Note Title 4/1/2008

Fermi's Golden rule

$$\boxed{\frac{1}{\tau_n} = \frac{2\pi}{\hbar} |W_{mn}|^2 D(E_m)\delta(E_m - E_n)}$$

Example

Consider a harmonic perturbation:

$$\hat{W}(t>0) = \hat{a} e^{i\omega t} + \hat{a}^{+} e^{-i\omega t}$$

Then the transition rate of scattering from state $|n\rangle$ to $|m\rangle$ is:

$$\frac{1}{\tau_n} = \frac{2\pi}{\hbar} |W_{mn}|^2 \delta(E_m - E_n) = \frac{2\pi}{\hbar} |\langle m| \hat{a} e^{i\omega t} + \hat{a}^{+} e^{-i\omega t} |n\rangle|^2 \delta(E_m - E_n)$$

$$\frac{1}{\tau_n} = \frac{2\pi}{\hbar} |\langle m|\hat{a}|n\rangle|^2 \delta(E_m - E_n + \hbar\omega) + \frac{2\pi}{\hbar} |\langle m|\hat{a}^{+}|n\rangle|^2 \delta(E_m - E_n - \hbar\omega)$$

Final energy $E_m = E_n - \hbar\omega$

Ex./ stimulated emission of a photon

Ex./ Phonon emission

$E_m = E_n + \hbar\omega$

Ex./ Photon absorption

Ex./ Phonon absorption

If there are continous energy states for the $|m\rangle$ (final state):

$$\frac{1}{\tau_n^{emi}} = \frac{2\pi}{\hbar} |\langle m|\hat{a}|n\rangle|^2 D(E_m)\delta(E_m - E_n + \hbar\omega)$$

$$\frac{1}{\tau_n^{abs}} = \frac{2\pi}{\hbar} |\langle m|\hat{a}^{+}|n\rangle|^2 D(E_m)\delta(E_m - E_n - \hbar\omega)$$

Since W_{mn} is hermitian (physical):

$$\langle m|\hat{a}|n\rangle = \langle m|\hat{a}|n\rangle^{+} = \langle n|\hat{a}^{+}|m\rangle$$

$$\Rightarrow \tau_n^{emi} D(E_m = E_n - \hbar\omega) = \tau_n^{abs} D(E_m = E_n + \hbar\omega)$$

What approximations we used to drive the Fermi Golden Rule?

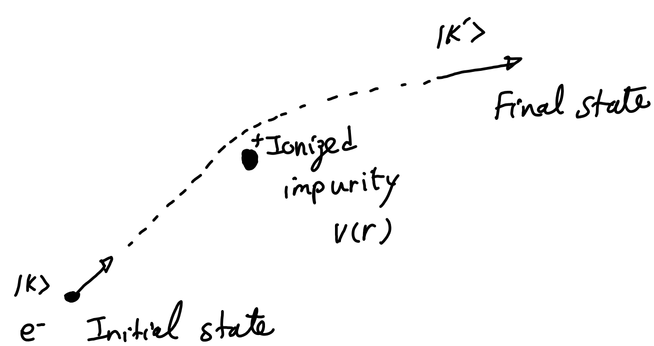
① $t \to \infty$ limit. So the collision must be complete before the next collision happens.

② We assumed the perturbation from $|n\rangle$ is so small that $|a_n|^2 = 1$ (conservation of number of particles ignored)

③ Also, we sometime assume that the incident wave is planwe $e^{ikx - i\omega t}$ and the final state also is planar $e^{ik'x - i\omega t}$. This means assuming that the collision is localized in real space.

All of these assumptions can be violated in modern semiconductor devices. So use FGR with caution!

Ionized Impurities scattering



$$\frac{1}{\tau(k,k')} = \frac{2\pi}{\hbar} |W_{kk'}|^2 D(E_{k'})\, \delta(E_{k'} - E_k)$$

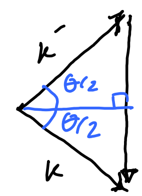
Must calculate the matrix element $W_{kk'}$:

$$W_{kk'} = \langle k' | v(r) | k \rangle = \int \varphi^*(k')\, v(r)\, \varphi(k)\, d^3r$$

Assume planar wave: $e^{i\vec{k}'\cdot\vec{r}}$ $\qquad e^{-i\vec{k}\cdot\vec{r}}$

(free electron wavefunction)

$$W_{kk'} = \int e^{-i\overbrace{(k-k')}^{\equiv q}\cdot r}\, v(r)\, d^3r$$



$\vec{k} - \vec{k}' = \vec{q}$

$|k| = |k'|$

$|q| = 2|k| \sin\frac{\theta}{2}$

$$= \int e^{-i\vec{q}\cdot\vec{r}}\, v(r)\, d^3r = v(q) \quad \text{Fourier transform}$$

So with planar wave assumption, the matrix element for the transition is the fourier transform of the peturbing potential:

$$\boxed{W_{kk'} = v(q) \quad \vec{q} \equiv \vec{k} - \vec{k}'}$$

This is a general argument for any potential with elastic scattering.

$$v(r) = \frac{-e^2}{4\pi\epsilon_r\epsilon_0}\frac{1}{r} \rightarrow v(q) = \int d^3r\, v(r)\, e^{-i\vec{q}\cdot\vec{r}} = \frac{-e^2}{4\pi\epsilon_r\epsilon_0}\int d^3r\, \frac{e^{-i\vec{q}\cdot\vec{r}}}{r}$$

$$= \frac{-e^2}{4\pi\epsilon_r\epsilon_0}\int_0^\infty dr \int_0^\pi d\theta \int_0^{2\pi} d\varphi\, \frac{e^{-iqr\cos\theta}}{r}\, r^2 \sin\theta$$

$$= \frac{-e^2 2\pi}{4\pi \epsilon_r \epsilon_0} \int_0^\infty dr \int_0^\pi d\theta \; r \sin\theta \; e^{-iqr\cos\theta} \qquad \begin{cases} x \equiv \cos\theta \\ dx = -\sin\theta \, d\theta \end{cases}$$

$$= \frac{-e^2}{2\epsilon_r \epsilon_0} \int_0^\infty dr \; r \int_{-1}^{1} dx \; e^{-iqrx} = \frac{-e^2}{2\epsilon_r\epsilon_0} \int_0^\infty dr \; r \frac{1}{-iqr} \left(e^{-iqr} - e^{iqr} \right)$$

$$= -\frac{e^2}{2\epsilon_r\epsilon_0} \int_0^\infty dr \frac{1}{-iq} (-2i \sin qr)$$

$$= \frac{-e^2}{\epsilon_r\epsilon_0 q} \int_0^\infty \sin qr \, dr = \frac{-e^2}{\epsilon_r\epsilon_0 q} \frac{-1}{q} \left[\cos(\infty) - \cos(0) \right]$$

$$\cos(\infty) \to 0 \qquad \cos(0) \to 1$$

$$V(r) = \frac{-e^2}{4\pi\epsilon_r\epsilon_0 r} \longrightarrow V(q) = \frac{e^2}{\epsilon_r\epsilon_0 q^2}$$

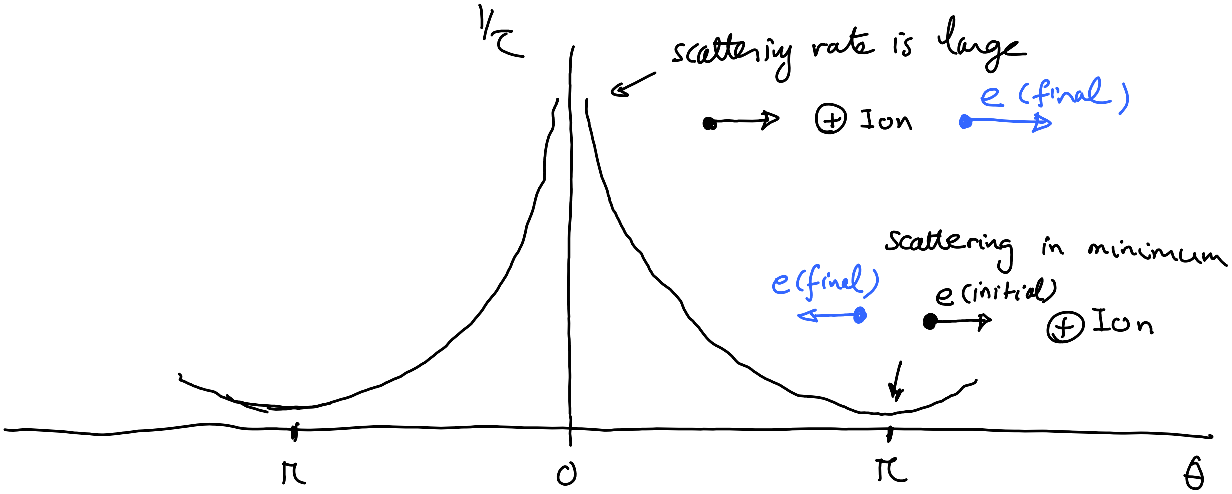
$$\frac{1}{\tau(k,k')} = \frac{2\pi}{\hbar} |V(q)|^2 \delta(E_k - E_{k'}) \qquad \begin{cases} \vec{q} = \vec{k} - \vec{k'} \\ |q| = 2|k| \sin\frac{\theta}{2} \end{cases}$$

$$= \frac{2\pi}{\hbar} \left(\frac{e^2}{\epsilon_r\epsilon_0 q^2} \right)^2 \delta(E_k - E_{k-q})$$

$$= \frac{2\pi e^4}{\hbar \epsilon_r^2 \epsilon_0^2} \frac{1}{16 k^4 \sin^4\frac{\theta}{2}} D(E_{k'}) \delta(E_{k'} - E_k)$$

Dielectric Constant often is a function of the wavevector q:

$$\epsilon_r = \epsilon_r(q)$$



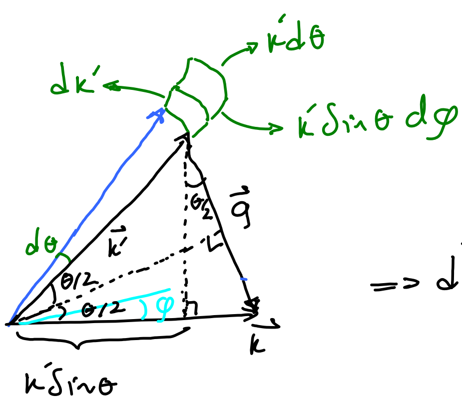
So most electrons are scattered without a significant change in their direction.

The total scattering rate is the integral of $\frac{1}{\tau(k,k')}$ over all possible final states k':

$$\frac{1}{\tau(k)} = \sum_q \frac{1}{\tau(k,q)} = \int \frac{d^3q}{(2\pi)^3} \frac{1}{\tau(k,q)} \qquad \vec{q} \equiv \vec{k} - \vec{k}'$$

$$= n \int \frac{d^3q}{(2\pi)^3} \frac{2\pi}{\hbar} \left(\frac{e^2}{\epsilon_r \epsilon_0 q^2} \right)^2 \delta(E_k - E_{k-q})$$

ions



$$\Rightarrow d^3q = k'^2 \sin\theta \, d\theta \, d\varphi \, dk$$

$$\frac{1}{\tau(k)} = \frac{2\pi n}{(2\pi)^3 \hbar}\left(\frac{e^2}{\epsilon_0}\right)^2 \underbrace{\int_0^{2\pi} d\varphi}_{2\pi} \int_0^{\pi} d\theta \int_0 dk' \, \delta(E_k - E_{k'}) \frac{k'^2}{\epsilon_r^2 q^4} \sin\theta$$

$$dk' \to \frac{dk'}{dE_{k'}} dE_{k'} = \frac{m}{\hbar^2 k'} dE_{k'}$$

$$= \frac{2\pi n}{(2\pi)^3 \hbar}\left(\frac{e^2}{\epsilon_0}\right)^2 (2\pi) \int_0^{\pi} d\theta \int dE_{k'} \, \delta(E_k - E_{k'}) \frac{m}{\hbar^2 k'} \frac{k'^2}{\epsilon_r^2 q^4} \sin\theta$$

$$= \frac{2\pi}{\hbar}\left(\frac{e^2}{2\pi\epsilon_0}\right)^2 \frac{m}{\hbar^2} \int_0^{\pi} d\theta \frac{k}{\epsilon_r^2 q^4} \sin\theta \qquad q = 2k\sin\frac{\theta}{2}$$

$$= \frac{2\pi n}{\hbar}\left(\frac{e^2}{2\pi\epsilon_0}\right)^2 \frac{m}{\hbar^2} \int_0^{\pi} d\theta \frac{k \sin\theta}{\epsilon_r^2 \, 16 k^4 \sin^4\frac{\theta}{2}} \qquad \sin\theta \to 2\sin\frac{\theta}{2}\cos\frac{\theta}{2}$$

$$= \frac{2\pi n}{\hbar}\left(\frac{e^2}{2\pi\epsilon_0}\right)^2 \frac{m}{\hbar^2} \frac{1}{8k^3} \int_0^{\pi} \frac{\cos\frac{\theta}{2} \, d\theta}{\epsilon_r^2 \sin^3\frac{\theta}{2}} \qquad \sin\frac{\theta}{2} = \eta, \quad \frac{1}{2}\cos\frac{\theta}{2}\, d\theta = d\eta$$

$$= \frac{2\pi n m}{\hbar^3 k^3}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2 \int_0^1 \frac{d\eta}{\epsilon_r^2 \eta^3}$$

$$\begin{cases} E = \frac{\hbar^2 k^2}{2m} \to k = \frac{\sqrt{2mE}}{\hbar} \\ k^3 = \frac{(2m)^{3/2}}{\hbar^3} E^{3/2} \end{cases}$$

$$= \frac{2\pi n m}{\hbar^3} \frac{\hbar^3 E^{-3/2}}{2^{3/2} m^{3/2}} \left(\frac{e^2}{4\pi\epsilon_0}\right)^2 \int_0^1 \frac{d\eta}{\epsilon_r^2 \eta^3}$$

$$\boxed{\frac{1}{\tau(E)} = \frac{\pi}{2^{1/2} m^{1/2}} n \left(\frac{e^2}{4\pi\epsilon_0}\right)^2 E^{-3/2} \int_0^1 \frac{d\eta}{\epsilon_r^2 \eta^3}}$$

If we assume $\epsilon_r(q) = \epsilon_r = \text{constant}$ =>

$$\frac{1}{\tau(E)} = \frac{\pi}{2^{1/2} m^{1/2}} n \left(\frac{e^2}{4\pi\epsilon_0 \epsilon_r}\right)^2 E^{-3/2} \underbrace{\int_0^1 \frac{d\eta}{\eta^3}}_{\left.\frac{-1}{2\eta^2}\right|_0^1 = \frac{-1}{2} + \infty \, !}$$

$$\Rightarrow \frac{1}{\tau(E)} = \infty \, !$$

So assuming ϵ_r to be constant, doesn't give a meaningful result.

Ex/ Calculat the electron meanfree path and mobility in GaAs doped to $n = 10^{18}\ cm^{-3}$ assuming that the dominant scattering for electrons is due to the ionized impurities.

Assume $\displaystyle\int_0^1 \frac{d\eta}{\epsilon_r^2(q)\, \eta^3} \simeq \frac{1}{\epsilon_{r_0}^2} = \frac{1}{100}$; $m_e^* = 0.07$

$$\frac{1}{\tau(E)} = \frac{\pi}{(2m)^{1/2}} n \left(\frac{e^2}{4\pi\epsilon_0}\right)^2 E^{-3/2} \frac{1}{100}$$

What is E? Most electrons are around Fermi energy – especially at low Temperature:

$$E \simeq E_f$$

At $T \simeq 0K$, we had: $k_F \simeq (3\pi^2 n)^{1/3} = (3\pi^2 \times 10^{18})^{1/3} = 3\times 10^{16}\ cm^{-1}$

$$E_f = \frac{\hbar^2 k_f^2}{2m_e} \quad \Rightarrow$$

$$\frac{1}{\tau(E)} \simeq \frac{\pi \times 10^{18} \times 10^{6}}{(2\times 0.07\times 9.1\times 10^{-31})^{1/2}} \left(\frac{1.6\times 10^{-19}}{4\pi \times 8.854\times 10^{-12}} \right)^2 \times \frac{E_f^{-3/2}}{100}$$

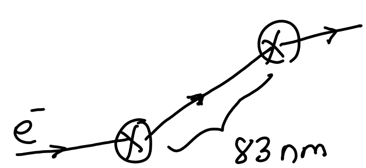
$$\cong 6.14\times 10^{12}\ s^{-1}$$

The electron scatters 6.14×10^{12} times per second!

The electron mean free path is:

$$l = v\tau \simeq v_F \tau(E_f) = 5\times 10^{7} \times \frac{1}{6.14\times 10^{12}} = 83\ nm$$

$$v_f = \frac{\hbar k_f}{m_e^*} = 5\times 10^{7}\ cm/s$$



Let's compare with electron wavelength:

$$\lambda = \frac{2\pi}{k} \simeq \frac{2\pi}{3\times 10^{6}\ cm^{-1}} \simeq 20\ nm$$

Note: This is comparable to l. So we cannot assume that scattering event is localized upon which the Fermi Golden Rulse is based on. We must have $l \gg \lambda$ so the scatterings to be independent.

Mobility calculation:

$$\mu = \frac{e\tau}{m^*}$$

$$= \frac{(1.6\times10^{-19})(6.14\times10^{12})^{-1}}{(0.07)(9.1\times10^{-31})}$$

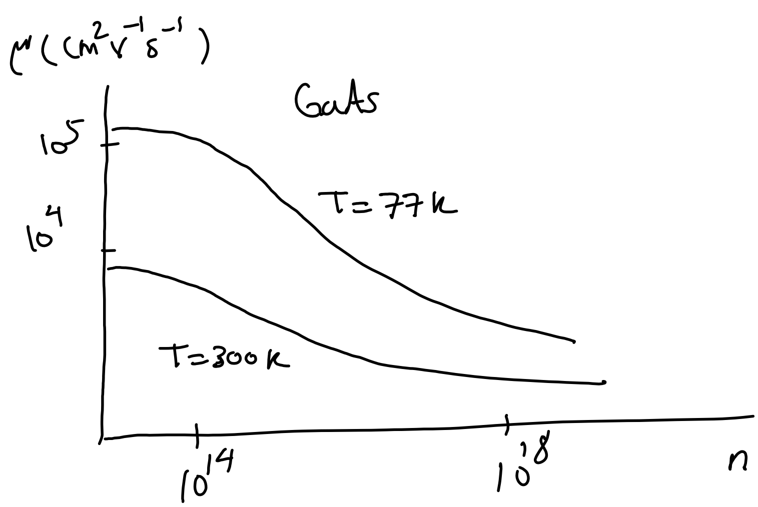
$$\mu = 4100 \ cm^2 V^{-1} s^{-1}$$

Conductivity:

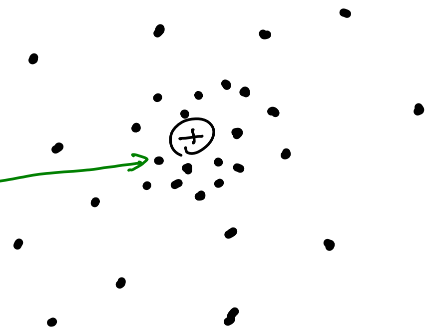
$$\sigma = en\mu$$

$$= (1.6\times10^{-19})(10^{18}\ cm^{-3})(4100\ cm^2V^{-1}s^{-1})$$

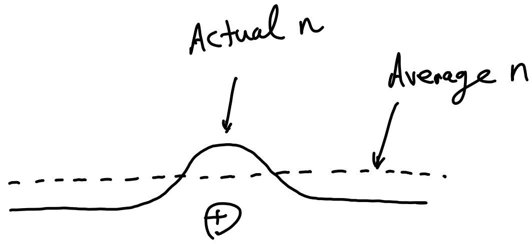
$$= 6560\ \Omega^{-1} cm^{-1}$$



Screening Effect



electron density increases around the ion



We should solve the poisson equation to find the potential V. Refer to the book for this. But the end result is interesting:

Solve the Poisson's Equation: $\nabla^2 V = -\dfrac{\rho}{\epsilon_r \epsilon_0} \Rightarrow$

$$V(r) = \frac{-e^2}{4\pi\epsilon_0\epsilon_r}\frac{1}{r} \xrightarrow[\text{effect}]{\text{screening}} V(r) = \frac{-e^2}{4\pi\epsilon_0\epsilon_r}\frac{e^{-r/r_0}}{r}$$

r_0 = the screening length

$$r_0 = \begin{cases} \dfrac{1}{q_D} = \left(\dfrac{\epsilon_r\epsilon_0 k_B T}{n_0 e^2}\right)^{1/2} & \text{Nondegenerate semicond. Debye screening length} \\[2ex] \dfrac{1}{q_{TF}} = \left(\dfrac{\epsilon\pi^2\hbar^2}{k_F m e^2}\right)^{1/2} & \text{Degenerate semicond. Thomas-Fermi screening length} \end{cases}$$

Fourier transform:

$$V(q) = \frac{-e^2}{\epsilon_0 \epsilon_r} \frac{1}{q^2} \xrightarrow{\text{Screening}} V(q) = \frac{-e^2}{\epsilon_0 \epsilon_r} \frac{1}{(q^2 + \frac{1}{r_0^2})}$$

or: $$V(q) = \frac{-e^2}{\epsilon_0 \epsilon_r} \frac{1}{q^2} \frac{1}{(1 + \frac{1}{q^2 r_0^2})}$$

$$= \frac{-e^2}{\epsilon_0 \epsilon_r(q)} \frac{1}{q^2}$$

$q_0 \equiv \frac{1}{r_0}$

As if : $$\boxed{\epsilon_r(q) = \epsilon_{r_0}\left(1 + \frac{1}{q^2 r_0^2}\right) = \epsilon_{r_0}\left(1 + \frac{q_0^2}{q^2}\right)}$$

Example

For the GaAs of the previous example:

$$q_{TF} = \left(\frac{k_F m e^2}{\epsilon \pi^2 \hbar^2}\right)^{1/2} = 2 \times 10^{16}\ cm^{-1}$$

$$\Rightarrow \frac{1}{q_{TF}} = 5\ nm$$

Compare it with $\frac{1}{k_F} \simeq 3nm$. This is not surprising that these are close to each other as they are both a measure of highest spatial frequency that can be used by electron to screen the coulomb interaction.

Ionized Impurity scattering — again!

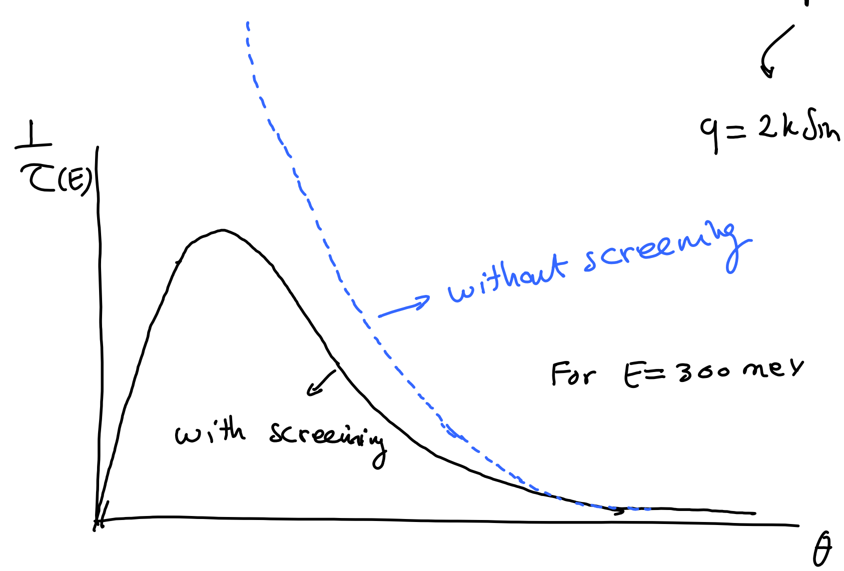
We now include the screening effect to our previous calculation:

$$\frac{1}{\tau(E)} = \frac{\pi}{2^{1/2} m^{1/2}} n \left(\frac{e^2}{4\pi\epsilon_0}\right)^2 E^{-3/2} \int_0^1 \frac{d\eta}{\epsilon_r^2 \eta^3}$$

$$\epsilon_r(q) = \epsilon_{r0}\left(1 + \frac{q_{TF}^2}{q_0^2}\right)$$

$$= \frac{\pi n}{2^{1/2} m^{1/2}} \left(\frac{e^2}{4\pi\epsilon_0\epsilon_{r0}}\right)^2 E^{-3/2} \int_0^1 \frac{d\eta}{\eta^3\left(1 + \frac{q_{TF}^2}{q^2}\right)^2}$$

$$q = 2k\sin\frac{\theta}{2} = 2k\eta$$



$$\boxed{\frac{1}{\tau(E)} = \frac{\pi}{\sqrt{2}}\left(\frac{e^2}{\epsilon_r\epsilon_0}\right)^2 \frac{E^{-3/2}}{m^{1/2}}\left[\ln\left(1 + \left(\frac{8mE}{\hbar^2 q_0}\right)^2\right) - \frac{1}{1 + \left(\frac{\hbar^2 q_0}{8mE}\right)^2}\right]}$$

$q_0 = q_{TF}$ if degenerate & $q_0 = q_D$ if non-degenerate.

Let's consider two limiting cases of very small and very large electron velocities:

Small initial velocity:

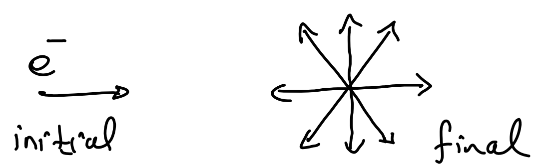
$k \to 0 \Rightarrow k r_0 \ll 1$.

The scattering amplitude $\propto V(q) = \int d^3r\, V(r)\, e^{-iq\cdot r}$

$k r_0 \ll 1 \Rightarrow e^{-iq\cdot r} \sim 1$ (since $q = 2k\sin\frac{\theta}{2}$ & $k \to 0$)

$V(q) = \int d^3r\, V(r) = 4\pi \int dr\, V(r)\, r^2$

So it doesn't depend on θ and is isotropic:



Low-energy electron

Large initial velocity:

$k \to \infty \Rightarrow k r_0 \gg 1$, you can show now it is highly anisotropic:

High energy

Stimulated Photon emission

Density of optical modes (states) in 3D:

$$D_3^{opt}(k) = 2 \times \frac{d^3k}{(2\pi)^3} = 2\times \frac{4\pi k^2 dk}{(2\pi)^3} = \frac{k^2}{\pi^2} dk$$

$2 \downarrow$ two orthogonal modes

For electron: $E = \frac{\hbar^2 k^2}{2m}$ For Photon: $\omega = ck$ or in a dielectric:

$$\omega = \underbrace{\frac{c}{n_r}}_{\text{reduced speed}} k$$

$$D_3^{opt}(\omega)\, d\omega = \frac{k^2}{\pi^2} dk$$

$$\Rightarrow D_3^{opt}(\omega) = \frac{k^2}{\pi^2}\frac{dk}{d\omega} = \frac{k^2}{\pi^2}\frac{n_r}{c} = \frac{\omega^2 n_r^2}{\pi^2 c^2}\frac{n_r}{c}$$

$$\boxed{D_3^{opt}(\omega) = \frac{n_r^3}{\pi^2 c^3}\omega^2}$$

mode density per unit energy per unit volume

Light intensity:

Pointing vector $\vec{S} = \vec{E} \times \vec{H}$ (power flux)

Average: $|S_{av}| = \frac{1}{2} |\vec{E}\times\vec{H}| = \frac{1}{2} |E_0||H_0|$

$$= \frac{1}{2}|E_0|\, \epsilon_0 c\, |E_0|$$

$$= \frac{1}{2} c\epsilon_0 |E_0|^2$$

Note: $\vec{H} = \sqrt{\frac{\epsilon_0}{\mu_0}}\, \hat{k}\times\vec{E} = \epsilon_0 c\, \hat{k}\times\vec{E}$

$\hat{k}$: propagation direction unit vector

$$|S_{av}| = \frac{1}{2} c \epsilon_0 |E_0|^2$$ Average power flux

(Average light intensity)

Energy density for photon per unit frequency interval in free space is,

$$\boxed{U(\omega) = \frac{1}{2} \epsilon_0 |E_0|^2}$$

Background photon energy density at thermal equilibrium;

$$U(\omega) = D_3^{opt}(\omega) \underbrace{f(\omega)}_{\text{Bose-Einstein dist.}} \hbar\omega$$

$$U(\omega) = \frac{\omega^2 n_r^3}{\pi^2 c^3} \frac{1}{e^{\hbar\omega/k_B T} - 1} \hbar\omega$$

$$\boxed{U(\omega) = \frac{\hbar\omega^3 n_r^3}{\pi^2 c^3} \frac{1}{e^{\hbar\omega/k_B T} - 1}}$$