Nonrelativistic dipole approximation

- **Since we are considering strongly *non-relativistic* case, we may (for the moment) take non-relativistic Schrödinger wavefunctions in our matrix element:**

$$M_{ab} = \int \psi_a^*(\boldsymbol{r})\, \boldsymbol{\alpha}\, \boldsymbol{\varepsilon}\, \psi_b(\boldsymbol{r})\, d\boldsymbol{r}$$

$$\Downarrow$$

$$M_{ab} = \int \psi_a^*(\boldsymbol{r})\, \boldsymbol{p}\, \boldsymbol{\varepsilon}\, \psi_b(\boldsymbol{r})\, d\boldsymbol{r} = m\boldsymbol{\varepsilon} \int \psi_a^*(\boldsymbol{r})\, \dot{\boldsymbol{r}}\, \boldsymbol{\varepsilon}\, \psi_b(\boldsymbol{r})\, d\boldsymbol{r}$$

- **For the further evaluation of this matrix element we shall recall Heisenberg equation:**

$$\frac{d\hat{Q}}{dt} = \frac{i}{\hbar}\left[\hat{H}_0, \hat{Q}\right] \quad \Longrightarrow \quad \dot{\boldsymbol{r}} = \frac{i}{\hbar}\left[\hat{H}_0, \boldsymbol{r}\right]$$

- **By using this equation, we finally may find:**

$$M_{ab} = \frac{\boldsymbol{\varepsilon}}{i\hbar}(E_a - E_b) \int \psi_a^*(\boldsymbol{r})\, \boldsymbol{r}\, \psi_b(\boldsymbol{r})\, d\boldsymbol{r} = -\frac{\boldsymbol{\varepsilon}}{i\hbar e}(E_a - E_b) \int \psi_a^*(\boldsymbol{r}) \underbrace{(-e\boldsymbol{r})}_{\text{electric dipole moment}} \psi_b(\boldsymbol{r})\, d\boldsymbol{r}$$

E1 selection rules

- **From our discussion above it is clear that in order to understand whether some particular transition from level *n_b, l_b, m_b* to level *n_a, l_a, m_a* is allowed we have to find whether transition matrix element is zero or not:**

$$M_{ab} = -\frac{1}{i\hbar e}(E_a - E_b)\int \psi^*_{n_a l_a m_a}(\mathbf{r})(-e\mathbf{r})\psi_{n_b l_b m_b}(\mathbf{r})d\mathbf{r} =$$

$$\propto \int_0^\infty R_{n_a l_a}(r)\, R_{n_b l_b}(r) r^3\, dr \int Y^*_{l_a m_a}(\theta,\varphi)\left(\boldsymbol{\varepsilon}\cdot\hat{\mathbf{r}}\right)Y_{l_b m_b}(\theta,\varphi)\, d\Omega$$

- **For the further evaluation of this matrix element let us write vector product *εr* in terms of spherical components:**

$$\boldsymbol{\varepsilon}\cdot\hat{\boldsymbol{r}} = \sum_q \varepsilon^*_q r_q$$

E1 selection rules

$$\hat{\epsilon}\cdot\hat{r} = \epsilon_x \sin\theta\cos\phi + \epsilon_y \sin\theta\sin\phi + \epsilon_z\cos\theta$$

$$= \sqrt{\frac{4\pi}{3}}\left(\epsilon_z Y_{10} + \frac{-\epsilon_x + i\epsilon_y}{\sqrt{2}} Y_{11} + \frac{\epsilon_x + i\epsilon_y}{\sqrt{2}} Y_{1-1}\right)$$

Y_{lm}	l = 0	l = 1	l = 2	l = 3
m = -3				$\sqrt{\frac{35}{64\pi}}\sin^3\vartheta\, e^{-3i\varphi}$
m = −2			$\sqrt{\frac{15}{32\pi}}\sin^2\vartheta\, e^{-2i\varphi}$	$\sqrt{\frac{105}{32\pi}}\sin^2\vartheta\cos\vartheta\, e^{-2i\varphi}$
m = −1		$\sqrt{\frac{3}{8\pi}}\sin\vartheta\, e^{-i\varphi}$	$\sqrt{\frac{15}{8\pi}}\sin\vartheta\ \cos\vartheta\, e^{-i\varphi}$	$\sqrt{\frac{21}{64\pi}}\sin\vartheta\left(5\cos^2\vartheta - 1\right)\ e^{-i\varphi}$
m = 0	$\sqrt{\frac{1}{4\pi}}$	$\sqrt{\frac{3}{4\pi}}\cos\vartheta$	$\sqrt{\frac{5}{16\pi}}\left(3\cos^2\vartheta - 1\right)$	$\sqrt{\frac{7}{16\pi}}\left(5\cos^3\vartheta - 3\cos\vartheta\right)$
m = 1		$-\sqrt{\frac{3}{8\pi}}\sin\vartheta\, e^{i\varphi}$	$-\sqrt{\frac{15}{8\pi}}\sin\vartheta\ \cos\vartheta\, e^{i\varphi}$	$-\sqrt{\frac{21}{64\pi}}\sin\vartheta\left(5\cos^2\vartheta - 1\right)\ e^{i\varphi}$
m = 2			$\sqrt{\frac{15}{32\pi}}\sin^2\vartheta\, e^{2i\varphi}$	$\sqrt{\frac{105}{32\pi}}\sin^2\vartheta\cos\vartheta\, e^{2i\varphi}$
m = 3				$-\sqrt{\frac{35}{64\pi}}\sin^3\vartheta\, e^{3i\varphi}$

E1 selection rules

So we „simply" have to calculate following integral

$$M_{ab} \propto \int Y^*_{l_a m_a}(\theta,\varphi)\left(\varepsilon_z Y_{10} + \frac{-\varepsilon_x + i\varepsilon_y}{\sqrt{2}} Y_{11} + \frac{\varepsilon_x + i\varepsilon_y}{\sqrt{2}} Y_{1-1}\right) Y_{l_b m_b}(\theta,\varphi)\, d\Omega$$

Reminder on spherical harmonics

Simple number

$$Y_{\ell_1 m_1}(\theta,\phi)Y_{\ell_2 m_2}(\theta,\phi) = \sum_{\ell=|\ell_1-\ell_2|}^{\ell_1+\ell_2} \overbrace{\sqrt{\frac{(2\ell_1+1)(2\ell_2+1)}{4\pi(2\ell+1)}}\langle \ell 0|\ell_1\ell_2 00\rangle}^{\text{Simple number}} \times$$

$$\times \underbrace{\langle \ell(m_1+m_2)|\ell_1\ell_2 m_1 m_2\rangle}_{\text{Clebsch – Gordan – coefficients (CGC)}} Y_{\ell(m_1+m_2)}(\theta,\phi)$$

Clebsch – Gordan – coefficients (CGC)

$$\langle JM \mid j_a m_a\, j_b m_b \rangle \neq 0, if$$

$$|j_a - j_b| \leq J \leq j_a + j_b$$

and

$$M = m_a + m_b$$

E1 selection rules

$$Y_{1m}(\theta,\phi)Y_{\ell_i m_i}(\theta,\phi) = \sum_{\ell=|\ell_i-1|}^{\ell_i+1}\sqrt{\frac{3(2\ell_i+1)}{4\pi(2\ell+1)}}\langle \ell 0|\ell_i 100\rangle \text{ x}$$

$$\text{x}\langle \ell(m+m_i)|\ell_i 1 m_i m\rangle Y_{\ell(m_i+m)}(\theta,\phi)$$

$$M_{ab} \propto \int Y^*_{l_a m_a}(\theta,\varphi)\,Y_{1m}(\theta,\varphi)Y_{l_b m_b}(\theta,\varphi)\,d\Omega =$$

$$= \sqrt{\frac{3(2l_b+1)}{4\pi(2l_n+1)}}\langle l_a 0|l_b 100\rangle\langle l_a m_a|l_b 1 l_b m\rangle$$

E1 selection rules

So we „simply“ have to calculate following integral

$$M_{ab} \propto \int Y^*_{l_a m_a}(\theta,\varphi)\left(\varepsilon_z Y_{10} + \frac{-\varepsilon_x + i\varepsilon_y}{\sqrt{2}} Y_{11} + \frac{\varepsilon_x + i\varepsilon_y}{\sqrt{2}} Y_{1-1}\right) Y_{l_b m_b}(\theta,\varphi)\, d\Omega$$

$$M_{ab} \propto = \sqrt{\frac{3(2l_b+1)}{4\pi(2l_n+1)}}\left\langle l_a 0 \middle| l_b 100 \right\rangle \times$$

$$\times\left(\varepsilon_z \left\langle l_a m_a \middle| l_b 1 m_b 0\right\rangle + \frac{-\varepsilon_x + i\varepsilon_y}{\sqrt{2}}\left\langle l_a m_a \middle| l_b 1 m_b 1\right\rangle + \frac{\varepsilon_x + i\varepsilon_y}{\sqrt{2}}\left\langle l_a m_a \middle| l_b 1 m_b -1\right\rangle\right)$$

E1 selection rules

So we „simply“ have to calculate following integral

$$M_{ab} \propto \int Y^{*}_{l_a m_a}(\theta,\varphi)\left(\varepsilon_z Y_{10} + \frac{-\varepsilon_x + i\varepsilon_y}{\sqrt{2}} Y_{11} + \frac{\varepsilon_x + i\varepsilon_y}{\sqrt{2}} Y_{1-1}\right) Y_{l_b m_b}(\theta,\varphi)\, d\Omega$$

$$M_{ab} \propto = \sqrt{\frac{3(2l_b+1)}{4\pi(2l_n+1)}}\,\overbrace{\left\langle l_a 0 \middle| l_b 100 \right\rangle}^{\Delta l=\cancel{0};\pm 1}\times$$

$$\times\left(\varepsilon_z \underbrace{\left\langle l_a m_a \middle| l_b 1 m_b 0\right\rangle}_{\Delta m=0} + \frac{-\varepsilon_x + i\varepsilon_y}{\sqrt{2}} \underbrace{\left\langle l_a m_a \middle| l_b 1 m_b 1\right\rangle}_{\Delta m=-1} + \frac{\varepsilon_x + i\varepsilon_y}{\sqrt{2}} \underbrace{\left\langle l_a m_a \middle| l_b 1 m_b -1\right\rangle}_{\Delta m=+1}\right)$$