Lecture 22:
Ionized Impurity Scattering

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scattering of plane waves

incident plane wave

\[ \psi_i = \frac{1}{\sqrt{\Omega}} e^{i \vec{p} \cdot \vec{r}/\hbar} \]

\[ \vec{p} \]

\[ U_s(\vec{r}, t) \]

\[ \vec{p}' \]

weak scattering

\[ \psi_f = \frac{1}{\sqrt{\Omega}} e^{i \vec{p}' \cdot \vec{r}/\hbar} \]

infrequent scattering

\[ S(\vec{p}, \vec{p}') = \frac{2\pi}{\hbar} \left| H_{\vec{p}', \vec{p}} \right|^2 \delta(E' - E - \Delta E) \]

\[ H_{\vec{p}', \vec{p}} = \int_{-\infty}^{+\infty} \psi^*_f U_s(\vec{r}) \psi_i d\vec{r} \]

\[ H_{\vec{p}', \vec{p}} = \frac{1}{\Omega} \int_{-\infty}^{+\infty} e^{-i \vec{p}' \cdot \vec{r}/\hbar} U_s(\vec{r}) e^{i \vec{p} \cdot \vec{r}/\hbar} d\vec{r} \]
examples

“short range potential”

\[ U_S(\vec{r}) = C \delta(0) \]

\[ S(\vec{p}, \vec{p}') = K \frac{1}{\Omega} \delta(E' - E) \]

\[ \frac{1}{\tau(E)} = \frac{1}{\tau_m(E)} \propto D_f(E) \]

“oscillating, propagating potential”

\[ U_S(\vec{r}, t) = \frac{U_{\beta}^{a,e}}{\sqrt{\Omega}} e^{\pm i(\vec{\beta} \cdot \vec{r} - \omega t)} \]

\[ S(\vec{p}, \vec{p}') = \frac{2\pi}{\hbar} \left| \frac{U_{\beta}^{a,e}}{\Omega} \right|^2 \delta(E' - E \mp \hbar \omega) \delta(\vec{p}', \vec{p} \pm \hbar \vec{\beta}) \]

\[ \frac{1}{\tau(E)} = \frac{1}{\tau_m(E)} \propto D_f(E \pm \hbar \omega) \]

\[ \frac{1}{\tau_E(\vec{p})} = \left( \frac{\hbar \omega}{E} \right) \frac{1}{\tau(\vec{p})} \]
acoustic vs. optical phonon scattering

\[ \frac{1}{\tau(\vec{p})} \sim D_f(E) \]

\[ \frac{1}{\tau(\vec{p})} \sim (n_\omega + 1) D_f(E - \hbar \omega_0) \]

\[ \frac{1}{\tau(\vec{p})} \sim n_\omega D_f(E + \hbar \omega_0) \]
summary

1) Characteristic times are derived from the transition rate, $S(p,p')$
2) $S(p,p')$ is obtained from Fermi’s Golden Rule
3) The scattering rate is proportional to the final DOS
4) Static potentials lead to elastic scattering
5) Time varying potentials lead to inelastic scattering
6) General features of scattering in common semiconductors can now be understood (almost)
covalent vs. polar semiconductors

Covalent

\[ E \]

\[ \langle 100 \rangle \]

\[ \frac{1}{\tau} \]

\[ E \]

\[ \langle 100 \rangle \rightarrow x \]

Polar

\[ E \]

\[ \langle 100 \rangle \rightarrow x \]

\[ \langle 111 \rangle \]

\[ \frac{1}{\tau} \]

\[ E \]

\[ 0.03 \rightarrow 0.30 \rightarrow E \]
II scattering potential

i) electrons in P-type material

\[ \mathbf{p} \rightarrow \mathbf{p}' \]

\[ N_A^- - b \]

“impact parameter”

ii) electrons in N-type material

\[ \mathbf{p} \rightarrow \mathbf{p}' \]

\[ N_D^+ + \]

\[ U_S(\mathbf{r}) = \pm \frac{q^2}{4\pi\kappa S \varepsilon_0 r} \]

According to FGR, the transition rate is independent of the sign of the scattering potential.
outline

1) Review
2) **Screening**
3) Brooks-Herring approach
4) Conwell-Weisskopf approach
5) Discussion
6) Summary / Questions

(Reference: Chapter 2, Lundstrom, FCT)
Bare Coulomb potential:

\[ U_S(\vec{r}) = \frac{q^2}{4\pi \kappa_s \varepsilon_0 r} \]

Screened Coulomb potential: ??

Mobile charges attracted to fixed charges “screen” out the fixed charge.
screening in 3D

\[ \nabla^2 V(\vec{r}) = -\frac{\rho}{\kappa_S \varepsilon_0} = -\frac{q [N_D^+ - n(\vec{r})]}{\kappa_S \varepsilon_0} \]

\[ n(\vec{r}) \approx N_D^+ = n_0 \]

\[ V(\vec{r}) = V_0 \]

\[ \delta n(\vec{r}) \approx n(\vec{r}) - n_0 \]

\[ \delta V(\vec{r}) \approx V(\vec{r}) - V_0 \]

\[ \nabla^2 \delta V(\vec{r}) = -\frac{q}{\kappa_S \varepsilon_0} \frac{\partial n_0(\vec{r})}{\partial V} \delta V(\vec{r}) \]

\[ \frac{1}{L_D^2} \equiv \frac{q}{\kappa_S \varepsilon_0} \frac{\partial n_0(\vec{r})}{\partial V} \]

\[ n_0(\vec{r}) = \frac{1}{\Omega} \sum_k f_0(k) \]

\[ f_0(k) = \frac{1}{1 + e^{(E_C(\vec{r}) + E(\vec{k}) - E_F)/k_B T}} \]

\[ \frac{\partial n_0(\vec{r})}{\partial V} = q \frac{\partial n_0(\vec{r})}{\partial E_F} \]

\[ \frac{1}{L_D^2} \equiv \frac{q^2}{\kappa_S \varepsilon_0} \frac{\partial n_0(\vec{r})}{\partial E_F} \]
screening in 3D

$$\nabla^2 \delta V (\vec{r}) = \frac{1}{L_D^2} \delta V (\vec{r})$$

$$\frac{1}{L_D^2} \equiv \frac{q^2}{\kappa_S \varepsilon_0} \frac{\partial n_0 (\vec{r})}{\partial E_F}$$

$$\frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{dV}{dr} \right) = \frac{1}{L_D^2} \delta V (\vec{r})$$

$$\delta V (r) = C \frac{e^{-r/L_D}}{r}$$

$$U_S (r) = -q \delta V (r) = \frac{q^2}{4\pi\kappa_S \varepsilon_0 r} e^{-r/L_D}$$
Debye length in 3D

\[ U_S(r) = \frac{q^2}{4\pi\kappa_S\varepsilon_0 r} e^{-r/L_D} \]

\[ \frac{1}{L_D^2} \equiv \frac{q^2}{\kappa_S\varepsilon_0} \frac{\partial n_0(\vec{r})}{\partial E_F} = \frac{q^2}{\kappa_S\varepsilon_0 k_B T} \frac{\partial n_0(\vec{r})}{\partial \eta_F} \]

\[ n_0 = N_{3D} \mathcal{F}^{1/2}(\eta_F) \]

\[ \frac{\partial n_0}{\partial \eta_F} = N_{3D} \mathcal{F}^{-1/2}(\eta_F) = n_0 \frac{\mathcal{F}^{-1/2}(\eta_F)}{\mathcal{F}^{1/2}(\eta_F)} = n_0 \]

Debye length (non-degenerate)

\[ L_D = \sqrt{\frac{\kappa_S \varepsilon_0 k_B T_L}{q^2 n_0}} \]
comments on screening

1) Our semi-classical approach assumes that the potential is slowly varying on the scale of the electron’s wavelength. For rapidly varying potentials, a more sophisticated approach is needed. (See Ashcroft and Mermin, pp. 340-343 for a discussion of the Lindhard theory.)

2) Our semi-classical approach also assumes that the potential is slowly in time. (See Ashcroft and Mermin, p. 344 for a brief discussion.)

3) For potentials that vary rapidly in space and time, a “dynamic screening” treatment is needed. (See chapter 9 in Ridley, Quantum Processes in Semiconductors, 4th Ed. and Chapter 10 in Ridley, Electrons and Phonons in Semiconductor Multilayers.)

4) Screening is generally less effective in 2D and in 1D. (See J.H. Davies, The Physics of Low-Dimensional Structures, pp. 350-356)
Outline

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(Reference: Chapter 2, Lundstrom, FCT)
transition rate and scattering potential

\[
S(\vec{p}, \vec{p}') = \frac{2\pi}{\hbar} |H_{p', p}|^2 \delta(E' - E)
\]

\[
H_{p', p} = \frac{1}{\Omega} \int_{-\infty}^{+\infty} e^{-i\vec{p}' \cdot r / \hbar} U_S(r) e^{i\vec{p} \cdot r / \hbar} \, dr = \frac{1}{\Omega} \int_{-\infty}^{+\infty} U_S(r) e^{-i(\vec{p}' - \vec{p}) \cdot \vec{r} / \hbar} \, dr
\]

\[
= \frac{1}{\Omega} \int_{-\infty}^{+\infty} U_S(r) e^{-i\vec{\beta} \cdot \vec{r}} \, d\vec{r} \equiv \frac{1}{\Omega} \tilde{U}_S(\vec{\beta})
\]

\[
\vec{p}' = \vec{p} + \hbar \vec{\beta}
\]
Il scattering (Brooks-Herring)

\[ U_S(r) = \frac{q^2}{4\pi \kappa_S \epsilon_0 r} e^{-r/L_D} \]

\[ L_D = \sqrt{\frac{\kappa_S \epsilon_0 k_B T}{q^2 n_0}} \] Debye length

\[ \tilde{U}_S(\beta) = \int_{-\infty}^{+\infty} U_S(r) e^{-i\beta \cdot \vec{r}} \, d\vec{r} \]

\[ \vec{p}' = \vec{p} + \hbar \vec{\beta} \]
Fourier transform of the screened Coulomb potential

\[ \tilde{U}_S (\beta) = \int_{-\infty}^{+\infty} \frac{q^2}{4\pi \kappa_S \varepsilon_0 r} e^{-r/L_D} e^{-i\vec{\beta} \cdot \vec{r}} \, d\vec{r} \]

\[ \tilde{U}_S (\beta) = \frac{q^2}{4\pi \kappa_S \varepsilon_0} \int_{0}^{2\pi} \int_{0}^{\pi} \int_{0}^{\infty} e^{-r/L_D} e^{-i\vec{\beta} \cdot \vec{r}} \, r \sin \theta \, d\theta \, dr \]

choose z-axis along \( \beta \):

\[ \tilde{U}_S (\beta) = \frac{q^2}{2\kappa_S \varepsilon_0} \int_{0}^{+1} e^{-r/L_D} r dr \int_{-1}^{+1} e^{-i\beta r \cos \theta} \, d(\cos \theta) \]

\[ \frac{2 \sin(\beta r)}{\beta r} \]

\[ \vec{p}' = \vec{p} + \hbar \vec{\beta} \]
Fourier transform (ii)

\[ \tilde{U}_S (\beta) = \frac{q^2}{\kappa_s \varepsilon_0} \int_0^{\infty} \frac{e^{-r/L_D}}{\beta} \sin(\beta r) \, dr \]

\[ \tilde{U}_S (\beta) = \frac{q^2}{\kappa_s \varepsilon_0} \left( \frac{1}{\beta^2 + 1/L_D^2} \right) \]

\[ \tilde{U}_S (\beta) = \frac{q^2}{\kappa_s \varepsilon_0} \left( \frac{1}{4(p/h)^2 \sin^2(\alpha/2) + 1/L_D^2} \right) \]

\[ \hbar \beta = 2p \sin(\alpha/2) \]

\[ \bar{\beta} \cdot \vec{r} = \beta r \cos \theta \]

\[ \sin \theta d\theta = -d (\cos \theta) \]

small angle scattering preferred!!
small angle scattering

\[ \tilde{U}_S(\beta) = \frac{q^2}{\kappa_S \varepsilon_0} \left( \frac{1}{\beta^2 + 1/L_D^2} \right) \]

\[ U_S(r) = \frac{q^2}{4\pi\kappa_S \varepsilon_0 r} e^{-r/L_D} \]
II. Scattering of high energy carriers

\[ \tilde{U}_S(\beta) = \frac{q^2}{\kappa_S \varepsilon_0} \left( \frac{1}{4(p/\hbar)^2 \sin^2(\alpha/2) + 1/L_D^2} \right) \]

For a given deflection angle, higher energies scatter less.

For a given deflection angle, higher energies scatter less.

Random charges introduce random fluctuations in \( E_C \), which act as scattering centers.

High energy electrons don’t “see” these fluctuations and are not scattered as strongly.
II scattering: recap

\[
S(\vec{p}, \vec{p}') = \frac{2\pi}{\hbar} |H_{p',p}|^2 \delta(E' - E) \quad H_{p,p'} = \frac{1}{\Omega} \tilde{U}_S(\beta) \quad \tilde{U}_S(\beta) = \frac{q^2}{\kappa_s \varepsilon_0} \left( \frac{1}{\beta^2 + 1/L_D^2} \right)
\]

Need to multiply by the total number of ionized impurities in the volume, \(\Omega\).

\[
S(\vec{p}, \vec{p}') = \frac{2\pi q^4 N_I}{\hbar \kappa_s^2 \varepsilon_0^2 \Omega} \frac{\delta(E' - E)}{\left( \beta^2 + 1/L_D^2 \right)^2}
\]

\[
\frac{\hbar \beta}{2} = p \sin \alpha / 2
\]

\[
\vec{p}' = \vec{p} + \hbar \beta
\]
\[ S(\vec{p}, \vec{p}') = \frac{2\pi q^4 N_I}{\hbar \kappa_0^2 \epsilon_0^2 \Omega} \frac{\delta(E' - E)}{\left( \frac{4p^2}{\hbar^2} \sin^2 \alpha/2 + 1/L_D^2 \right)^2} \]

1) \( S(\vec{p}, \vec{p}') \sim N_I \)

2) \( S(\vec{p}, \vec{p}') \sim q^4 \)

3) \( S(\vec{p}, \vec{p}') \sim 1/E^2 \)

4) favors small angle scattering
4) angular dependence

\[
S(\vec{p}, \vec{p}') = \frac{2\pi q^4 N_I}{\hbar \kappa_S^2 \varepsilon_0^2 \Omega} \frac{\delta(E' - E)}{\left(\frac{4p^2}{\hbar^2} \sin^2 \alpha/2 + 1/L_D^2\right)^2}
\]

\[
S(\vec{p}, \vec{p}') \rightarrow \frac{2\pi q^4 N_I L_D^4}{\hbar \kappa_S^2 \varepsilon_0^2 \Omega} \delta(E' - E)
\]
momentum relaxation time

\[
\frac{1}{\tau_m} = \sum_{\vec{p}'} S(\vec{p}, \vec{p}') \left( 1 - \frac{p'}{p} \cos \alpha \right)
\]

favors small angles

\[
S(\vec{p}, \vec{p}')
\]

expect:

\[
\frac{1}{\tau_m} < \frac{1}{\tau} \quad \tau_m > \tau
\]
momentum relaxation time

\[
\frac{1}{\tau_m(E)} = \sum_{\vec{p}'} S(\vec{p}, \vec{p}')(1 - \cos \alpha)
\]

\[
\tau_m(E) = \frac{16\sqrt{2m^* \pi \kappa^2 \varepsilon_0^2}}{N_l q^4} \left[ \ln \left(1 + \gamma^2\right) - \frac{\gamma^2}{1 + \gamma^2} \right] E^{3/2}
\]

\[
\gamma^2 = 8m^* EL_D^2 / \hbar^2
\]

See Lundstrom, pp. 69-70

\[
\tau_m(E) \sim E^{3/2}
\]

\[
\tau_m(E) \approx \tau_0 \left(\frac{E}{k_B T_L}\right)^{3/2}, \quad \tau_0 \sim T_L^{3/2}, \quad s = 3/2
\]
to be continued in next lecture

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