n\rangle) = \hat{N}\sqrt{n}\,|n-1\rangle = \sqrt{n}\,(n-1)\,|n-1\rangle = (n-1)\sqrt{n}\,|n-1\rangle = (n-1)(\hat{a}|n\rangle)$$

η' $$\hat{N}(\hat{a}^{+}|n\rangle) = \hat{N}\sqrt{n+1}\,|n+1\rangle = \sqrt{n+1}\,\hat{N}|n+1\rangle = \sqrt{n+1}\,(n+1)|n+1\rangle =$$
$$(n+1)\sqrt{n+1}\,|n+1\rangle$$
$$(n+1)(\hat{a}^{+}|n\rangle)$$