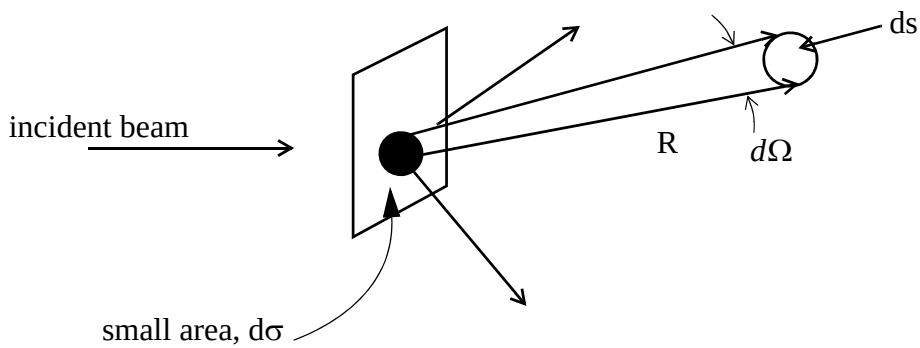
Scattering theory
(read Lundstrom 1.4, 1.5, 2.1, 2.2, See also, Schiff, Quantum Mechanics)



$d\Omega$ – small solid $\measuredangle$

$$= \frac{ds}{R^2}$$

$I_{inc} \equiv$ incident flux

$$= \begin{bmatrix} \text{\# particles passing unit} \\ \text{area transverse to beam} \end{bmatrix} / \text{sec}$$

if particle goes thru dσ - an "event" occurs

# of events / sec $= I_{inc} \cdot d\sigma$

Elastic scattering - an event is defined as elastic scattering into a solid angle dΩ

$$d\sigma = \frac{\text{\# events/sec}}{I_{inc}} \underset{\text{scatt}}{\overset{\text{elastic}}{=}} \frac{\text{\# particles scattered into } (d\Omega)/\text{sec}}{I_{inc}}$$

$$\boxed{d\sigma = \frac{\text{flux thru ds}}{\text{incident flux}}}$$

This is a ratio of fluxes. We can get this from quantum mechanics.

incident state Ψ_{inc} - plane wave

scattered state Ψ_{scatt}
far away from the scattering site:

$$\Psi_{r\to\infty} = \frac{1}{\sqrt{V}}\left[e^{i\vec{k}\cdot\vec{r}} + f(\theta,\varphi)\frac{e^{ikr}}{r}\right]$$

outgoing wave

We will drop the Bloch functions for simplicity. For isotropic, parabolic bands, the Bloch function part of the wavefunctions will integrate to 1.
Recall QM current density:

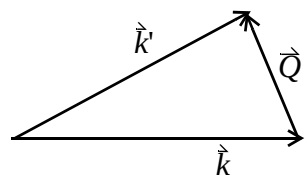
$$\vec{j}_{inc} = \frac{1}{V}\frac{\hbar\vec{k}}{m^*} \qquad I_{inc} = \vec{j}_{inc}\cdot\hat{z} = \left(\frac{\hbar k}{m^*}\right)\frac{1}{V}$$

$$\Psi_{scatt} \underset{r\to\infty}{\to} \frac{1}{\sqrt{V}} f(\theta,\varphi)\frac{e^{ikr}}{r}$$

$$\vec{j}_{scatt}\cdot d\vec{s} = R^2 d\Omega\left[\frac{\hbar}{2im^*}\left(\Psi^*_{scatt}\frac{d\Psi_{scatt}}{dr} - \Psi_{scatt}\frac{d\Psi^*_{scatt}}{dr}\right)\Bigg|_{r=R}\right] \qquad (d\vec{s} = \hat{r}R^2 d\Omega)$$

$$\underset{R\to\infty}{=} R^2 d\Omega\left[\frac{\hbar k}{m^*}|f(\theta,\varphi)|^2\frac{1}{R^2}\right]\frac{1}{V}$$

$$d\sigma = \frac{\vec{j}_{scatt}\cdot d\vec{s}}{\vec{j}_{inc}\cdot\hat{z}} = \frac{\frac{1}{V}\frac{\hbar k}{m^*}|f(\theta,\varphi)|^2 d\Omega}{\frac{1}{V}\frac{\hbar k}{m^*}}$$



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

momentum transfer vector

elastic scattering: $|\vec{k}| = |\vec{k}'|$

First Born approximation (derivation can be found in most advanced quantum texts)

$$f(\vec{Q}) = -\frac{2m^*}{4\pi\hbar^2}\int e^{i\vec{Q}\cdot\vec{y}} V(\vec{y})\, d^3y$$

scattering potential

$$= -\frac{2m^*}{4\pi\hbar^2}\tilde{V}(-Q)$$

Fourier transform
of the scattering potential

<u>Applications</u>

Ionized impurity scattering:

Bare Coulomb potential (I'm using esu units here, while Lundstrom uses MKS)

<u>Screening</u>

In an electron gas, carriers screen the potential. Solve Poisson's eqn, with density given by Maxwell-Boltzmann:

$$\nabla^2 V(r) = \rho$$

(n-type)

Using the Maxwell-Boltzmann function, we can relate the density to the local electrostatic potential:

$$n = N_C e^{[E_F - E_c(r)]/kT}$$

$$E_F - E_c(r) = \text{constant} + qV(r)$$

Now consider a perturbation in V denoted by δV. This leads to a perturbation in n, denoted by δn. Poisson's equation relates these:

$$\frac{1}{r^2}\frac{d}{dr}\left[r^2 \frac{d(\delta V)}{dr}\right] = q\delta n$$

Using: $\delta n = \frac{\partial n}{\partial V}\delta V$ and defining the unperturbed electron density:

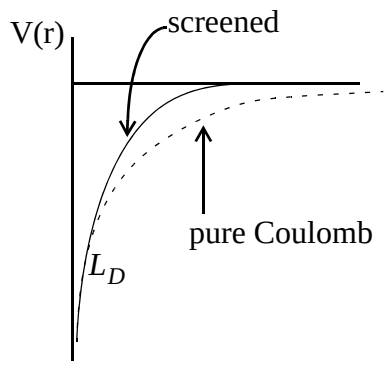
Then, $\frac{\partial n}{\partial V} = \frac{q}{kT}n$ and therefore, $\delta n = \frac{qn_o}{kT}\delta V$. Inserting this into Poisson's equation, we now get an equation for δV:

$$\frac{1}{r^2}\frac{d}{dr}\left[r^2 \frac{d(\delta V)}{dr}\right] = \frac{q^2 n_o}{kT}\delta V = \frac{\delta V}{L_D^2}$$

with $L_D \equiv \sqrt{\frac{kT}{q^2 n_o}}$, which is known as the "Debye screening length".

The solution to this equation is : $\delta V = \frac{A}{r}e^{-r/L_D}$

To match the Coulumb potential at small r:



Now calculate the scattering amplitude for the screened Coulomb potential using the Born approximation:

$$\vec{Q} \cdot \vec{x} = Qx\cos\theta \equiv Qx\mu$$

$$\tilde{V}(Q) = \int_0^\infty \int_0^{2\pi} d\varphi \int_{-1}^{1} d\mu e^{iQx\mu} \frac{e^{-x/L_D}}{x} x^2 dx$$

$$= 2\pi \int_0^\infty \frac{1}{iQx}(e^{iQx} - e^{-iQx}) \frac{e^{-x/L_D}}{x} x^2 dx$$

$$= \frac{2\pi}{iQ} \int_0^\infty e^{-x/L_D}[e^{iQx} - e^{-iQx}] dx$$

$$= \frac{2\pi}{iQ}\left[-\frac{1}{iQ - 1/L_D} + \frac{1}{-iQ - 1/L_D}\right]$$

$$= \frac{2\pi}{iQ}\left[\frac{2iQ}{Q^2 + (1/L_D)^2}\right]$$

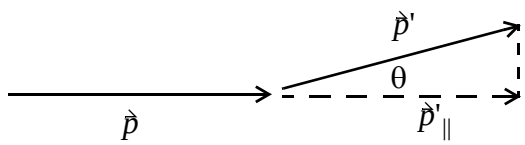
$$= \frac{4\pi}{Q^2 + (1/L_D)^2}$$

Since $Q = |\vec{k} - \vec{k}'| = 2k\sin\left(\frac{\theta}{2}\right)$

we obtain for the differential cross section:

$$\frac{d\sigma}{d\Omega} = \frac{4m^{*2}e^4}{\hbar^4}\left[\frac{1}{4k^2\sin^2\left(\frac{\theta}{2}\right) + \left(\frac{1}{L_D}\right)^2}\right]^2$$

<u>Momentum relaxation</u>



$$p'_{\parallel} = p'\cos\Theta$$
$$\Delta p'_{\parallel} = p'(1 - \cos\Theta)$$

Momentum relaxation is weighted by (1- cosθ). So, large angle scattering is more effective than small scattering.

Therefore the total **momentum relaxation** cross-section is:

$$\boxed{}$$

$$= \frac{4m^{*2}e^4}{\hbar^4}2\pi\int_0^{\pi}\frac{1}{\left(4\frac{p^2}{\hbar}\sin^2\frac{\theta}{2} + \frac{1}{L_D^2}\right)^2}(1-\cos\theta)\sin\theta\, d\theta$$

$$= \frac{8\pi m^{*2}e^4}{\hbar^4}\int_{-1}^{1}\frac{(1-\cos\theta)d(\cos\theta)}{\left[4\left(\frac{p}{\hbar}\right)^2\sin^2\frac{\theta}{2} + \frac{1}{L_D^2}\right]^2}$$

let $x = 1 - \cos\theta \quad \frac{1}{2}x = \sin^2\frac{\theta}{2}$

θ integral:

$$\int_0^2 \frac{x\,dx}{\left[2\left(\frac{p}{\hbar}\right)^2 x + \frac{1}{L_D^2}\right]^2}$$

Tabulated value of this integral is:

$$= \frac{1}{4(p/\hbar)^4}\left[\ln\left\{\frac{1}{L_D^2} + 2\left(\frac{p}{\hbar}\right)^2 x\right\} + \frac{1/L_D^2}{1/L_D^2 + 2\left(\frac{p}{\hbar}\right)^2 x}\right]\Bigg|_0^2$$

$$= \frac{1}{4(p/\hbar)^4}\left[\ln\left(\frac{1}{L_D^2} + 4\left(\frac{p}{\hbar}\right)^2\right) - \ln\left(\frac{1}{L_D^2}\right) + \frac{1/L_D^2}{1/L_D^2 + 4\left(\frac{p}{\hbar}\right)^2} - 1\right]$$

$$= \frac{1}{4(p/\hbar)^4}\left[\ln\left\{1 + 4L_D^2\left(\frac{p}{\hbar}\right)^2\right\} - \frac{4\left(\frac{p}{\hbar}\right)^2}{1/L_D^2 + 4\left(\frac{p}{\hbar}\right)^2}\right]$$

let $\boxed{}$ a dimensionless parameter. In terms of γ, the intergral is expressed:

$$\frac{1}{4(p/\hbar)^4}\left[\ln(1+\gamma^2) - \frac{\gamma^2}{1+\gamma^2}\right]$$

inserting back to the momentum relaxation cross-section,

$$\sigma_m(p) = \frac{8\pi m^{*2} e^4}{\cancel{\hbar^4}} \frac{1}{4(p/\cancel{\hbar})^4}\left[\ln(1+\gamma^2) - \frac{\gamma^2}{1+\gamma^2}\right]$$

We want the scattering rate:

$$\text{Scattering rate per ion} = \frac{\#\ \text{events}}{\text{sec}} = I_{inc} \cdot d\sigma = \frac{\hbar k}{m^*}\frac{1}{V}\sigma$$

The total scattering rate = . This is then:

$$S(p) = \frac{2\pi m^{*2} e^4}{p^4}\left(\frac{N_d}{V}\right)\frac{p}{m^*}\left[\ln(1+\gamma^2) - \frac{\gamma^2}{1+\gamma^2}\right]$$

The relaxation time $\tau(p) = S^{-1}(p)$. So,

$$\tau(p) = \left(\frac{N_d}{V}\right)^{-1}\frac{1}{2\pi m^* e^4}\left[\ln(1+\gamma^2) - \frac{\gamma^2}{1+\gamma^2}\right]^{-1} p^3$$

Since $E = \frac{p^2}{2m}$, $p^3 = (2m^*E)^{3/2}$

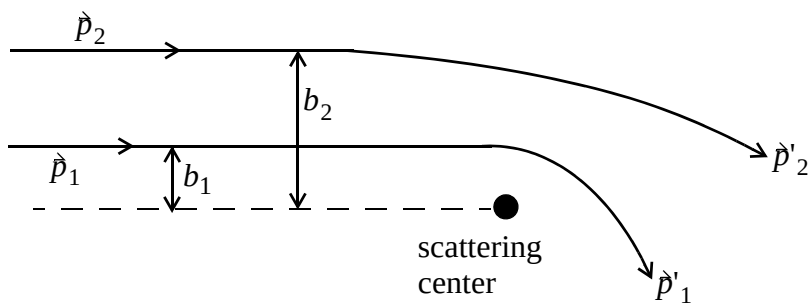
This is called the Brooks - Herring formula. It gives a $E^{3/2}$ law!

Unscreened Coulomb scattering

With no screening, $L_D \to \infty$. In this limit, we get the Rutherford scattering cross section, which was first derived to describe nuclear scattering at moderate energy..

This diverges strongly for $\theta \to 0$, which leads to a divergent total cross section. There are several practical approaches to dealing with this. We will use the so-called Conwell-Weisskopf approach.

Define the impact parameter, b:



Smaller impact paramater leads to larger angle scattering. We impose a cutoff on b, namely half the spacing between impurities. This is plausible, since at that point, the electron will tend to scatter from the nearest adjacent impurity.

$$b_{max} = \frac{1}{2} N_D^{-1/3}$$

Using classical theory in which we compute the classical "orbit" in $\frac{1}{r}$ potential, we can relate the impact parameter to the scattering angle:

$$b = \frac{e^2}{2\mathrm{E}(p)} \cot\left(\frac{\theta}{2}\right)$$

Defining:

$$\gamma_{CW} = \frac{E}{e^2 N_d^{1/3}} = \frac{b_{max}}{e^2/2\mathrm{E}}$$

We can now let $L_D \to \infty$, and integrate the Rutherford differential cross section from $\theta_{min} \to \pi$. The result, for the momentum relaxation time, is:

$$\tau_m = \frac{\sqrt{2m^*}}{\pi N_d e^4}\left[\frac{1}{\ln(1+\gamma_{CW}^2)}\right]E^{3/2}.$$

Again we see an $E^{3/2}$ power law, just with a different coefficient than for the screened scattering case.

<u>Strong screening limit</u>

In this limit, $L_D \to 0$ and we have a δ - function potential. Taking the appropriate limit of the screened Coulomb scattering cross section, this time we get:

which is flat - as expected for FT of δ - fn. The scattering is isotropic. In calculating the momentum relaxation cross-section, the cos θ term integrates to zero.

$$\sigma_m(p) = \frac{4m^{*2}e^4 L_D^4}{\hbar^4}\cdot(4\pi)$$

$$S(p) = N_D\frac{16\pi m^{*2}e^4 L_D^4}{\hbar^4}\frac{p}{m^*}$$

$$= N_D\frac{16\pi m^{*3/2}e^4 L_D^4}{\hbar^4}E^{1/2}$$

$$\tau_m = N_d^{-1}\frac{\hbar^4}{16\pi(m^*)^{3/2}e^4 L_D^4}E^{-1/2}$$

Again, we obtain a power law in E, but notice that now it has a negative exponent!