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

incident beam

small area, dσ

if particle goes thru dσ - an “event” occurs

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

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

$ds = \frac{# \text{ events/sec}}{I_{inc}} \cdot dσ = \frac{# \text{ particles scattered into (dΩ)/sec}}{I_{inc}}$

This is a ratio of fluxes. We can get this from quantum mechanics.
incident state $\Psi_{inc}$ - plane wave

scattered state $\Psi_{scatt}$

far away from the scattering site:

$$\Psi_{r \to \infty} = \frac{1}{\sqrt{V}} \left[ e^{ik \cdot \hat{r}} + f(\theta, \phi) \left( e^{ikr} \right) \right]$$

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:

$$j_{inc} = \frac{\hbar}{m^*} \Psi_{inc} \cdot \hat{z} = \left( \frac{\hbar k}{m^*} \right) \frac{1}{V}$$

$$\Psi_{scatt} \rightarrow \frac{1}{\sqrt{V}} f(\theta, \phi) e^{ikr}$$

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

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

$$(d\hat{s} = R^2 d\Omega)$$

$$d\sigma = \frac{\jmath_{scatt} \cdot d\hat{s}}{j_{inc} \cdot \hat{z}} = \frac{1}{V m^*} \frac{\hbar k f(\theta, \phi)^2}{\hbar k} d\Omega$$
First Born approximation  
(derivation can be found in most advanced quantum texts)

\[ f(\tilde{Q}) = \frac{2m^*}{4\pi\hbar^2} \int e^{i\tilde{Q} \cdot \hat{r}} V(\hat{r}) d^3y \]

scattering potential

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

Fourier transform of the scattering potential

Applications

Ionized impurity scattering:

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

Screening

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:

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

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

Now consider a perturbation in V denoted by \( \delta V \). This leads to a perturbation in n, denoted by \( \delta n \). 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, \( \delta n = \frac{q n_o}{kT} \delta V \). Inserting this into Poisson’s equation, we now get an equation for \( \delta V \):

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

with \( L_D = \sqrt{\frac{kT}{q n_o}} \), which is known as the “Debye screening length”.

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

To match the Coulomb potential at small r:
Now calculate the scattering amplitude for the screened Coulomb potential using the Born approximation:

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

\[
\tilde{V}(Q) = \int \int d\phi \int d\mu e^{iQx\mu} e^{-x/L_D} x^2 dx
\]

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

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

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

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

\[
= \frac{4\pi}{Q^2 + (1/L_D)^2}
\]
Since \( Q = |\mathbf{k} - \mathbf{k}'| = 2k\sin\left(\frac{\theta}{2}\right) \)

we obtain for the differential cross section:

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

Momentum relaxation

\[
\Delta p'_{||} = p'(1 - \cos \Theta)
\]

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

Therefore the total momentum relaxation cross-section is:

\[
\begin{align*}
\int_{0}^{\pi} & \left( \frac{1}{4k^2 \sin^2\left(\frac{\theta}{2}\right) + \left(\frac{1}{L_D}\right)^2} \right) \sin \theta d\theta \\
= & \frac{8\pi m^* e^4}{\hbar^4} \int_{-1}^{1} \left(1 - \cos \theta\right) d\left(\cos \theta\right) \\
= & \frac{8\pi m^* e^4}{\hbar^4} \left[ \left(\frac{p}{h}\right)^2 \sin^2\left(\frac{\theta}{2}\right) + \left(\frac{1}{L_D^2}\right) \right]^{1/2}
\end{align*}
\]

let \( x = 1 - \cos \theta \quad \frac{1}{2}x = \sin\frac{\theta}{2} \)
\( \theta \) integral:

\[
\int_{0}^{2} \frac{x \, dx}{2 \left( \frac{p}{\hbar} \right)^2 x + \frac{1}{L_D^2}}
\]

Tabulated value of this integral is:

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

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

Let \( a \) be a dimensionless parameter. In terms of \( \gamma \), the integral is expressed:

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

inserting back to the momentum relaxation cross-section,

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

We want the scattering rate:

Scattering rate per ion \( \frac{\text{# events}}{\text{sec}} \) = \( I_{inc} \cdot d\sigma = \frac{\hbar k}{m^* V} \sigma \)
The total scattering rate $S(p) = \frac{2\pi m^* e^4}{p^4} \left( \frac{N_d}{V} \right) \frac{p}{m^*} \ln\left(1 + \frac{\gamma^2}{1 + \gamma^2}\right)$.

This is then:

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

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

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

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

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 parameter 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.

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

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:

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

Defining:
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.

**Strong screening limit**

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

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

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

$$\sigma_{m}(p) = \frac{4m*^{2} e^{4} L_{D}^{4}}{h^{4}} \cdot (4\pi)$$

$$S(p) = N_{D} \frac{16\pi m*^{2} e^{4} L_{D}^{4} p}{h^{4} m*}$$

$$= N_{D} \frac{16\pi m^{3/2} e^{4} L_{D}^{4}}{h^{4}} E^{1/2}$$

$$\tau_{m} = N_{d}^{-1} \frac{h^{4}}{16\pi (m*)^{3/2} e^{4} L_{D}} E^{-1/2}$$

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