ECE-656: Fall 2011

Lecture 26:

Phonon Scattering: III

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transition rate for phonon scattering

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

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

$$U_S(\vec{r}) = K_\beta\, u_\beta \qquad u_\beta(\vec{r}) = A_\beta e^{\pm i\vec{\beta}\bullet\vec{r}}$$

$$\left|H_{p',p}\right|^2 = \left|K_\beta\right|^2 \left|A_\beta\right|^2 \delta_{\vec{p}\,',\vec{p}\pm\hbar\vec{\beta}}$$

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

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

transition rate for phonon scattering

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

ADP $\quad \left|K_\beta\right|^2 = \beta^2 D_A^2$

PZ $\quad \left|K_\beta\right|^2 = \left(q e_{PZ}/\kappa_S \varepsilon_0\right)^2$

ODP $\quad \left|K_\beta\right|^2 = D_0^2$

POP $\quad \left|K_\beta\right|^2 = \frac{\rho q^2 \omega_0^2}{\beta^2 \kappa_0 \varepsilon_0}\left(\frac{\kappa_0}{\kappa_\infty} - 1\right)$

energy-momentum conservation

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

$$\vec{p}\,'=\vec{p}\pm\hbar\vec{\beta} \qquad E'=E\pm\hbar\omega_\beta$$

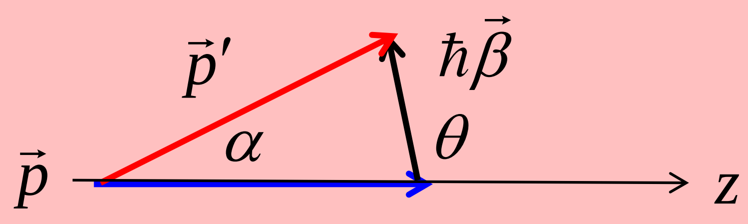
$$\delta_{\vec{p}\,',\vec{p}\pm\hbar\vec{\beta}}\,\delta\left(E'-E\mp\hbar\omega_\beta\right)\rightarrow\frac{1}{\hbar\upsilon\beta}\delta\left(\pm\cos\theta+\frac{\hbar\beta}{2p}\mp\frac{\omega_\beta}{\upsilon\beta}\right)$$

final answer: transition rate

$$S(\vec{p},\vec{p}\,') = \frac{2\pi}{\hbar}\left|K_\beta\right|^2 \frac{\hbar}{2\rho\Omega\omega}\frac{1}{\hbar\upsilon\beta}\left(N_\omega + \frac{1}{2} \mp \frac{1}{2}\right)\delta\left(\pm\cos\theta + \frac{\hbar\beta}{2p} \mp \frac{\omega}{\upsilon\beta}\right)$$

$$S(\vec{p},\vec{p}\,') = \frac{1}{\Omega} C_\beta \left(N_\omega + \frac{1}{2} \mp \frac{1}{2}\right)\delta\left(\pm\cos\theta + \frac{\hbar\beta}{2p} \mp \frac{\omega}{\upsilon\beta}\right)$$

$$C_\beta = \frac{\pi}{\hbar\rho\upsilon\omega\beta}\left|K_\beta\right|^2 \qquad N_\omega = \frac{1}{e^{\hbar\omega/k_B T} - 1}$$



general expression for the phonon scattering rate

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

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

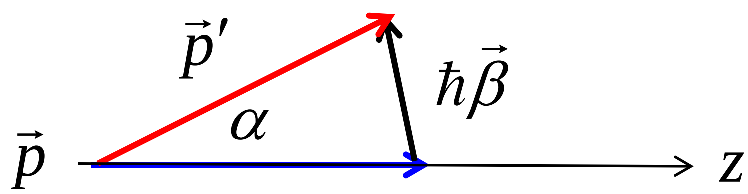
$$\beta_{\min} < \beta < \beta_{\max}$$

$$\frac{1}{\tau} = \frac{1}{4\pi^2} \int_{\beta_{\min}}^{\beta_{\max}} C_\beta \left(N_\omega + \frac{1}{2} \mp \frac{1}{2} \right) \beta^2 \, d\beta$$

$$C_\beta = \frac{\pi}{\hbar \rho \upsilon \, \omega \, \beta} \left| K_\beta \right|^2 \qquad N_\omega = \frac{1}{e^{\hbar\omega / k_B T} - 1}$$

momentum relaxation rate

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



$$\frac{1}{\tau_m} = \frac{1}{4\pi^2}\int_{\beta_{\min}}^{\beta_{\max}} C_\beta\left(N_\omega + \frac{1}{2} \mp \frac{1}{2}\right)\left(\frac{\hbar\beta}{2p} \mp \frac{\omega_\beta}{\upsilon\beta}\right)\frac{\hbar\beta^3}{p}\,d\beta$$

outline

1) Review
2) **Example**
3) POP and IV scattering
4) Scattering in common semiconductors
5) Electron-electron scattering
6) Summary

(Reference: Chapter 2, Lundstrom, FCT)

acoustic phonon scattering

$$\frac{1}{\tau} = \frac{1}{4\pi^2} \int_{\beta_{\min}}^{\beta_{\max}} C_\beta \left(N_\omega + \frac{1}{2} \mp \frac{1}{2} \right) \beta^2 \, d\beta$$

$$C_\beta = \frac{\pi m^* D_A^2}{\hbar \rho \upsilon_s p}$$ (Lundstrom, FCT, p. 79)

$$N_\omega = \frac{1}{e^{\hbar\omega_s / k_B T_L} - 1} \qquad \hbar\omega_s << k_B T_L \rightarrow N_{\omega_s} \approx \frac{k_B T_L}{\hbar \omega_s} \approx N_{\omega_s} + 1$$

"equipartition"

$$\frac{1}{\tau_{abs}} = \frac{1}{\tau_{ems}} = \frac{1}{4\pi^2} \int_{\beta_{\min}}^{\beta_{\max}} \frac{\pi m^* D_A^2}{\hbar \rho \upsilon_s p} \frac{k_B T_L}{\hbar \omega_s} \beta^2 \, d\beta$$

acoustic phonon scattering (ii)

$$\frac{1}{\tau_{abs}} = \frac{1}{\tau_{ems}} = \frac{m^* D_A^2 k_B T_L}{4\pi\hbar^2 \rho \upsilon_s p} \int_{\beta_{\min}}^{\beta_{\max}} \frac{\beta}{\omega_s} \beta \, d\beta \qquad \upsilon_s = \sqrt{c_l / \rho}$$

$$\frac{1}{\tau_{abs}} = \frac{1}{\tau_{ems}} = \frac{m^* D_A^2 k_B T_L}{4\pi\hbar^2 c_l p} \int_{\beta_{\min}}^{\beta_{\max}} \beta \; d\beta = \frac{m^* D_A^2 k_B T_L}{4\pi\hbar^2 c_l p} \left(\frac{\beta_{\max}^2}{2} - \frac{\beta_{\min}^2}{2} \right)$$

elastic scattering:

$$\hbar\beta_{\max} = 2p$$

$$\hbar\beta_{\min} = 0$$

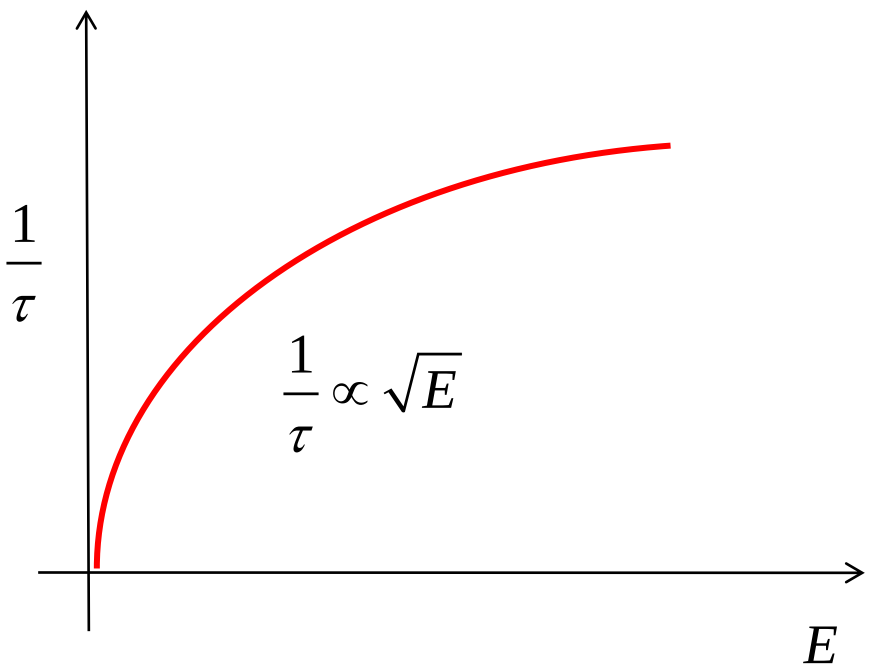
$$\frac{1}{\tau_{abs}} = \frac{1}{\tau_{ems}} \qquad \frac{1}{\tau} = \frac{1}{\tau_{abs}} + \frac{1}{\tau_{ems}}$$

acoustic phonon scattering (iii)

$$\frac{1}{\tau} = \frac{1}{\tau_{abs}} + \frac{1}{\tau_{ems}} = \frac{2\pi}{\hbar}\left(\frac{D_A^2 k_B T}{c_l}\right)\frac{D_{3D}(E)}{2}$$

$$\frac{1}{\tau} = \frac{1}{\tau_m}$$

(isotropic)



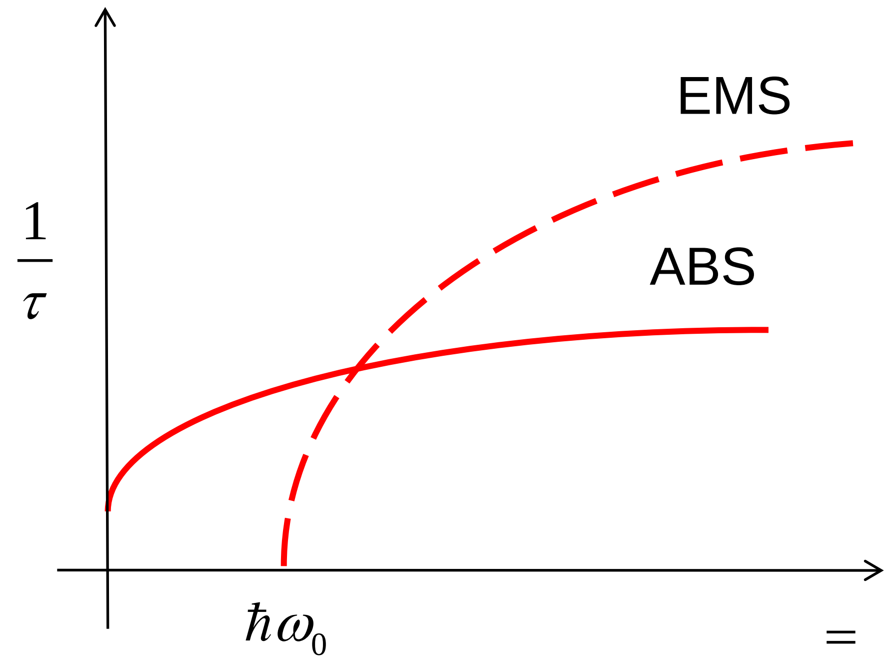
optical deformation potential scattering

$$\frac{1}{\tau}=\frac{1}{4\pi^2}\int_{\beta_{\min}}^{\beta_{\max}} C_\beta\left(N_\omega+\frac{1}{2}\mp\frac{1}{2}\right)\beta^2\,d\beta$$

$$C_\beta=\frac{\pi m^* D_O^2}{\hbar\rho\omega_0\beta p}$$

(Lundstrom, FCT, p. 79)

$$N_0=\frac{1}{e^{\hbar\omega_o/k_B T_L}-1}$$



$$\frac{1}{\tau}=\frac{1}{\tau_m}=\frac{2\pi}{\hbar}\left(\frac{\hbar D_O^2}{2\rho\omega_0}\right)\left(N_0+\frac{1}{2}\mp\frac{1}{2}\right)\frac{D_{3D}\left(E\pm\hbar\omega_0\right)}{2}$$

$$\frac{1}{\tau_{abs}}\neq\frac{1}{\tau_{ems}}$$

isotropic vs. anisotropic scattering

$$\frac{1}{\tau} = \frac{1}{4\pi^2} \int_{\beta_{\min}}^{\beta_{\max}} C_\beta \left(N_\omega + \frac{1}{2} \mp \frac{1}{2} \right) \beta^2 \, d\beta \qquad C_\beta = \frac{\pi m^* D_O^2}{\hbar \rho \omega_0 \beta p}$$

How do we determine whether scattering is isotropic?

Go back to the matrix element:

$$\left| H_{p',p} \right|^2 = \frac{1}{\Omega} \left| K_\beta \right|^2 \frac{\hbar}{2\rho\,\omega_0} \left(N_0 + \frac{1}{2} \mp \frac{1}{2} \right) \delta_{\vec{p}',\vec{p} \pm \hbar\vec{\beta}}$$

$$\left| K_\beta \right|^2 = D_0^2 \qquad N_0 = \frac{1}{e^{\hbar\omega_o / k_B T} - 1}$$

No dependence on β → isotropic scattering.

short cut for isotropic scattering

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

$$U_S(\vec{r}) = K_\beta u_\beta \qquad u_\beta(\vec{r}) = A_\beta e^{\pm i\vec{\beta}\bullet\vec{r}} \qquad \left|H_{p',p}\right|^2 = \left|K_\beta\right|^2 \left|A_\beta\right|^2 \delta_{\vec{p}\,',\vec{p}\pm\hbar\vec{\beta}}$$

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

For isotropic scattering:

$$S(\vec{p},\vec{p}\,') = \frac{2\pi}{\hbar}\left|K_\beta\right|^2 \left|A_\beta\right|^2 \delta\left(E' - E \mp \hbar\omega\right)$$

outline

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2) Example
3) **POP and IV scattering**
4) Scattering in common semiconductors
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(Reference: Chapter 2, Lundstrom, FCT)

POP scattering

$$S(\vec{p}, \vec{p}') \approx \frac{2\pi}{\hbar} \left| H_{p,p'} \right|^2 \delta\left(E' - E \pm \hbar\omega_0\right)$$ (inelastic at RT and below)

$$\left| H_{p',p} \right|^2 = \frac{1}{\Omega} \left| K_\beta \right|^2 \frac{\hbar}{2\rho\ \omega_0} \left(N_0 + \frac{1}{2} \mp \frac{1}{2} \right) \delta_{\vec{p}', \vec{p} \pm \hbar\vec{\beta}} \qquad N_0 = \frac{1}{e^{\hbar\omega_0/k_B T} - 1} < N_0 + 1$$

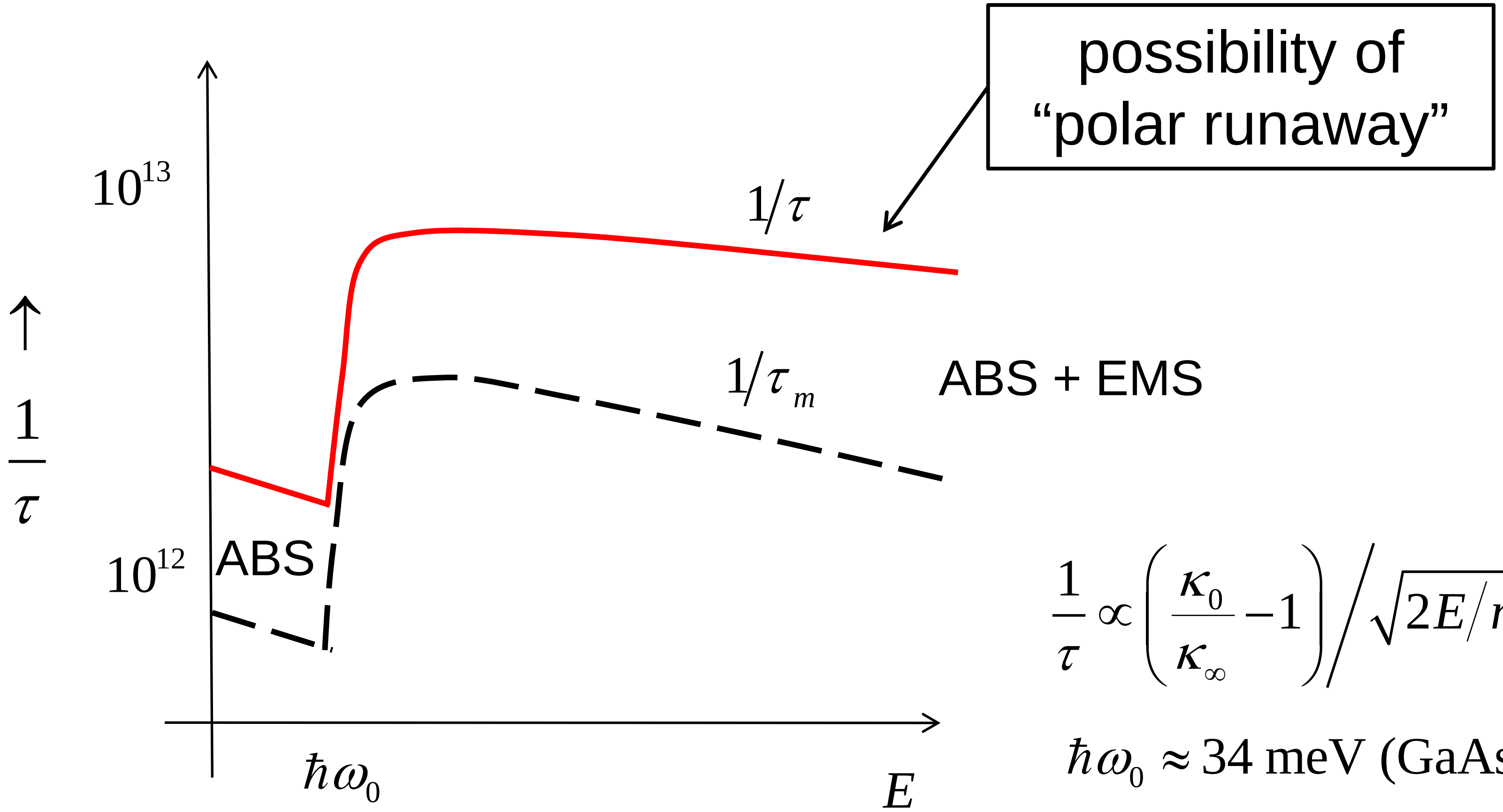
$$\left| K_\beta \right|^2 = \frac{\rho q^2 \omega_0^2}{\beta^2 \kappa_0 \varepsilon_0} \left(\frac{\kappa_0}{\kappa_\infty} - 1 \right)$$ (favors small angle scattering)

$$\frac{1}{\tau} = \frac{1}{\tau_{abs}} + \frac{1}{\tau_{ems}} = \frac{q^2 \omega_0^2 \left(\frac{\kappa_0}{\kappa_\infty} - 1 \right)}{2\pi\kappa_0 \varepsilon_0 \hbar \sqrt{2E/m^*}} \left[N_0 \sinh^{-1}\left(\frac{E}{\hbar\omega_0} \right) + \left(N_0 + 1\right) \sinh^{-1}\left(\frac{E}{\hbar\omega_0} - 1 \right) \right]$$

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

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

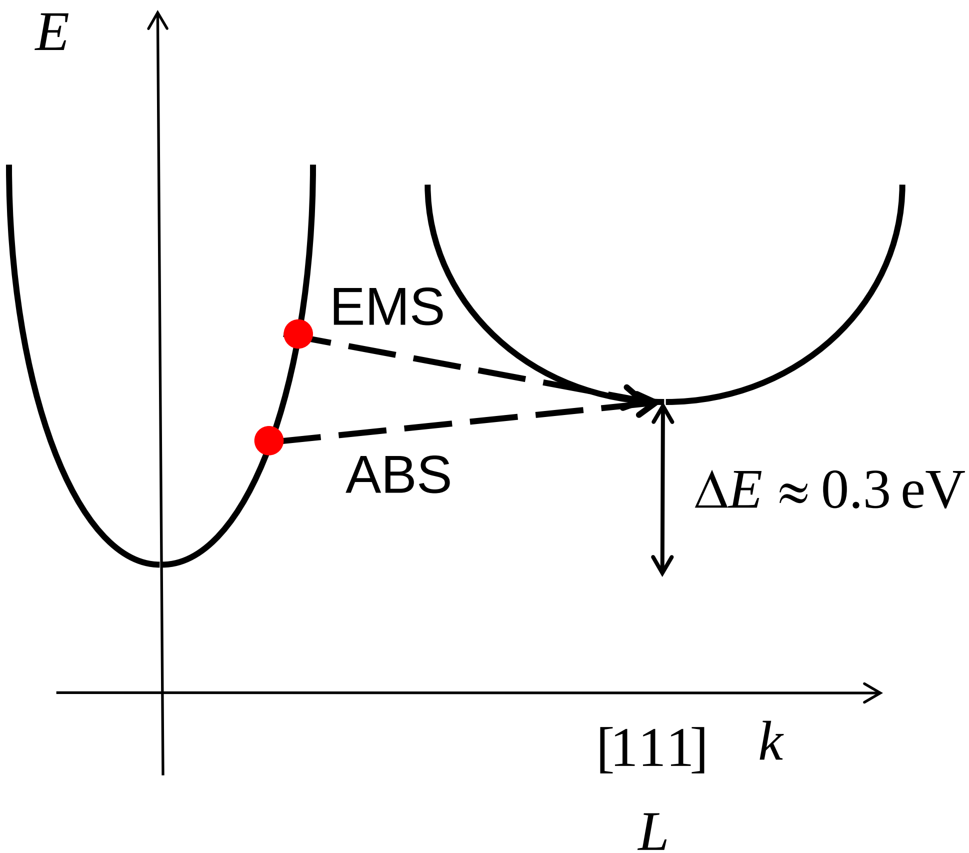
POP scattering

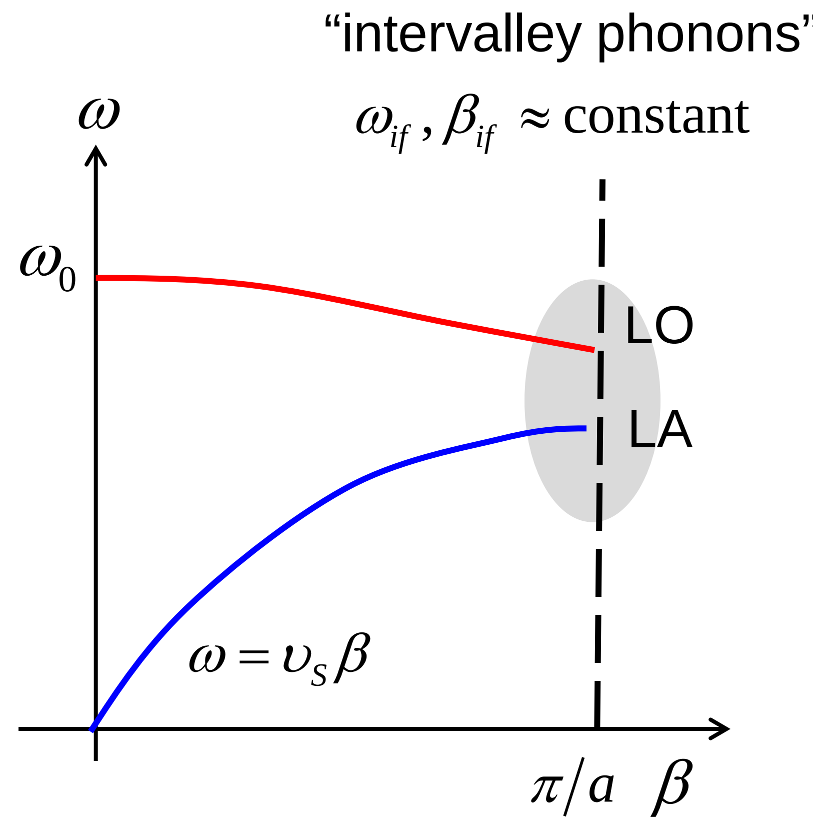


$$\frac{1}{\tau} \propto \left(\frac{\kappa_0}{\kappa_\infty} - 1\right) \Big/ \sqrt{2E/m^*}$$

$$\hbar\omega_0 \approx 34 \text{ meV (GaAs)}$$

IV scattering (GaAs)





Requires phonons with momentum near the zone boundary.

IV scattering (GaAs)

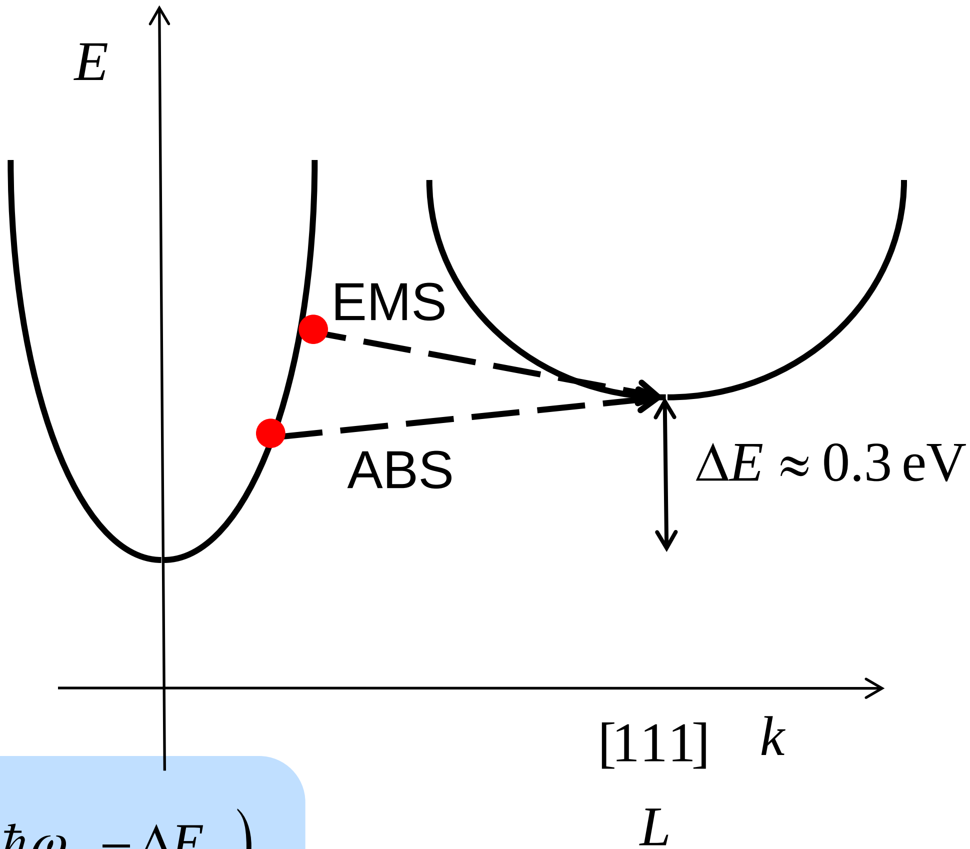
Postulate:

$$U_S = D_{if} u_\beta$$

Then IV scattering looks like ODP scattering

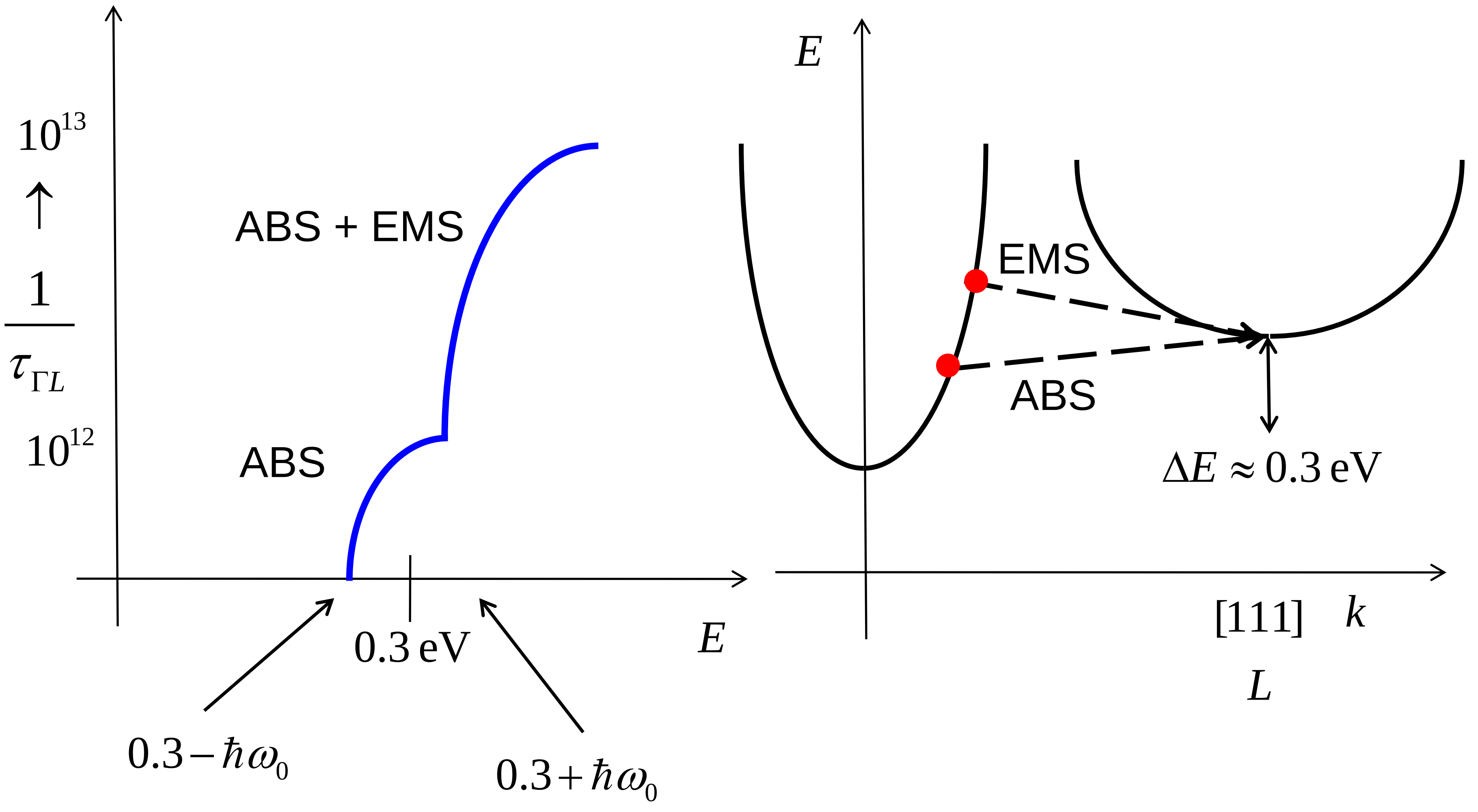
Isotropic: $\dfrac{1}{\tau} = \dfrac{1}{\tau_m}$

Number of final valleys: Z_f

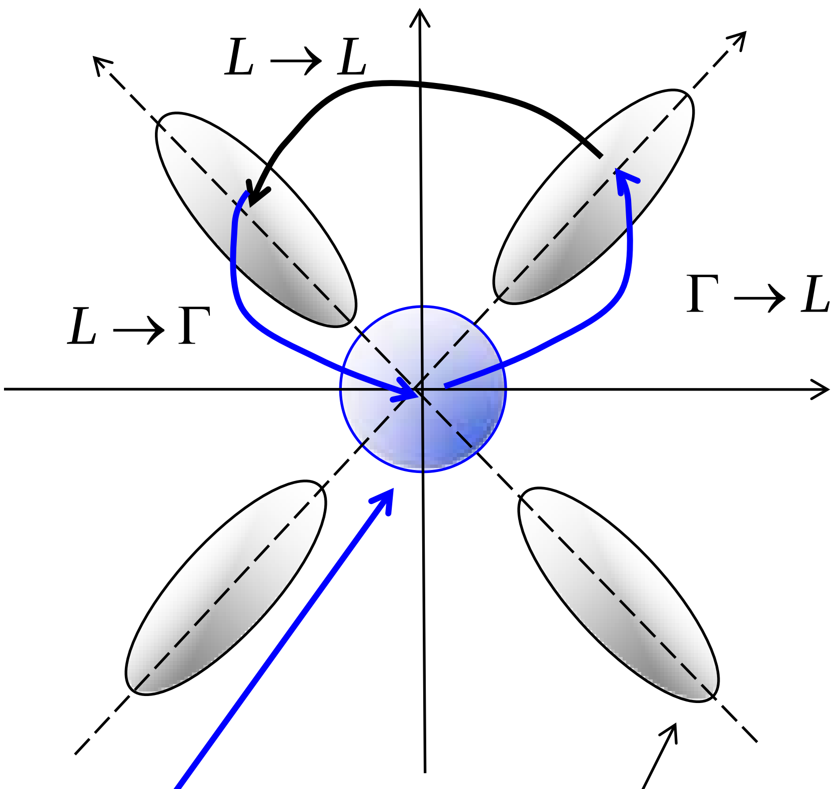


$$\frac{1}{\tau} = \frac{2\pi}{\hbar}\left(\frac{\hbar D_{if}^2 Z_f}{2\rho\omega_{if}}\right)\left(N_{if} + \frac{1}{2} \mp \frac{1}{2}\right)\frac{D_f\left(E \pm \hbar\omega_{if} - \Delta E_{fi}\right)}{2}$$

IV scattering (GaAs)



L-L and L-Γ IV scattering (GaAs)



Γ valley constant energy surface.

L valley constant energy surfaces.

$$\frac{1}{\tau} \propto D_{if}^2 Z_f \frac{D_f\left(E \pm \hbar\omega_{if} - \Delta E_{fi}\right)}{2}$$

$$\Gamma \rightarrow L: \quad Z_f = 4 \quad \Delta E_{fi} = 0.3\,\text{eV}$$

$$L \rightarrow L: \quad Z_f = 3 \quad \Delta E_{fi} = 0\,\text{eV}$$

$$L \rightarrow \Gamma: \quad Z_f = 1 \quad \Delta E_{fi} = -0.3\,\text{eV}$$

Compare rates:

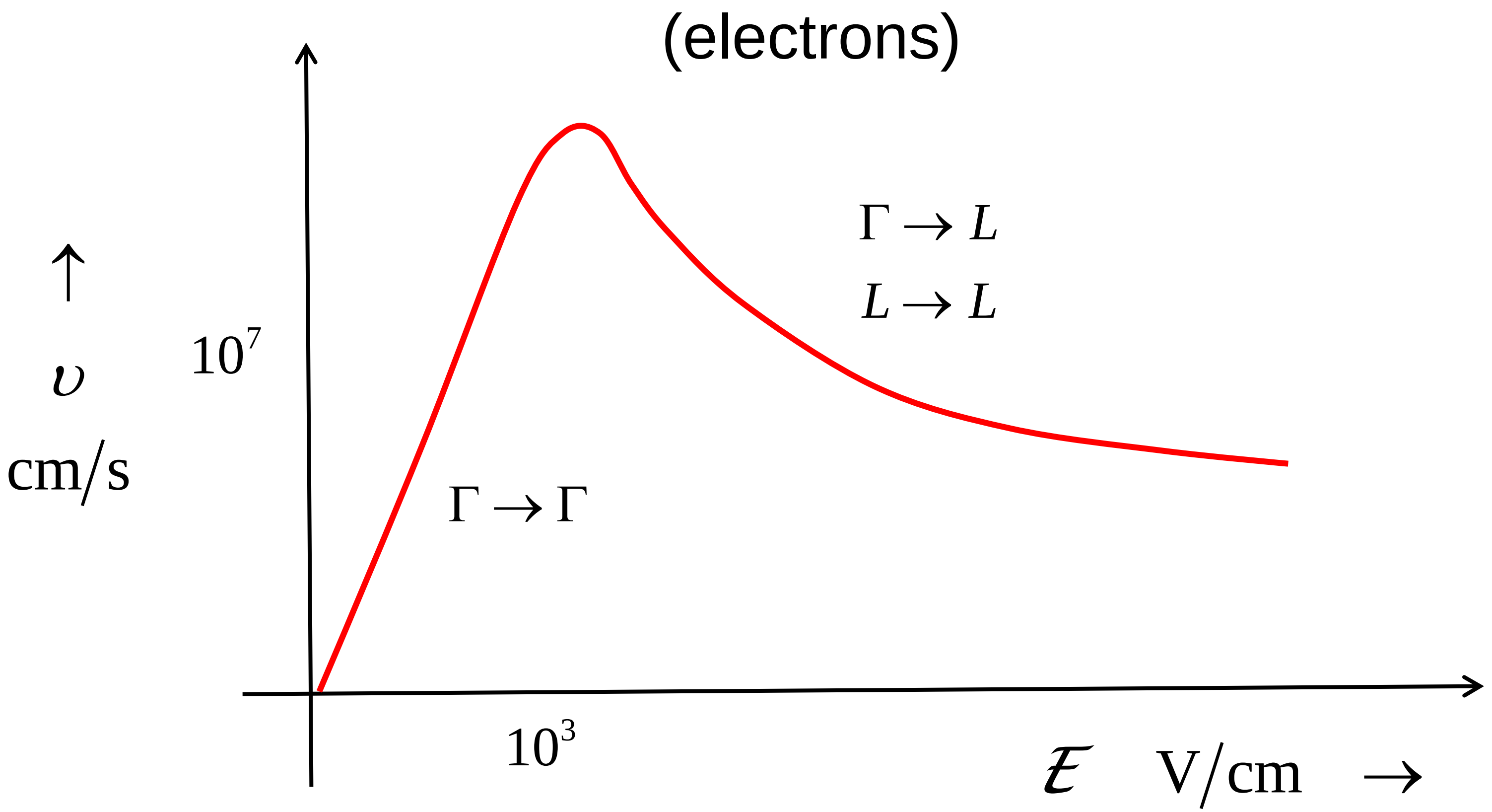
$1/\tau_{\Gamma\rightarrow\Gamma}$ (POP)

$1/\tau_{\Gamma\rightarrow L}$

$1/\tau_{L\rightarrow L}$

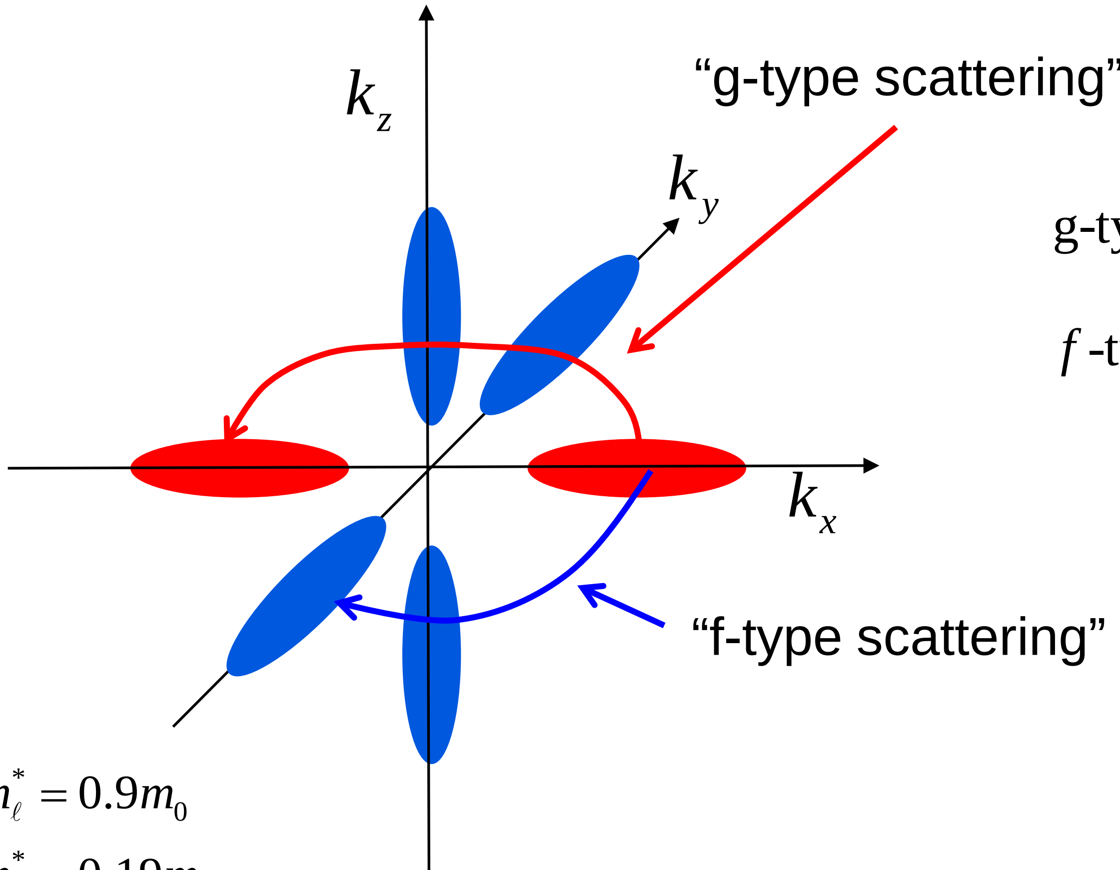
$1/\tau_{L\rightarrow\Gamma}$

velocity vs. electric field: GaAs



equivalent IV scattering (Si)

Si conduction band



$$\text{g-type}: \quad Z_f = 1 \quad \Delta E_{fi} = 0 \text{ eV}$$

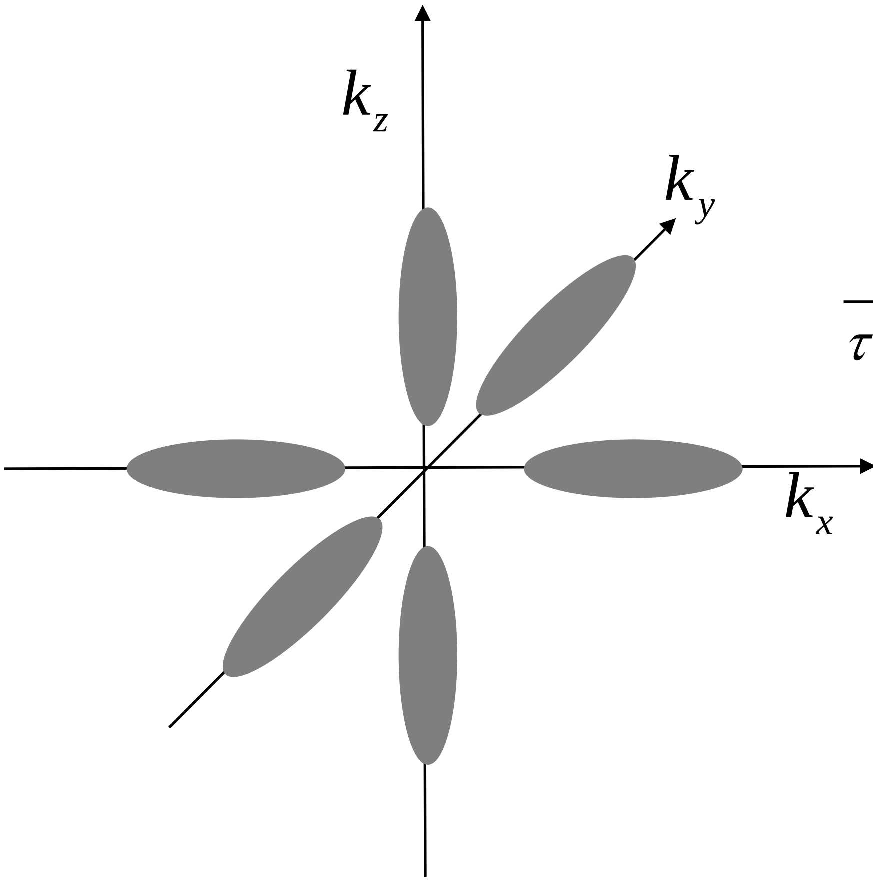
$$f\text{-type}: \quad Z_f = 4 \quad \Delta E_{fi} = 0 \text{ eV}$$

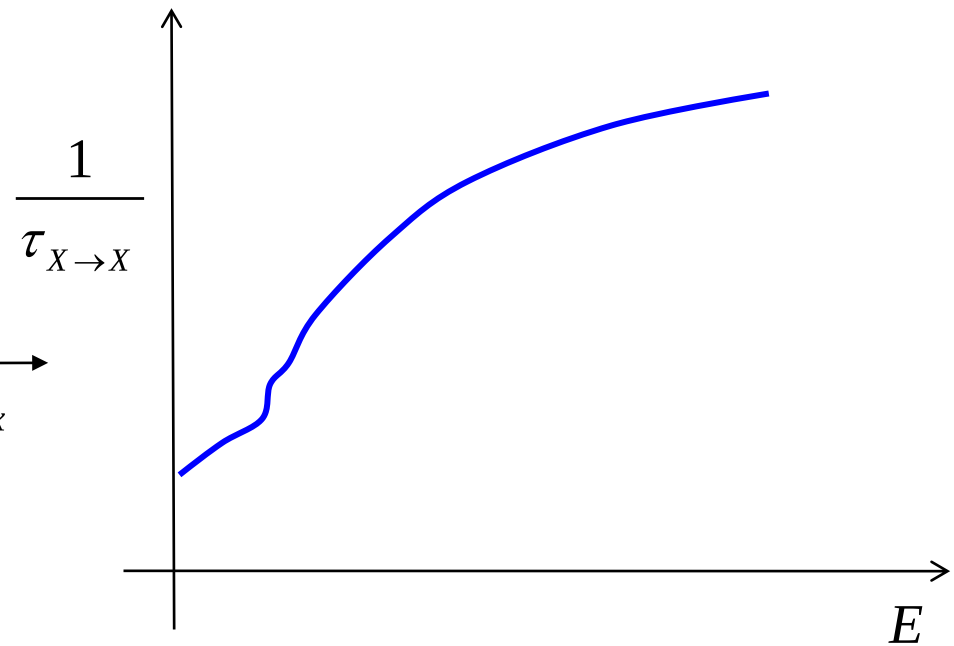
$$m_\ell^* = 0.9 m_0$$

$$m_t^* = 0.19 m_0$$

equivalent IV scattering (Si)

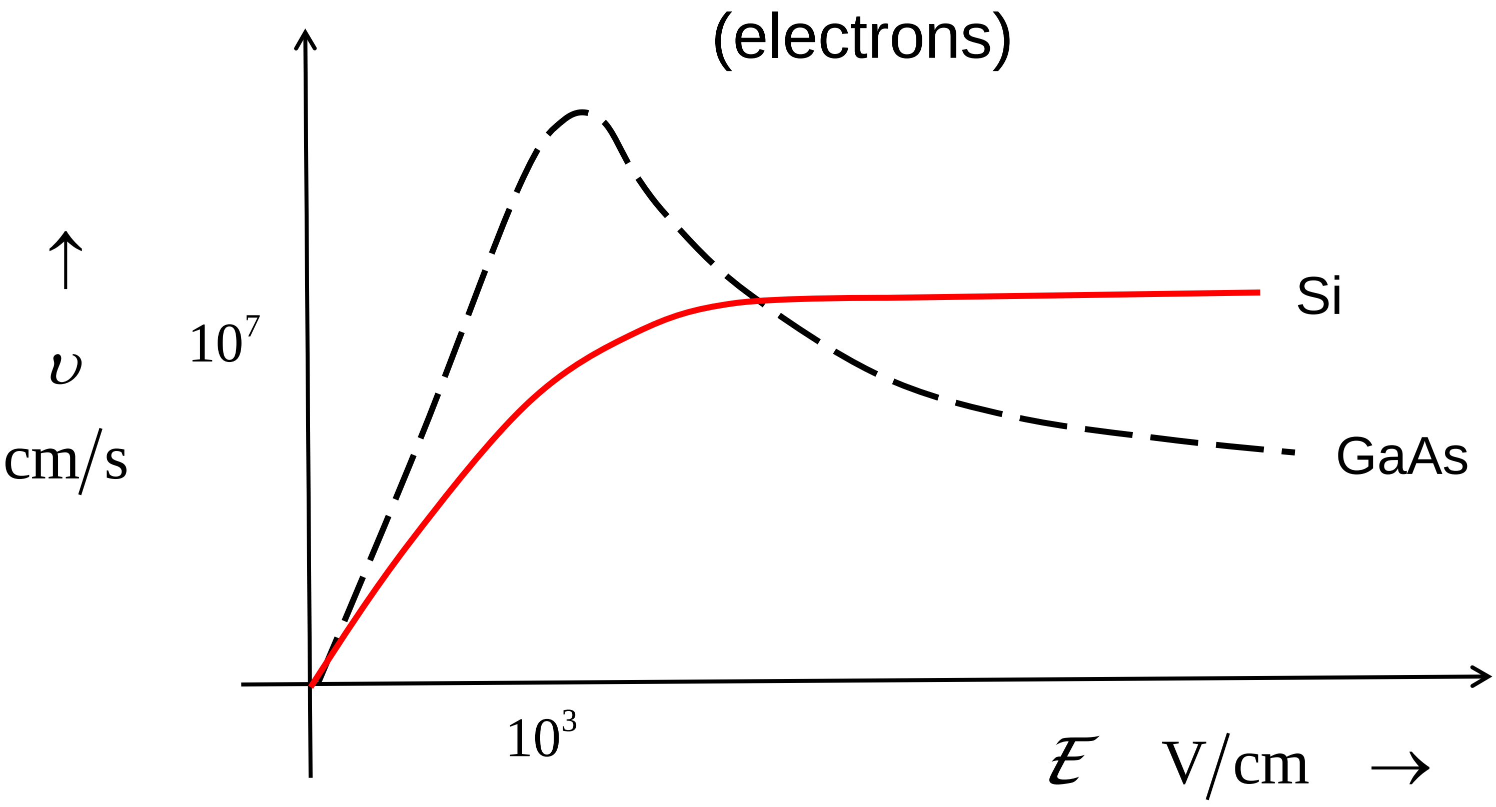
Si conduction band



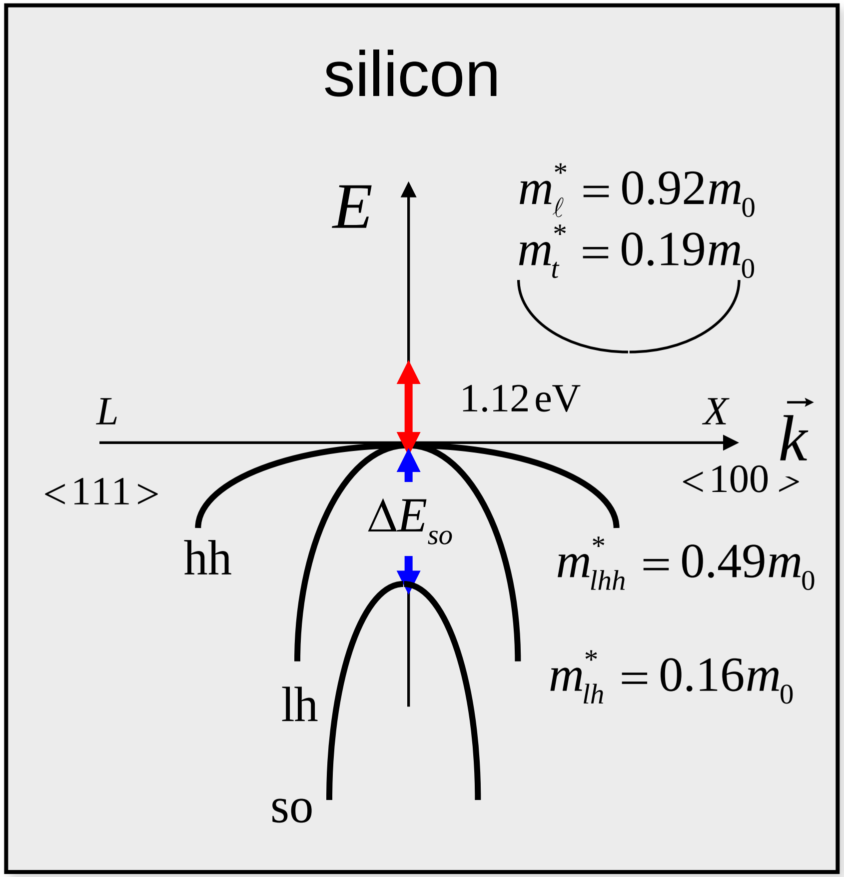


Important at room temperature in Si

velocity vs. electric field: Si



about holes



$$\Delta E_{so} = 44 \text{ meV (Si)}$$
$$= 290 \text{ meV (Ge)}$$

Intravalley:

$$\frac{1}{\tau_{hh \to hh}} \quad \frac{1}{\tau_{lh \to lh}} \quad \frac{1}{\tau_{so \to so}}$$

Intervalley:

$$\frac{1}{\tau_{hh \to lh}} \quad \frac{1}{\tau_{lh \to hh}}$$

$$\frac{1}{\tau_{hh \to so}} \quad \frac{1}{\tau_{so \to hh}} \quad \frac{1}{\tau_{lh \to so}} \quad \frac{1}{\tau_{so \to lh}}$$

Valence band is complex (warped) and can be engineered by strain.

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(Reference: Chapter 2, Lundstrom, FCT)

key questions

1) What is the total scattering rate vs. energy for common semiconductors?

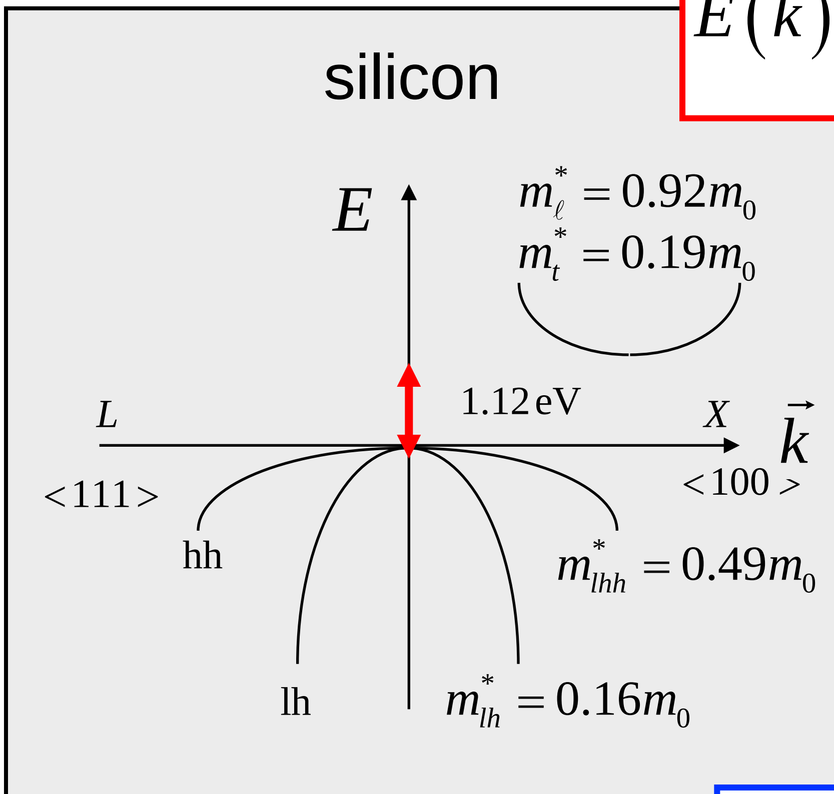
$$\Gamma = \sum_i \frac{1}{\tau_i}$$

2) How do covalent semicondictors (e.g. Si, Ge) differ from polar semiconductors (e.g. GaAs, InP, InGaAs, ZnSe)?

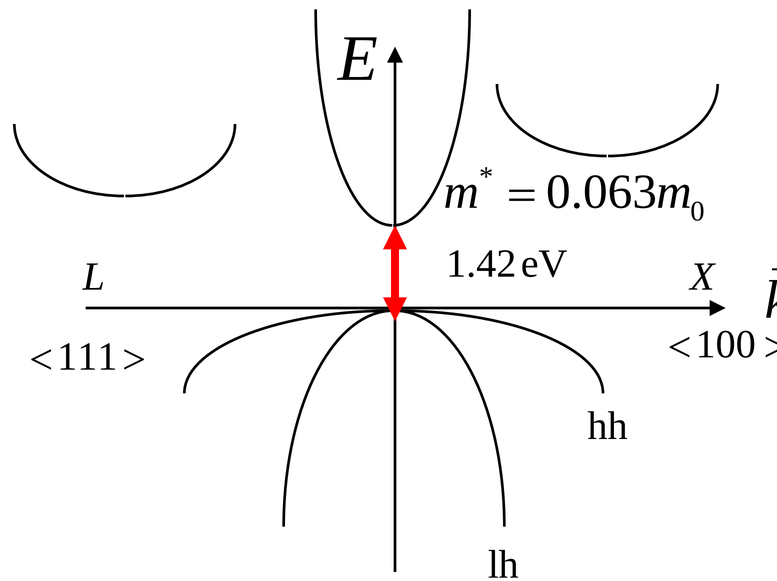
model bandstructure (for analytical calculations)

Si, covalent, indirect BG

$$E(k) = E_C + \frac{\hbar^2 k^2}{2m_n^*}$$

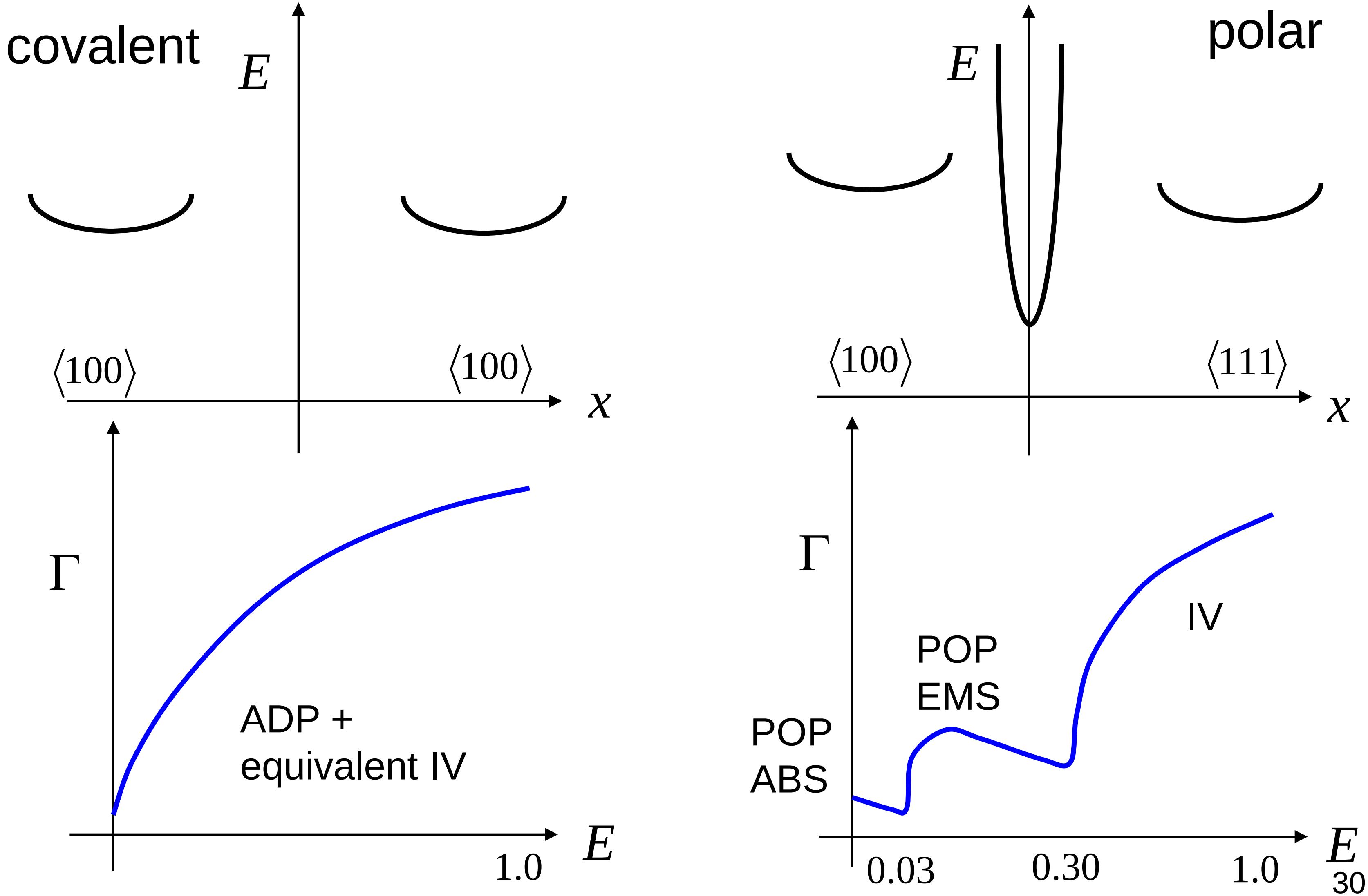


GaAs



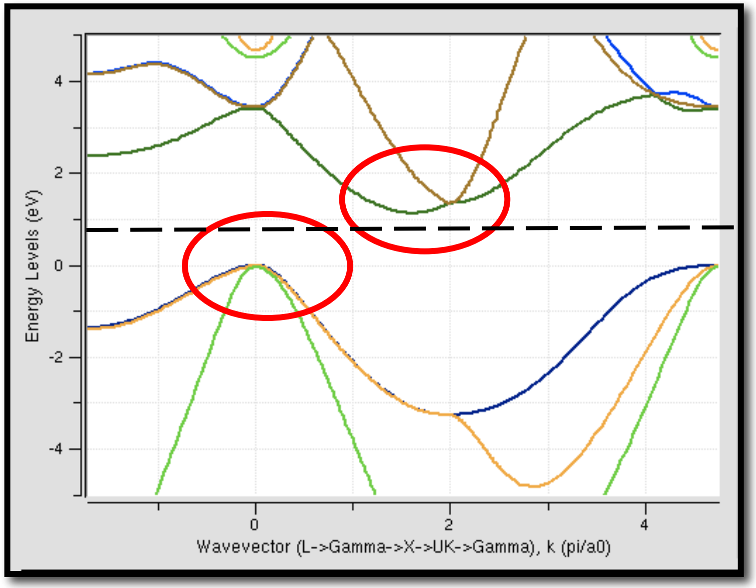
$$E(k) = E_V - \frac{\hbar^2 k^2}{2m_p^*}$$

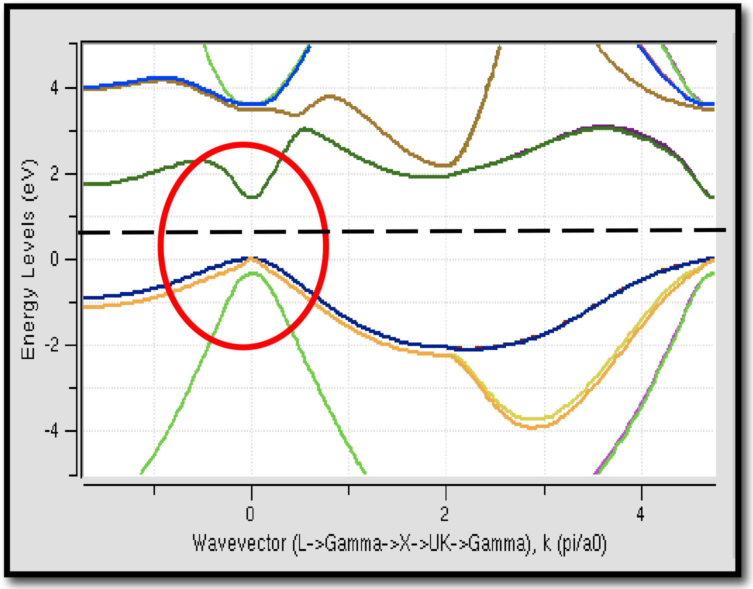
covalent vs. polar semiconductors



energy bands

Si, covalent, indirect bandgap





(“Bandstructure Lab” at www.nanoHUB.org)

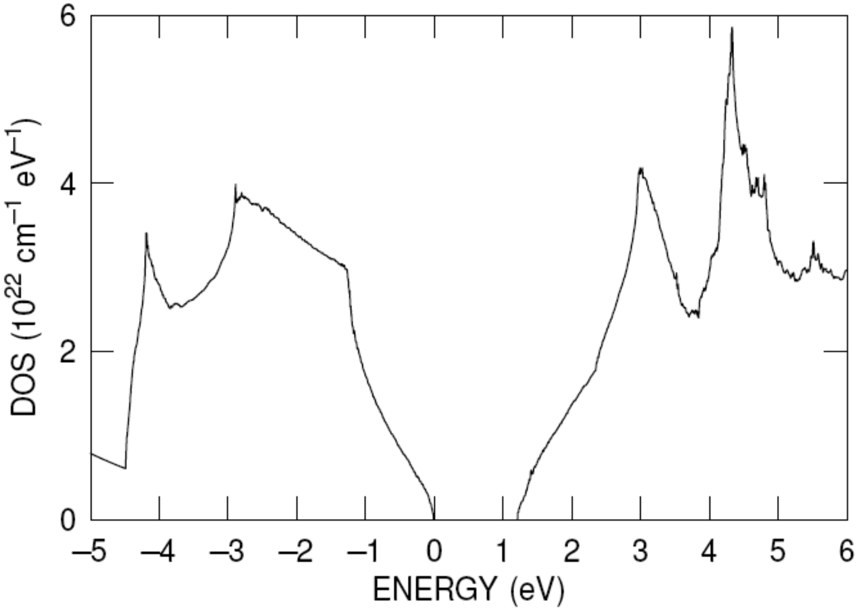
"full band" scattering rates

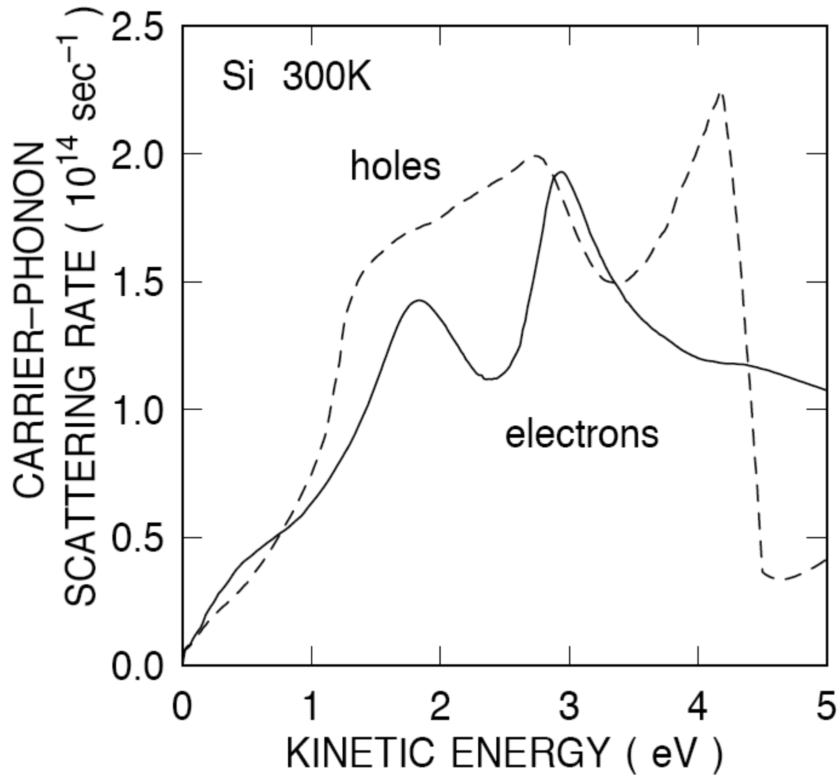
For a good, general reference on the numerical evaluation of scattering rates in common semiconductors, see:

[1] Massimo V. Fischetti, Monte Carlo Simulation of Transport in Technologically Significant Semiconductors of the Diamond and Zinc-Blende Structures-Part I: Homogeneous Transport," *IEEE Trans. Electron Dev*., **38**, pp. 634-649, 1991

[2] M. V. Fischetti, N. Sano, S. E. Laux, and K. Natori, "Full-bandstructure theory of high-field transport and impact ionization of electrons and holes in Ge, Si, GaAs, InAs, and $In_{0.53}Ga_{0.47}As$," *unpublished manuscript*., January 3, 2001.

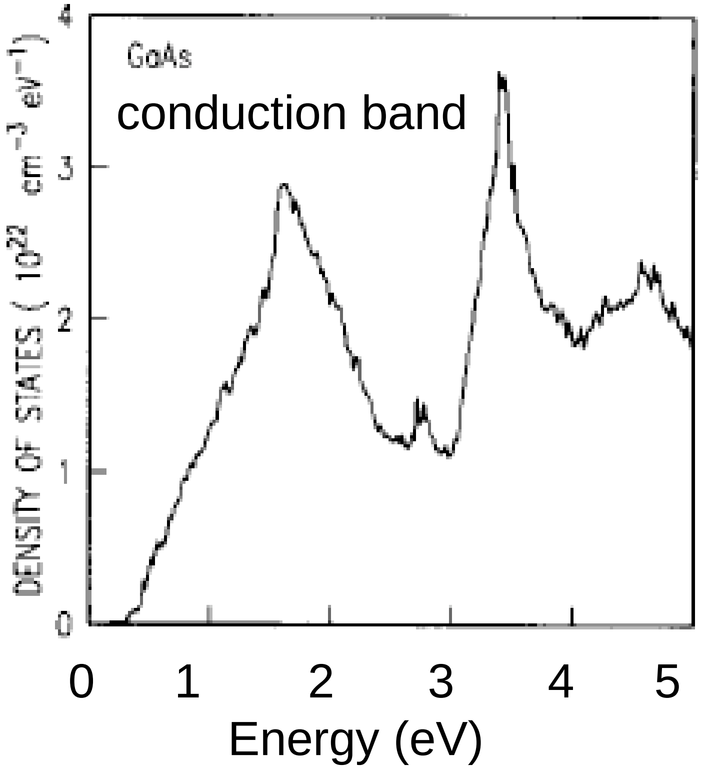
electrons and holes in Si

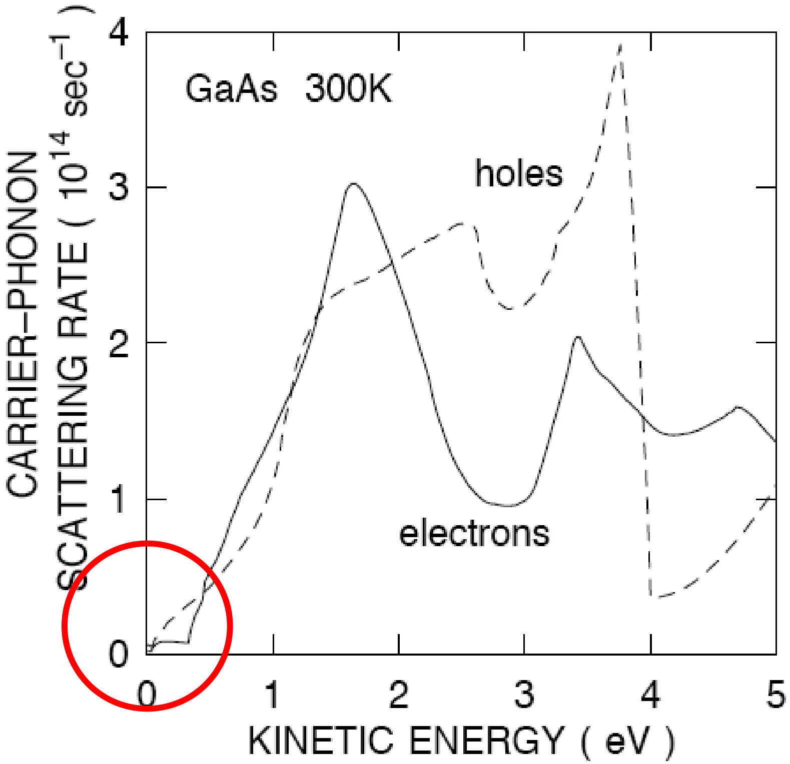




[2] Figures provided by Massimo V. Fischetti, October, 2009.

electrons and holes in GaAs





DOS: [1] M. V. Fischetti," *IEEE Trans. Electron Dev*., **38**, pp. 634-649, 1991
Scattering rate: [2] Provided by M. V. Fischetti, October, 2009)

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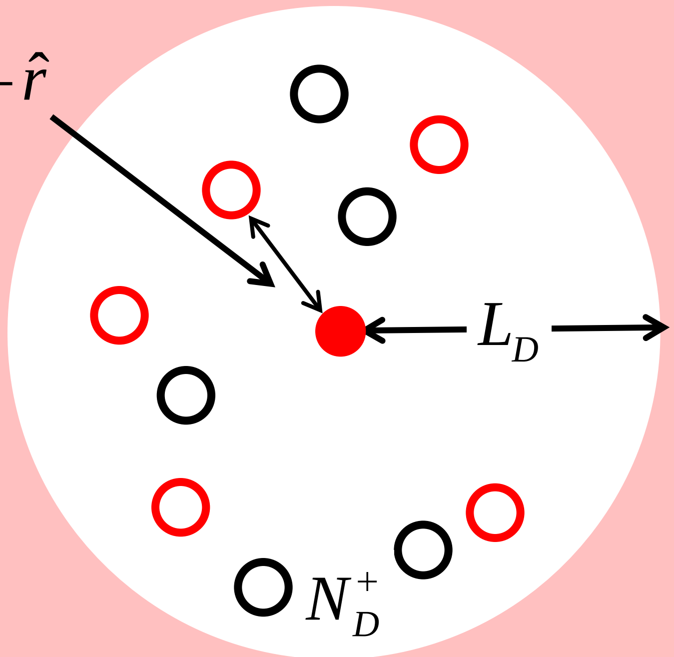
long and short range Coulomb effects

$$\vec{F}_e\left(\vec{r},t\right) = -q\vec{\mathcal{E}}\left(\vec{r},t\right)$$

$$\nabla \bullet \left[\kappa_S \varepsilon_0 \vec{\mathcal{E}}\left(\vec{r},t\right)\right] = \rho\left(\vec{r},t\right)$$

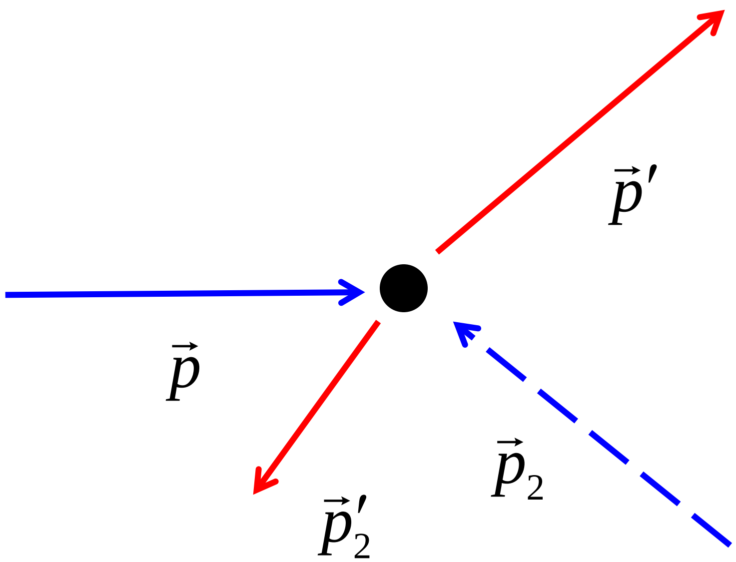
$$\vec{F}_e\left(\vec{r},t\right) = \frac{q_1 q_2}{4\pi\kappa_S\varepsilon_0 r^2}\hat{r}$$



n_0 cm^{-3}

$$\rho = q\left(N_D^+ - n_0\right) \text{ C/cm}^{-3}$$

binary e-e scattering



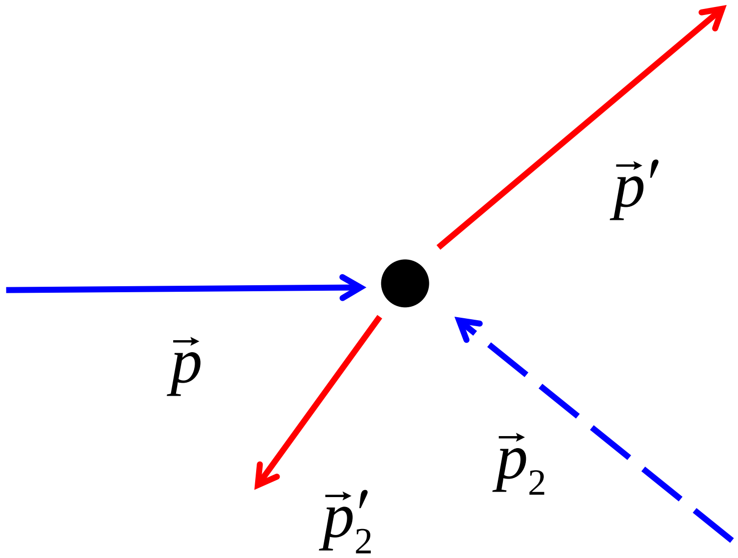
$$\vec{p} + \vec{p}_2 = \vec{p}\,' + \vec{p}_2'$$

$$E + E_2 = E' + E_2'$$

Important when $n > \sim 10^{17}$ cm^{-3}

$$S\left(\vec{p}, \vec{p}\,'\right) \rightarrow S\left(\vec{p}, \vec{p}_2; \vec{p}\,', \vec{p}_2'\right)$$

binary e-e scattering rate



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

Important when $n >\sim 10^{17}$ cm^{-3}

$$\frac{1}{\tau_{e-e}} = \sum_{\vec{p}\,', \vec{p}_2} S(\vec{p}, \vec{p}_2; \vec{p}\,', \vec{p}_2') f(\vec{p}_2)\left[1 - f(\vec{p})\right]\left[1 - f(\vec{p}_2')\right]$$

(a very difficult problem to solve)

e-e scattering

When e-e- scattering dominates, electrons exchange energy among themselves and an equilibrium shape (Maxwellian or Fermi-Dirac) distribution is established.

$$f\left(\vec{p}\right) \propto e^{p^2 / 2mk_BT_e}$$

The electron temperature, however, may be quite different from the lattice temperature.

To first order, electron-electron scattering does not lower the mobility, because the total momentum of the electron system is conserved, but there can be an indirect effect because the shape of the distribution affects the average scattering rate for other scattering processes.

outline

1) Review
2) Example
3) POP and IV scattering
4) Scattering in common semiconductors
5) Electron-electron scattering
6) Summary

(Reference: Chapter 2, Lundstrom, FCT)