

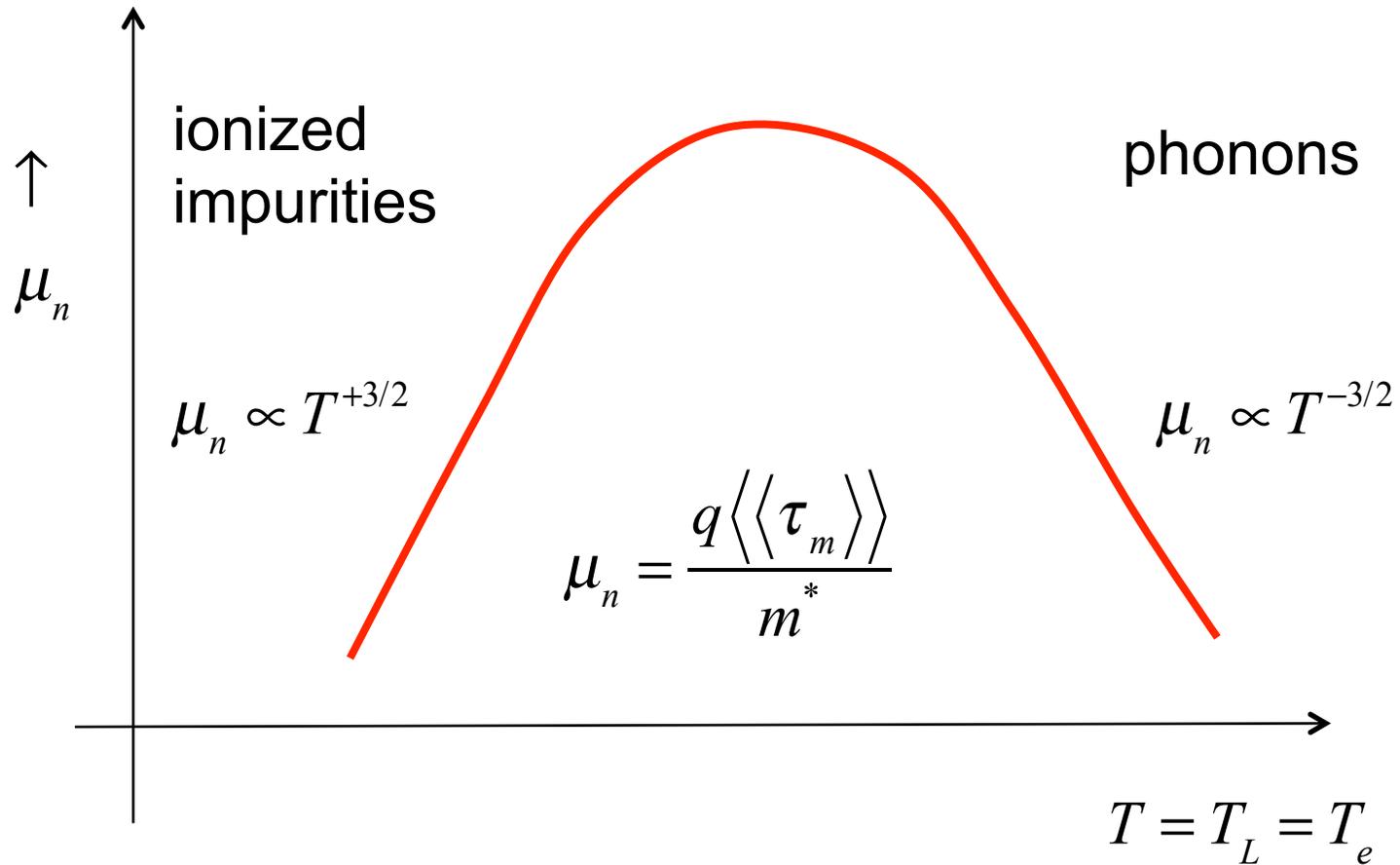
Ionized Impurity Scattering: Brooks Herring Approach

Mark Lundstrom

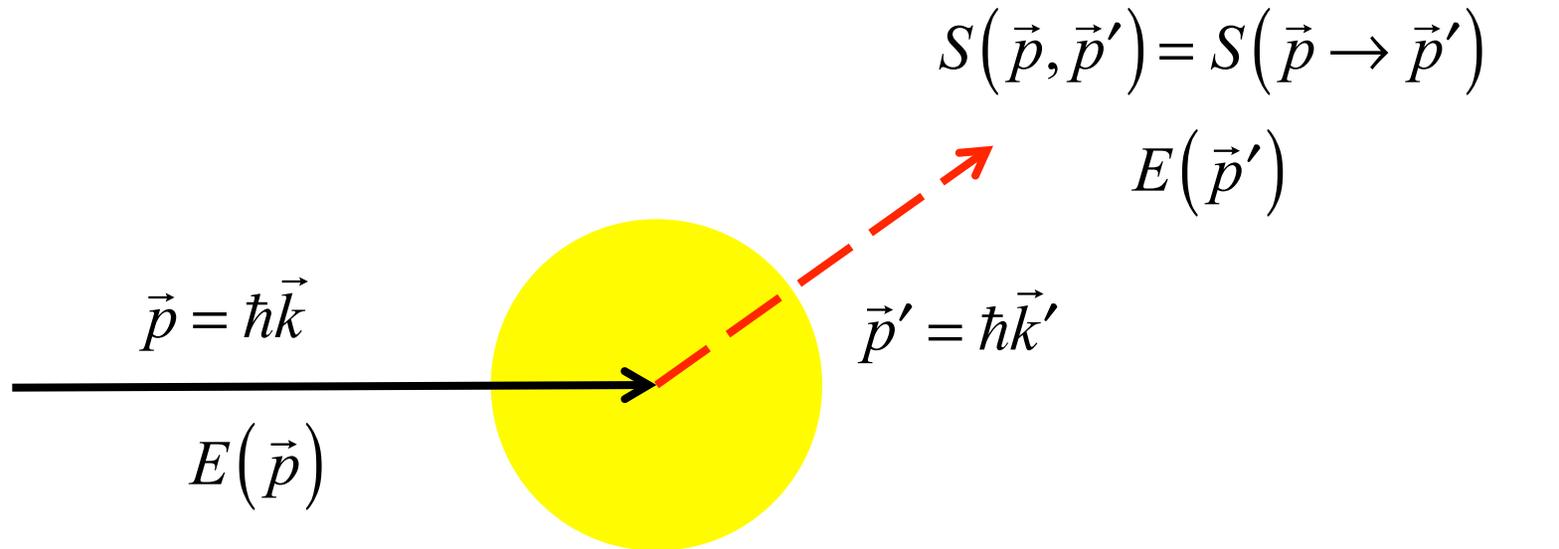
Electrical and Computer Engineering
Purdue University
West Lafayette, IN USA

(revised 9/5/17)

Mobility vs. temperature



Fermi's Golden Rule



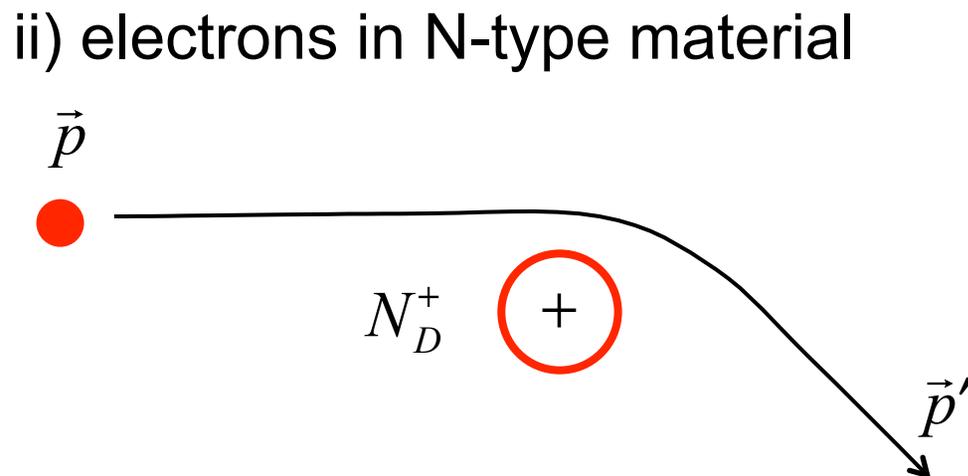
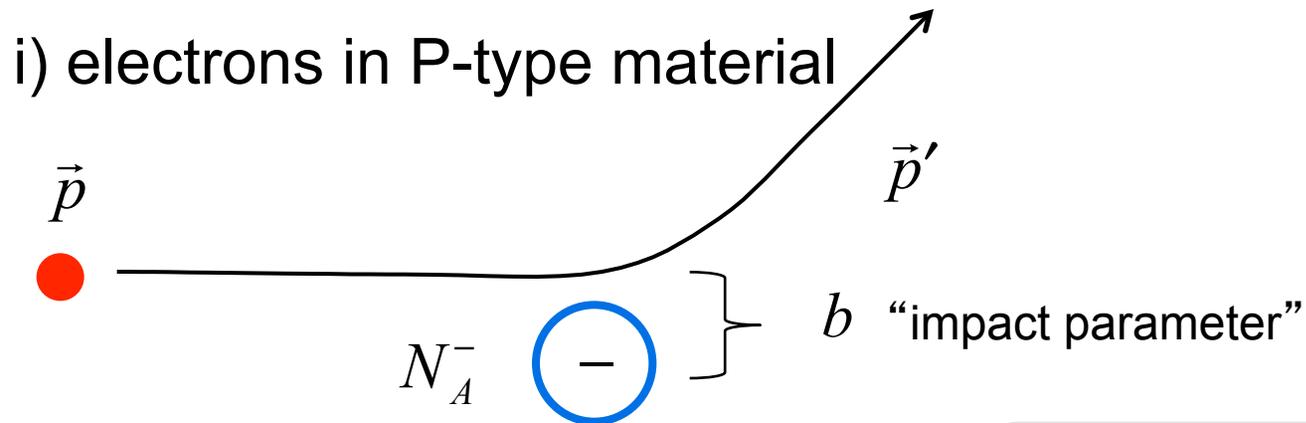
$$S(\vec{p} \rightarrow \vec{p}') = \frac{2\pi}{\hbar} |H_{\vec{p}', \vec{p}}|^2 \delta(E' - E)$$

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

$$U_S(\vec{r}) = \pm \frac{q^2}{4\pi\kappa_S \epsilon_0 r}$$

Coulomb potential

Sign of the scattering potential



$$U_s(\vec{r}) = \pm \frac{q^2}{4\pi\kappa_s\epsilon_0 r}$$

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

In fact, attractive potentials scatter more strongly.

II scattering: Approaches

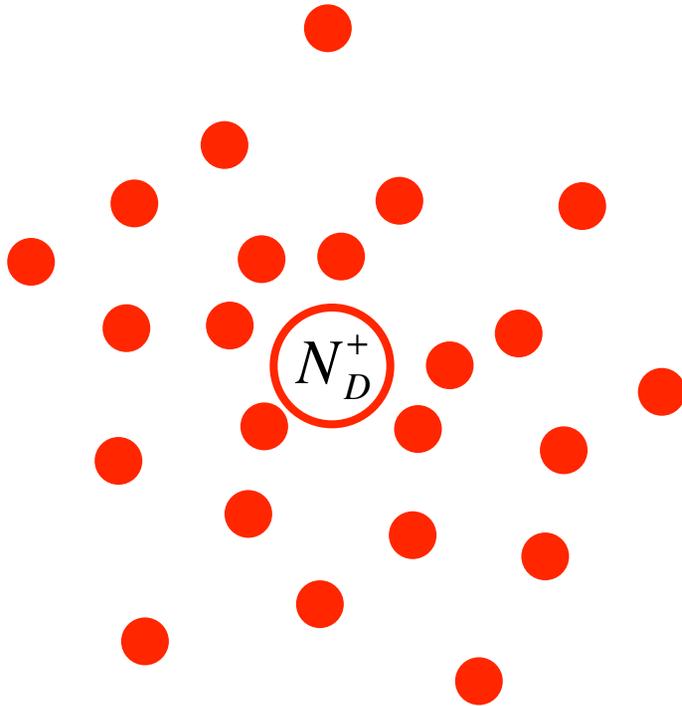
- 1) II scattering (Brooks-Herring - *screened*)
- 2) II scattering (Conwell-Weisskopf - *unscreened*)

Historically, the CW approach came first, but we will discuss the BH approach first, then CW.

Outline

- 1) Introduction
- 2) Screening**
- 3) Transition rate
- 4) Characteristic times

Screened Coulomb potential



Bare Coulomb potential:

$$U_S(\vec{r}) = \frac{q^2}{4\pi\kappa_S\epsilon_0 r}$$

Screened Coulomb potential:

??

Mobile charges attracted to fixed charges “screen” out the fixed charge.

Screening in 3D

$$\nabla^2 V(\vec{r}) = -\frac{\rho}{\kappa_S \epsilon_0} = -\frac{q [N_D^+ - n(\vec{r})]}{\kappa_S \epsilon_0}$$

$$\frac{1}{L_D^2} \equiv \frac{q}{\kappa_S \epsilon_0} \frac{\partial n(\vec{r})}{\partial V}$$

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

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

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

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

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

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

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

$$\frac{1}{L_D^2} \equiv \frac{q^2}{\kappa_S \epsilon_0} \frac{\partial n(\vec{r})}{\partial E_F}$$

$$\nabla^2 \delta V(\vec{r}) = -\frac{q}{\kappa_S \epsilon_0} \frac{\partial n(\vec{r})}{\partial V} \delta V(\vec{r})$$

Lundstrom ECE-656 F17

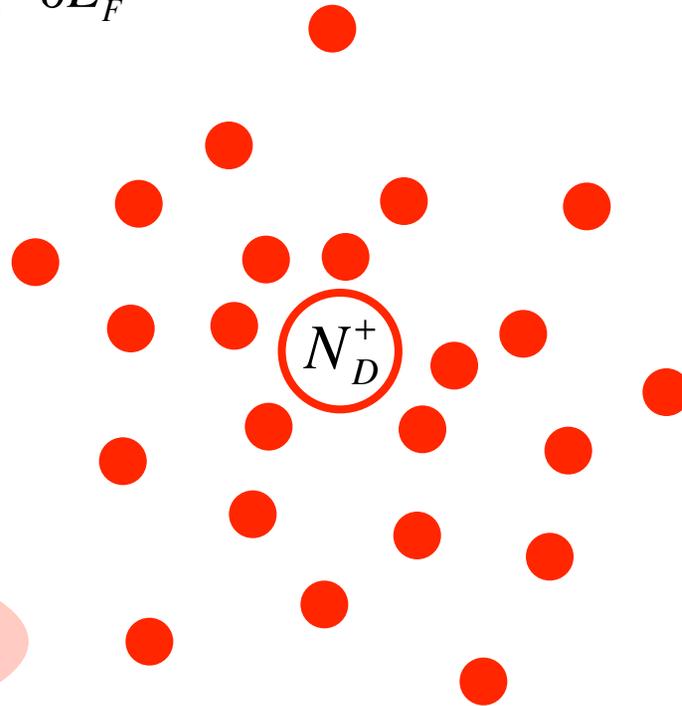
Screening in 3D

$$\nabla^2 \delta V(\vec{r}) = \frac{1}{L_D^2} \delta V(\vec{r}) \quad \frac{1}{L_D^2} \equiv \frac{q^2}{\kappa_S \epsilon_0} \frac{\partial n(\vec{r})}{\partial E_F}$$

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

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

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



Debye length in 3D

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

$$\frac{1}{L_D^2} \equiv \frac{q^2}{\kappa_S\epsilon_0} \frac{\partial n(\vec{r})}{\partial E_F} = \frac{q^2}{\kappa_S\epsilon_0 k_B T} \frac{\partial n(\vec{r})}{\partial \eta_F}$$

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

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

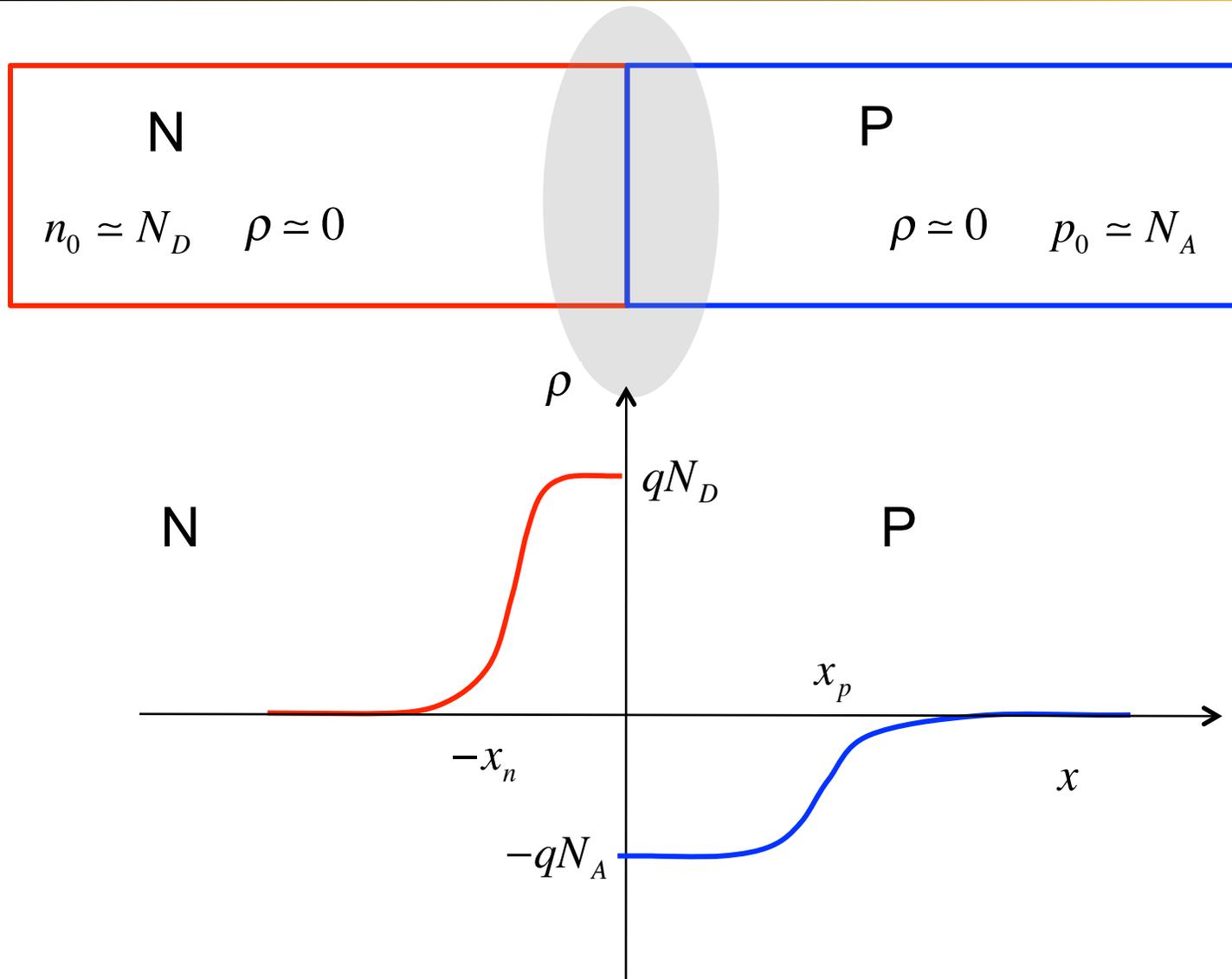
$$L_D = \sqrt{\frac{\kappa_S \epsilon_0 k_B T}{q^2 n_0}}$$

Debye length
(non-degenerate)

Comments

- 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)

Example: Rapid variation in space

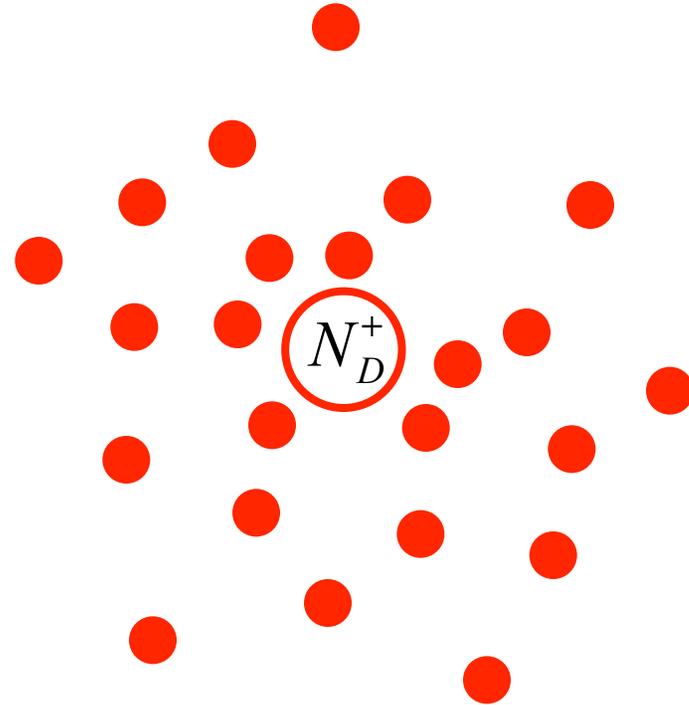


Screened Coulomb potential

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

$$L_D = \sqrt{\frac{\kappa_S \epsilon_0 k_B T_L}{q^2 n_0}}$$

Debye length
(non-degenerate)



Screened Coulomb potential:

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

Outline

- 1) Introduction
- 2) Screening
- 3) Transition rate**
- 4) Characteristic times

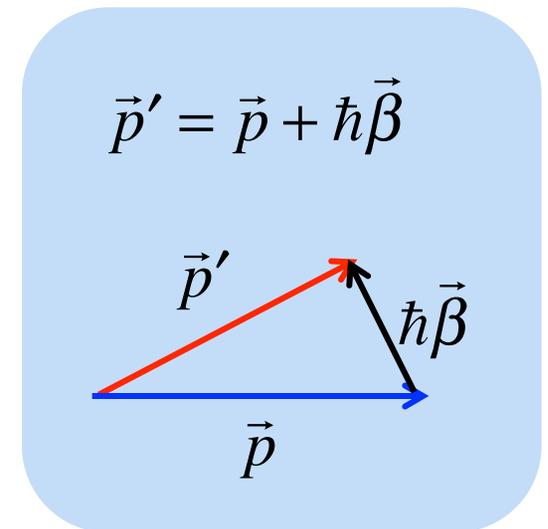
Transition rate

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

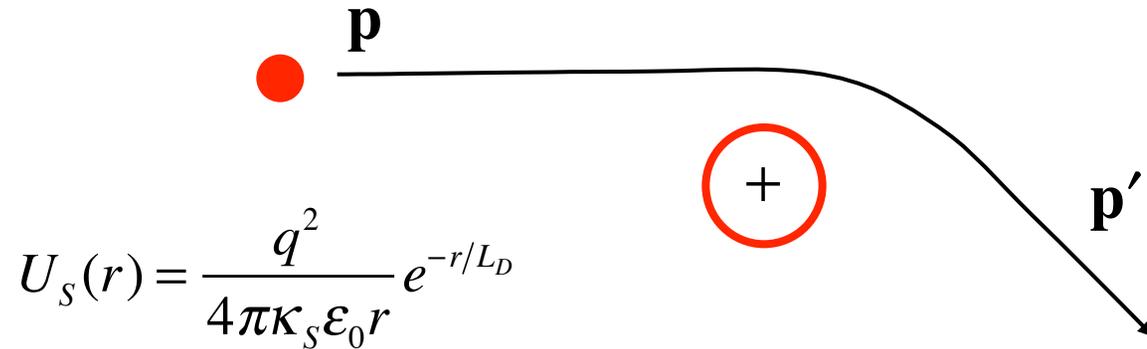
$$\begin{aligned} H_{p',p} &= \frac{1}{\Omega} \int_{-\infty}^{+\infty} e^{-i\vec{p}'\cdot\vec{r}/\hbar} U_S(r) e^{i\vec{p}\cdot\vec{r}/\hbar} d\vec{r} = \frac{1}{\Omega} \int_{-\infty}^{+\infty} U_S(r) e^{-i(\vec{p}'-\vec{p})\cdot\vec{r}/\hbar} d\vec{r} \\ &= \frac{1}{\Omega} \int_{-\infty}^{+\infty} U_S(r) e^{-i\vec{\beta}\cdot\vec{r}} d\vec{r} \equiv \frac{1}{\Omega} \tilde{U}_S(\vec{\beta}) \end{aligned}$$

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

Transition rate is proportional to the square of the Fourier transform of the screened Coulomb potential

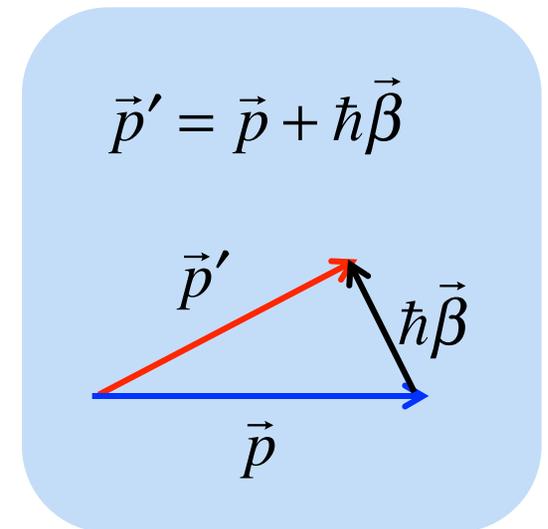


Recap



$$L_D = \sqrt{\frac{\kappa_S \epsilon_0 k_B T}{q^2 n_0}} \quad \text{Debye length}$$

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



Fourier transform

$$\tilde{U}_s(\beta) = \int_{-\infty}^{+\infty} \frac{q^2}{4\pi\kappa_s\epsilon_0 r} e^{-r/L_D} e^{-i\vec{\beta}\cdot\vec{r}} d\vec{r}$$

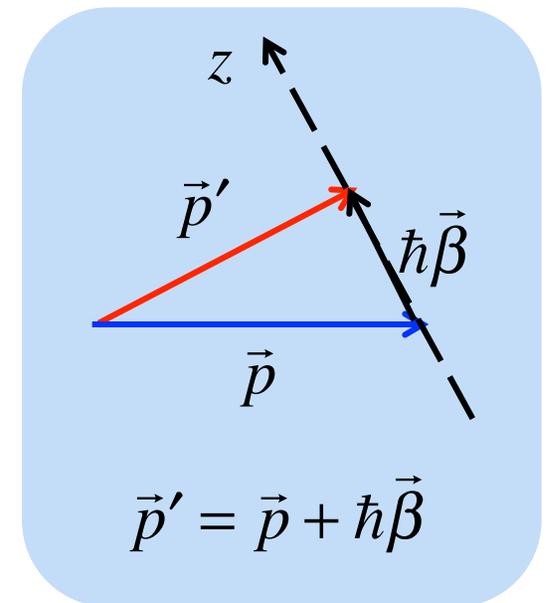
$$\tilde{U}_s(\beta) = \frac{q^2}{4\pi\kappa_s\epsilon_0} \int_0^{2\pi} d\phi \int_0^\pi \int_0^\infty e^{-r/L_D} e^{-i\vec{\beta}\cdot\vec{r}} r \sin\theta d\theta dr$$

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

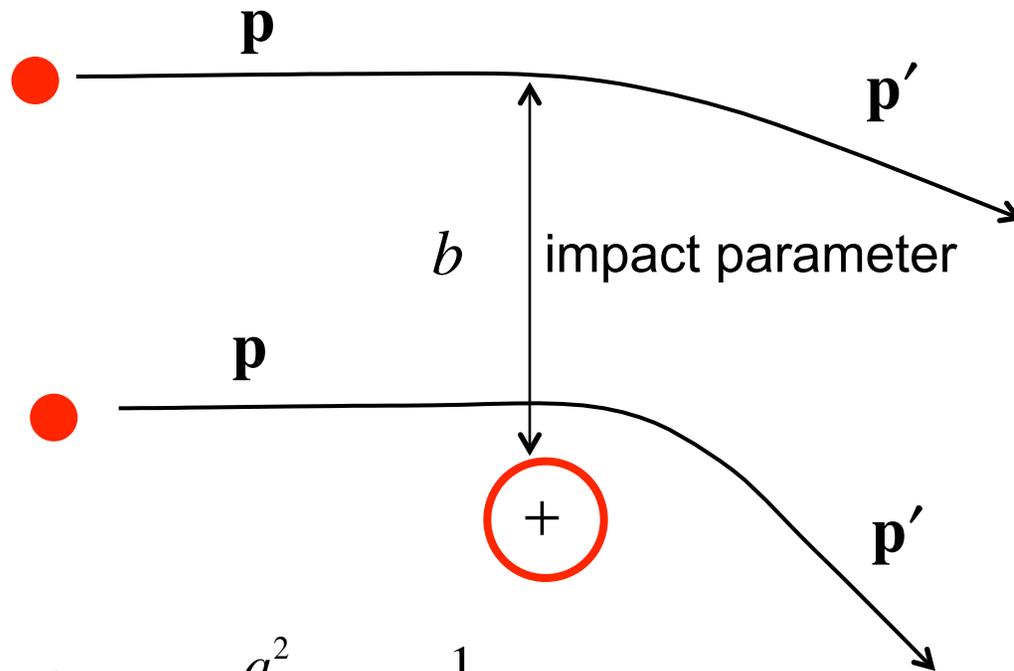
$$\sin\theta d\theta = -d(\cos\theta)$$

choose z-axis along β :

$$\tilde{U}_s(\beta) = \frac{q^2}{2\kappa_s\epsilon_0} \int_0^\infty e^{-r/L_D} r dr \underbrace{\int_{-1}^{+1} e^{-i\beta r \cos\theta} d(\cos\theta)}_{\frac{2 \sin(\beta r)}{\beta r}}$$



Relation to impact parameter



A small angle scattering event implies a large impact parameter.

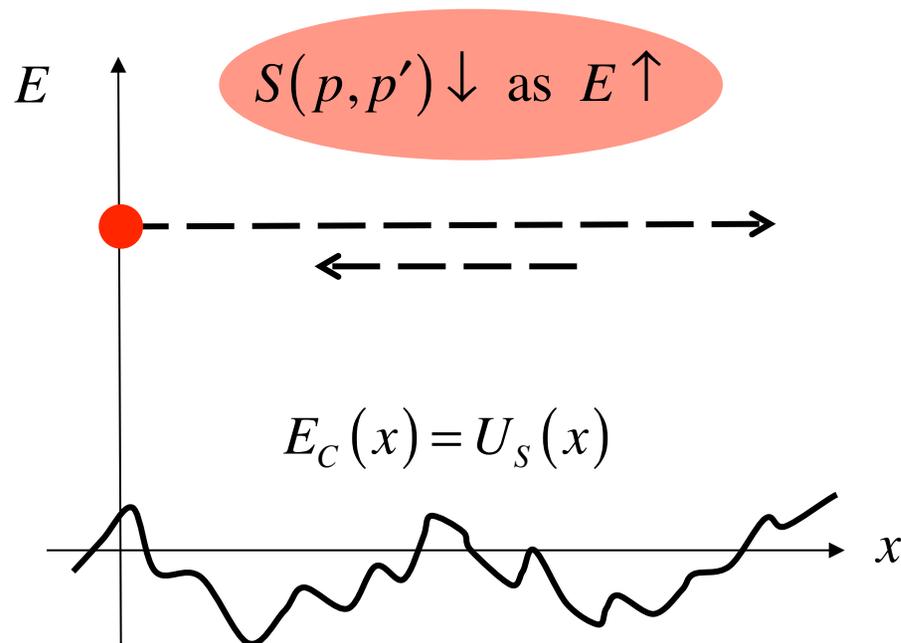
$$\tilde{U}_s(\beta) = \frac{q^2}{\kappa_s \epsilon_0} \frac{1}{(\beta^2 + 1/L_D^2)}$$

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

II scattering of high energy electrons

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

For a given deflection angle, higher energies scatter less.



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

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

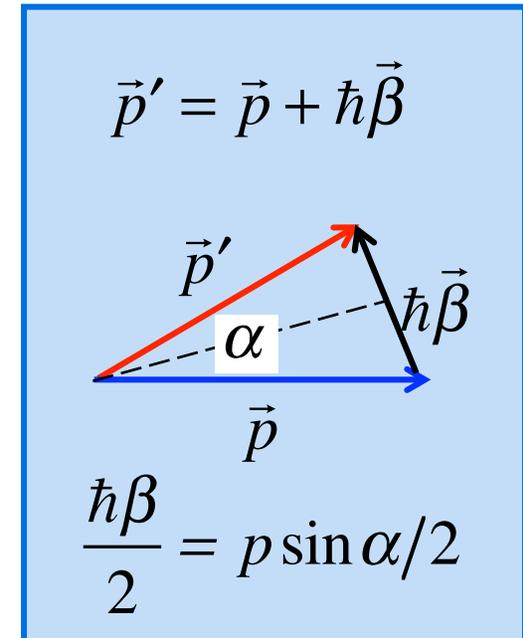
Recap

$$S(\vec{p}, \vec{p}') = \frac{2\pi}{\hbar} |H_{p',p}|^2 \delta(E' - E) \quad H_{p,p'} = \frac{1}{\Omega} \tilde{U}_s(\beta) \quad \tilde{U}_s(\beta) = \frac{q^2}{\kappa_s \epsilon_0} \frac{1}{(\beta^2 + 1/L_D^2)}$$

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

$$S(\vec{p}, \vec{p}') = \frac{2\pi q^4 N_I}{\hbar \kappa_s^2 \epsilon_0^2 \Omega} \frac{\delta(E' - E)}{(\beta^2 + 1/L_D^2)^2}$$

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



Examine result

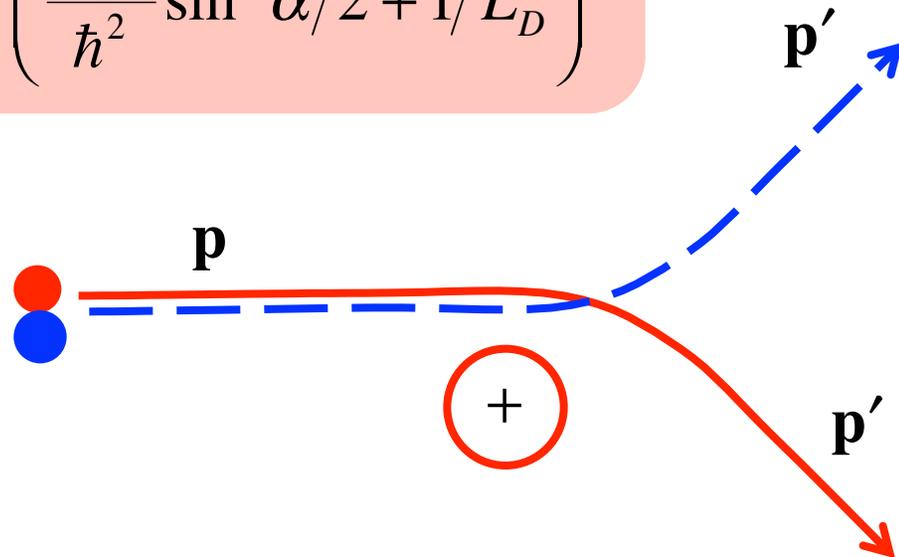
$$S(\vec{p}, \vec{p}') = \frac{2\pi q^4 N_I}{\hbar \kappa_S^2 \epsilon_S^2 \Omega} \frac{\delta(E' - E)}{\left(\frac{4p^2}{\hbar^2} \sin^2 \alpha/2 + 1/L_D^2 \right)^2}$$

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

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

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

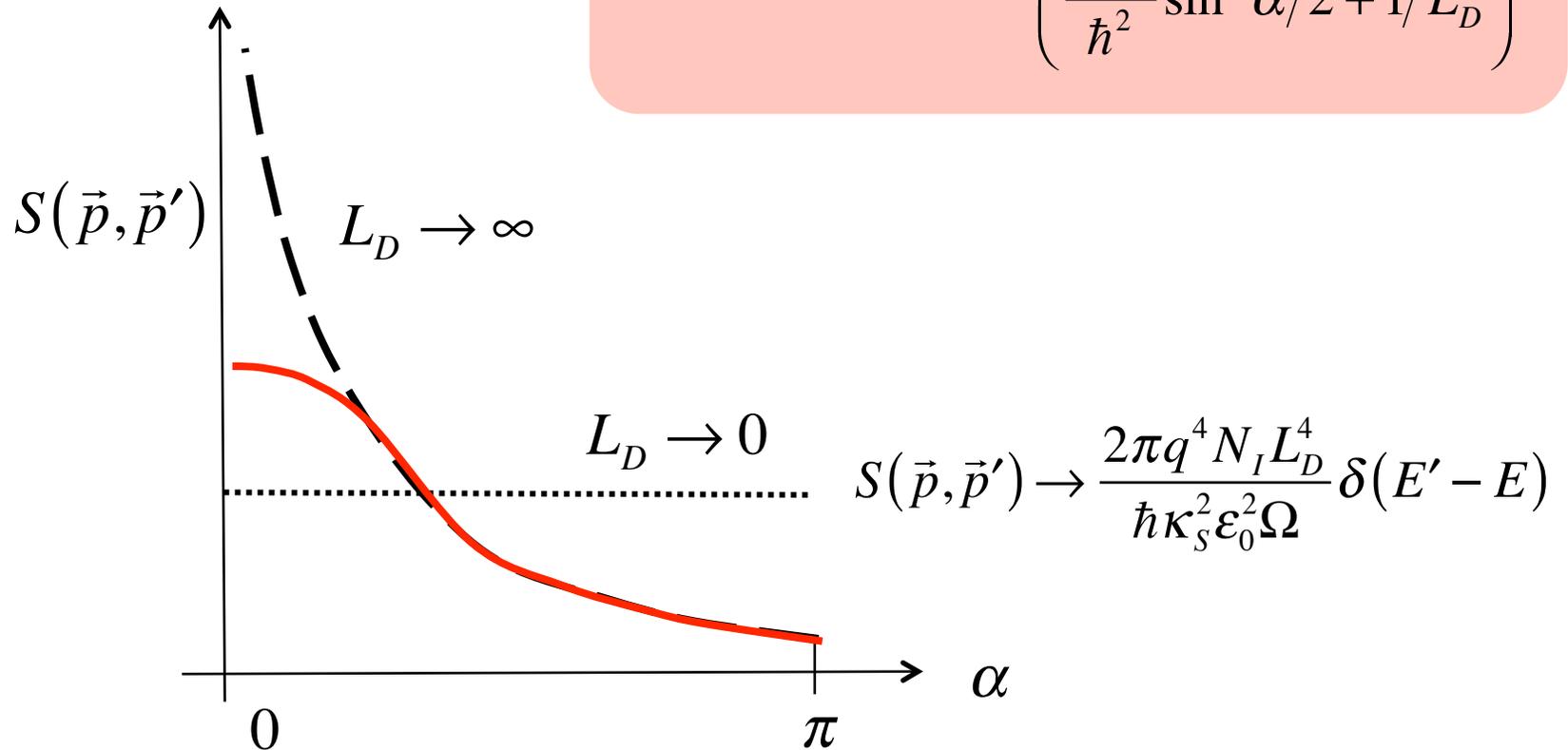
4) Favors small angle scattering



Examine result

4) angular dependence

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

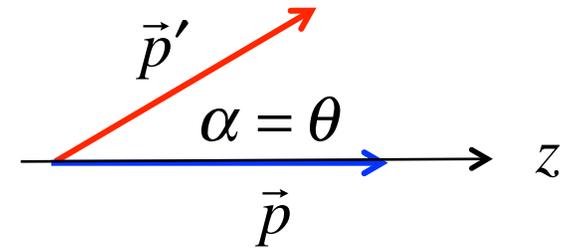


Outline

- 1) Introduction
- 2) Screening
- 3) Transition rate**
- 4) Characteristic times

Characteristic times

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



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

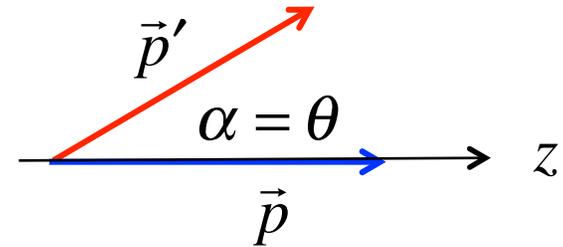
$S(\vec{p}, \vec{p}')$ favors small angles

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

$$1/\tau_E = 0 \quad \tau_E > \tau$$

Momentum relaxation time

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



$$\tau_m(E) = \frac{16\sqrt{2m^*} \pi \kappa_s^2 \epsilon_0^2}{N_I q^4} \left[\ln(1 + \gamma^2) - \frac{\gamma^2}{1 + \gamma^2} \right] E^{3/2}$$

$$\gamma^2 = 8m^* EL_D^2 / \hbar^2 \quad \text{See Lundstrom (FCT) pp. 69-70}$$

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

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

Questions?

- 1) Introduction
- 2) Screening
- 3) Transition rate
- 4) Characteristic times

