J08Q3 - Photoelectric Effect (Solution by Jim Wu)

Compute the differential cross section for the photoelectric effect, i.e., the scattering process by which a photon is absorbed by an atom while kicking an electron out of its orbit. Assume that the initially the electron is in the ground state $|\psi_{100}\rangle$ of an H-atom,

$$\psi_{100}(\vec{r}) = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}$$

where a_0 denotes the Bohr radius. The incoming photon beam consists of N photons, all in a momentum and polarization eigenstate $|\vec{k}, \hat{\epsilon}\rangle$. The beam and atom are inside a periodic box with volume V. The final state has $N-1$ photons, and you may assume that the electron ends up in a momentum eigenstate $|\vec{k}_f\rangle$.

Hint: Use the dipole approximation, where the interaction describing the coupling between the photon field and the electron is given by $(e/m)\vec{A} \cdot \vec{p}$ with

$$\vec{A} = \sqrt{\frac{2\pi\hbar}{V}} \sum_{\vec{k},\hat{\epsilon}} \frac{1}{\sqrt{c|\vec{k}|}} (a_{\vec{k},\hat{\epsilon}} + a^{\dagger}_{\vec{k},\hat{\epsilon}})\hat{\epsilon}$$

Here, $a_{\hat{k},\hat{\epsilon}}$ and $a^{\dagger}_{\hat{k},\hat{\epsilon}}$ are the photon creation and annihilation operators, $\hbar\vec{k}$ is the momentum and $\hat{\epsilon}$ the polarization of a photon.

Solution:

The initial state of the system consists of an electron in the ground state of a hydrogen atom and N photons with momentum $\hbar\mathbf{k}$ and polarization $\hat{\epsilon}$, which can be written as

$$|\psi_i\rangle = |\psi_{100}\rangle \otimes |N_{\mathbf{k},\hat{\epsilon}}\rangle$$

The electron absorbs one photon and is ejected out in a momentum eigenstate $|\mathbf{k}_f\rangle$, and so the final state is

$$|\psi_f\rangle = |\mathbf{k}_f\rangle \otimes |(N-1)_{\mathbf{k},\hat{\epsilon}}\rangle$$

where $\langle \mathbf{r}|\mathbf{k}_f\rangle = \frac{1}{\sqrt{V}} e^{i\mathbf{k}_f\cdot\mathbf{r}}$ is the position space representation of the plane wave.

Then, from the dipole approximation,

$$\langle\psi_i|H|\psi_f\rangle = \frac{e}{m}\sqrt{\frac{2\pi\hbar}{V}} \int d^3r \langle N_{\mathrm{k},\hat{\epsilon}}| \otimes \left(\frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}\right)^* \left(\sum_{\vec{k}',\hat{\epsilon}'} \frac{1}{\sqrt{c|\mathbf{k}'|}} (a_{\mathbf{k}',\hat{\epsilon}'} + a^{\dagger}_{\mathbf{k}',\hat{\epsilon}'})\hat{\epsilon}'\right) \cdot \vec{p} \left(\frac{e^{i\mathbf{k}_f\cdot\mathbf{r}}}{\sqrt{V}}\right) \otimes |(N-1)_{\mathbf{k},\hat{\epsilon}}\rangle$$

Note that the only term left in the sum is the one that matches the momentum and polarization of the photons, i.e. $\mathbf{k}' = \mathbf{k}$ and $\hat{\epsilon}' = \hat{\epsilon}$. Furthermore, we are doing $\langle\psi_i|H|\psi_f\rangle$ instead of $\langle\psi_f|H|\psi_i|rangle$ as the calculations are much easier using the former. In the end, either will give the same answer for the differential cross sections as the two amplitudes are only complex conjugates of each other.

The momentum operator $\vec{p}$ acting on the momentum eigenstate yields $\vec{p}|\mathbf{k}_f\rangle = \hbar\mathbf{k}_f|\mathbf{k}_f\rangle$. Furthermore, only the creation operator survives from the vector potential operator, and we will use the fact that $a^{\dagger}_{\mathbf{k}_f,\hat{\epsilon}}|(N-1)_{\mathbf{k_f},\hat{\epsilon}}\rangle = \sqrt{N}|(N-1)_{\mathbf{k_f},\hat{\epsilon}}\rangle$. This simplifies the above amplitude to

$$\langle\psi_i|H|\psi_f\rangle = \frac{e}{m}\sqrt{\frac{2\pi\hbar}{Vc|\mathbf{k}|}}\int d^3r\ \frac{1}{\sqrt{\pi a_0^3}}e^{-r/a_0}\hat{\epsilon}\cdot\hbar\mathbf{k}_f\left(\frac{1}{\sqrt{V}}e^{i|\mathbf{k}|r\cos\theta}\right)\ \langle N_{\mathbf{k},\hat{\epsilon}}|a^\dagger_{\mathbf{k},\hat{\epsilon}}|(N-1)_{\mathbf{k},\hat{\epsilon}}\rangle$$

$$= \frac{e\hbar}{m}\sqrt{\frac{2\pi\hbar N}{V^2\omega}}(\hat{\epsilon}\cdot\mathbf{k}_f)\int\ e^{i|\mathbf{k}_f|r\cos\theta}\left(\frac{1}{\sqrt{\pi a_0^3}}e^{-r/a_0}\right)2\pi r^2\sin\theta\ drd\theta$$

$$= \frac{e\hbar}{m}\sqrt{\frac{2\pi\hbar N}{V^2\omega}}(\hat{\epsilon}\cdot\mathbf{k}_f)\left(\frac{2\pi}{\sqrt{\pi a_0^3}}\right)\int_0^\infty -\left(\frac{e^{-i|\mathbf{k}_f|r}-e^{i|\mathbf{k}_f|r}}{i|\mathbf{k}_f|r}\right)e^{-r/a_0}\ r^2\ dr$$

$$= \frac{2\pi e\hbar}{im|\mathbf{k}_f|}\sqrt{\frac{2\hbar N}{\omega V^2a_0^3}}(\hat{\epsilon}\cdot\mathbf{k}_f)\int_0^\infty e^{\left(i|\mathbf{k}_f|-(1/a_0)\right)r}-e^{-\left(i|\mathbf{k}_f|+(1/a_0)\right)r}r\ dr$$

Note that I replaced $c|\mathbf{k}|$ with ω, the frequency of light, to prevent confusion between $|\mathbf{k}_f|$ and $|\mathbf{k}|$.

Splitting the integral and using $u = \left(-i|\mathbf{k}|_f + (1/a_0)\right)r$ for the first integral and $u = \left(i|\mathbf{k}_f| + (1/a_0)r\right)r$, we get

$$\langle\psi_i|H|\psi_f\rangle = \frac{2\pi e\hbar}{im|\mathbf{k}|_f}\sqrt{\frac{2\hbar N}{\omega V^2a_0^3}}(\hat{\epsilon}\cdot\mathbf{k}_f)\left(\int_0^\infty\frac{ue^{-u}}{(-i|\mathbf{k}_f|+(1/a_0))^2}du-\int_0^\infty\frac{ue^{-u}}{(i|\mathbf{k}_f|+(1/a_0))^2}\ du\right)$$

$$= \frac{2\pi e\hbar}{im|\mathbf{k}_f|}\sqrt{\frac{2\hbar N}{\omega V^2a_0^3}}(\hat{\epsilon}\cdot\mathbf{k}_f)\left(\frac{1}{(-i|\mathbf{k}_f|+(1/a_0))^2}-\frac{1}{(i|\mathbf{k}_f|+(1/a_0))^2}\right)$$

$$= \frac{2\pi e\hbar}{im|\mathbf{k}_f|}\sqrt{\frac{2\hbar N}{\omega V^2a_0^3}}(\hat{\epsilon}\cdot\mathbf{k}_f)\left(\frac{4i|\mathbf{k}_f|/a_0}{(|\mathbf{k}_f|^2+(1/a_0)^2)^2}\right)$$

$$= \frac{8\pi e\hbar}{ma_0}\sqrt{\frac{2\hbar N}{\omega V^2a_0^3}}\left(\frac{\hat{\epsilon}\cdot\mathbf{k}_f}{(|\mathbf{k}_f|^2+(1/a_0)^2)^2}\right)$$

The transition probability per unit time into a solid angle, from Fermi's golden rule, is

$$dR = \frac{2\pi}{\hbar}|\langle f|H|i\rangle|^2\rho d\Omega$$

where $\rho\ dEd\Omega$ is the electronic density of states between energy E and $E+dE$ in solid angle $d\Omega$. Note that

$$\rho\ dkd\Omega = \frac{V}{(2\pi)^3}k^2dkd\Omega \to \frac{V}{(2\pi)^3\hbar^3}p^2dpd\Omega$$

Since $E = \frac{p^2}{2m}$, then

$$\rho\ dEd\Omega = \frac{V}{(2\pi)^3\hbar^3}mp\ dEd\Omega = \frac{V}{(2\pi)^3\hbar^2}m|\mathbf{k}_f|\ dEd\Omega$$

So, the transition probability per unit time into a solid angle, representing the scattered flux times $d\Omega$, is

$$dR = \frac{2\pi}{\hbar}\left(\frac{V}{(2\pi)^3\hbar^2}m|\mathbf{k}_f|\right)\left[\frac{8\pi e\hbar}{ma_0}\sqrt{\frac{2\hbar N}{\omega V^2a_0^3}}\left(\frac{\hat{\epsilon}\cdot\mathbf{k}_f}{(|\mathbf{k}_f|^2+(1/a_0)^2)^2}\right)\right]^2 d\Omega$$

$$= \frac{32e^2N|\mathbf{k}_f|}{ma_0^5V\omega}\left(\frac{(\hat{\epsilon}\cdot\mathbf{k}_f)^2}{(|\mathbf{k}_f|^2+(1/a_0)^2)^4}\right)d\Omega$$

$$= \frac{32\alpha\hbar cN|\mathbf{k}_f|}{ma_0^5V\omega}\left(\frac{(\hat{\epsilon}\cdot\mathbf{k}_f)^2}{(|\mathbf{k}_f|^2+(1/a_0)^2)^4}\right)d\Omega$$

where the fine structure constant is $\alpha = \frac{e^2}{\hbar c}$. The incident flux is the number of particles crossing per unit area per unit time through our volume is equal to

$$\text{incident flux } = \frac{Nc}{V}$$

since there are N photons in our beams going into our box. Our differential cross section is the ratio of the scattered flux over the incident flux, or

$$\frac{d\sigma}{d\Omega} = \left(\frac{V}{Nc}\right)\frac{32\alpha\hbar c N|\mathbf{k}_f|}{ma_0^5 V\omega}\left(\frac{(\hat{\epsilon}\cdot\mathbf{k}_f)^2}{(|\mathbf{k}_f|^2 + (1/a_0)^2)^4}\right) = \boxed{32\alpha\frac{\hbar|\mathbf{k}_f|}{ma_0^5\omega}\left(\frac{(\hat{\epsilon}\cdot\mathbf{k}_f)^2}{(|\mathbf{k}_f|^2 + (1/a_0)^2)^4}\right)}$$

Note that using the dipole approximation was somewhat unnecessary and we could have gotten an exact answer. If we do the calculations with $e^{-i\mathbf{k}\cdot\mathbf{r}}$, where $\mathbf{k}$ is the wave vector of the photons, then the $|\mathbf{k}_f|^2$ in the denominator of the differential cross section would map to $|\mathbf{k}_f - \mathbf{k}|$, and we would have

$$\frac{d\sigma}{d\Omega} = 32\alpha\frac{\hbar|\mathbf{k}_f|}{ma_0^5\omega}\left(\frac{(\hat{\epsilon}\cdot\mathbf{k}_f)^2}{(|\mathbf{k}_f - \mathbf{k}|^2 + (1/a_0)^2)^4}\right)$$

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