Photon absorption and emission

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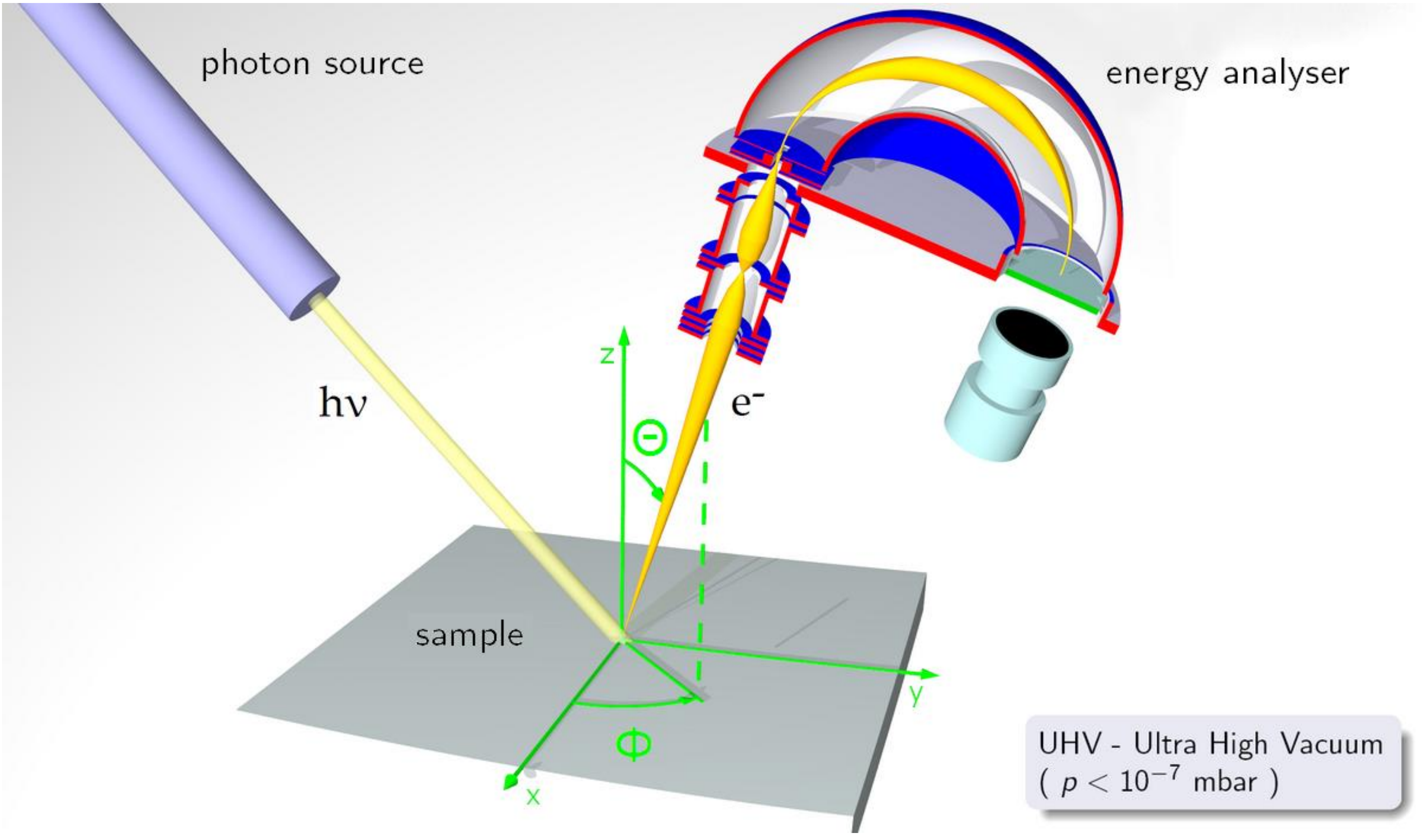
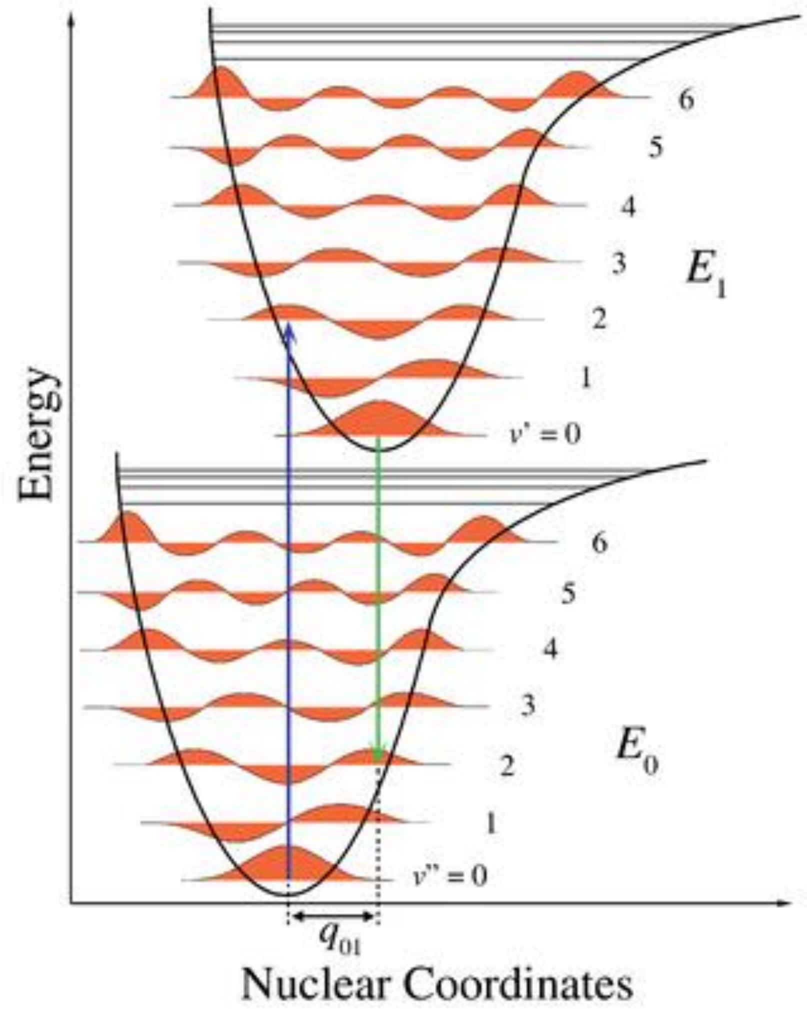
Photoelectric effect





Hamiltonian

- $\mathrm{H} = H_m + H_{rad} + H_I$

$$H_m = \sum_i \frac{p_i^2}{2m_i} + \frac{1}{2}\sum_{i,j} \frac{e_i e_j}{4\pi\left|r_i - r_j\right|}$$

$$H_{rad} = \frac{1}{2}\int (E_T^2 + B^2) d^3x$$

$$H_I = \sum_i (-\frac{e_i}{m_i c} A_i \cdot p_i + \frac{e_i^2}{2m_i c^2} A_i^2)$$

A(x,t)= $\sum_k \sum_r \left(\frac{\hbar c^2}{2V\omega_k}\right)^{\frac{1}{2}} \varepsilon_r(k)[a_r(k,t)e^{ik\cdot x} + a_r^*(k,t)e^{-ik\cdot x}]$

Quantize radiation field

- Take A into hamiltonian $H_{rad} = \sum_k \sum_r \hbar\omega_k a_r^*(k) a_r(k)$
- Similar to oscillator Hamiltonian

$$H_{osc} = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2 = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right), \text{taking } a = \frac{1}{(2\hbar m\omega)^{\frac{1}{2}}}(m\omega q + ip)$$

Commutation relation $[a_r(k), a_s^\dagger(k')] = \delta_{rs}\delta_{kk'}, [a_r(k), a_s\ (k')] = 0$

So $H_{rad} = \sum_k \sum_r \hbar\omega_k a_r^\dagger(k) a_r(k)$

Eigenstate $|n_r(k)\rangle = \frac{[a_r^\dagger(k)]^{n_r(k)}}{\sqrt{n_r(k)!}}|0\rangle, with\ energy\ \sum_k \sum_r \hbar\omega_k n_r(k)$

Transition rate

- Photon emission, initial electronic state $|A\rangle, photonic\ state\ |n_r(k)\rangle$

$$\langle B, n_r(k)+1|H_I|A, n_r(k)\rangle = \left\langle B, n_r(k)+1\middle|\sum_i -\frac{e_i}{m_i c} A\cdot p_i\middle|A, n_r(k)\right\rangle$$

$$= -\frac{e}{m}\left(\frac{\hbar}{2V\omega_k}\right)^{\frac{1}{2}} \left\langle n_r(k)+1\middle|a_r^\dagger(k)\middle|n_r(k)\right\rangle \langle B|\varepsilon_r(k)\cdot p_i|A\rangle e^{i\omega_k t}$$

$$= -\frac{e}{m}\left(\frac{\hbar}{2V\omega_k}\right)^{\frac{1}{2}} (n_r(k)+1)^{\frac{1}{2}} \varepsilon_r(k)\cdot\langle B|p_i|A\rangle e^{i\omega_k t}$$

- Since $i\hbar\dot{r}_i = [r_i, H], so\ \langle B|p_i|A\rangle = -im\omega\langle B|r_i|A\rangle$
- Transition rate from time-dependent perturbation

$$w = \frac{2\pi}{\hbar}|\langle B, n_r(k)+1|H_I|A, n_r(k)\rangle|^2 \delta(E_A - E_B - \hbar\omega_k)$$

Integral over dk and d$\mathbf{\Omega}$ $\quad w_{total} = \frac{e^2\omega^3}{3\pi\hbar c^3}\langle B|r_i|A\rangle^2$

Transition matrix element

- $|A\rangle = |R_A\rangle|Y_{lm}\rangle, |B\rangle = |R_B\rangle|Y_{l'm'}\rangle, x = rsin\theta cos\varphi, y = rsin\theta sin\varphi, z = rcos\theta$

Angular matrix

- $sin\theta e^{\pm i\varphi}|Y_{lm}\rangle = \pm\alpha|Y_{l+1,m\pm1}\rangle \mp \beta|Y_{l-1,m\pm1}\rangle, cos\theta|Y_{lm}\rangle = \gamma|Y_{l+1,m}\rangle + \vartheta|Y_{l-1,m}\rangle$
- So $l' = l \pm 1, m' = m \pm 1\ or\ m$

Selection rules: $\Delta l = \pm 1, \Delta m = 0, \pm 1$

But for intersystem transition, selection rule can be ignored, transition is only forbidden by Spin direction.