ECE-656: Fall 2009

Lecture 22: Charged Impurity Scattering

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outline

1) **Review**

2) Screening

3) Brooks-Herring approach

4) Conwell-Weisskopf approach

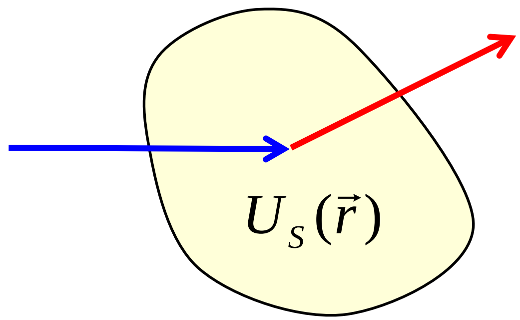
5) Discussion

6) Summary / Questions

prescription

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

$$\vec{p} = \hbar\vec{k}$$



$$\vec{p}\,' = \hbar\vec{k}\,'$$

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

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

Time-independent scattering potential → elastic scattering.

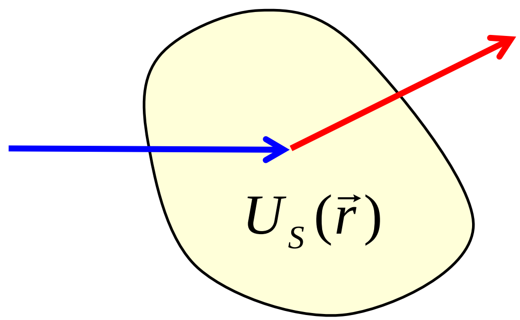
$$H_{\vec{p}\,',\vec{p}} = \int_{-\infty}^{+\infty} \psi_f^* U_S(\vec{r}) \psi_i d\vec{r}$$

Matrix element.

Initial and final states are plane waves → assume that the overlap factor is 1.

prescription (ii)

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



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

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

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

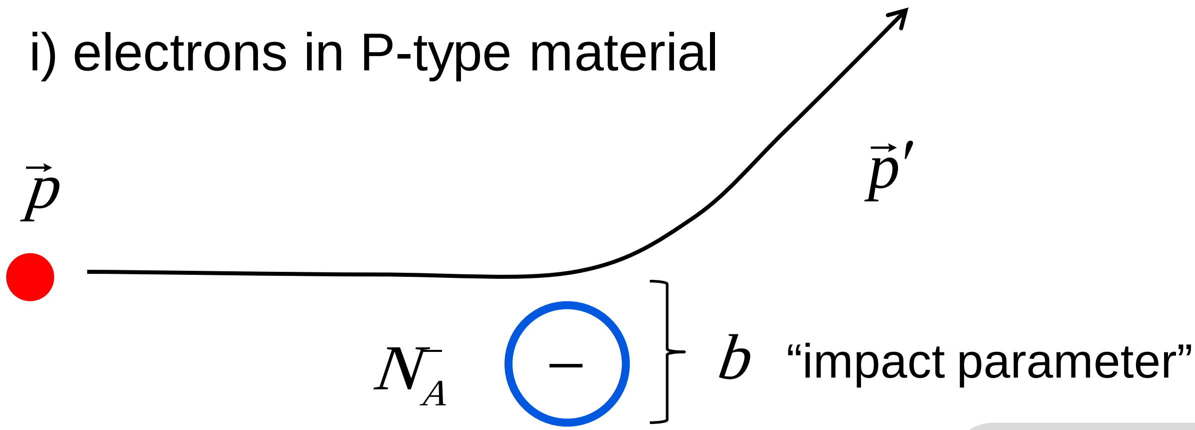
1) Identify the scattering potential

2) Compute the matrix element

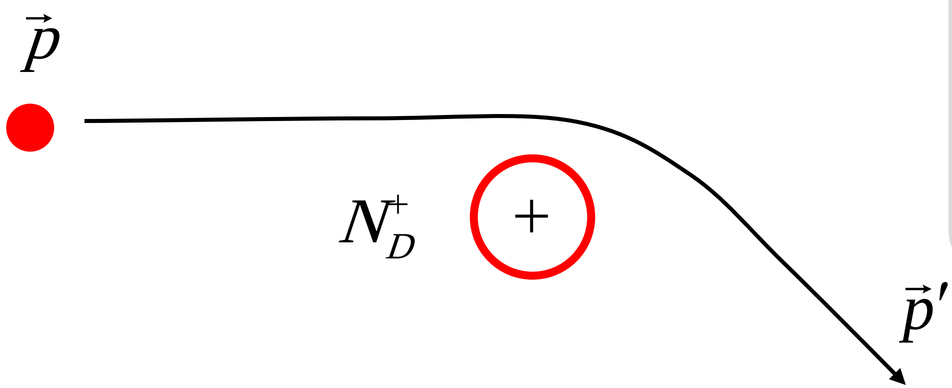
3) Compute characteristic times

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.

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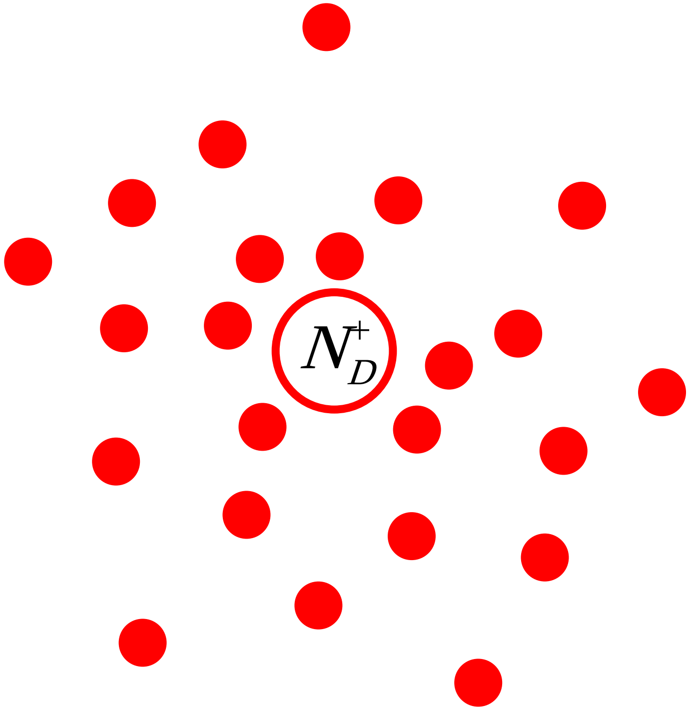
screening



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

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

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

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

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

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

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

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

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

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

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

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

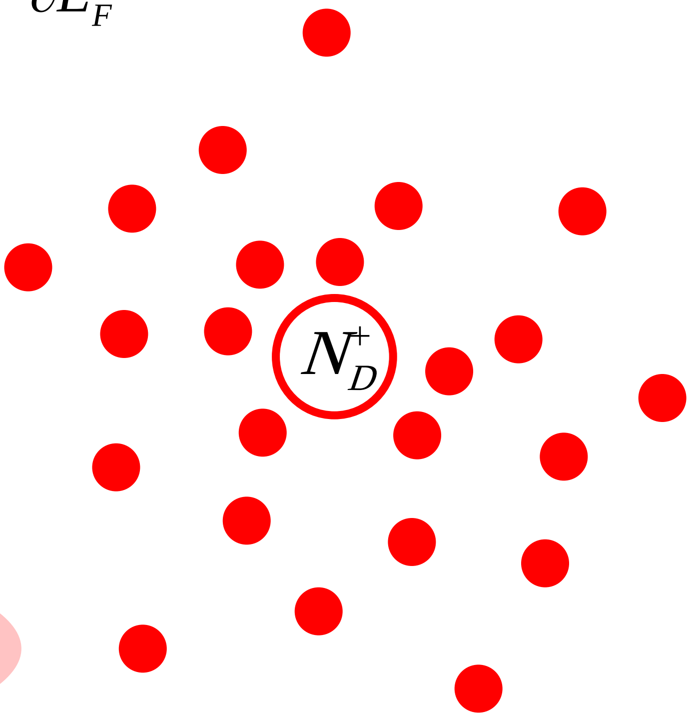
screening in 3D

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

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

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

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



Debye length in 3D

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

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

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

$$\frac{\partial n_{3D}}{\partial \eta_F} = N_{3D}\mathcal{F}_{-1/2}(\eta_F) = n_{3D}\frac{\mathcal{F}_{-1/2}(\eta_F)}{\mathcal{F}_{1/2}(\eta_F)} = n_{3D}$$ (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

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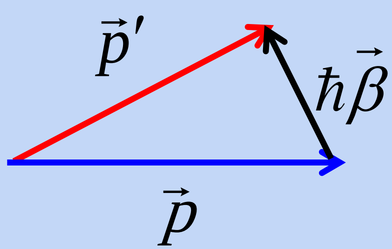
transition rate and scattering potential

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

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

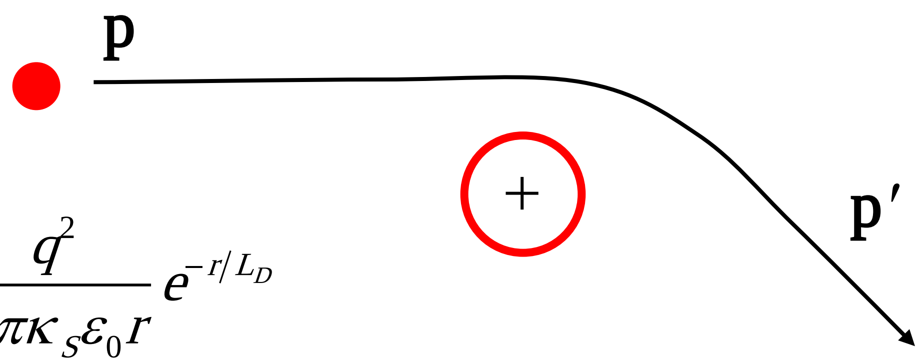
$$= \frac{1}{\Omega}\int_{-\infty}^{+\infty} U_S(r) e^{-i\vec{\beta}\bullet\vec{r}}\, d\vec{r} \equiv \frac{1}{\Omega}\tilde{U}_S(\vec{\beta})$$

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



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

II scattering (Brooks-Herring)

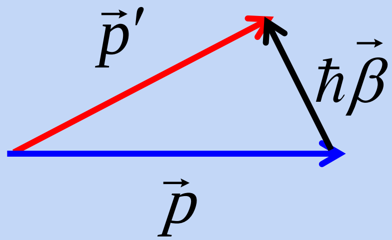


$$U_S(r) = \frac{q^2}{4\pi\kappa_S\varepsilon_0 r}e^{-r/L_D}$$

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

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

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



Fourier transform of the screened Coulomb potential

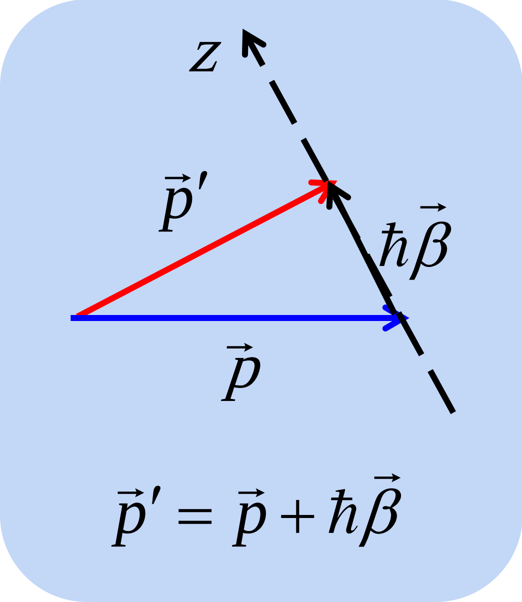
$$\tilde{U}_S(\beta) = \int_{-\infty}^{+\infty} \frac{q^2}{4\pi\kappa_S\varepsilon_0 r} e^{-r/L_D} e^{-i\vec{\beta}\bullet\vec{r}}\, d\vec{r}$$

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

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

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

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)

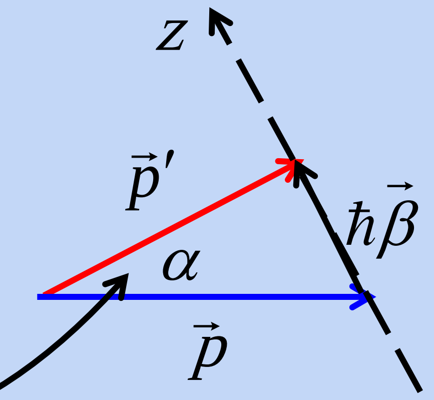
$$\tilde{U}_S(\beta) = \frac{q^2}{\kappa_S \varepsilon_0} \int_0^\infty \frac{e^{-r/L_D}\sin(\beta r)}{\beta}\, dr$$

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

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

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

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

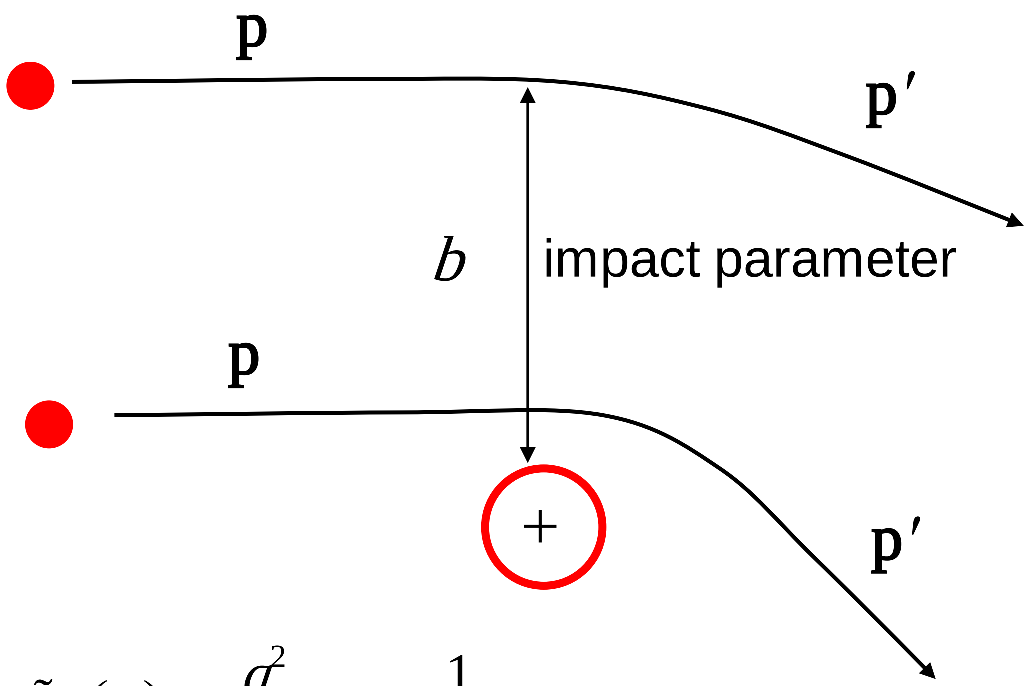


$$\vec{p}' = \vec{p} + \hbar\vec{\beta}$$

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

small angle scattering preferred!!

small angle scattering



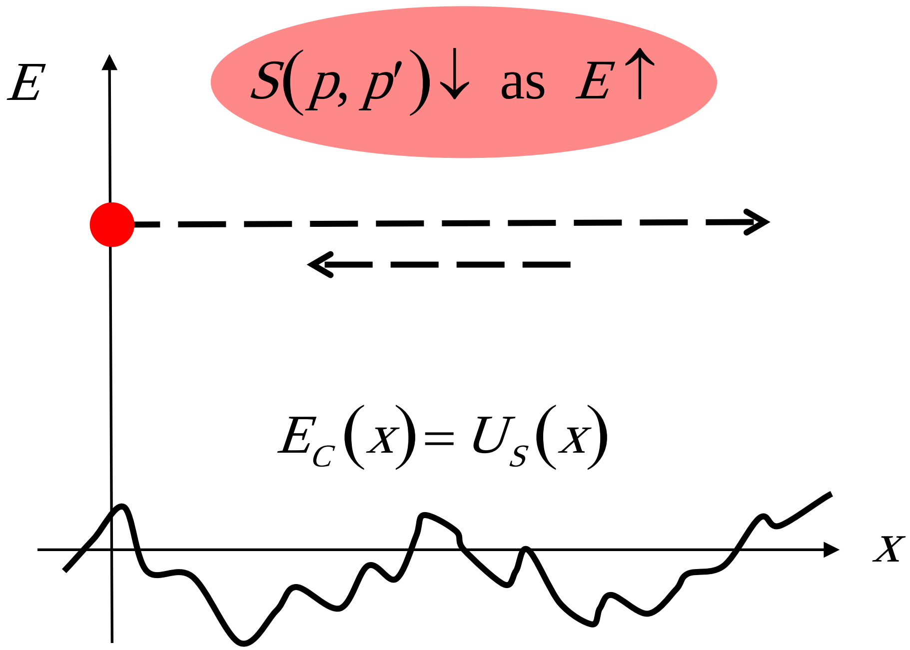
$$\tilde{U}_S(\beta) = \frac{q^2}{\kappa_S \varepsilon_0} \frac{1}{\left(\beta^2 + 1/L_D^2\right)}$$

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

II scattering of high energy carriers

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

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

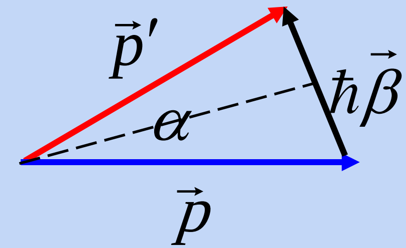
$$S(\vec{p},\vec{p}\,') = \frac{2\pi}{\hbar}\left|H_{p',p}\right|^2 \delta(E'-E) \quad H_{p,p'} = \frac{1}{\Omega}\tilde{U}_S(\beta) \quad \tilde{U}_S(\beta) = \frac{q^2}{\kappa_S\varepsilon_0}\frac{1}{\left(\beta^2 + 1/L_D^2\right)}$$

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

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

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

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



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

examine result

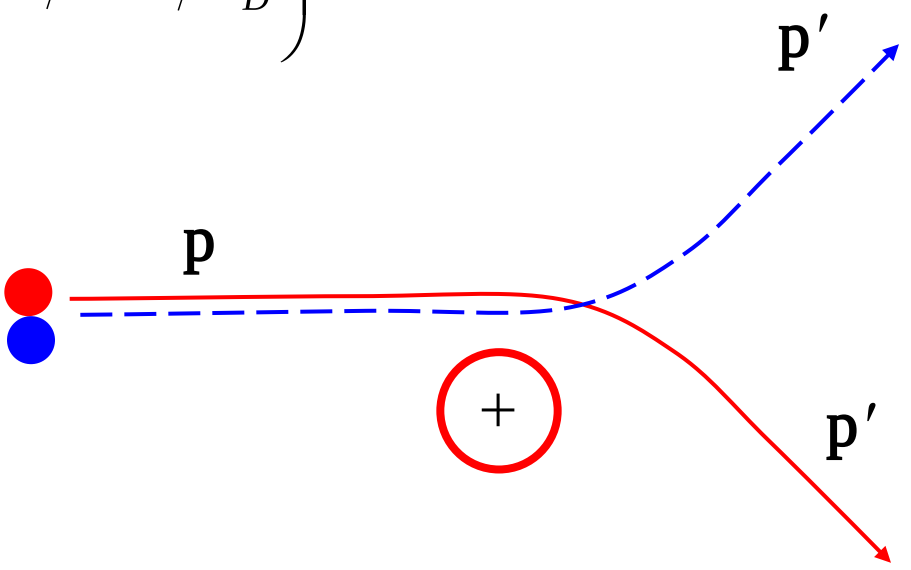
$$S(\vec{p},\vec{p}') = \frac{2\pi q^4 N_I}{\hbar \kappa_S^2 \varepsilon_0^2 \Omega} \frac{\delta(E'-E)}{\left(\frac{4p^2}{\hbar^2}\sin^2\alpha/2 + 1/L_D^2\right)^2}$$

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

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

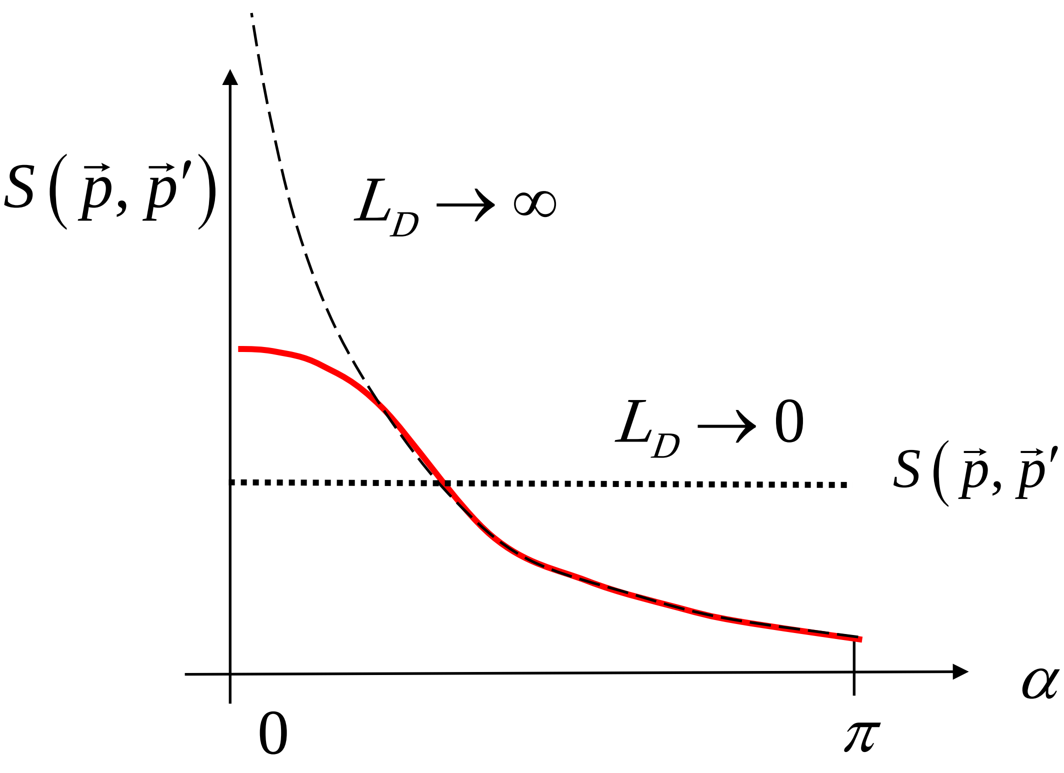
3) $S(\vec{p},\vec{p}') \sim 1/E^2$

4) favors small angle scattering



examine result

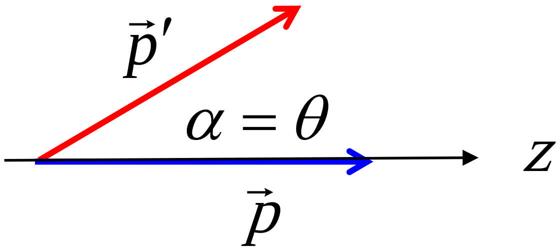
4) angular dependence $S(\vec{p},\vec{p}\,') = \dfrac{2\pi q^4 N_I}{\hbar \kappa_S^2 \varepsilon_0^2 \Omega} \dfrac{\delta(E'-E)}{\left(\dfrac{4p^2}{\hbar^2}\sin^2\alpha/2 + 1/L_D^2\right)^2}$



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

momentum relaxation time

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



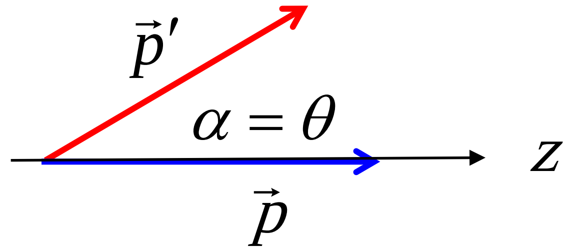
$$\frac{1}{\tau_m} = \sum_{\vec{p}'} S(\vec{p}, \vec{p}')(1 - \cos\alpha)$$

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

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

momentum relaxation time

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



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

$$\gamma^2 = 8m^* E L_D^2 / \mathrm{h}^2$$

See Lundstrom, pp. 69-70

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

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

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BH vs.CW

Brook-Herring means “screened Coulomb scattering.”

Conwell-Weisskopf means “unscreened Coulomb scattering.”

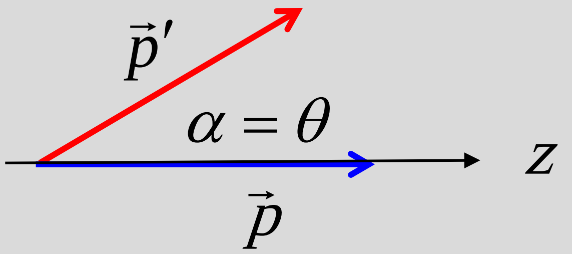
Conwell-Weiskopf approach

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

unscreened Coulomb potential

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

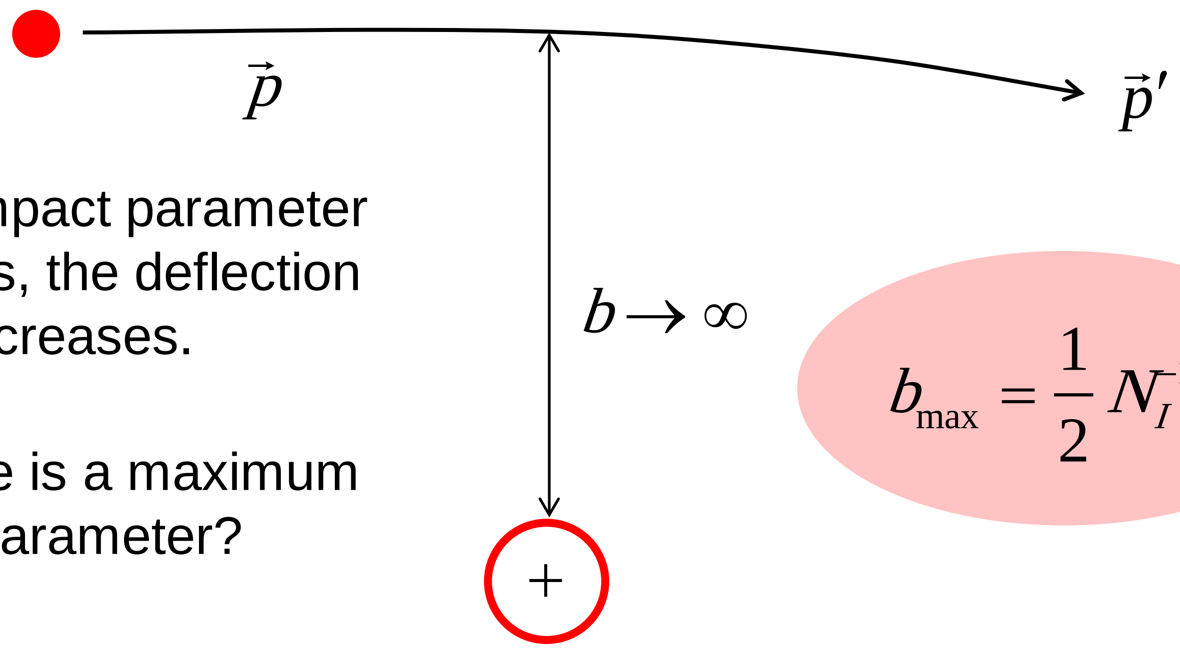
$$\frac{1}{\tau_m} = \sum_{\vec{p}\,'} S(\vec{p},\vec{p}\,')(1-\cos\alpha)$$



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

Conwell-Weiskopf approach

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



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

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

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

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

Conwell-Weisskopf approach

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

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

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

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

Much like the Brooks-Herring result.

CW vs. BH

Compare b_{MAX} to L_D

Use BH if:

$$b_{\max} > L_D$$

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

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

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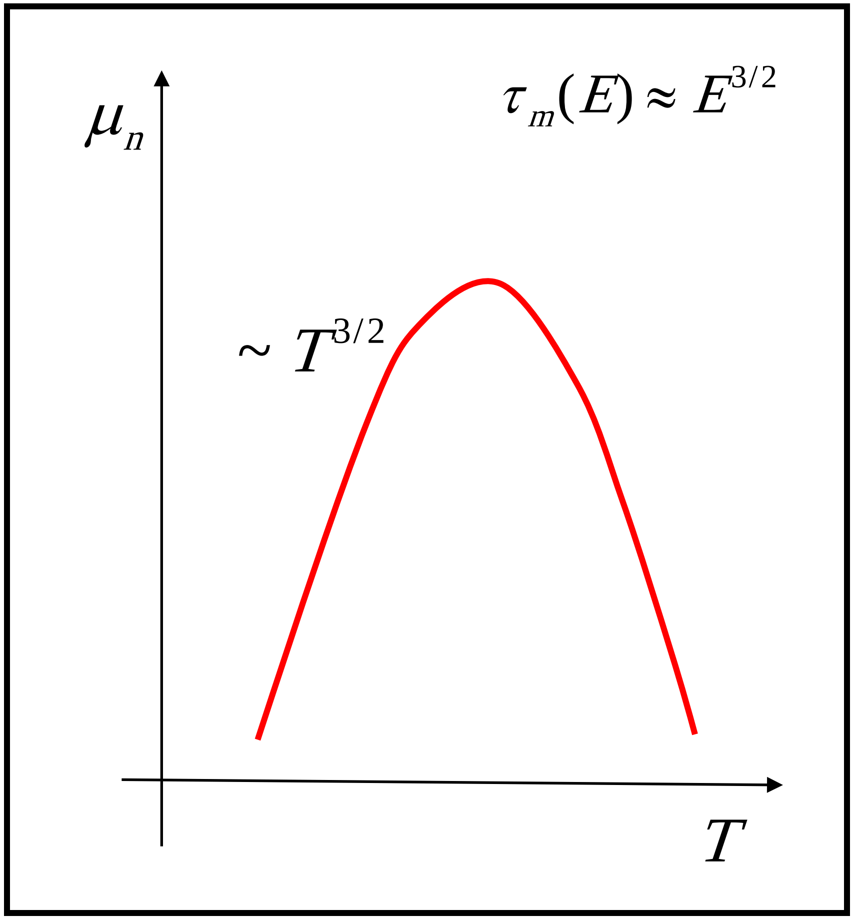
mobility

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

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

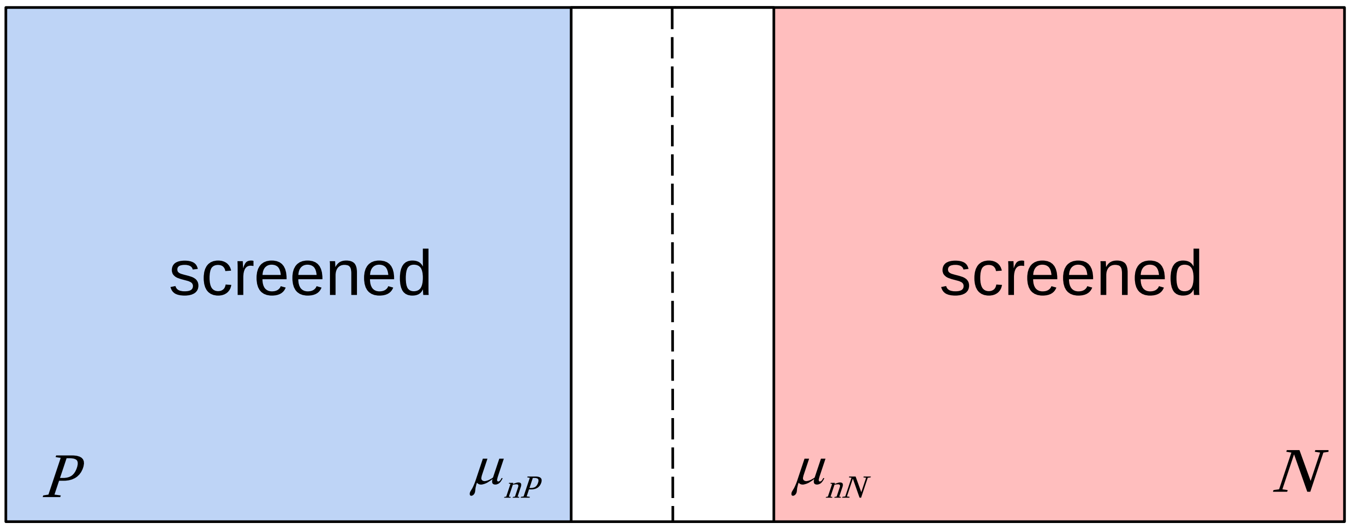
$$\mu_n = \frac{q\tau_0}{m^*}\frac{3\sqrt{\pi}}{4} \sim T^{3/2}$$

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



PN junction

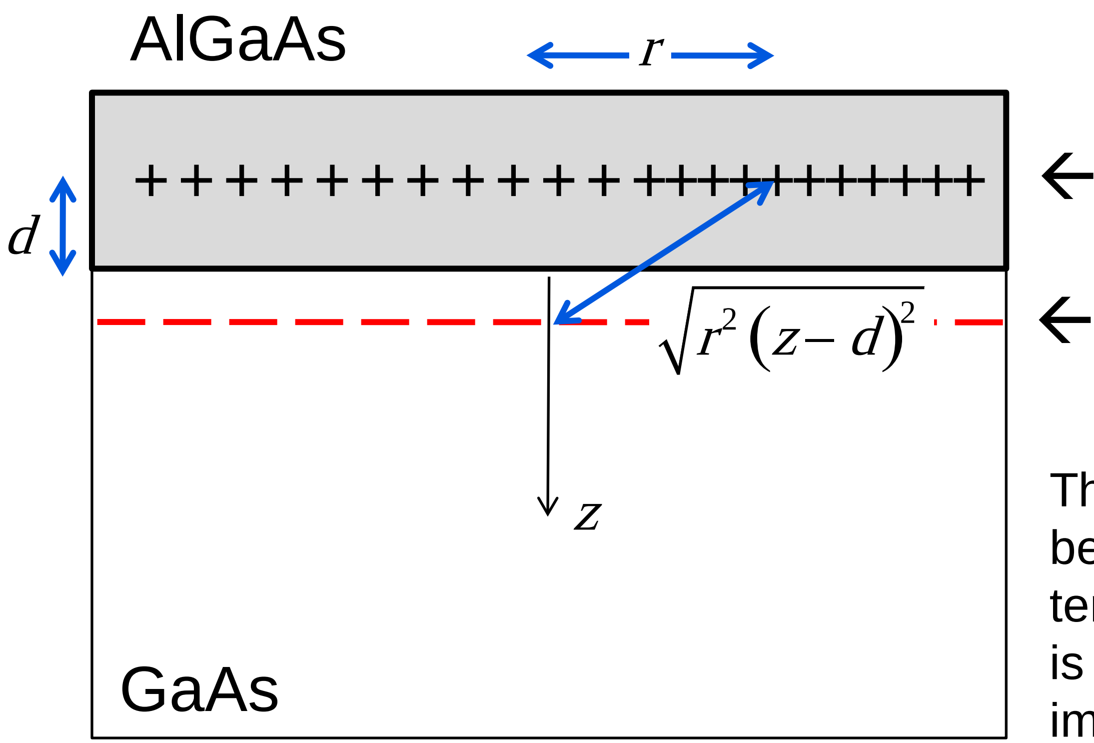
$$U_S(r) = +\frac{q^2}{4\pi\kappa_S\varepsilon_0 r}e^{-r/L_D} \qquad U_S(r) = -\frac{q^2}{4\pi\kappa_S\varepsilon_0 r}e^{-r/L_D}$$



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

unscreened

screening 2D modulation-doped layers



The heterojunction interface can be atomically smooth and at low temperatures, phonon scattering is absent, so scattering by remove impurities dominates. Extraordinarlly 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.

questions

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