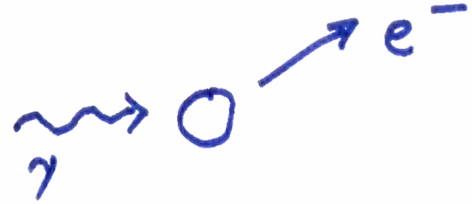
Photoelectric effect



atomic core

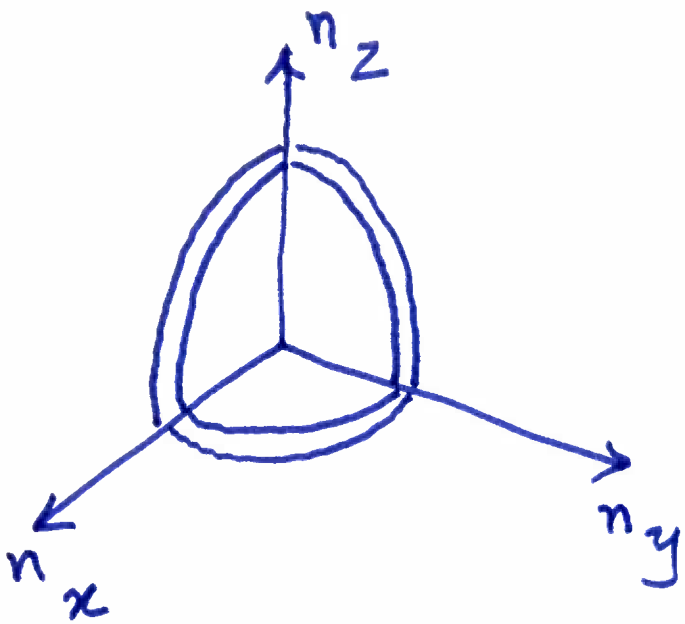
Using time dependent, harmonic perturbation formalism, we found

$$\sigma_{abs} \propto \omega \frac{e^2}{m^2} \left| \langle n | e^{i \frac{\omega}{c} \hat{n}\cdot\vec{x}} \, \hat{\epsilon}\cdot\vec{p} \, | i \rangle \right|^2 \cancel{\rho(E_n - E_i - \hbar\omega)}$$

$$\times \rho(E_n - E_i - \hbar\omega)$$

For ρ calculation, use periodic boundary conditions $\vec{k} = \frac{2\pi}{L}(n_x \hat{i} + n_y \hat{j} + n_z \hat{k})$ $\quad \left.\begin{matrix} n_x \\ n_y \\ n_z \end{matrix}\right\} = 0, \pm 1, \pm 2, \ldots$

$$\psi_{\vec{k}} = \langle \vec{x} | \vec{k} \rangle = \frac{1}{L^{3/2}} e^{i\vec{k}\cdot\vec{x}}$$ remains periodic



$$E = \frac{\hbar^2 |\vec{k}|^2}{2m}$$

$$= \frac{\hbar^2}{2m}\left(\frac{2\pi}{L}\right)^2 (n_x^2 + n_y^2 + n_z^2)$$

$$\frac{dE}{d|\vec{k}_f|} \approx \frac{\Delta|\vec{n}|}{\Delta|k_f|} \frac{dE}{d|n|}$$

$$\vec{n} = n_x \hat{i} + n_y \hat{j} + n_z \hat{k} \qquad \Delta|\vec{n}| \approx 1 \text{ for sample calculation}$$

Volume of a shell with fixed $|\vec{n}|$ is

$$\underbrace{n^2 dn \, d\Omega_n}_{\text{solid angle element in } n \text{ space}} = \left(\frac{L}{2\pi}\right)^3 k_f^2 \, dk_f \, d\Omega_k = \left(\frac{L}{2\pi}\right)^3 k_f^2 \underbrace{\frac{m}{\hbar^2 k_f} dE}_{dk = \text{"}\frac{dk}{dE}\text{"} dE} d\Omega$$

Note : (1) $\vec{n} \to \vec{k}$ conversion requires the Jacobian $\left|\dfrac{\partial n_i}{\partial k_j}\right|$

$$\text{"}d^3n\text{"} \equiv \underbrace{dn_x\,dn_y\,dn_z}_{n^2\,dn\,d\Omega_n} = \underbrace{\left|\frac{\partial n}{\partial k}\right|}_{\left(\frac{L}{2\pi}\right)^2}\underbrace{dk_x\,dk_y\,dk_z}_{k^2\,dk\,d\Omega_k}$$

(2) $dk = \dfrac{1}{dE/dk}\,dE$ i.e. "$\dfrac{dk}{dE}$" $\to \dfrac{1}{dE/dk}$

$E = \dfrac{\hbar^2}{2m}k^2 \quad \therefore \quad dE = \dfrac{\hbar^2}{m}k\,dk \qquad \dfrac{dE}{dk} = \dfrac{\hbar^2 k}{m}$

Thus $\underbrace{n^2\,dn\,d\Omega_n}_{\text{no. of states}} \equiv \rho(E_n)\,dE \implies \rho \sim$ no. of states per energy interval

We now look for

$$\frac{d\sigma}{d\Omega} = \frac{4\pi^2 \alpha \hbar}{m^2 \omega} \left| \langle \vec{k}_f | e^{i\frac{\omega}{c}\hat{n}\cdot\vec{x}} \hat{\epsilon}\cdot\vec{p} | i \rangle \right|^2 \times \underbrace{\frac{m k_f}{\hbar^2}\left(\frac{L}{2\pi}\right)^3}_{\rho(E_n)/d\Omega}$$

Next, to calculate the atomic matrix element, consider K-shell electron

$$\psi_K = e^{-Zr/a_0}\left(\frac{Z}{a_0}\right)^{3/2} \qquad a_0 \to \text{Bohr radius}$$

Thus we need

$$\int d^3x \, \frac{e^{-i\vec{k}_f\cdot\vec{x}}}{L^{3/2}} \, e^{i\frac{\omega}{c}\hat{n}\cdot\vec{x}} \, \hat{\epsilon}\cdot\vec{p} \, \psi_K$$

Now we have $\int e^{i\vec{k}_f\cdot\vec{x}}\, e^{i\frac{\omega}{c}\hat{n}\cdot\vec{x}}\, \hat{\epsilon}\cdot(-i\hbar\vec{\nabla})\,\psi_k$

Integrate by parts, giving a term

$$\cancel{(-i\hbar)\oint e^{i\vec{k}_f\cdot\vec{x}}\, e^{i\frac{\omega}{c}\hat{n}\cdot\vec{x}}\, \hat{\epsilon}\cdot \underbrace{d\vec{S}}_{\text{boundary area element}}\,\psi_k} \to 0 \quad \left\{ \begin{array}{l} \psi_k \text{ zero} \\ \text{at boundary} \end{array} \right.$$

on the boundary

$$\int u\left(\frac{d}{dx}v\right)dx = uv\Big|_{\text{boundary}} - \int \frac{du}{dx}\, v\, dx$$

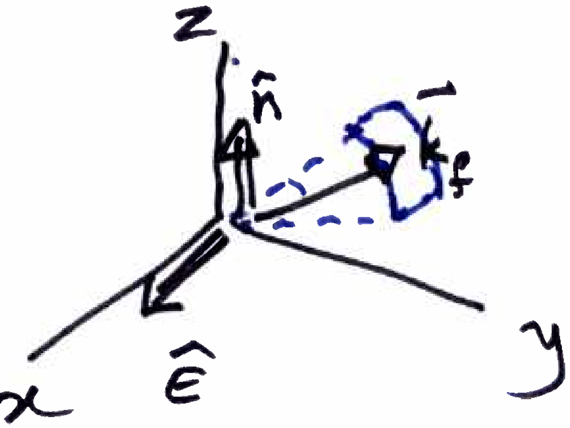
Remaining term :

$$-\frac{(i\hbar)}{L^{3/2}}\int d^3x\, \psi_k\, \hat{\epsilon}\cdot\vec{\nabla}\left(e^{-i\vec{k}_f\cdot\vec{x}}\, e^{i\frac{\omega}{c}\hat{n}\cdot\vec{x}}\right)$$

Note $\hat{\epsilon}\cdot\vec{\nabla}\left(e^{i\frac{\omega}{c}\hat{n}\cdot\vec{x}}\right) = \hat{\epsilon}\cdot\hat{n}\left(i\frac{\omega}{c}\right)e^{i\frac{\omega}{c}\hat{n}\cdot\vec{x}} = 0 \quad \because \hat{\epsilon}\cdot\hat{n} = 0$

plane E-M wave

$$= \frac{\hbar\, \vec{k}_f \cdot \hat{\epsilon}}{L^{3/2}} \int \psi_k \, d^3x \; e^{-i\left(\vec{k}_f - \frac{\omega}{c}\hat{n}\right)\cdot \vec{x}}$$



Note the $d\Omega$ in $\frac{d\sigma}{d\Omega}$ is the solid angle into which $\vec{k}_f$ emerges : $\cos\theta_k \, d\theta_k \, d\phi_k$

Now use $\psi_k = e^{-Zr/a_0}\left(\frac{Z}{a_0}\right)^{3/2}$; write $\vec{q} = \vec{k}_f - \frac{\omega}{c}\hat{n}$

Need the integral $\int d^3x \; e^{-Zr/a_0} e^{-i\vec{q}\cdot\vec{x}} = \int \sin\theta \, d\theta \, d\phi \, dr \, r^2 \; e^{-Zr/a_0} e^{-iqr\cos\theta}$

$$\frac{d\sigma}{d\Omega} = 32\, e^2 k_f \frac{(\hat{\epsilon}\cdot k_f)^2}{mc\omega} \frac{Z^5}{a_0^5} \frac{1}{\left(\left(Z/a_0\right)^2 + q^2\right)^4}$$