

# Phonon Scattering in Polar Semiconductors

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# Outline

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- 1) Quick re-cap
- 2) POP coupling constant
- 3) POP Transition rate and scattering time
- 4) PZ scattering
- 5) Summary

# Transition rate for phonon scattering

$$S(\vec{p}, \vec{p}') = \frac{2\pi}{\hbar} |H_{p,p'}|^2 \delta(E' - E \mp \hbar\omega) \quad H_{p',p} = \frac{1}{\Omega} \int_{-\infty}^{+\infty} e^{-i\vec{p}'\cdot\vec{r}/\hbar} U_S(\vec{r}) e^{i\vec{p}\cdot\vec{r}/\hbar} d\vec{r}$$

$$U_S(\vec{r}) = K_q u_q \quad u_q(\vec{r}) = A_q e^{\pm i\vec{q}\cdot\vec{r}} \quad |H_{p',p}|^2 = |K_q|^2 |A_q|^2 \delta_{\vec{p}', \vec{p} \pm \hbar\vec{q}}$$

$$|A_q|^2 \rightarrow \frac{\hbar}{2\rho\Omega\omega} \left( N_\omega + \frac{1}{2} \mp \frac{1}{2} \right)$$

$$S(\vec{p}, \vec{p}') = \frac{\pi}{\Omega\rho\omega} |K_q|^2 \left( N_\omega + \frac{1}{2} \mp \frac{1}{2} \right) \delta(\vec{p}' - \vec{p} \mp \hbar\vec{q}) \delta(E' - E \mp \hbar\omega)$$

# Scattering times

$$S(\vec{p}, \vec{p}') = \frac{\pi}{\Omega \rho \omega} |K_q|^2 \left( N_\omega + \frac{1}{2} \mp \frac{1}{2} \right) \delta(\vec{p}' - \vec{p} \mp \hbar \vec{q}) \delta(E' - E \mp \hbar \omega)$$

Coupling constant  
has a **strong q-**  
**dependence.**

$$\frac{1}{\tau(\vec{p})} = \sum_{\vec{p}', \uparrow} S(\vec{p}, \vec{p}')$$

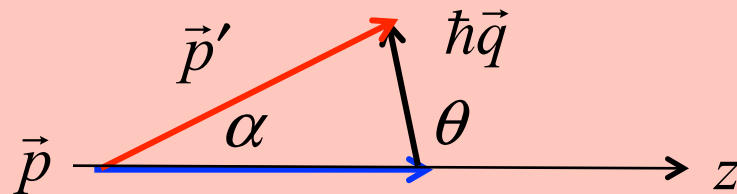
$$\frac{1}{\tau_m(\vec{p})} = \sum_{\vec{p}', \uparrow} S(\vec{p}, \vec{p}') \frac{\Delta p_z}{p_{z0}}$$

# Including E-M conservation

$$S(\vec{p}, \vec{p}') = \frac{2\pi}{\hbar} |K_q|^2 \frac{\hbar}{2\rho\Omega\omega_0} \frac{1}{\hbar v q} \left( N_q + \frac{1}{2} \mp \frac{1}{2} \right) \delta \left( \pm \cos\theta + \frac{\hbar q}{2p} \mp \frac{\omega_0}{vq} \right)$$

$$S(\vec{p}, \vec{p}') = \frac{1}{\Omega} C_q \left( N_\omega + \frac{1}{2} \mp \frac{1}{2} \right) \delta \left( \pm \cos\theta + \frac{\hbar q}{2p} \mp \frac{\omega_0}{vq} \right)$$

$$C_q = \frac{\pi}{\hbar\rho v\omega_0 q} |K_q|^2 \quad N_\omega = \frac{1}{e^{\hbar\omega_0/k_B T} - 1}$$



# General expression for scattering time

$$\frac{1}{\tau} = \sum_{\vec{p}', \uparrow} S(\vec{p}, \vec{p}') = \sum_{\vec{q}, \uparrow} S(\vec{p}, \vec{p}') \quad \vec{p}' = \vec{p} \pm \hbar \vec{q}$$

Integration of the delta function simply restricts  $q$  to those values that satisfy energy and momentum conservation.

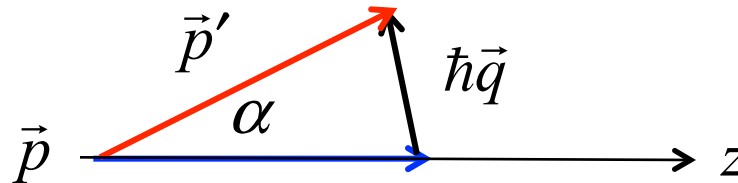
$$q_{\min} < q < q_{\max}$$

$$\frac{1}{\tau} = \frac{1}{4\pi^2} \int_{q_{\min}}^{q_{\max}} C_q \left( N_{\omega} + \frac{1}{2} \mp \frac{1}{2} \right) q^2 dq$$

$$C_q = \frac{\pi}{\hbar \rho v \omega_0 q} |K_q|^2 \quad N_{\omega} = \frac{1}{e^{\hbar \omega_0 / k_B T} - 1}$$

# Momentum relaxation time

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



$$\frac{1}{\tau_m} = \frac{1}{4\pi^2} \int_{q_{\min}}^{q_{\max}} C_q \left( N_\omega + \frac{1}{2} \mp \frac{1}{2} \right) \left( \frac{\hbar q}{2p} \mp \frac{\omega_q}{vq} \right) \frac{\hbar q^3}{p} dq$$

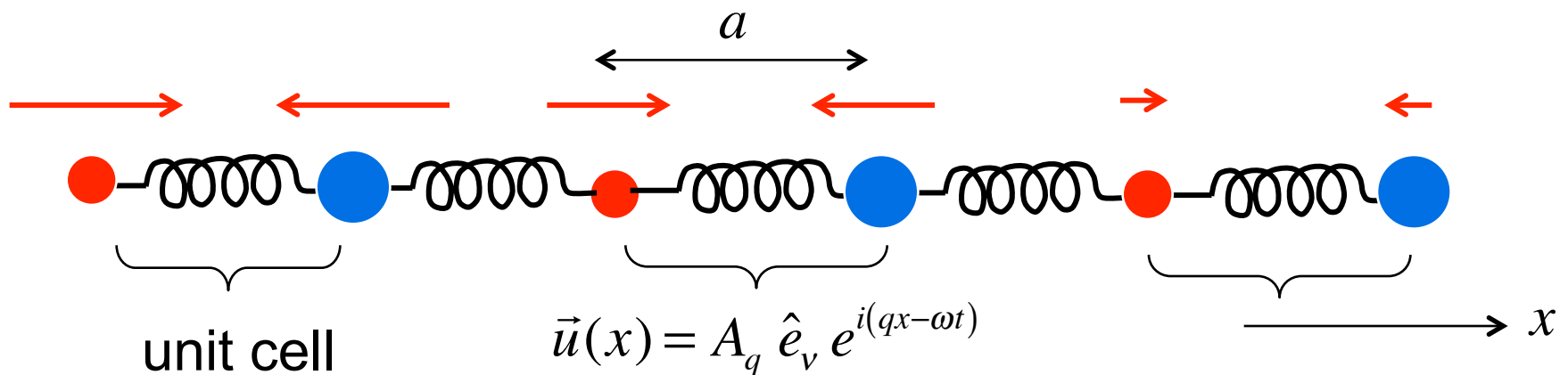
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# LO phonons

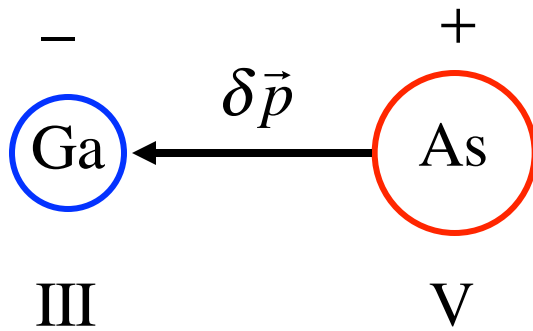


In covalent semiconductors (e.g. Si, Ge), all atoms are the same.

In II-VI and III-V semiconductors, the bonds are partially ionic, which gives rise to internal dipole moments.

Oscillating dipole moments produce strong scattering potentials.

# POP coupling constant

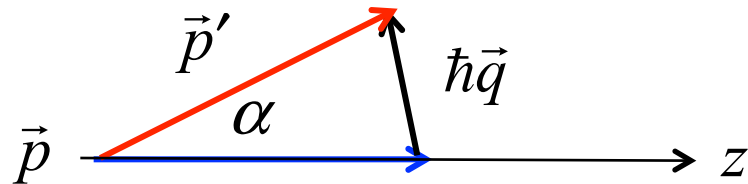


$$U_s = K_q u_q$$

$$u_q(x, t) = A_q e^{\pm i(qz - \omega t)}$$

$$|K_q|^2 = \frac{\rho e^2 \omega_0^2}{q^2 \kappa_0 \epsilon_0} \left( \frac{\kappa_0}{\kappa_\infty} - 1 \right)$$

*small angle scattering dominates*



See Lundstrom, FCT, Sec. 2.2.2

# Outline

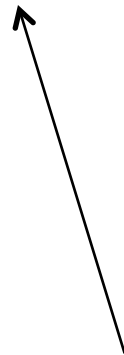
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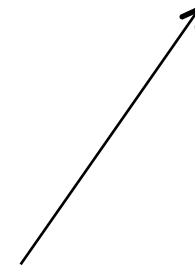
# Transition rate

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$$S(\vec{p}, \vec{p}') = \frac{\pi}{\Omega \rho \omega} |K_q|^2 \left( N_\omega + \frac{1}{2} \mp \frac{1}{2} \right) \delta(\vec{p}' - \vec{p} \mp \hbar \vec{q}) \delta(E' - E \mp \hbar \omega_0)$$



**scattering is anisotropic**



**scattering is inelastic**

$$|K_q|^2 = \frac{\rho e^2 \omega_0^2}{q^2 \kappa_0 \epsilon_0} \left( \frac{\kappa_0}{\kappa_\infty} - 1 \right)$$

# Scattering times

$$\frac{1}{\tau} = \frac{1}{4\pi^2} \int_{q_{\min}}^{q_{\max}} C_q \left( N_\omega + \frac{1}{2} \mp \frac{1}{2} \right) q^2 dq \quad C_q = \frac{\pi}{\hbar \rho v \omega_0 q} |K_q|^2$$

$$\frac{1}{\tau_m} = \frac{1}{4\pi^2} \int_{q_{\min}}^{q_{\max}} C_q \left( N_\omega + \frac{1}{2} \mp \frac{1}{2} \right) \left( \frac{\hbar q}{2p} \mp \frac{\omega_q}{vq} \right) \frac{\hbar q^3}{p} dq$$

$$q_{\min} = \frac{p}{m^*} \left[ \mp 1 \pm \left( 1 \pm \hbar \omega_0 / E_k \right)^{1/2} \right] \quad (\text{ABS/EMS})$$

$$q_{\max} = \frac{p}{m^*} \left[ 1 + \left( 1 \pm \hbar \omega_0 / E_k \right)^{1/2} \right] \quad (\text{For EMS: } E_k > \hbar \omega_0 )$$

# Scattering rate

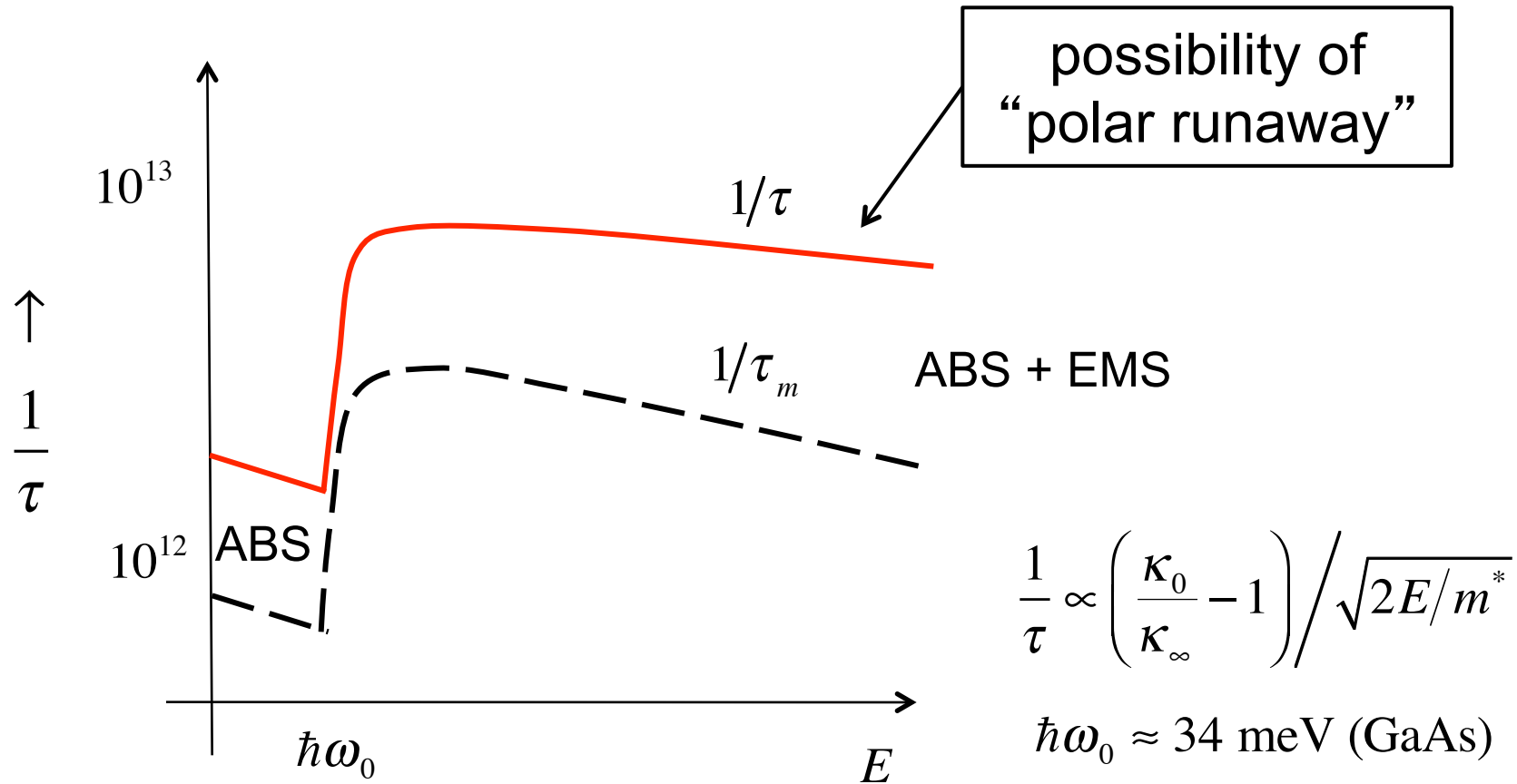
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$$\frac{1}{\tau} = \frac{1}{\tau_{abs}} + \frac{1}{\tau_{ems}} = \frac{q^2 \omega_0^2 \left( \frac{\kappa_0}{\kappa_\infty} - 1 \right)}{2\pi \kappa_0 \epsilon_0 \hbar \sqrt{2E/m^*}} \left[ N_0 \sinh^{-1} \left( \frac{E}{\hbar \omega_0} \right) + (N_0 + 1) \sinh^{-1} \left( \frac{E}{\hbar \omega_0} - 1 \right) \right]$$

$$\frac{1}{\tau} > \frac{1}{\tau_m} > \frac{1}{\tau_E}$$

See Lundstrom (FCT) , pp. 84 – 86 for momentum and energy relaxation rates.

# POP scattering



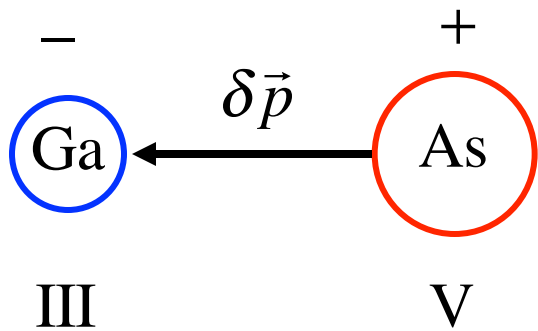
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# Acoustic phonons in polar materials



$$u_q(x, t) = A_q e^{\pm i(qx - \omega t)}$$

$$U_s = K_q u_q$$

$$|K_q|^2 = \frac{e^2 e_{PZ}^2}{\kappa_0^2 \epsilon_0^2}$$

Isotropic and elastic near room temperature.

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# Intra-band phonon scattering

$$u_q(\vec{r}, t) = A_q e^{\pm i(\vec{q} \cdot \vec{r} - \omega_q t)} \quad U_S = K_q u_q$$

$$\text{ADP} \quad |K_q|^2 = q^2 D_A^2$$

$$\text{ODP} \quad |K_q|^2 = D_0^2$$

$$\text{PZ} \quad |K_q|^2 = (ee_{PZ}/\kappa_S \epsilon_0)^2$$

$$\text{POP} \quad |K_q|^2 = \frac{\rho e^2 \omega_0^2}{q^2 \kappa_0 \epsilon_0} \left( \frac{\kappa_0}{\kappa_\infty} - 1 \right)$$

# Questions?

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