# Electric dipole approximation (E1)

- **We have shown that for interaction of low-Z ions with visible light we may apply electric dipole (long-wave) approximation**

$$e^{i\boldsymbol{kr}} \approx 1$$

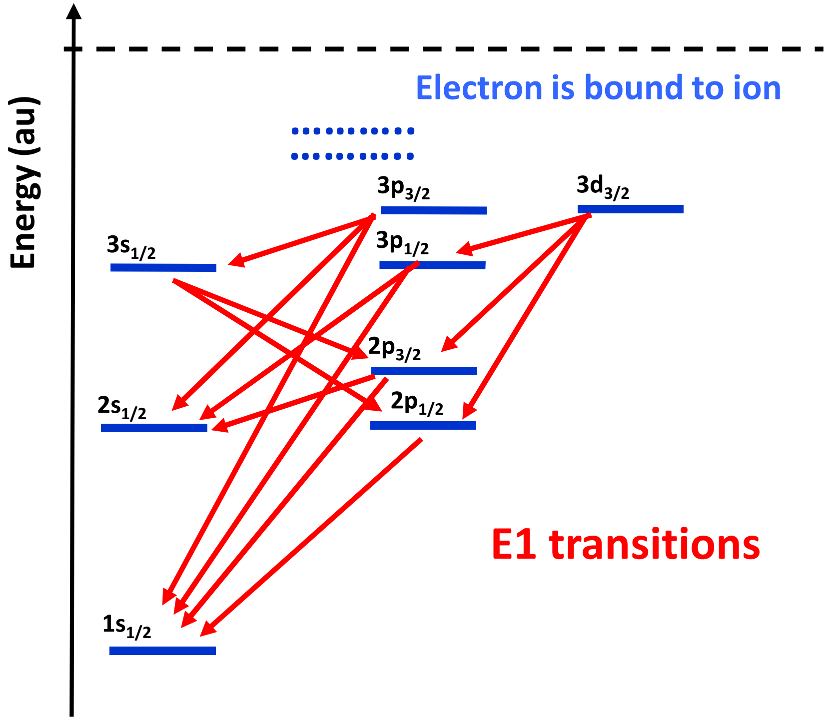
- **In this approximation transition amplitude reads as:**

$$M_{ab}^{(E1)} = \int \psi_a^*(\boldsymbol{r})\, \boldsymbol{\alpha}\, \boldsymbol{\varepsilon}\, \psi_b(\boldsymbol{r})\, d\boldsymbol{r}$$

- **Evaluation of this amplitude leads us to set of selection rules:**

$$\left| j_a - j_b \right| = 0, \pm 1$$

$$\pi_a = -\pi_b$$



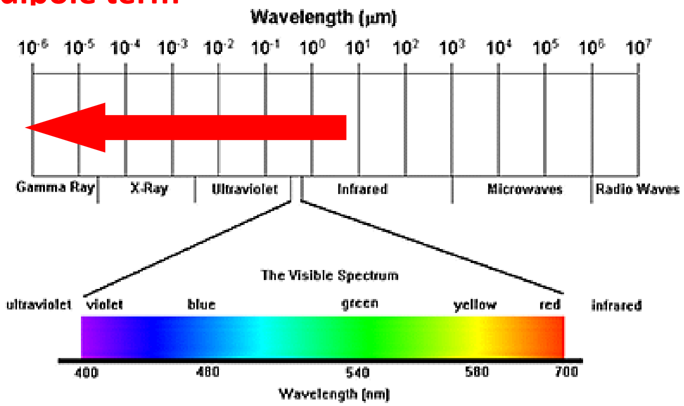
# Higher multipoles contributions

- **Transition matrix element can be evaluated by making "multipole expansion" of the electron-photon interaction operator:**

$$M_{ab} = \int \psi_a^+(\mathbf{r})\, \boldsymbol{\alpha}\, \boldsymbol{\varepsilon}\, e^{i\mathbf{kr}}\, \psi_b(\mathbf{r})\, d\mathbf{r}$$

$$e^{i\mathbf{kr}} = 1 + i\mathbf{kr} + \frac{1}{2}(i\mathbf{kr})^2 + \ldots$$

electric dipole term




X-rays: $k \approx 10^8\ cm^{-1}$

γ-rays: $k > 10^9\ cm^{-1}$

- **For interaction of heavy ions with energetic photons we may find that:**

$$kr \approx 1$$

- **Which means that electric dipole approximation is not longer valid!**

We have to take into account higher (non-dipole) terms!

# Beyound the E1 approximation

(first correction)

- **Let us consider the next term in the multipole decomposition of electron-photon interaction:**

$$e^{i\boldsymbol{kr}} = 1 + \underbrace{i\boldsymbol{kr}} + \frac{1}{2}\left(i\boldsymbol{kr}\right)^2 + \ldots$$

- **And let us analyze matrix element containing this term:**

$$M'_{ab} = \int \psi_a^+(\boldsymbol{r})\, \boldsymbol{\alpha}\, \boldsymbol{\varepsilon} \left(i\boldsymbol{kr}\right) \psi_b(\boldsymbol{r})\, d\boldsymbol{r}$$

- **Again, to make mathematical analysis more "clear" let us restrict ourselves now to the non-relativistic formulation of this matrix element:**

$$M'_{ab} \propto \int \psi_a^+(\boldsymbol{r})\, \boldsymbol{p}\, \boldsymbol{\varepsilon} \left(i\boldsymbol{kr}\right) \psi_b(\boldsymbol{r})\, d\boldsymbol{r}$$

By assuming photon propagating along z-axis ($\boldsymbol{k} \uparrow\uparrow O_z$), we can choose photon polarization in x-direction (remember: $\boldsymbol{k} \cdot \boldsymbol{\varepsilon} = 0$).

$$\Rightarrow \quad M'_{ab} \propto \int \psi_a^+(\boldsymbol{r})\, p_x\, z\, \psi_b(\boldsymbol{r})\, d\boldsymbol{r}$$

# Beyound the E1 approximation

(magnetic dipole and electric quadrupole transitions)

- **Let us re-write our matrix element as:**

$$M'_{ab} \propto \int \psi_a^+(\mathbf{r})\, p_x\, z\, \psi_b(\mathbf{r})d\mathbf{r} = \int \psi_a^+(\mathbf{r})(p_x\, z - x\, p_z)\psi_b(\mathbf{r})d\mathbf{r}$$

$$+ \int \psi_a^+(\mathbf{r})\, x\, p_z\, \psi_b(\mathbf{r})d\mathbf{r}$$

- **By using the fact that:** $\hat{L}_y = zp_x - xp_z$
- **and:** $\dot{z} = \frac{i}{\hbar}\left[\hat{H}_0, z\right]$

$\Downarrow$ (in a.u.)

$$M'_{ab} \propto \int \psi_a^+(\mathbf{r})\, L_y\, \psi_b(\mathbf{r})d\mathbf{r} + i\,\omega_{ab} \int \psi_a^+(\mathbf{r})\, x\, z\, \psi_b(\mathbf{r})d\mathbf{r}$$

# Higher multipoles contributions

(M1 and E2 terms)

- **We just have found that:**

$$M_{ab}^{(M1,E2)} \propto \underbrace{\int \psi_a^+(\mathbf{r})\, L_y\, \psi_b(\mathbf{r})\, d\mathbf{r}}_{\text{magnetic dipole (M1) term}} + i\omega_{ab} \underbrace{\int \psi_a^+(\mathbf{r})\, x\, z\, \psi_b(\mathbf{r})\, d\mathbf{r}}_{\text{electric quadrupole (E2) term}}$$

Proportional to magnetic moment of the ion

$$\hat{\boldsymbol{\mu}} = -\mu_0 (\hat{\mathbf{L}} + g\hat{\mathbf{S}})/\hbar$$

Proportional to electric quadrupole moment of the ion

$$Q_{ij} = \sum_n q_n \left(3x_i x_j - x^2 \delta_{ij}\right)$$

deviation from spherical shape!

⇒ After some algebra, selection rules for these transitions can be found!

# Magnetic dipole and electric quadrupole transitions

(Selection rules)

- **We just have found that:**

$$M_{ab}^{(M1,E2)} \propto \underbrace{\int \psi_a^+(\mathbf{r})\, L_y\, \psi_b(\mathbf{r})\, d\mathbf{r}}_{\text{magnetic dipole (M1) term}} + i\omega_{ab} \underbrace{\int \psi_a^+(\mathbf{r})\, x\, z\, \psi_b(\mathbf{r})\, d\mathbf{r}}_{\text{electric quadrupole (E2) term}}$$

$$\boxed{\begin{array}{c} |j_a - j_b| = 0, \pm 1 \\ \pi_a = \pi_b \end{array}} \qquad \boxed{\begin{array}{c} |j_a - j_b| = 0, \pm 1, \pm 2 \\ \pi_a = \pi_b \end{array}}$$

- **By making further multipole decomposition of the electron-photon interaction we can obtain even higher terms:**

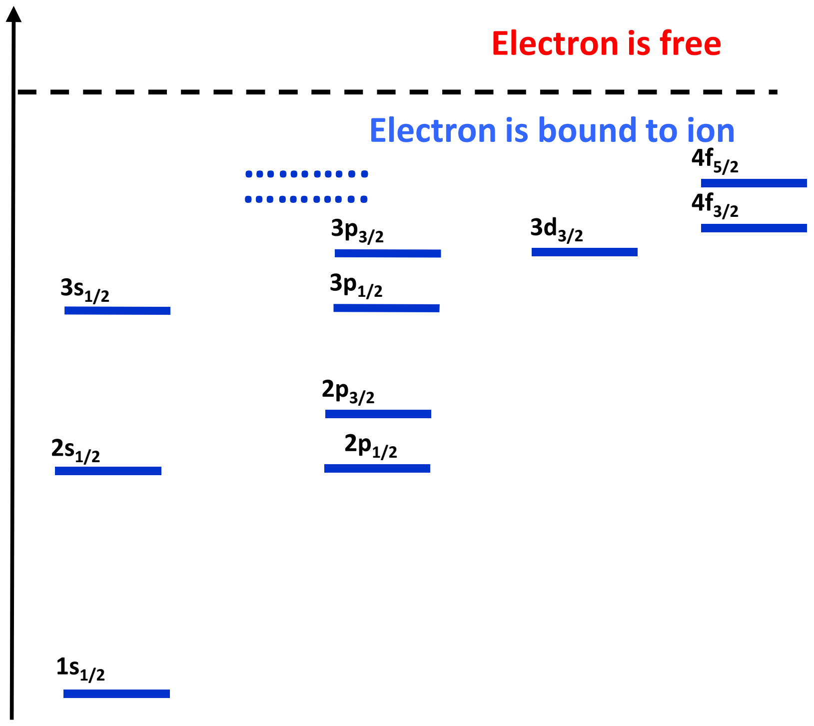
$$e^{i\mathbf{kr}} = 1 + i\mathbf{kr} + \frac{1}{2}(i\mathbf{kr})^2 + \ldots = E1 + M1 + E2 + M2 + E3 + \ldots.$$

# Multipole transitions

(selection rules)

| transition | selection rules |
|---|---|
| Electric dipole (E1) | $\left\lvert j_a - j_b \right\rvert = 0, \pm 1$ <br> $\pi_a = -\pi_b$ |
| Magnetic dipole (M1) | $\left\lvert j_a - j_b \right\rvert = 0, \pm 1$ <br> $\pi_a = \pi_b$ |
| Electric quadrupole (E2) | $\left\lvert j_a - j_b \right\rvert = 0, \pm 1, \pm 2$ <br> $\pi_a = \pi_b$ |
| Magnetic quadrupole (M2) | $\left\lvert j_a - j_b \right\rvert = 0, \pm 1, \pm 2$ <br> $\pi_a = -\pi_b$ |

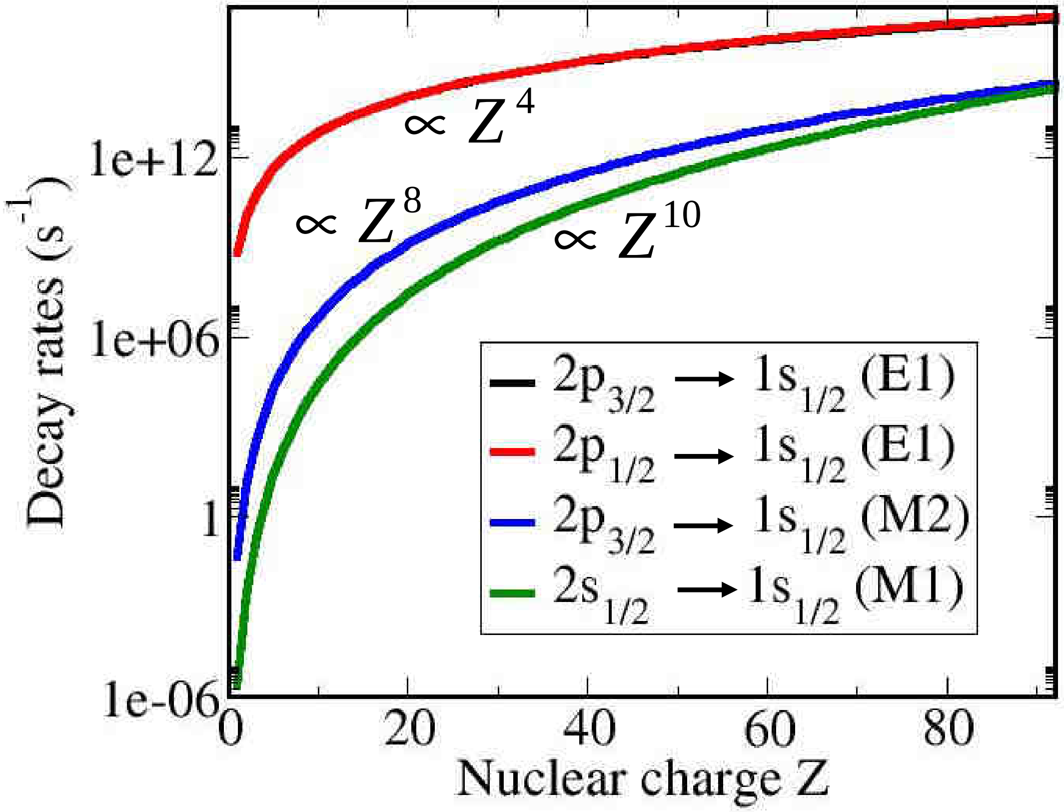
**(for all transitions** $0 \to 0$ **is forbidden and triangle rule** $\left\lvert j_a - j_b \right\rvert \le L \le j_a + j_b$ **should be satisfied)**

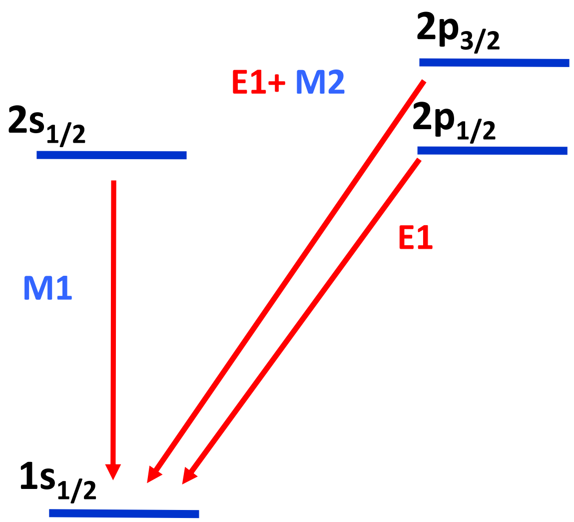



**Higher multipoles become more pronounced for heavy ions (large nuclear charges)!**

**(Remind yourself our discussion on value of *kr*)!**

# Z-scaling of multipole decay rates




- For low-Z higher multipole transition are orders of magnitude smaller than the leading electric dipole (E1) term.
- However, higher terms are enhanced with Z faster than E1 due to the increasing role of relativistic effects.

# Atomic photoionization

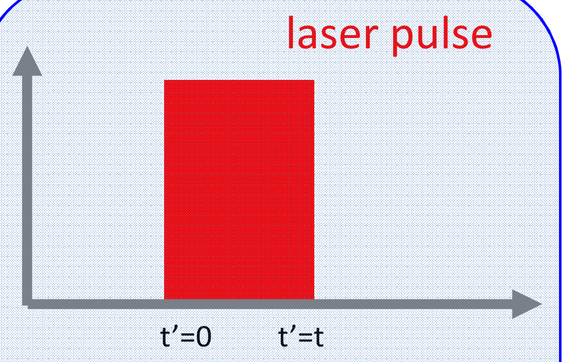
(theory background)

- For the case of the photoabsorption:

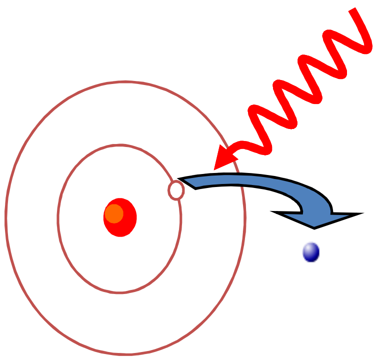
$$c_b^{(1)}(t) = \frac{ce}{i\hbar} \int_{\Delta_\omega} d\omega\, A_0(\omega)\, \mathrm{e}^{i\delta_\omega} \left\langle \psi_b \middle| \boldsymbol{\alpha}\, \boldsymbol{\varepsilon}\, e^{i\boldsymbol{kr}} \middle| \psi_a \right\rangle \int_0^t dt'\, \mathrm{e}^{i(E_b - E_a - \hbar\omega)t'/\hbar}$$

- We can get total cross section as:

$$d\sigma_{ab} = C \frac{1}{\omega_{ba}} \left| \left\langle \psi_b \middle| \boldsymbol{\alpha}\, \boldsymbol{\varepsilon}\, e^{i\boldsymbol{kr}} \middle| \psi_a \right\rangle \right|^2 \rho_b\, d\Omega$$




We assume that laser pulse is independent on time except for being "switched on" at t=0.



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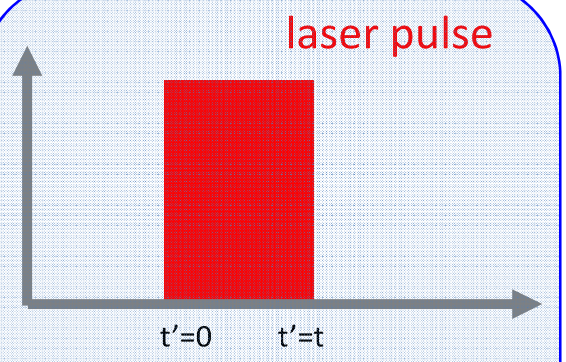


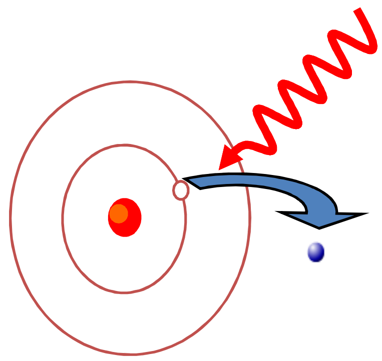

We assume that laser pulse is independent on time except for being "switched on" at t=0.

- Bound-free transition matrix element is:

$$M_{ab} = \langle \psi_b | \boldsymbol{\alpha}\, \boldsymbol{\varepsilon}\, e^{i\boldsymbol{kr}} | \psi_a \rangle \equiv \int \psi_b^+(\boldsymbol{r})\, \boldsymbol{\alpha}\, \boldsymbol{\varepsilon}\, e^{i\boldsymbol{kr}}\, \psi_a(\boldsymbol{r}) d\boldsymbol{r}$$

continuum wave function

bound wave function



# K-shell atomic photoionization

(non-relativistic framework)

- We shall consider evaluation of the bound-free matrix element for the moment in the non-relativistic framework:

$$M_{ab} = \int \psi_b^{+}(\boldsymbol{r})\ \boldsymbol{\varepsilon}\, e^{i\boldsymbol{kr}}\ \nabla\ \psi_{1s}(\boldsymbol{r})d\boldsymbol{r}$$

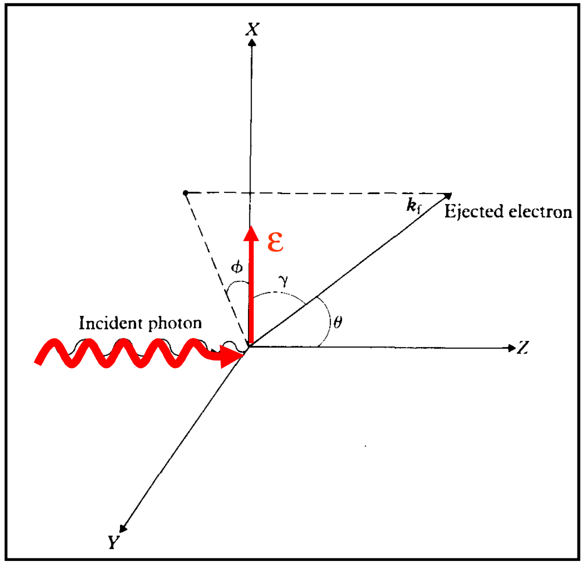
- And let us make an approximation in which continuum electron will be decsribed by the plane wave! (We neglected the interaction of a nucleus with electron in continuum):

$$M_{ab} = C \cdot \int e^{-i\boldsymbol{k}_b\boldsymbol{r}}\ \ \boldsymbol{\varepsilon}\, e^{i\boldsymbol{kr}}\ \nabla\ \psi_{1s}(\boldsymbol{r})d\boldsymbol{r}$$

$$\Downarrow$$

Angular differential photoionization cross section

$$\frac{d\sigma}{d\Omega} = C \cdot \left|M_{ab}\right|^2 \approx C \cdot \sin^2\theta \cos^2\varphi$$

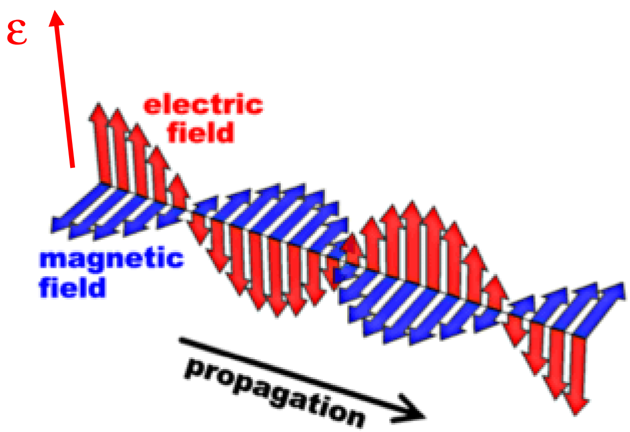


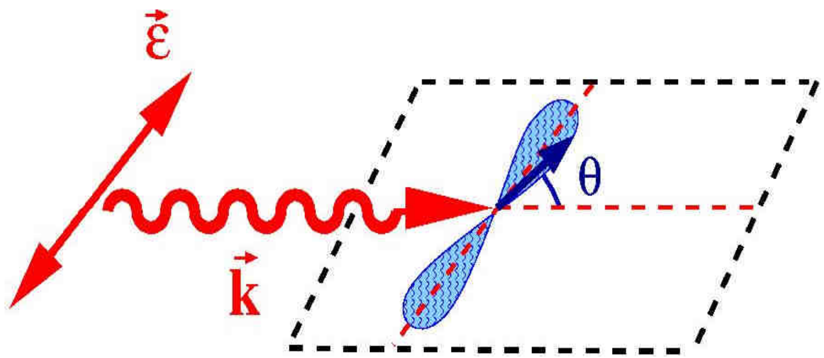
# K-shell atomic photoionization

(non-relativistic framework)

- Simple physical interpretation can be obtained for the derived cross section:

$$\frac{d\sigma}{d\Omega} = C \cdot \left| M_{ab} \right|^2 \approx C \cdot \sin^2 \theta \cos^2 \varphi$$




- Obviously: in non-relativistic electric-dipole (E1) approximation electron should be emitted along the electric field vector = polarization vector of EM wave.

For the case of unpolarized light:

$$\left. \frac{d\sigma}{d\Omega} \right|_{unp} \approx C \cdot \sin^2 \theta$$

# Summary of Effects with light and matter

(non-relativistic framework)

| Effect | Initial wavefunction | Final wavefunction |
|---|---|---|
| Photoabsorption (Excitation) | bound state | bound state |
| Photoionization | bound state | continuous state |
| Radiative electron capture | bound | bound state |
| Radiative recombination | continuous state | bound state |
| bremsstrahlung | continuous state | continuous state |
| pair production | neg. continuous state | bound state |