ECE-656: Fall 2011

Lecture 22:

Ionized Impurity Scattering

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10/19/11

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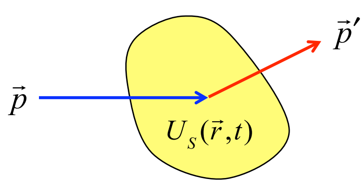
scattering of plane waves

$$\psi_i = \frac{1}{\sqrt{\Omega}} e^{i\vec{p}\bullet\vec{r}/\hbar}$$

incident plane wave



$$\psi_f = \frac{1}{\sqrt{\Omega}} e^{i\vec{p}\,'\bullet\vec{r}/\hbar}$$

weak scattering

infrequent scattering

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

$$H_{\vec{p}\,',\vec{p}} = \int_{-\infty}^{+\infty} \psi_f^* U_S(\vec{r})\psi_i d\vec{r}$$

$$H_{\vec{p}\,',\vec{p}} = \frac{1}{\Omega}\int_{-\infty}^{+\infty} e^{-i\vec{p}\,'\bullet r/\hbar} U_S(\vec{r}) e^{i\vec{p}\bullet\vec{r}/\hbar} d\vec{r}$$

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"

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

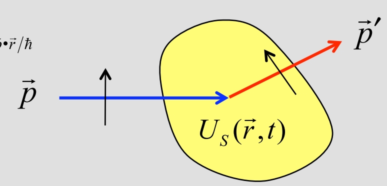
$$S(\vec{p},\vec{p}\,') = \frac{2\pi}{\hbar}\frac{\left|U_\beta^{a,e}\right|^2}{\Omega}\delta(E'-E\mp\hbar\omega)\delta_{\vec{p}\,',\vec{p}\pm\hbar\vec{\beta}}$$

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

$$\frac{1}{\tau_E(\vec{p})} = \left(\frac{\hbar\omega}{E}\right)\frac{1}{\tau(\vec{p})}$$

static potential summary

$$\psi_i = \frac{1}{\sqrt{\Omega}} e^{i\vec{p}\bullet\vec{r}/\hbar}$$



$$\psi_f = \frac{1}{\sqrt{\Omega}} e^{i\vec{p}\,'\bullet\vec{r}/\hbar}$$

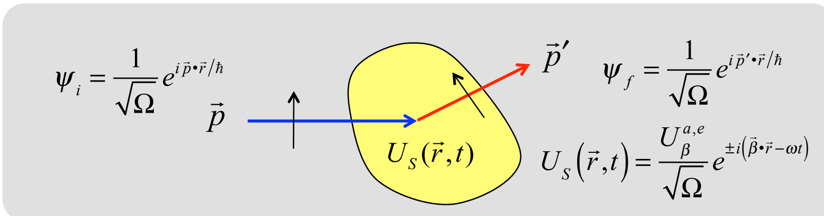
$$U_S(\vec{r}) = C\delta(0)$$

$$\frac{1}{\tau(\vec{p})} \sim \frac{D(E)}{2}$$

$$\frac{1}{\tau_m(\vec{p})} = \frac{1}{\tau(\vec{p})} \quad \text{(isotropic)}$$

$$\frac{1}{\tau_E(\vec{p})} = 0 \quad \text{(elastic)}$$

oscillating potential summary

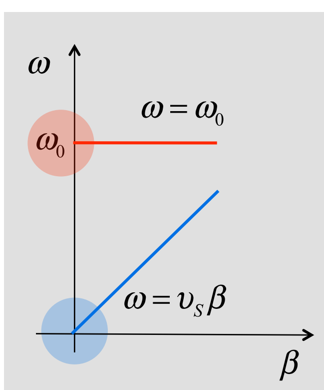


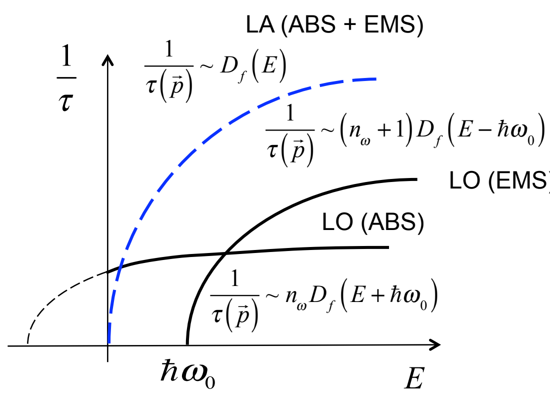
$$\frac{1}{\tau(\vec{p})} \sim \frac{D_f(E \pm \hbar\omega)}{2}$$

$$\frac{1}{\tau_m(\vec{p})} = \frac{1}{\tau(\vec{p})} \quad \text{(isotropic)}$$

$$\frac{1}{\tau_E(\vec{p})} = \frac{\hbar\omega}{E}\frac{1}{\tau(\vec{p})} \quad \text{(inelastic)}$$

acoustic vs. optical phonon scattering

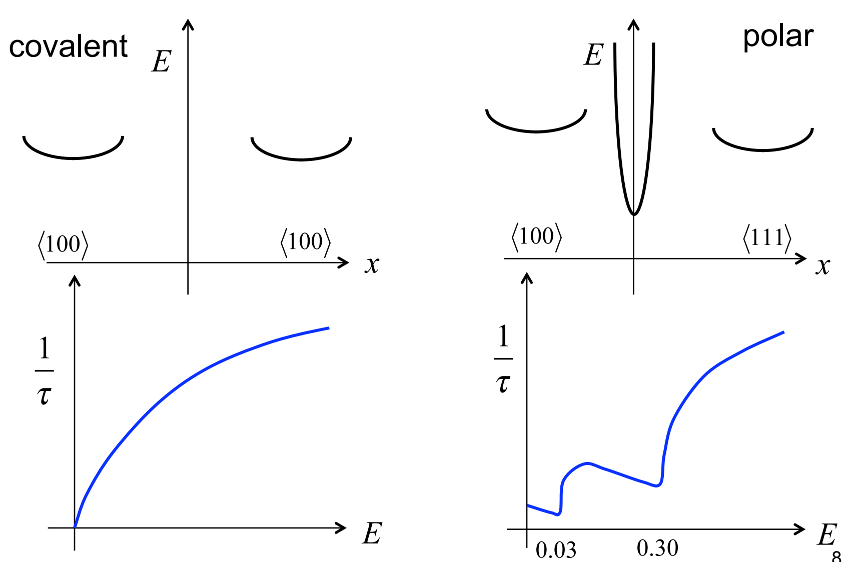




summary

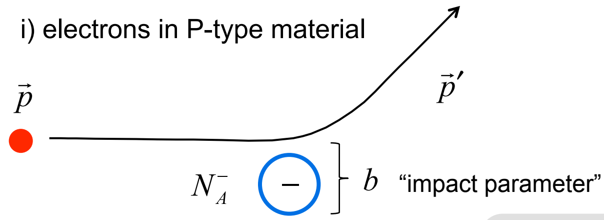
1) Characteristic times are derived from the transition rate, $S(p,p')$
2) $S(p,p')$ is obtained from Fermi's Golden Rule
3) The scattering rate is proportional to the final DOS
4) Static potentials lead to elastic scattering
5) Time varying potentials lead to inelastic scattering
6) General features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

covalent vs. polar semiconductors

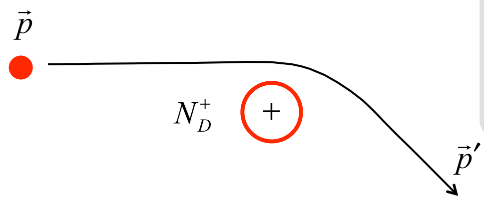


II scattering potential

i) electrons in P-type material



ii) electrons in N-type material



$$U_S(\vec{r}) = \pm \frac{q^2}{4\pi\kappa_S\varepsilon_0 r}$$

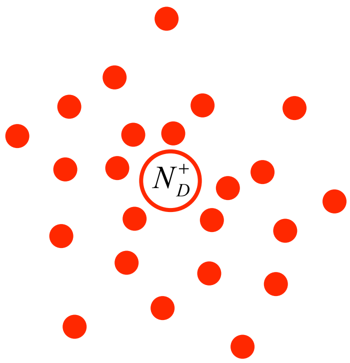
According to FGR, the transition rate is independent of the sign of the scattering potential.

outline

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

(Reference: Chapter 2, Lundstrom, FCT)

screening



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

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

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

$$V(\vec{r}) = V_0$$

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

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

$$\nabla^2 \delta V(\vec{r}) = -\frac{q}{\kappa_S\varepsilon_0}\frac{\partial n(\vec{r})}{\partial V}\delta V(\vec{r})$$

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

$$n(\vec{r}) = \frac{1}{\Omega}\sum_{\vec{k}} f_0(k)$$

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

$$\frac{\partial n(\vec{r})}{\partial V} = q\frac{\partial n(\vec{r})}{\partial E_F}$$

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

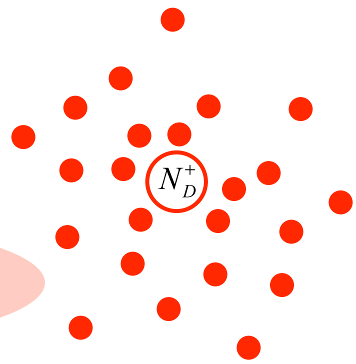
screening in 3D

$$\nabla^2 \delta V(\vec{r}) = \frac{1}{L_D^2}\delta V(\vec{r}) \qquad \frac{1}{L_D^2} \equiv \frac{q^2}{\kappa_S \varepsilon_0}\frac{\partial n(\vec{r})}{\partial E_F}$$

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

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

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



Debye length in 3D

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

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

$$n_0 = N_{3D}\mathcal{F}_{1/2}(\eta_F)$$

$$\frac{\partial n_0}{\partial \eta_F} = N_{3D}\mathcal{F}_{-1/2}(\eta_F) = n_0\frac{\mathcal{F}_{-1/2}(\eta_F)}{\mathcal{F}_{1/2}(\eta_F)} = n_0 \qquad \text{(non-degenerate)}$$

$$L_D = \sqrt{\frac{\kappa_S \varepsilon_0 k_B T}{q^2 n_0}}$$

Debye length

(non-degenerate)

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

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

(Reference: Chapter 2, Lundstrom, FCT)

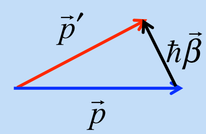
transition rate and scattering potential

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

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

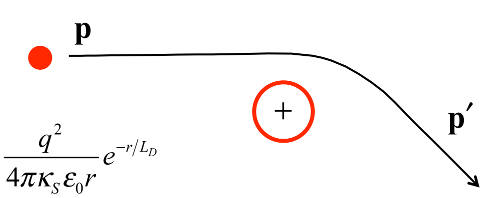
$$= \frac{1}{\Omega}\int_{-\infty}^{+\infty} U_S(r) e^{-i\vec{\beta}\bullet\vec{r}}\, d\vec{r} \equiv \frac{1}{\Omega}\tilde{U}_S\left(\vec{\beta}\right)$$

$$\vec{p}\,' = \vec{p} + \hbar\vec{\beta}$$



$$S(\vec{p},\vec{p}\,') = \frac{2\pi}{\hbar}\frac{1}{\Omega^2}\left|\tilde{U}_S(\beta)\right|^2 \delta(E'-E)$$

II scattering (Brooks-Herring)

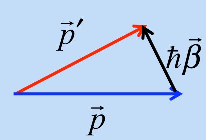


$$U_S(r) = \frac{q^2}{4\pi\kappa_S\varepsilon_0 r} e^{-r/L_D}$$

$$L_D = \sqrt{\frac{\kappa_S\varepsilon_0 k_B T}{q^2 n_0}} \quad \text{Debye length}$$

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

$$\vec{p}\,' = \vec{p} + \hbar\vec{\beta}$$



Fourier transform of the screened Coulomb potential

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

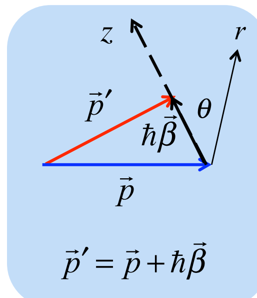
$$\tilde{U}_S(\beta) = \frac{q^2}{4\pi\kappa_S\varepsilon_0} \int_0^{2\pi} d\phi \int_0^{\pi} \int_0^{\infty} e^{-r/L_D} e^{-i\vec{\beta}\bullet\vec{r}}\, r\sin\theta\, d\theta\, dr$$

$$\vec{\beta}\bullet\vec{r} = \beta r\cos\theta$$

$$\sin\theta\, d\theta = -d(\cos\theta)$$

choose z-axis along β:

$$\tilde{U}_S(\beta) = \frac{q^2}{2\kappa_S\varepsilon_0} \int_0^{\infty} e^{-r/L_D}\, r\,dr \underbrace{\int_{-1}^{+1} e^{-i\beta r\cos\theta}\, d(\cos\theta)}_{\frac{2\sin(\beta r)}{\beta r}}$$



Fourier transform (ii)

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

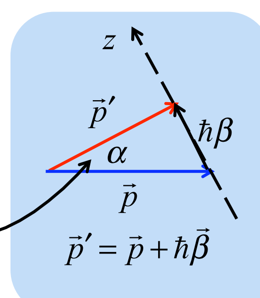
$$\tilde{U}_S(\beta) = \frac{q^2}{\kappa_S\varepsilon_0}\left(\frac{1}{\beta^2 + 1/L_D^2}\right)$$

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

$$\vec{\beta}\bullet\vec{r} = \beta r\cos\theta$$

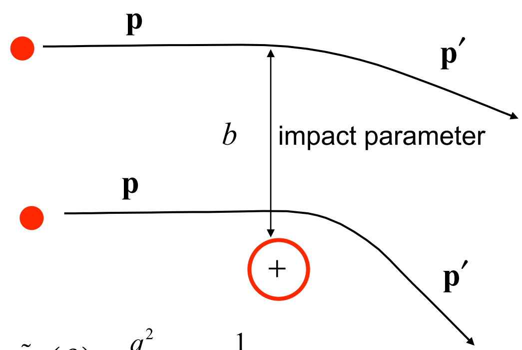
$$\sin\theta\, d\theta = -d(\cos\theta)$$

$$\hbar\beta = 2p\sin(\alpha/2)$$



small angle scattering preferred!!

small angle scattering



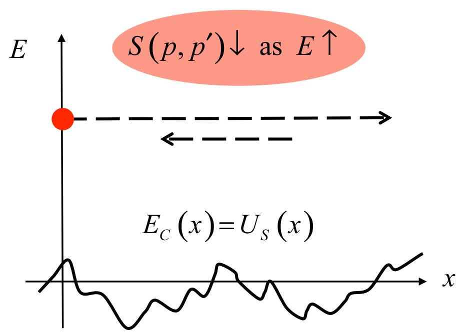
$$\tilde{U}_S(\beta) = \frac{q^2}{\kappa_S \epsilon_0} \frac{1}{\left(\beta^2 + 1/L_D^2\right)}$$

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

II scattering of high energy carriers

$$\tilde{U}_S(\beta) = \frac{q^2}{\kappa_S \epsilon_0} \left(\frac{1}{4(p/\hbar)^2 \sin^2(\alpha/2) + 1/L_D^2} \right)$$

For a given deflection angle, higher energies scatter less.



Random charges introduce random fluctuations in E_C, which act a scattering centers.

High energy electrons don't "see" these fluctuations and are not scattered as strongly.

II scattering: recap

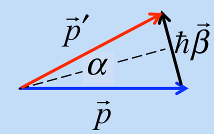
$$S(\vec{p},\vec{p}\,')=\frac{2\pi}{\hbar}\left|H_{p',p}\right|^2\delta(E'-E)\quad H_{p,p'}=\frac{1}{\Omega}\tilde{U}_S(\beta)\quad \tilde{U}_S(\beta)=\frac{q^2}{\kappa_S\varepsilon_0}\frac{1}{\left(\beta^2+1/L_D^2\right)}$$

Need to multiple by the total number of ionized impurities in the volume, Ω.

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

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

$$\vec{p}\,'=\vec{p}+\hbar\vec{\beta}$$



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

examine result

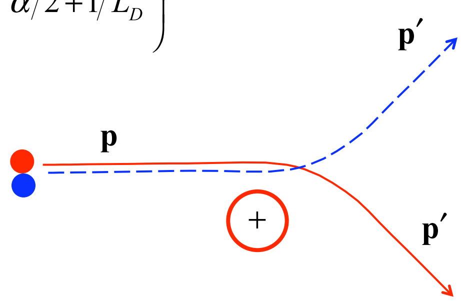
$$S(\vec{p},\vec{p}\,')=\frac{2\pi q^4 N_I}{\hbar\kappa_S^2\varepsilon_0^2\Omega}\frac{\delta(E'-E)}{\left(\frac{4p^2}{\hbar^2}\sin^2\alpha/2+1/L_D^2\right)^2}$$

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

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

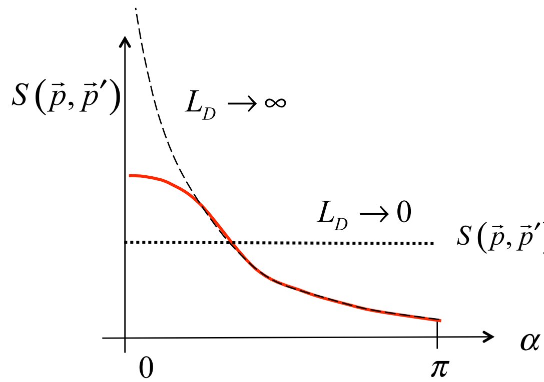
3) $S(\vec{p},\vec{p}\,')\sim 1/E^2$

4) favors small angle scattering



examine result

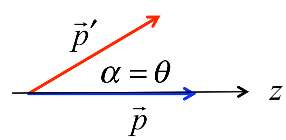
4) angular dependence $S(\vec{p},\vec{p}\,')=\dfrac{2\pi q^4 N_I}{\hbar\kappa_S^2\varepsilon_0^2\Omega}\dfrac{\delta(E'-E)}{\left(\dfrac{4p^2}{\hbar^2}\sin^2\alpha/2+1/L_D^2\right)^2}$



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

momentum relaxation time

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



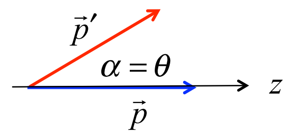
$$\frac{1}{\tau_m}=\sum_{\vec{p}\,'}S(\vec{p},\vec{p}\,')(1-\cos\alpha)$$

$S(\vec{p},\vec{p}\,')$ favors small angles

expect: $1/\tau_m<1/\tau \quad \tau_m>\tau$

momentum relaxation time

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



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

$$\gamma^2 = 8m^* EL_D^2/\hbar^2$$

See Lundstrom, pp. 69-70

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

$$\tau_m(E) \approx \tau_0\left(E/k_B T_L\right)^{3/2} \qquad \tau_0 \sim T_L^{3/2} \qquad s = 3/2$$

outline

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

(Reference: Chapter 2, Lundstrom, FCT)

BH vs.CW

Brook-Herring means “screened Coulomb scattering.”

Conwell-Weisskopf means “unscreened Coulomb scattering.”

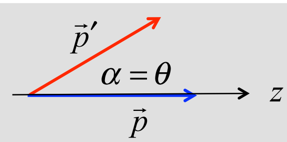
Conwell-Weiskopf approach

$$S(\vec{p},\vec{p}\,')=\frac{2\pi q^4 N_I}{\hbar\kappa_S^2\epsilon_0^2\Omega}\frac{\delta(E'-E)}{\left(\frac{4p^2}{\hbar^2}\sin^2\alpha/2\right)^2}$$

unscreened Coulomb potential

$$S(\vec{p},\vec{p}\,')\rightarrow\infty \quad \text{as} \quad \alpha\rightarrow 0$$

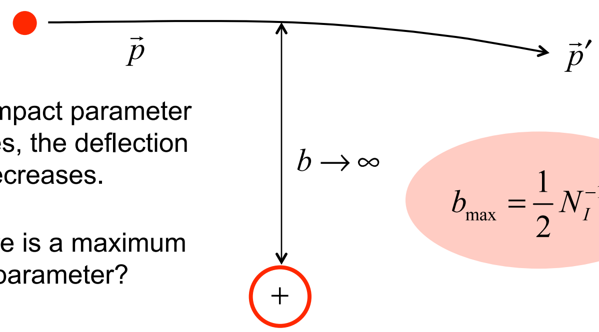
$$\frac{1}{\tau_m}=\sum_{\vec{p}\,'}S(\vec{p},\vec{p}\,')(1-\cos\alpha)$$



Can we specify a minimum angle, so that the integral does not blow up?

Conwell-Weiskopf approach

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



As the impact parameter increases, the deflection angle decreases.

But there is a maximum impact parameter?

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

Conwell-Weisskopf approach

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

$$\frac{1}{\tau_m} = \frac{\Omega}{(2\pi)^3} \int_0^{2\pi} d\phi \int_{\alpha_{\min}}^{\pi} S(\vec{p},\vec{p}\,')(1-\cos\alpha)\sin\alpha d\alpha\, p'^2 dp' =$$

$$b_{\max} = \frac{q^2}{8\pi\kappa_S \varepsilon_0 E(p)} \cot(\alpha_{\min}/2) \qquad \text{(Rutherford)}$$

Conwell-Weisskopf approach

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

$$\tau_m(E) = \frac{16\pi\sqrt{2m^*}\kappa_S^2\varepsilon_0^2}{N_I q^4}\left[\frac{1}{\ln\left(1+\gamma_{CW}^2\right)}\right]E^{3/2} \qquad \gamma_{CW}^2 = b_{\max}\Big/\left(q^2/8\pi\kappa_S\varepsilon_0 E\right)$$

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

$$\tau_m(E) \approx \tau_0\left(E/k_B T_L\right)^{3/2} \qquad \tau_0 \sim T_L^{3/2} \qquad s = 3/2$$

Much like the Brooks-Herring result.

CW vs. BH

Compare b_{MAX} to L_D

Use BH if:

$$b_{\max} > L_D$$

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

$$L_D = \sqrt{\frac{\kappa_S\varepsilon_0 k_B T}{q^2 n_0}}$$

B. K. Ridley, "Reconciliation of the Conwell-Weisskopf and Brooks-Herring formulae for charged-impurity scattering in semiconductors: Third-body interference," *J. Phys. C: Solid State Phys.* **10,** p. 1589 doi:10.1088/0022-3719/10/10/003, 1977.

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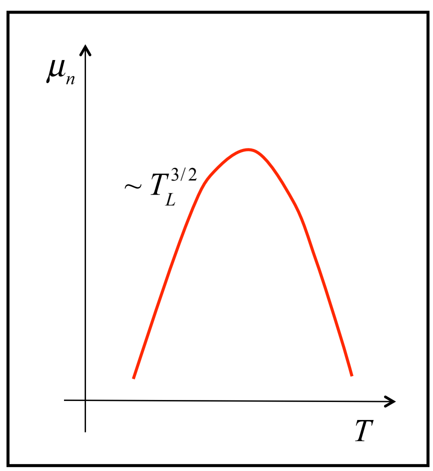
mobility

$$\mu_n = \frac{q\langle\langle\tau_m\rangle\rangle}{m^*}$$

$$\langle\langle\tau_m\rangle\rangle = \tau_0 \frac{\Gamma(s+5/2)}{\Gamma(5/2)} \qquad s = 3/2$$

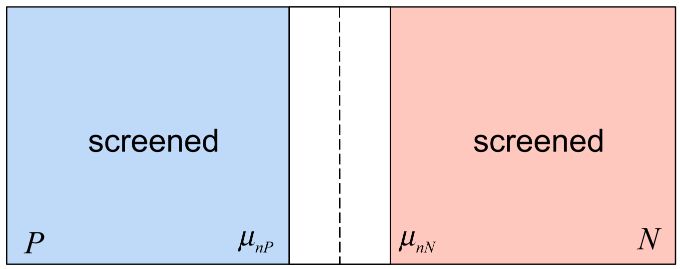
$$\mu_n = \frac{q\tau_0}{m^*}\frac{3\sqrt{\pi}}{4} \sim T_L^{3/2}$$

$T^{3/2}$ temperature dependence is the "signature" of charged impurity scattering.



PN junction

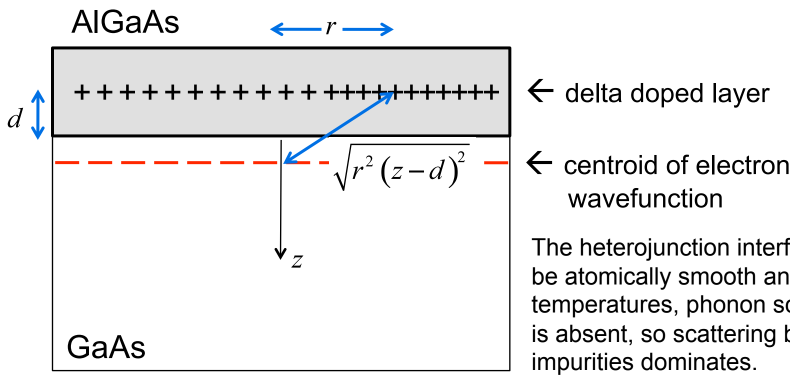
$$U_S(r) = +\frac{q^2}{4\pi\kappa_S\varepsilon_0 r}e^{-r/L_D} \qquad U_S(r) = -\frac{q^2}{4\pi\kappa_S\varepsilon_0 r}e^{-r/L_D}$$



$$U_S(r) = +\frac{q^2}{4\pi\kappa_S\varepsilon_0 r} \qquad U_S(r) = -\frac{q^2}{4\pi\kappa_S\varepsilon_0 r}$$

unscreened

screening 2D modulation-doped layers



The heterojunction interface can be atomically smooth and at low temperatures, phonon scattering is absent, so scattering by remote impurities dominates. Extraordinarily high mobilities (e.g. > 10^6 cm^2/V-s) can be achieved at about T = 1K.

modulation-doped structures

For a discussion of modulation doping, screening in 2D, and remote impurity scattering in 2D, see:

J.H. Davies, *The Physics of Low-Dimensional Semiconductors*, Chapter 8, Cambridge Univ. Press, 1998.

outline

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

(Reference: Chapter 2, Lundstrom, FCT)

summary

1) The two classic treatments of II scattering are Brooks-Herring and Conwell-Weiskopf

2) II scattering is actually difficult to treat properly because:

   FGR does not account for the difference in sign of the scattering potential

   “multiple scattering” occurs at heavy doping.

questions

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