Photoelectric effect

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The photoelectric effect was discovered by Heinrich Hertz in 1887 during the course of the experiment that discovered radio waves. It remained unexplained until 1905 when Albert Einstein postulated the existence of quanta of light - photons - which, when absorbed by an electron near the surface of a metal, could give the electron enough energy to escape from the metal. Robert Milliken carried out a careful set of experiments and that verified the predictions of Einstein's photon theory of light. Einstein was awarded the 1921 Nobel Prize in physics for his discovery of the law of the photoelectric effect. Milliken received the Prize in 1923 for his work on the elementary charge of electricity (the oil drop experiment) and on the photoelectric effect.

Here the photoelectric effect is discussed using the time dependent perturbation. Note that the photoelectric effect can be explained in a semi-classical approach without the quantization of the electromagnetic field,

1. Sinusoidal perturbation

We consider the case of interaction between photon and electron. The perturbation can be given by

$$\begin{aligned}\hat{H}_1 &= \frac{e}{mc}|\boldsymbol{A}_0|[e^{i(\boldsymbol{k}\cdot\boldsymbol{r}-\omega t)} + e^{-i(\boldsymbol{k}\cdot\boldsymbol{r}-\omega t)}](\boldsymbol{\varepsilon}\cdot\hat{\boldsymbol{p}}) \\ &= \hat{V}^{+}e^{-i\omega t} + \hat{V}e^{i\omega t}\end{aligned}$$

with

$$\hat{V}^{+} = \frac{e}{mc}|\boldsymbol{A}_0|e^{i\boldsymbol{k}\cdot\boldsymbol{r}}(\boldsymbol{\varepsilon}\cdot\hat{\boldsymbol{p}}) .$$

where $\boldsymbol{A}_0$ is the vector potential. The matrix element is given by

$$\langle\varphi_f|\hat{V}^{+}|\varphi_i\rangle = \langle\varphi_i|\hat{V}|\varphi_f\rangle^{*} = \frac{e}{mc}|\boldsymbol{A}_0|\langle\varphi_f|e^{i\boldsymbol{k}\cdot\boldsymbol{r}}(\boldsymbol{\varepsilon}\cdot\hat{\boldsymbol{p}})|\varphi_i\rangle$$

In conclusion, the transition probability is proportional to

$$\frac{e^2}{m^2c^2}|\boldsymbol{A}_0|^2|\langle\varphi_f|e^{i\boldsymbol{k}\cdot\boldsymbol{r}}(\boldsymbol{\varepsilon}\cdot\hat{\boldsymbol{p}})|\varphi_i\rangle|^2$$

The absorption cross section σ_{abs} is

σ_{abs} = absorption cross section

$$= \frac{\text{(energy/unit time) absorpted by the atom } (i \to f)}{\text{Energy flux of the radiation field (erg/cm}^2\text{s)}}$$

$$= \frac{\hbar\omega W_{i\to f}\,\text{(erg/s)}}{\frac{1}{2\pi}\frac{\omega^2}{c}|\boldsymbol{A}_0|^2\,\text{(erg/cm}^2\text{s)}}[\text{cm}^2]$$

or

$$\sigma_{abs} = \frac{\hbar\omega\frac{2\pi}{\hbar}\frac{e^2}{m^2c^2}|\boldsymbol{A}_0|^2\left|\left\langle\varphi_f\left|e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\boldsymbol{\varepsilon}\cdot\hat{\boldsymbol{p}}\right|\varphi_i\right\rangle\right|^2\delta\left(E_f - E_i - \hbar\omega\right)}{\frac{1}{2\pi}\frac{\omega^2}{c}|\boldsymbol{A}_0|^2}$$

$$= \frac{4\pi^2\hbar}{m^2\omega}\left(\frac{e^2}{\hbar c}\right)\left|\left\langle\varphi_f\left|e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\boldsymbol{\varepsilon}\cdot\hat{\boldsymbol{p}}\right|\varphi_i\right\rangle\right|^2\delta\left(E_f - E_i - \hbar\omega\right)$$

Note that the energy flux (energy per area per unit time) is given by

$$cu = \frac{1}{2\pi}\frac{\omega^2}{c}|\boldsymbol{A}_0|^2$$

The fine structure constant is defined by

$$\alpha = \frac{e^2}{\hbar c}.$$

2. Photoelectric effect

In the photoelectric effect, electrons are emitted from metals when they absorb energy from light. Electrons emitted in this manner may be called photoelectrons.

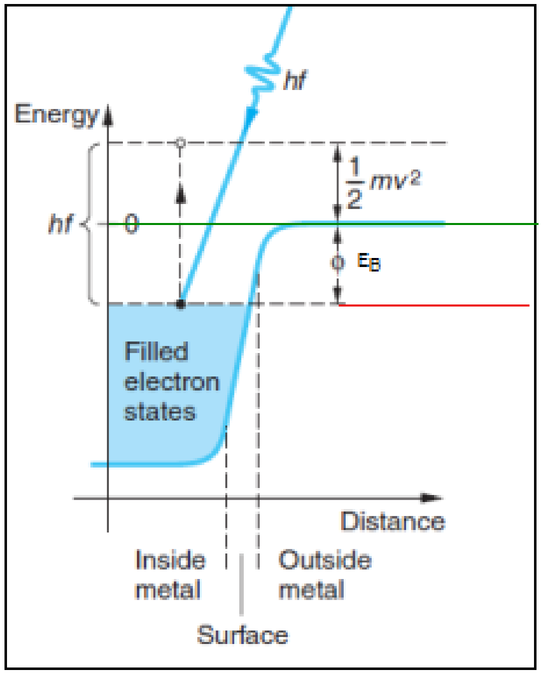

Fig. Photoelectric effect in metal. Electron potential energy across the metal surface. An electron with the highest energy in the metal absorps a photon of energy $\hbar\omega$ Conservation of energy requires that its kinetic energy after leaving the surface be $\hbar\omega - E_B$, where E_B is the work function of metal (the energy difference between the vacuum state and the Fermi energy of the metal.

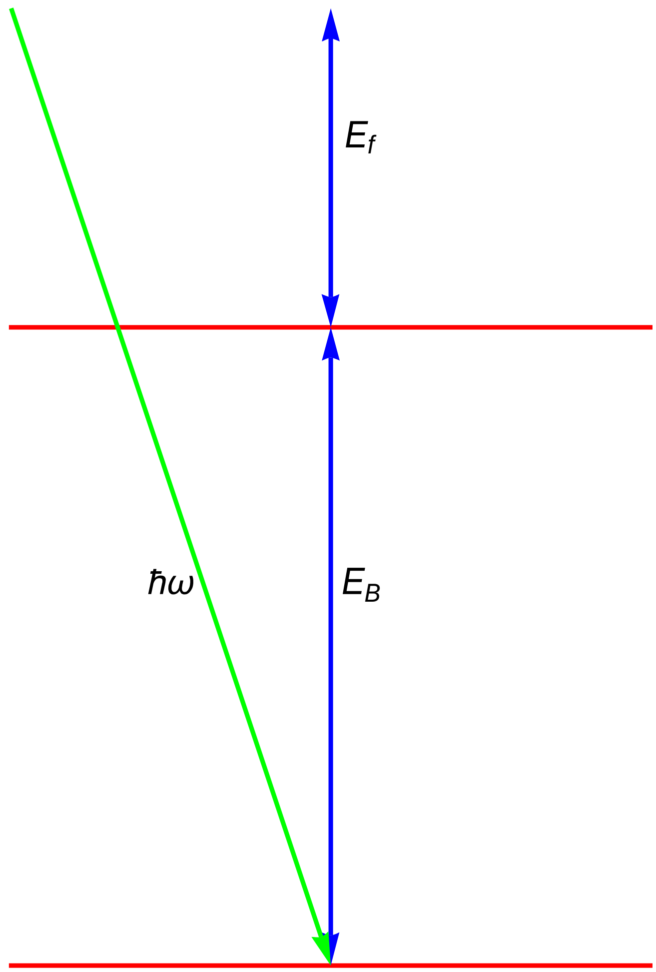

Fig. Our model on the photoelectric effect. The binding energy E_B. The kinetic energy E_f of free electron. $\hbar\omega$ is the energy of photon absorbed,

((**Note**))

The energy conservation:

$$\hbar\omega = \frac{1}{2} m v_f{}^2 + E_B$$

where $\hbar\omega$ is the photon energy, $\frac{1}{2} m v_f{}^2 = \frac{\hbar^2 k_f{}^2}{2m}$ is the kinetic energy of free electron, and

$$E_B = \frac{1}{2} m c^2 (Z\alpha)^2$$

is the bound energy.

Ejection of an electron when an atom is placed in the radiation field.

$|i\rangle$: atomic (bound) state
$|n\rangle$: continum state ($E > 0$)

Plane-wave state $|\boldsymbol{k}_f\rangle$, an approximation that is valid if the final electron is not too slow.

$$\langle \boldsymbol{r}|\boldsymbol{k}_f\rangle = \frac{1}{L^{3/2}} e^{i\boldsymbol{k}_f \cdot \boldsymbol{r}}$$

with the periodic boundary condition

$$k_x = \frac{2\pi}{L} n_x,\ k_y = \frac{2\pi}{L} n_y,\ k_z = \frac{2\pi}{L} n_z .$$

$$\begin{aligned} E &= \frac{\hbar^2}{2m}\left(k_x^2 + k_y^2 + k_z^2\right) \\ &= \frac{\hbar^2}{2m}\left(\frac{2\pi}{L}\right)^2 \left(n_x^2 + n_y^2 + n_z^2\right) \\ &= \frac{\hbar^2}{2m}\left(\frac{2\pi}{L}\right)^2 n^2 \end{aligned}$$

where

$$\begin{cases} n_x = 0, \pm 1, \pm 2, \cdots \\ n_y = 0, \pm 1, \pm 2, \cdots \\ n_z = 0, \pm 1, \pm 2, \cdots \end{cases}$$

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

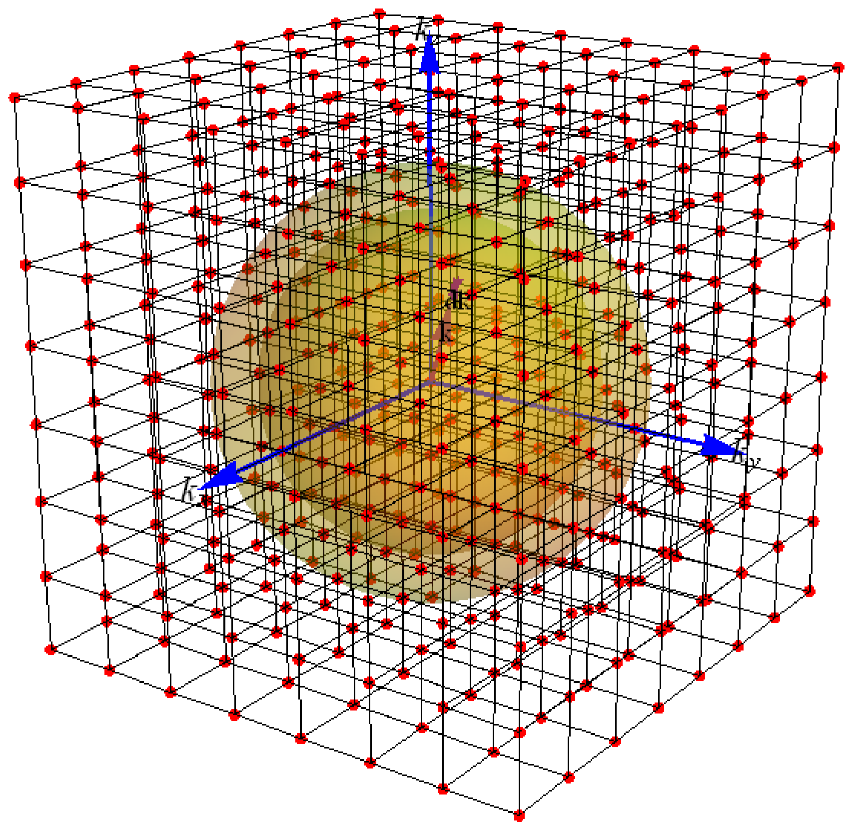

Fig. Density of states in the 3D ***k***-space. There is one state per $(2\pi/L)^3$. We use the periodic boundary condition for the wave function.

The number of states for $k \sim k+dk$ and solid angle element $d\Omega$

$$\frac{k^2 dk d\Omega}{\left(\frac{2\pi}{L}\right)^3} = \left(\frac{L}{2\pi}\right)^3 k^2 dk d\Omega$$

$$= \left(\frac{L}{2\pi}\right)^3 \frac{1}{2}\left(\frac{2m}{\hbar^2}\right)^{3/2} \sqrt{E} dE d\Omega$$

since

$$E = \frac{\hbar^2 k^2}{2m}, \qquad k = \sqrt{\frac{2m}{\hbar^2}}\sqrt{E}, \qquad \frac{dk}{dE} = \sqrt{\frac{2m}{\hbar^2}}\frac{1}{2\sqrt{E}}$$

$$k^2 dk = k^2 \frac{dk}{dE} dE = \frac{1}{2}\left(\frac{2m}{\hbar^2}\right)^{3/2} \sqrt{E} dE$$

3. Fermi's golden rule

We note that

$$\int \left(\frac{L}{2\pi}\right)^3 \frac{1}{2}\left(\frac{2m}{\hbar^2}\right)^{3/2} \sqrt{E} dE \delta(E - E_i - \hbar\omega) = \left(\frac{L}{2\pi}\right)^3 \frac{1}{2}\left(\frac{2m}{\hbar^2}\right)^{3/2} \sqrt{E_f}$$

$$= \left(\frac{L}{2\pi}\right)^3 \frac{m}{\hbar^2}\left(\frac{2mE_f}{\hbar^2}\right)^{1/2}$$

$$= \left(\frac{L}{2\pi}\right)^3 \frac{mk_f}{\hbar^2}$$

Using the Fermi's golden rule, we have the differential cross section as

$$d\sigma = \frac{4\pi^2\hbar}{m^2\omega}\left(\frac{e^2}{\hbar c}\right)\left|\langle \boldsymbol{k}_f \right| e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \boldsymbol{\varepsilon}\cdot\hat{\boldsymbol{p}} \left| i\rangle\right|^2 \left(\frac{L}{2\pi}\right)^3 \frac{mk_f}{\hbar^2} d\Omega$$

or

$$\frac{d\sigma}{d\Omega} = \frac{4\pi^2\alpha\hbar}{m^2\omega}\left|\langle \boldsymbol{k}_f \right| e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \boldsymbol{\varepsilon}\cdot\hat{\boldsymbol{p}} \left| i\rangle\right|^2 \frac{mk_f}{\hbar^2}\frac{L^3}{(2\pi)^3}$$

$$= \frac{4\pi^2\alpha k_f}{m\hbar\omega}\left|\langle \boldsymbol{k}_f \right| e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \boldsymbol{\varepsilon}\cdot\hat{\boldsymbol{p}} \left| i\rangle\right|^2 \frac{L^3}{(2\pi)^3}$$

To be specific, let us consider the ejection of a *K*-shell (the innermost shell) electron caused by absorption of light. $|i\rangle$: essentially the same as the ground state hydrogen atom wave function except that the Bohr radius a_0 is replaced by a_0/Z;

$$\langle \boldsymbol{r} | i\rangle = R_{10}(r) Y_0^0(\theta,\phi) = \frac{2}{\sqrt{4\pi}} e^{-Zr/a_0}\left(\frac{Z}{a_0}\right)^{3/2}$$

The matrix element is given by

$$\langle \boldsymbol{k}_f \left| e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \boldsymbol{\varepsilon}\cdot\hat{\boldsymbol{p}} \right| i\rangle = \boldsymbol{\varepsilon}\cdot\int d^3\boldsymbol{r} \frac{e^{-i\boldsymbol{k}_f\cdot\boldsymbol{r}}}{L^{3/2}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\left(\frac{\hbar}{i}\nabla\right)\left[\frac{2}{\sqrt{4\pi}} e^{-Zr/a_0}\left(\frac{Z}{a_0}\right)^{3/2}\right]$$

$$= i\hbar\int d^3\boldsymbol{r}\, \boldsymbol{\varepsilon}\cdot\nabla\left[\frac{e^{-i\boldsymbol{k}_f\cdot\boldsymbol{r}}}{L^{3/2}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\right]\frac{2}{\sqrt{4\pi}} e^{-Zr/a_0}\left(\frac{Z}{a_0}\right)^{3/2}$$

Here note that

$$I_1 = \boldsymbol{\varepsilon} \cdot \nabla \left[\frac{e^{-i\boldsymbol{k}_f \cdot \boldsymbol{r}}}{L^{3/2}} e^{i\boldsymbol{k} \cdot \boldsymbol{r}} \right]$$

$$= \boldsymbol{\varepsilon} \cdot \nabla \left(\frac{e^{-i\boldsymbol{k}_f \cdot \boldsymbol{r}}}{L^{3/2}} \right) e^{i\boldsymbol{k} \cdot \boldsymbol{r}} + \boldsymbol{\varepsilon} \cdot \nabla (e^{i\boldsymbol{k} \cdot \boldsymbol{r}}) \frac{e^{-i\boldsymbol{k}_f \cdot \boldsymbol{r}}}{L^{3/2}}$$

We have

$$\boldsymbol{\varepsilon} \cdot \nabla \left(e^{i\boldsymbol{k} \cdot \boldsymbol{r}} \right) = 0$$

because

$$\boldsymbol{\varepsilon} \cdot \boldsymbol{k} = 0 .$$

Using

$$\nabla \left(e^{-i\boldsymbol{k}_f \cdot \boldsymbol{r}} \right) = e^{-i\boldsymbol{k}_f \cdot \boldsymbol{r}} \left(-i\boldsymbol{k}_f \right)$$

we get

$$I_1 = -i\boldsymbol{k}_f \cdot \boldsymbol{\varepsilon} \frac{e^{-i\boldsymbol{k}_f \cdot \boldsymbol{r}}}{L^{3/2}} e^{i\boldsymbol{k} \cdot \boldsymbol{r}} = -i\boldsymbol{k}_f \cdot \boldsymbol{\varepsilon} \frac{1}{L^{3/2}} e^{-i\boldsymbol{q} \cdot \boldsymbol{r}}$$

with

$$\boldsymbol{q} = \boldsymbol{k}_f - \boldsymbol{k} . \qquad \text{(scattering vector)}$$

All we need to do is to take the Fourier transform of the atomic wave function.

$$\left\langle \boldsymbol{k}_f \left| e^{i\boldsymbol{k} \cdot \boldsymbol{r}} \boldsymbol{\varepsilon} \cdot \hat{\boldsymbol{p}} \right| i \right\rangle = i\hbar (-i\boldsymbol{k}_f \cdot \boldsymbol{\varepsilon}) \frac{1}{L^{3/2}} \int d^3\boldsymbol{r} e^{-i\boldsymbol{q} \cdot \boldsymbol{r}} \left[\frac{2}{\sqrt{4\pi}} e^{-Zr/a_0} \left(\frac{Z}{a_0} \right)^{3/2} \right]$$

Here we calculate

$$I_2 \equiv \int d^3\boldsymbol{r} e^{-i\boldsymbol{q} \cdot \boldsymbol{r}} \left[\frac{2}{\sqrt{4\pi}} e^{-Zr/a_0} \left(\frac{Z}{a_0} \right)^{3/2} \right]$$

$$= \frac{2}{\sqrt{4\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \int_0^\infty 2\pi r^2 dr \int_0^\pi \sin\theta d\theta e^{-iqr\cos\theta} e^{-Zr/a_0}$$

Using the Mathematica, we get

$$\int_0^\infty 2\pi r^2 dr \int_0^\pi \sin\theta d\theta e^{-iqr\cos\theta} e^{-Zr/a_0} = \frac{8\pi \frac{Z}{a_0}}{(q^2 + \frac{Z^2}{a_0{}^2})^2}$$

((**Mathematica**))

```
Clear["Global`*"];

f1 = 2 π r^2 Sin[θ] Exp[- i q r Cos[θ] ] Exp[-Z r/a0];

Integrate[Integrate[f1, {θ, 0,  π}], {r, 0, ∞}] //
 Simplify[#, {Abs[Im[q]] ≤ Re[Z/a0] && Re[Z/a0] > 0}] &

8 a0^3 π Z/(a0^2 q^2 + Z^2)^2
```

Thus we get

$$\langle \boldsymbol{k}_f | e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \boldsymbol{\varepsilon}\cdot\hat{\boldsymbol{p}} | i \rangle = \hbar(\boldsymbol{k}_f\cdot\boldsymbol{\varepsilon}) \frac{1}{L^{3/2}} \frac{16\pi}{\sqrt{4\pi}} \left(\frac{Z}{a_0}\right)^{5/2} \frac{1}{\left[\left(\frac{Z}{a_0}\right)^2 + q^2\right]^2}$$

Since

$$\frac{d\sigma}{d\Omega} = \frac{4\pi^2\alpha k_f}{m\hbar\omega} \left| \langle \boldsymbol{k}_f | e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \boldsymbol{\varepsilon}\cdot\hat{\boldsymbol{p}} | i \rangle \right|^2 \frac{L^3}{(2\pi)^3},$$

the differential cross section is obtained as

$$\frac{d\sigma}{d\Omega} = \frac{4\pi^2 \alpha k_f}{m\hbar\omega} \frac{L^3}{(2\pi)^3} \hbar^2 (\boldsymbol{k}_f \cdot \boldsymbol{\varepsilon})^2 \frac{1}{L^3} \frac{16^2 \pi^2}{4\pi} \left(\frac{Z}{a_0}\right)^5 \frac{1}{\left[\left(\frac{Z}{a_0}\right)^2 + q^2\right]^4}$$

$$= \frac{32\alpha\hbar}{m\omega} k_f (\boldsymbol{k}_f \cdot \boldsymbol{\varepsilon})^2 \left(\frac{Z}{a_0}\right)^5 \frac{1}{\left[\left(\frac{Z}{a_0}\right)^2 + q^2\right]^4}$$

where

$$q^2 = k_f^{\ 2} - 2k_f k \cos\theta + k^2$$

$$= k_f^{\ 2} - 2k_f \frac{\omega}{c} \cos\theta + \frac{\omega^2}{c^2}$$

and

$$\boldsymbol{k}_f \cdot \boldsymbol{\varepsilon} = k_f \sin\theta \cos\phi$$

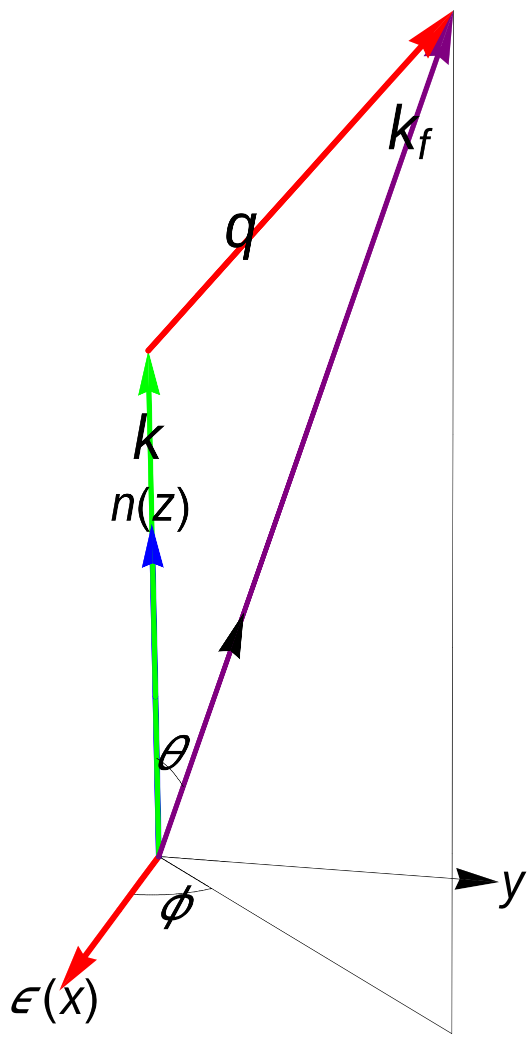

Fig. Experimental configuration for the photoelectric effect. $\boldsymbol{\varepsilon}$ is the polarization vector. $\boldsymbol{n}$ is the unit vector is $\boldsymbol{k}$ of incident photon. $\boldsymbol{k}_f$ is the wavevector of the outgoing electron. $\boldsymbol{q} = \boldsymbol{k} - \boldsymbol{k}_f$. $\hbar\boldsymbol{q}$ is the momentum transfer between the initial photon and the final electron.

2. Energy conservation in the photoelectric effect

Energy is conserved in the system,

$$\hbar ck = E_B + \frac{\hbar^2 k_f^{\ 2}}{2m}$$

$$q^2 = k^2 + k_f^{\ 2} - 2kk_f \cos\theta$$

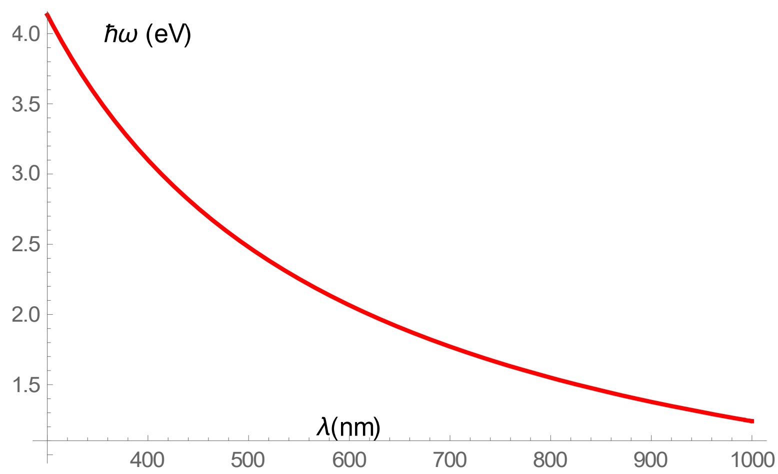

Fig. The energy (eV) vs wave length (nm) for visible light.

Note that k_f is only dependent on k. k_f is constant when k is fixed. We use the following approximation, for simplicity,

(i)

$$\hbar ck >> E_B \qquad \text{or} \qquad \frac{2mck}{\hbar} >> \left(\frac{Z}{a_B}\right)^2$$

$$\hbar ck \approx \frac{\hbar^2 {k_f}^2}{2m} >> E_B = \frac{\hbar^2}{2m}\left(\frac{Z}{a_B}\right)^2$$

$${k_f}^2 >> \left(\frac{Z}{a_B}\right)^2$$

where the binding energy is given by

$$E_B = \frac{1}{2}mc^2(Z\alpha)^2 = \frac{1}{2}mc^2 Z^2 \frac{\hbar^2}{m^2c^2{a_B}^2} = \frac{\hbar^2}{2m}\left(\frac{Z}{a_B}\right)^2$$

α is the fine structure constant:

$$\alpha = \frac{e^2}{\hbar c}$$

The Bohr radius is

$$a_B = \frac{\hbar^2}{me^2}$$

(ii) In the nonrelativistic case:

$$E_e^{\ 2} = m^2c^4 + c^2 p_e^{\ 2}, \quad m^2c^2 >> p_e^{\ 2} = \hbar^2 k_f^{\ 2} = 2mck\hbar^2$$

or

$$mc^2 >> 2c\hbar k$$

Since

$$k_f^{\ 2} = \frac{p_e^{\ 2}}{\hbar^2} \approx \frac{2m\hbar ck}{\hbar^2} = \frac{2mck}{\hbar} = \frac{2mc^2}{\hbar ck}k^2 >> 4k^2 > k^2$$

and

$$k_f^{\ 2} >> \left(\frac{Z}{a_B}\right)^2$$

we get

$$\begin{aligned} q^2 + \left(\frac{Z}{a_B}\right)^2 &\approx \left(\frac{Z}{a_B}\right)^2 + k^2 + k_f^{\ 2} - 2kk_f\cos\theta \\ &\approx k_f^{\ 2} - 2kk_f\cos\theta \\ &= \frac{2mck}{\hbar} - 2kk_f\cos\theta \\ &= \frac{2mck}{\hbar}(1 - \frac{2\hbar kk_f}{2mck}\cos\theta) \\ &= \frac{2mck}{\hbar}(1 - \frac{\hbar k_f}{mc}\cos\theta) \\ &= \frac{2mck}{\hbar}(1 - \frac{v_f}{c}\cos\theta) \end{aligned}$$

Then we have

$$\frac{d\sigma}{d\Omega} \approx \frac{32e^2 k_f^{\ 3}}{mc\omega}\left(\frac{Z}{a_B}\right)^5 \left(\frac{\hbar}{2mck}\right)^4 \frac{\sin\theta^2 \cos^2\phi}{(1-\frac{v_f}{c}\cos\theta)^4}$$

$$= \frac{32e^2}{mc\omega k_f^{\ 5}}\left(\frac{Z}{a_B}\right)^5 \frac{\sin\theta^2 \cos^2\phi}{(1-\frac{v_f}{c}\cos\theta)^4}$$

$$= \frac{32\alpha\hbar}{m\omega k_f^{\ 5}}\left(\frac{Z}{a_B}\right)^5 \frac{\sin\theta^2 \cos^2\phi}{(1-\frac{v_f}{c}\cos\theta)^4}$$

If the incident wave is not polarized, the contributions of the polarization in the x and y directions must be incoherently and averaged over ϕ.

$$\left\langle \cos^2\phi \right\rangle = \frac{1}{2\pi}\int_0^{2\pi} d\phi \cos^2\phi = \frac{1}{2}$$

Then we get

$$\frac{d\sigma}{d\Omega} = \frac{16\alpha\hbar}{m\omega k_f^{\ 5}}\left(\frac{Z}{a_B}\right)^5 \frac{\sin\theta^2}{(1-\frac{v_f}{c}\cos\theta)^4}$$

which is proportional to Z^5/ω in the high energy photon.

For simplicity we put

$$f(\theta) = \frac{\sin^2\theta}{(1-\frac{v_f}{c}\cos\theta)^4}$$

The derivative of $f(\theta)$ with respect to θ is

$$f'(\theta) = \frac{\sin\theta}{(1-\frac{v_f}{c}\cos\theta)^5}[2\cos\theta + \frac{v_f}{c}(-3+\cos(2\theta)]$$

In the limit of small $\frac{v_f}{c}$, $f(\theta)$ has a local maximum when

$$\cos\theta = \frac{\sqrt{1+8\frac{v_f{}^2}{c^2}}-1}{2\frac{v_f}{c}} \approx 2\frac{v_f}{c}$$

or

$$\theta = \arccos[2\frac{v_f}{c}]$$

When $\frac{v_f}{c} << 1$, $\cos\theta = 0$, or $\theta = \pi/2$. As $\frac{v_f}{c}$ increases, θ decreases.

3. Angular dependence of $\frac{d\sigma}{d\Omega}$

((**Mathematica**)) We make a plot of a part of $\frac{d\sigma}{d\Omega}$ using the SphericalPlot3D

The cross section vanishes in the forward direction. This is a consequence of the fact that photons are transversely polarized. The matrix element is proportional to $(\boldsymbol{k}_f \cdot \boldsymbol{\varepsilon})^2$. When $\boldsymbol{k}_f$ is parallel to the photon momentum $\boldsymbol{k} = k\boldsymbol{n}$, this factor vanishes.

We assume that the formula

$$\frac{d\sigma}{d\Omega} = \frac{16\alpha\hbar}{m\omega k_f{}^5}\left(\frac{Z}{a_B}\right)^5 \frac{\sin\theta^2}{(1-\frac{v_f}{c}\cos\theta)^4}$$

is valid for $v_f < c$. We make a plot of $\frac{d\sigma}{d\Omega}$ using Mathematica, where v_f is changed as a parameter.

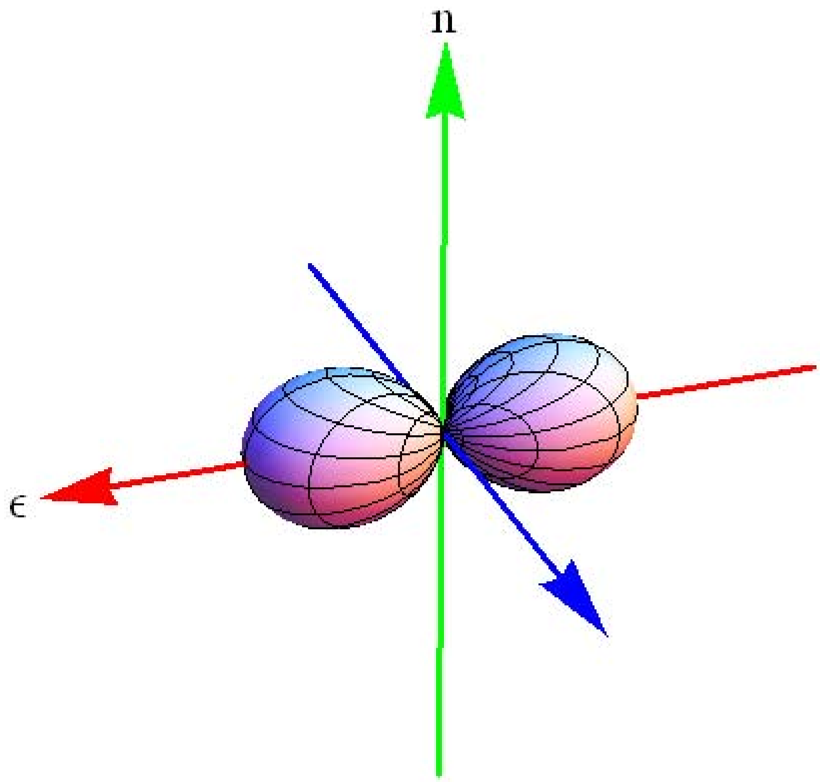

Fig. $v_f / c = 0$. Angular distribution of photoelectric electrons. The green line (the direction of photon). The red line (the direction of polarization vector for photon).

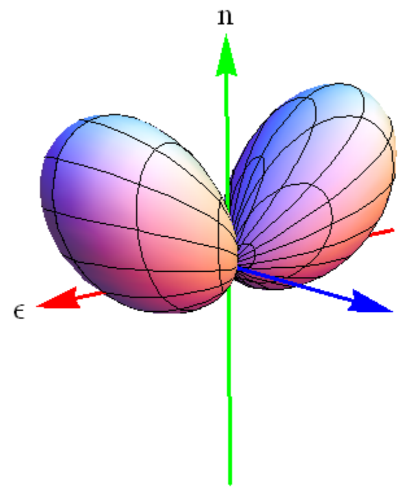

Fig. The case of $v_f / c = 0.6$.

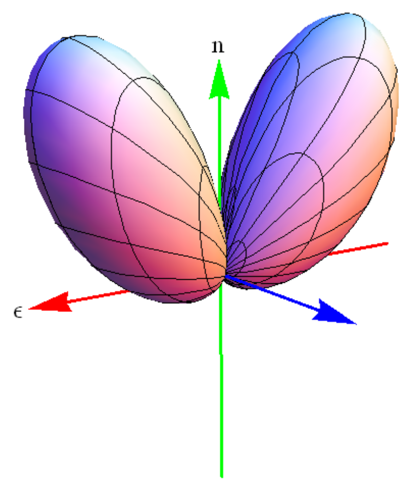

Fig. The case of $v_f / c = 0.8$.

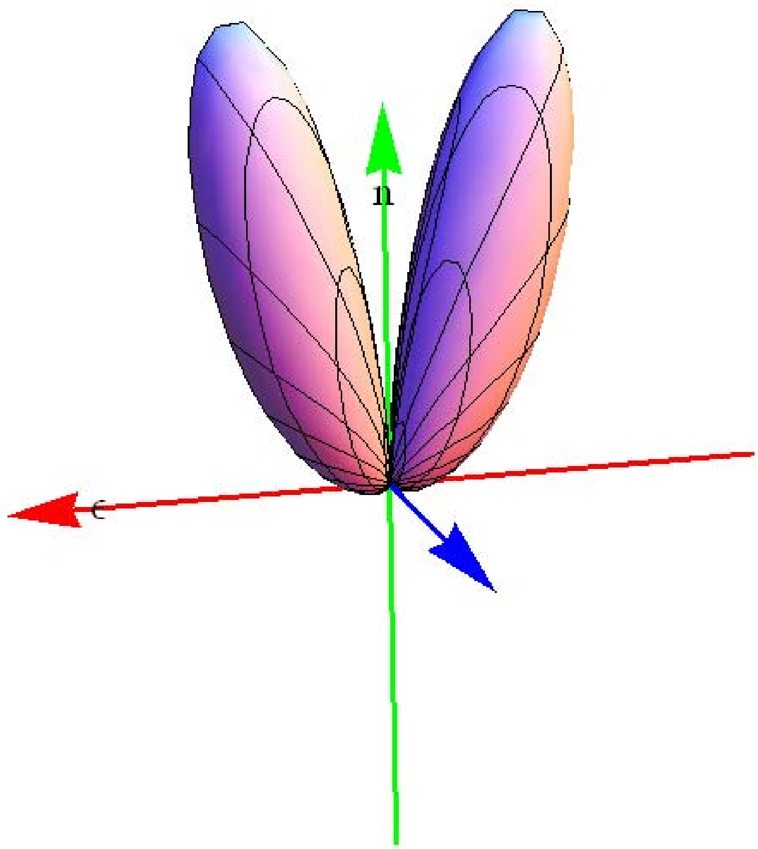

Fig. The case of $v_f / c = 0.95$.

((**David Park QM**))

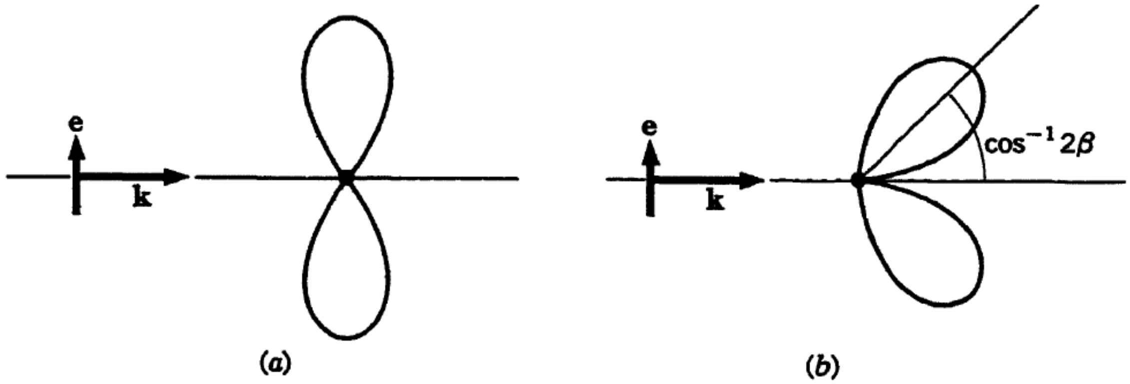

Fig. Angular distribution of photons at (a) low and (b) high photon energies. The electrons are ejected into two lobes whose maximum line lie in the plane of the polarization vector ***ε***. ***k*** is the wave vector of incident photon.

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APPENDIX

A1. Free electron gas in three dimensions

We consider the Schrödinger equation of an electron confined to a cube of edge *L*.

$$H\psi_{\mathbf{k}} = \frac{\mathbf{p}^2}{2m}\psi_{\mathbf{k}} = -\frac{\hbar^2}{2m}\nabla^2\psi_{\mathbf{k}} = \varepsilon_{\mathbf{k}}\psi_{\mathbf{k}} .$$

It is convenient to introduce wavefunctions that satisfy periodic boundary conditions.

Boundary condition (Born-von Karman boundary conditions).

$$\psi_{\mathbf{k}}(x+L, y, z) = \psi_{\mathbf{k}}(x, y, z) ,$$
$$\psi_{\mathbf{k}}(x, y+L, z) = \psi_{\mathbf{k}}(x, y, z) ,$$
$$\psi_{\mathbf{k}}(x, y, z+L) = \psi_{\mathbf{k}}(x, y, z) .$$

The wavefunctions are of the form of a traveling plane wave.

$$\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} ,$$

with

$k_x = (2\pi/L)\, n_x$, ($n_x = 0, \pm 1, \pm 2, \pm 3, \ldots..$),
$k_y = (2\pi/L)\, n_y$, ($n_y = 0, \pm 1, \pm 2, \pm 3, \ldots..$),
$k_z = (2\pi/L)\, n_z$, ($n_z = 0, \pm 1, \pm 2, \pm 3, \ldots..$).

The components of the wavevector ***k*** are the quantum numbers, along with the quantum number m_s of the spin direction. The energy eigenvalue is

$$\varepsilon(\mathbf{k}) = \frac{\hbar^2}{2m}(k_x{}^2 + k_y{}^2 + k_z{}^2) = \frac{\hbar^2}{2m}\mathbf{k}^2 .$$

Here

$$\mathbf{p}\psi_k(\mathbf{r}) = \frac{\hbar}{i}\nabla_{\mathbf{k}}\psi_k(\mathbf{r}) = \hbar\mathbf{k}\psi_k(\mathbf{r}) .$$

So that the plane wave function $\psi_{\mathbf{k}}(\mathbf{r})$ is an eigenfunction of $\boldsymbol{p}$ with the eigenvalue $\hbar\mathbf{k}$. The ground state of a system of N electrons, the occupied orbitals are represented as a point inside a sphere in $\boldsymbol{k}$-space.

Because we assume that the electrons are noninteracting, we can build up the N-electron ground state by placing electrons into the allowed one-electron levels we have just found.

A2. The Pauli's exclusion principle

The one-electron levels are specified by the wavevectors $\boldsymbol{k}$ and by the projection of the electron's spin along an arbitrary axis, which can take either of the two values $\pm\hbar/2$. Therefore associated with each allowed wave vector k are two levels:

$$|\boldsymbol{k},\uparrow\rangle,\ |\boldsymbol{k},\downarrow\rangle .$$

In building up the N-electron ground state, we begin by placing two electrons in the one-electron level $k = 0$, which has the lowest possible one-electron energy $\varepsilon = 0$. We have

$$N = 2\frac{L^3}{(2\pi)^3}\frac{4\pi}{3}k_F{}^3 = \frac{V}{3\pi^2}k_F{}^3 ,$$

A3 Density of states

There is one state per volume of $\boldsymbol{k}$-space $(2\pi/L)^3$. We consider the number of one-electron levels in the energy range from ε to ε+dε; $D(\varepsilon)$dε

$$D(\varepsilon)d\varepsilon = 2\frac{L^3}{(2\pi)^3}4\pi k^2 dk ,$$

where $D(\varepsilon)$ is called a density of states. Since $k = (2m/\hbar^2)^{1/2}\sqrt{\varepsilon}$, we have $dk = (2m/\hbar^2)^{1/2}d\varepsilon/(2\sqrt{\varepsilon})$. Then we get the density of states

$$D(\varepsilon) = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{\varepsilon} . \qquad (14)$$

B. Pythagorean relationship (relativistic dynamics)

Relativistic dynamics

$$\frac{E^2}{c^2} = m^2c^2 + \boldsymbol{p}^2$$

with

$$E = \frac{mc^2}{\sqrt{1-\frac{v^2}{c^2}}}, \qquad \boldsymbol{p} = \frac{mv}{\sqrt{1-\frac{v^2}{c^2}}}$$

$$\frac{E^2}{c^2} - m^2c^2 = \frac{m^2c^2}{1-\frac{v^2}{c^2}} - m^2c^2 = m^2c^2\left(\frac{1}{1-\frac{v^2}{c^2}} - 1\right) = \frac{m^2v^2}{1-\frac{v^2}{c^2}} = \boldsymbol{p}^2$$

Kinetic energy K is defined by

$$K = E - mc^2 = \frac{E^2 - m^2c^4}{E + mc^2} = \frac{c^2}{E + mc^2}\boldsymbol{p}^2$$

When $E \approx mc^2$, K is equal to

$$K \approx \frac{\boldsymbol{p}^2}{2m}$$

Pythagorean relationship

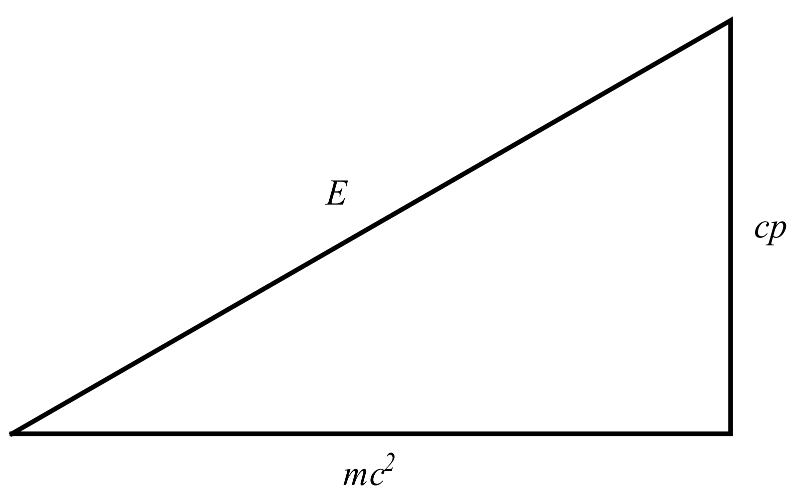

Fig. Pythagorean relationship. $\frac{E^2}{c^2} = m^2c^2 + \boldsymbol{p}^2$

C. Application — interaction with the classical radiation field

We consider the absorption and emission of light which is caused through the interaction between atoms and electromagnetic fields. The light is the electromagnetic field which periodically varies with time. Here we discuss the absorption and stimulated emission, where the electromagnetic field is semi-classically treated and the atoms are quantum-mechanically treated. There is another emission, so-called the spontaneous emission, where the electromagnetic field should be quantum-mechanically treated.

Classical radiation field

⇒ electric or magnetic field derivable from a classical radiation field as opposed to quantized field

$$\hat{H} = \frac{1}{2m}\hat{\boldsymbol{p}}^2 + e\phi(\hat{\boldsymbol{r}}) + \frac{e}{mc}\boldsymbol{A}\cdot\hat{\boldsymbol{p}}$$

which is justified if

$$\nabla\cdot\boldsymbol{A} = 0\,. \qquad \text{(Coulomb gauge)}$$

We work with a monochromatic field of the plane wave

$$\boldsymbol{A} = 2|\boldsymbol{A}_0|\boldsymbol{\varepsilon}\cos(\boldsymbol{k}\cdot\boldsymbol{r} - \omega t)$$

$$\boldsymbol{k} = \frac{\omega}{c}\boldsymbol{n}\,, \qquad \boldsymbol{\varepsilon}\cdot\boldsymbol{k} = 0$$

($\boldsymbol{\varepsilon}$ and $\boldsymbol{n}$ are the (linear) polarization and propagation directions.)

or

$$\boldsymbol{A} = |\boldsymbol{A}_0|\boldsymbol{\varepsilon}\left[e^{i(\boldsymbol{k}\cdot\boldsymbol{r}-\omega t)} + e^{-i(\boldsymbol{k}\cdot\boldsymbol{r}-\omega t)}\right]$$

The Hamiltonian is given by

$$\hat{H} = \hat{H}_0 + \hat{H}_1$$

where $\hat{H}_1$ is the time dependent perturbation

$$\hat{H}_1 = \frac{e}{mc}|\boldsymbol{A}_0|\left[e^{i(\boldsymbol{k}\cdot\boldsymbol{r}-\omega t)} + e^{-i(\boldsymbol{k}\cdot\boldsymbol{r}-\omega t)}\right](\boldsymbol{\varepsilon}\cdot\hat{\boldsymbol{p}})$$
$$= \hat{H}_1^{+}e^{-i\omega t} + \hat{H}_1 e^{i\omega t}$$

The first term: responsible for stimulated emission,
The second term: responsible for absorption

$$\left(\hat{H}_1^+\right)_{fi} = \frac{e\left|\boldsymbol{A}_0\right|}{mc}\left\langle \varphi_f \left| e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\boldsymbol{\varepsilon}\cdot\hat{\boldsymbol{p}} \right| \varphi_i \right\rangle$$

and

$$W_{i\to f} = \frac{2\pi}{\hbar}\frac{e^2}{m^2c^2}\left|\boldsymbol{A}_0\right|^2\left|\left\langle \varphi_f \left| e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\boldsymbol{\varepsilon}\cdot\hat{\boldsymbol{p}} \right| \varphi_i \right\rangle\right|^2 \delta\left(E_f - E_i - \hbar\omega\right)$$

((**Fermi's golden rule**))

where the energy is conserved during the process; $E_f - E_i = \hbar\omega$