Κανόνες επιλογής συνέχεια :

Διπολική προσ. $\exists \ \langle f | \vec{r} | i \rangle = \vec{d}_{fi}$

$$= \underbrace{\int \psi_f^*(\vec{r}) \, \vec{r} \, \psi_i(\vec{r}) \, d^3\vec{r}}_{\vec{p} \simeq [H, \vec{r}]}$$

Διπολ. προσ. $e^{i\vec{k}\cdot\vec{r}} = 1 + i\vec{k}\vec{r} + \cdots \simeq 1$

διπολ. προσ.

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

$$\psi_i(\vec{r}) = R_{nl}(r) \, Y_{lm}(\vartheta, \varphi)$$

$$\psi_f(\vec{r}) = R_{n'l'}(r) \, Y_{l'm'}(\vartheta, \varphi)$$

Κανόνες επιλογής

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

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

$$\int Y_{l'm'}^*(\vartheta, \varphi) \, Y_{lm}(\vartheta, \varphi) \, d\Omega = \delta_{mm'} \, \delta_{ll'}$$

$$Y_{1,1} = -\frac{1}{2}\sqrt{\frac{3}{2\pi}}\, e^{i\varphi} \sin\theta = -\frac{1}{2}\sqrt{\frac{3}{2\pi}} \left(\frac{x+iy}{r}\right).$$

$$Y_{1,0} = \frac{1}{2}\sqrt{\frac{3}{\pi}}\; \frac{z}{r}$$

$$Y_{1,-1} = \frac{1}{2}\sqrt{\frac{3}{2\pi}} \left(\frac{x-iy}{r}\right).$$

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

$$\frac{x}{r}, \frac{y}{r}, \frac{z}{r}$$

$$\frac{z}{r} = 2\sqrt{\frac{\pi}{3}}\, Y_{10}$$

$$\frac{x}{r} = -\sqrt{\frac{2\pi}{3}} \left(Y_{11} + Y_{11}^* \right) = \sqrt{\frac{2\pi}{3}} \left(Y_{11} - Y_{1,-1} \right)$$

$$\frac{y}{r} = i\sqrt{\frac{2\pi}{3}} \left(Y_{11} - Y_{11}^* \right) = i\sqrt{\frac{2\pi}{3}} \left(Y_{11} + Y_{1-1} \right)$$

$$\frac{\vec{r}}{r} = \hat{r} = \frac{x}{r}\hat{x} + \frac{y}{r}\hat{y} + \frac{z}{r}\hat{z}$$

$$\Rightarrow \boxed{\vec{r} = r\sqrt{\frac{4\pi}{3}}\left\{ \hat{z}\, Y_{10} - \frac{\hat{x} - i\hat{y}}{\sqrt{2}} Y_{11} + \frac{\hat{x} + i\hat{y}}{\sqrt{2}} Y_{1,-1} \right\}} \;*$$

$$\hat{r} = \frac{\vec{r}}{r} = f\left\{ Y_{10}, Y_{1,\pm 1} \right\}$$

$$Y_{\ell=1,\, m=0,\pm 1}$$

$$\vec{r}$$

$$\langle f | \vec{r} | i \rangle$$

$$Y^*_{\ell' m'} \left\{ Y_{10}, Y_{1\pm1} \right\} Y_{\ell m} \rightsquigarrow \begin{array}{l} \Delta \ell = \pm 1 \\ \Delta m = 0, \pm 1 \end{array}$$

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

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

$\psi_f \sim Y_{l'm'}$

$\psi_i \sim Y_{lm}$

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

$P|l'm'\rangle = (-1)^{l'} |l'm'\rangle$

$P_i \cdot P_f = -1 \Leftrightarrow$ διπ. προσεγ.

$\rightarrow (-1)^{l'+l} = -1$

$\Delta l = l' - l \Rightarrow (-1)^{\Delta l + \overset{\text{άρτιος}}{\overline{2l}}} = -1$

$\Rightarrow$ $\Delta l =$ περιττός

$\Delta l = \pm 1$

$$\vec{d}_{fi} = \langle \psi_f | \vec{r} | \psi_i \rangle = \int d^3\vec{r}\, \psi_f^*(\vec{r})\, \underset{r\hat{r}}{\vec{r}}\, \psi_i(\vec{r}) \leftarrow \psi_i(\vec{r}) = R_{nl}(r) Y_{lm}(\underbrace{\theta,\varphi}_{\hat{r}})$$

$$d^3\vec{r} \to r^2 dr\, \underline{d\Omega}$$

$\sin\vartheta\, d\vartheta\, d\varphi = -d\cos\vartheta\, d\varphi$

$f \ldots n', l', m'$

$$= \int_0^\infty r^3 dr\, R_{n'l'}(r)\, R_{nl}(r) \leftarrow \text{ακτινικό μέρος } I_{rad}$$

$$\underbrace{\times \sqrt{\frac{4\pi}{3}} \int d\Omega\, Y_{l'm'}^*\, \{Y_{1m''}\}\, Y_{lm}}_{J_{m''}} \leftarrow \text{γωνιακό μέρος}$$

$$\{Y_{10}, Y_{11}, Y_{1,-1}\}$$

$$\to (-1)^{l'+l+1} = +1 \to (-1)^{\Delta l+1} = +1 \rightsquigarrow \Delta l = \text{περιττός}$$

$\Delta l = \text{περιττός}$

$Y_{\ell m} \sim e^{im\varphi}$

$J_{m''}$ θα περιέχει τον όρο $\int_0^{2\pi} d\varphi\, e^{i\varphi(m-m'+m'')}$

επειδή $m'-m \equiv \Delta m$ ο όρος γίνεται

$$\int_0^{2\pi} d\varphi\, e^{i\varphi(m''-\Delta m)}$$

και επειδή $\int_0^{2\pi} d\varphi\, e^{i\varphi(m_\alpha - m_\beta)} = 2\pi\,\delta_{m_\alpha, m_\beta}$

$$\int_0^{2\pi} d\varphi\, e^{i\varphi(m''-\Delta m)} = 2\pi\,\delta_{m'', \Delta m}$$

Άρα το $\langle \psi_f | \vec{r} | \psi_i \rangle = \vec{d}_{fi}$

θα είναι μηδέν εκτός αν $\boxed{\Delta m = m'' = 0, \pm 1}$

Αυτό σημαίνει ότι

$$\vec{d}_{fi} = I_{rad} \left\{ \hat{z} \, \overset{J_{m''}}{J_0} \, \delta_{m', m} - \frac{\hat{x} - i\hat{y}}{\sqrt{2}} J_1 \, \delta_{m', m+1} + \frac{\hat{x} + i\hat{y}}{\sqrt{2}} J_{-1} \, \delta_{m', m-1} \right\}$$

με $J_{m''} = \frac{\sqrt{4\pi}}{3} \int Y^*_{\ell' m'}(\theta,\varphi) \underbrace{Y_{1m''}(\theta,\varphi) Y_{\ell m}(\theta,\varphi) \, d\Omega}_{*}$

Αν $|i\rangle$ ήταν s-state, $\ell = 0$

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

$$J_{m''} = \sqrt{\frac{1}{3}} \int Y^*_{\ell' m'} Y_{1 m''} \, d\Omega = \sqrt{\frac{1}{3}} \, \delta_{\ell', 1} \, \delta_{m', m''}$$

$$\to \boxed{\ell' = 1}$$

Γενικότερα $\ell > 1$

στο $J_{m''}$ περιέχεται όρος $\underbrace{Y_{1m''}}_{\ell_1 = 1} \underbrace{Y_{\ell m}}_{\ell_2 = \ell}$

$$\ell_1 = 1 \oplus \ell_2 = \ell$$

$$Y_{1m''} Y_{lm} = C_1 Y_{l+1,m+m''} + C_2 Y_{l-1,m+m''} \quad (*)$$

$$\cancel{+ C_0 Y_{l,m+m''}}_{0} \quad \Delta l = 0$$

Επειδή ξέρω ότι $\Delta l =$ περιττ.

Clebsch-Gordan

(*) Επειδή

$$Y_{l_1 m_1}(\theta,\varphi)\, Y_{l_2 m_2}(\theta,\varphi) = \sum_{L=|l_1-l_2|}^{l_1+l_2} C(L, m_1+m_2; l_1, l_2, m_1, m_2)\, Y_{L,m_1+m_2}(\theta,\varphi)$$

$$(*) \rightsquigarrow J_{m''} = \sqrt{\frac{4\pi}{3}} \int Y^{+}_{l'm'} \left\{ C_1 Y_{l+1,m+m''} + C_2 Y_{l-1,m+m''} \right\} d\Omega$$

$$= C_1 \delta_{l',l+1} \delta_{m',m+m''} + C_2 \delta_{l',l-1} \delta_{m',m+m''}$$

Άρα $\vec{d}_{fi} \neq 0$ αν $l' = l+1$ ή $l' = l-1$

δηλ. $\boxed{\Delta l = \pm 1}$ → διότι εκπέμπεται ή απορ. 1 γ

και $\boxed{\Delta m = m''}$

Βιβλιογραφία: Modern QM, Sakurai

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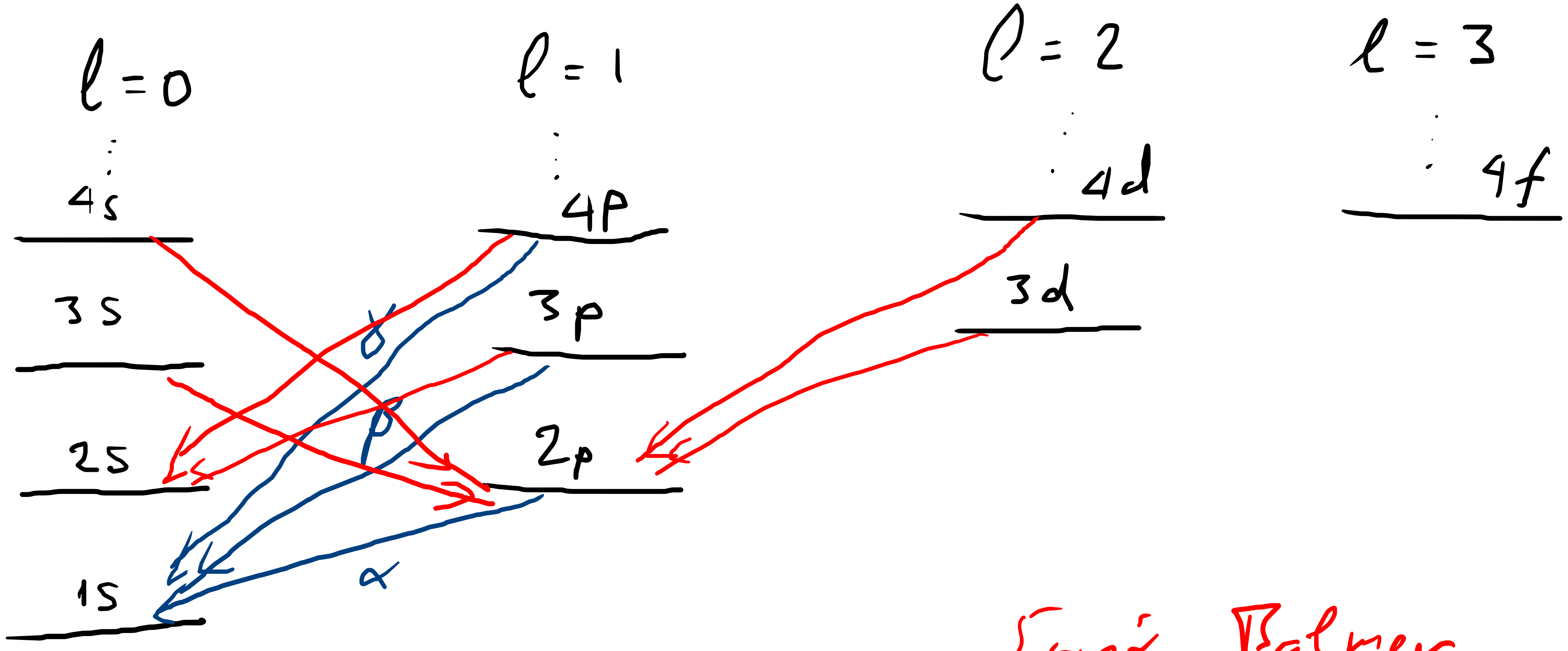
Gasiorowicz, Quantum Physics

Παραδείγματα από το H



Σειρά Balmer

Σειρά Lyman α, β, γ
μετάβαση στο 1s από
τα 2p, 3p, 4p