ECE 656: Electronic Transport in Semiconductors Fall 2017

Electron Scattering in Common Semiconductors

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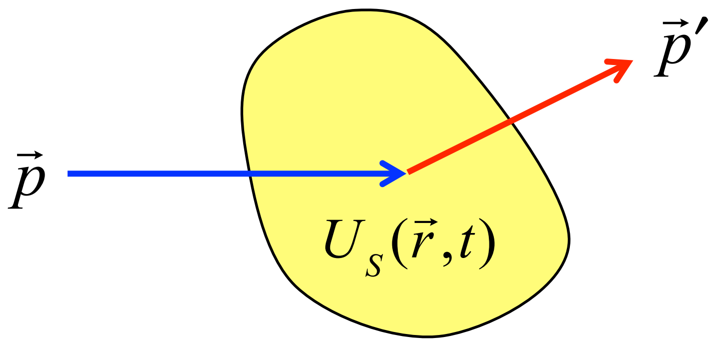
Outline

1) Review of Approach
2) II Scattering
3) Phonon Scattering
4) Other scattering mechanisms
5) Summary

Fermi's Golden Rule

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



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

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

$$\Delta E = \pm\hbar\omega$$

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

$$\vec{p}\,' = \vec{p} \pm \hbar\vec{q}$$

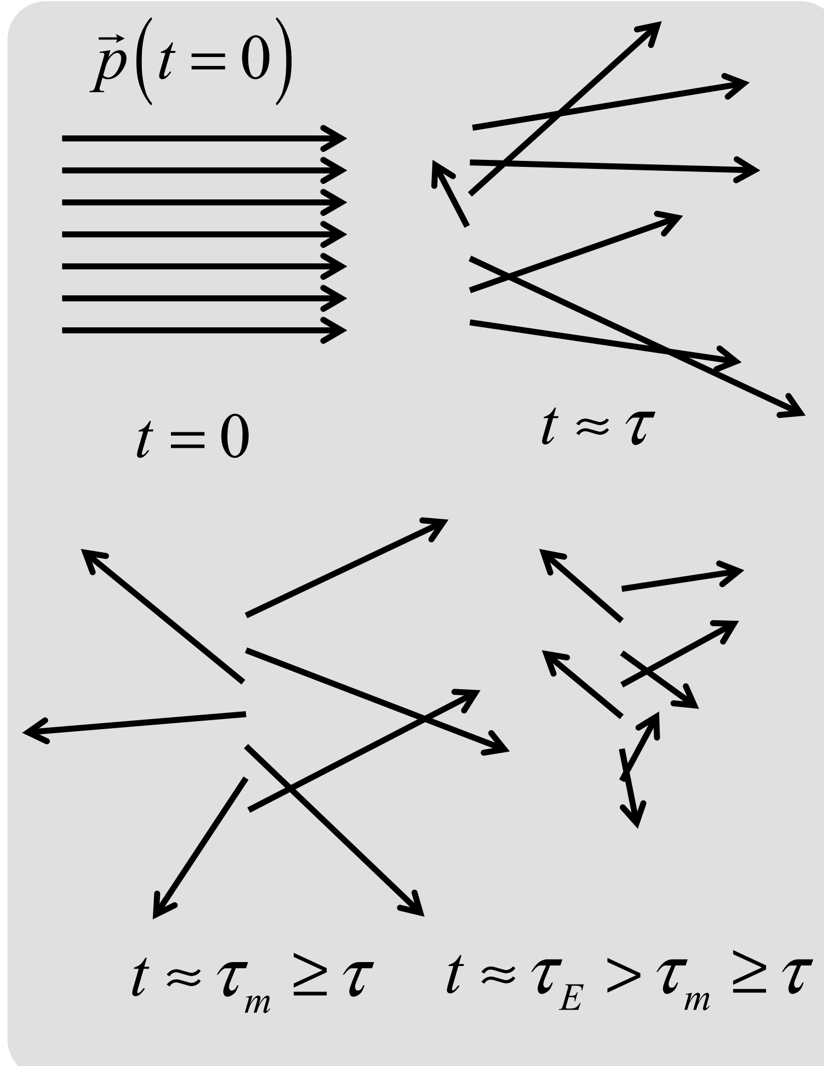
Characteristic times

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

(τ, single particle lifetime)

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

$$\frac{1}{\tau_E(\vec{p})} = \sum_{\vec{p}',\uparrow} S(\vec{p},\vec{p}')\frac{\Delta E}{E_0}$$



Characteristic times

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

(τ, single particle lifetime)

Note that these are "out-scattering" times – they assume that the final state is empty. To actually compute the rate, we need to weight by the probability that the final state is empty.

$$\frac{1}{\tau(\vec{p})} = \sum_{\vec{p}',\uparrow} S(\vec{p},\vec{p}')\left[1 - f(\vec{p}')\right]$$

General observations

Expect: $$\frac{1}{\tau(E_i)} \propto D(E_f) \qquad E_f = E_i + \Delta E$$

Isotropic scattering: $$\frac{1}{\tau(E_i)} = \frac{1}{\tau_m(E_i)}$$

Anisotropic scattering selects certain preferred final states, e.g. electrostatic interactions emphasize small angle scattering.

$$\frac{1}{\tau(E_i)} > \frac{1}{\tau_m(E_i)}$$

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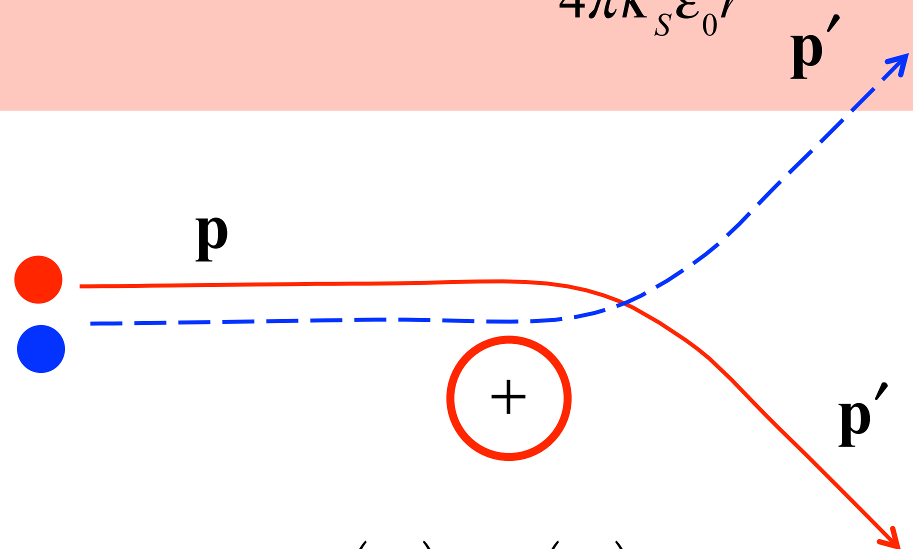
II summary

CW: $U_S(\vec{r}) = \pm \dfrac{q^2}{4\pi\kappa_S\varepsilon_0 r}$ BH: $U_S(r) = -\dfrac{q^2}{4\pi\kappa_S\varepsilon_0 r} e^{-r/L_D}$



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

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

3) favors small angle scattering $\tau_m(E) > \tau(E)$

4) $\tau_m(E) \approx \tau_0 (E - E_C)^{3/2}$ $\tau_0 \propto T^{3/2}$ (power law scattering)

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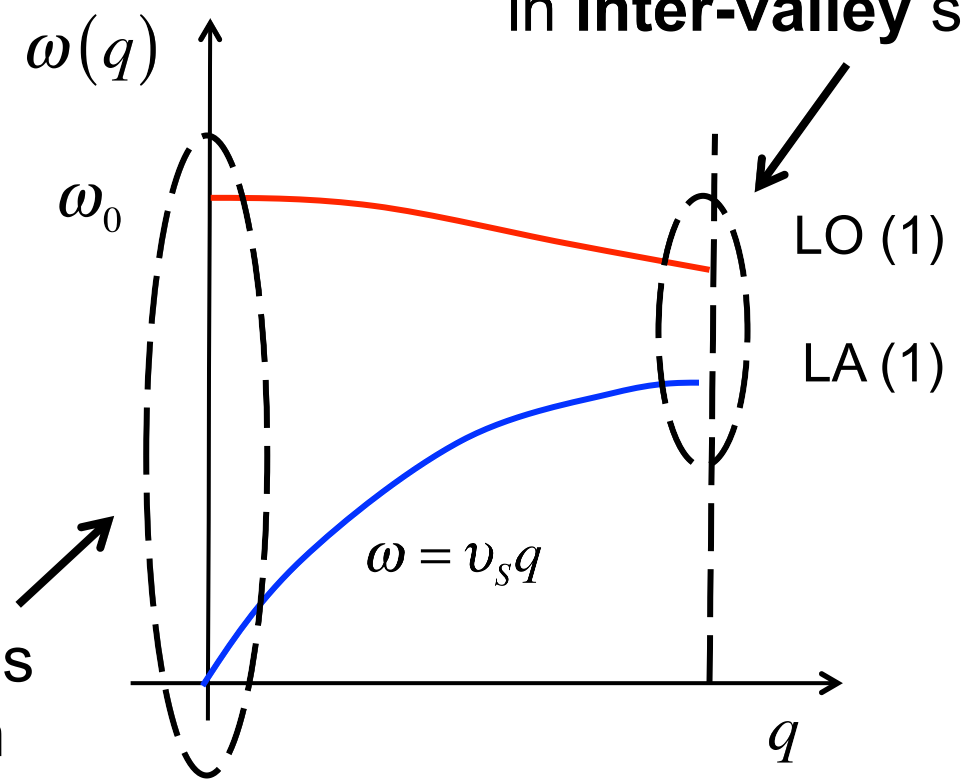
Phonon dispersion

Longitudinal modes couple most strongly to electrons.

These phonons are involved in **inter-valley** scattering



These phonons are involved in **intra-valley** scattering

Transition rate for phonon scattering

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

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

$$U_S(\vec{r}) = K_q u_q \qquad u_q(\vec{r}) = A_q e^{\pm i\vec{q}\bullet\vec{r}}$$

$$\left|H_{p',p}\right|^2 = \left|K_q\right|^2 \left|A_q\right|^2 \delta\left(\vec{p}\,' - \vec{p} \mp \hbar\vec{q}\right)$$

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

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

Electron-phonon coupling

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

ADP $\quad |K_q|^2 = q^2 D_A^2$

ODP $\quad |K_q|^2 = D_0^2$

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

POP $\quad |K_q|^2 = \dfrac{\rho e^2 \omega_0^2}{q^2 \kappa_0 \varepsilon_0}\left(\dfrac{\kappa_0}{\kappa_\infty} - 1\right)$

Simplified Transition Rate

$$S(\vec{p},\vec{p}\,') = \frac{2\pi}{\hbar}\left|K_q\right|^2\left|A_q^{a,e}\right|^2 \delta\left(p' - \vec{p} \mp \hbar\vec{q}\right)\delta\left(E' - E \mp \hbar\omega_0\right)$$

$$\left|K_q\right| \qquad \left|A_q^{a,e}\right|^2 = \left(N_\omega + \frac{1}{2} \mp \frac{1}{2}\right)\frac{\hbar}{2\Omega\rho\omega_0}$$

When there is no preference for one momentum or another, then there is no need to explicitly consider momentum conservation.

$$\boxed{S(\vec{p},\vec{p}\,') = \frac{2\pi}{\hbar}\left|K_q\right|^2\left|A_q^{a,e}\right|^2 \delta\left(E' - E \mp \hbar\omega_0\right)}$$

Isotropic scattering times

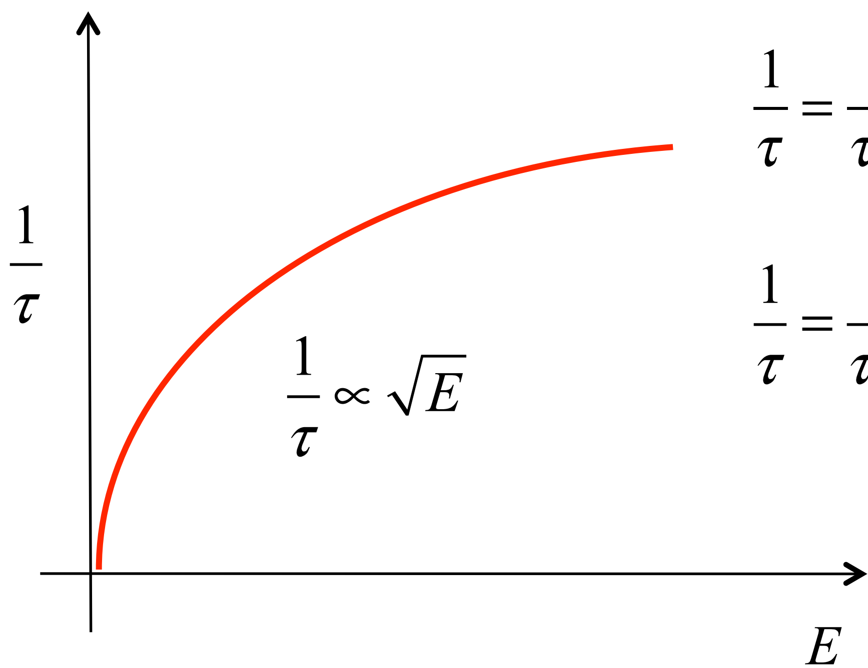
$$S\left(\vec{p},\vec{p}'\right)=\frac{2\pi}{\hbar}\left|K_q\right|^2\left|A_q^{a,e}\right|^2\delta\left(E'-E\mp\hbar\omega_0\right)$$

$$\left|K_q\right| \qquad \left|A_q^{a,e}\right|^2=\left(N_\omega+\frac{1}{2}\mp\frac{1}{2}\right)\frac{\hbar}{2\Omega\rho\omega_0}$$

$$\frac{1}{\tau\left(\vec{p}\right)}=\frac{1}{\tau_m\left(\vec{p}\right)}=\sum_{\vec{p}',\uparrow}S\left(\vec{p},\vec{p}'\right) \qquad \frac{1}{\tau_m\left(E\right)}\propto\frac{1}{\Omega}\sum_{\vec{p}',\uparrow}\delta\left(E'-E\mp\hbar\omega_0\right)$$

$$\boxed{\frac{1}{\tau_m\left(E\right)}\propto\left(N_\omega+\frac{1}{2}\mp\frac{1}{2}\right)\frac{D\left(E\pm\hbar\omega\right)}{2}}$$

Acoustic phonon scattering



$$N_\omega \approx N_\omega + 1 \approx \frac{k_B T}{\hbar\omega}$$

(elastic)

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

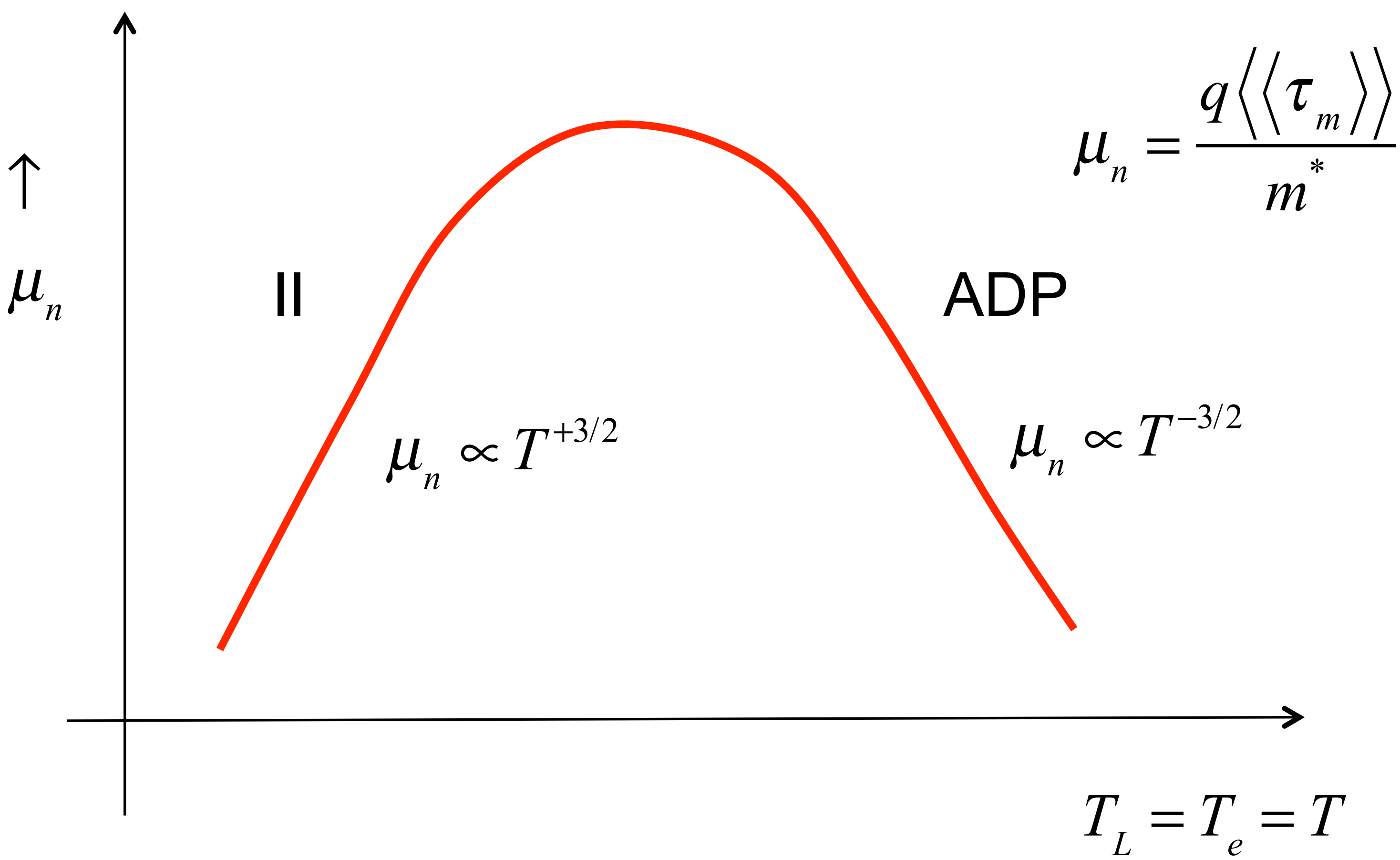
$$\frac{1}{\tau} = \frac{1}{\tau_m}$$

(isotropic)

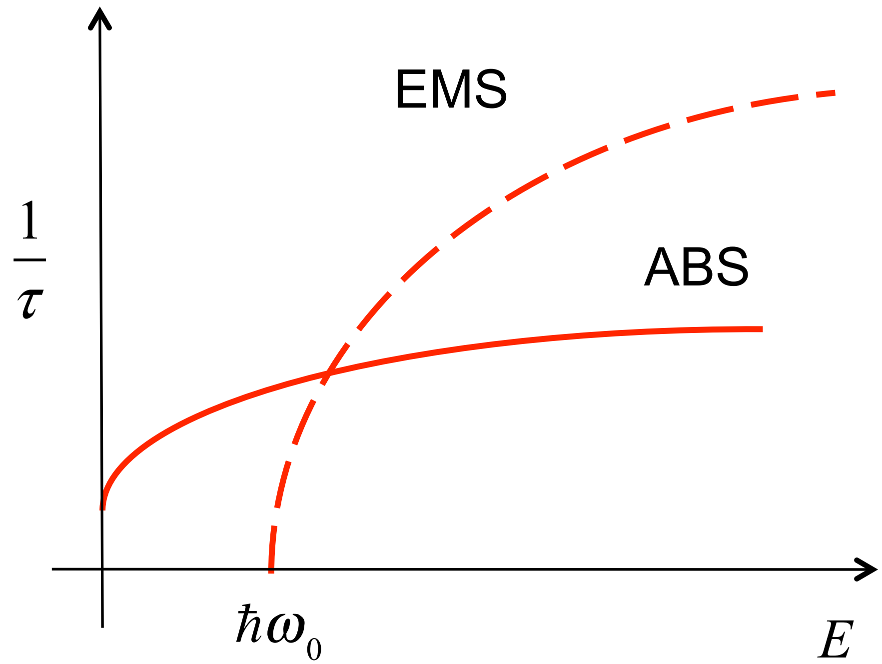
$$\tau_m\left(E\right) = \tau_0\left[\left(E - E_C\right)/k_B T\right]^{-1/2}$$

$$\tau_0 \propto T^{-3/2}$$

Mobility vs. temperature



ODP scattering



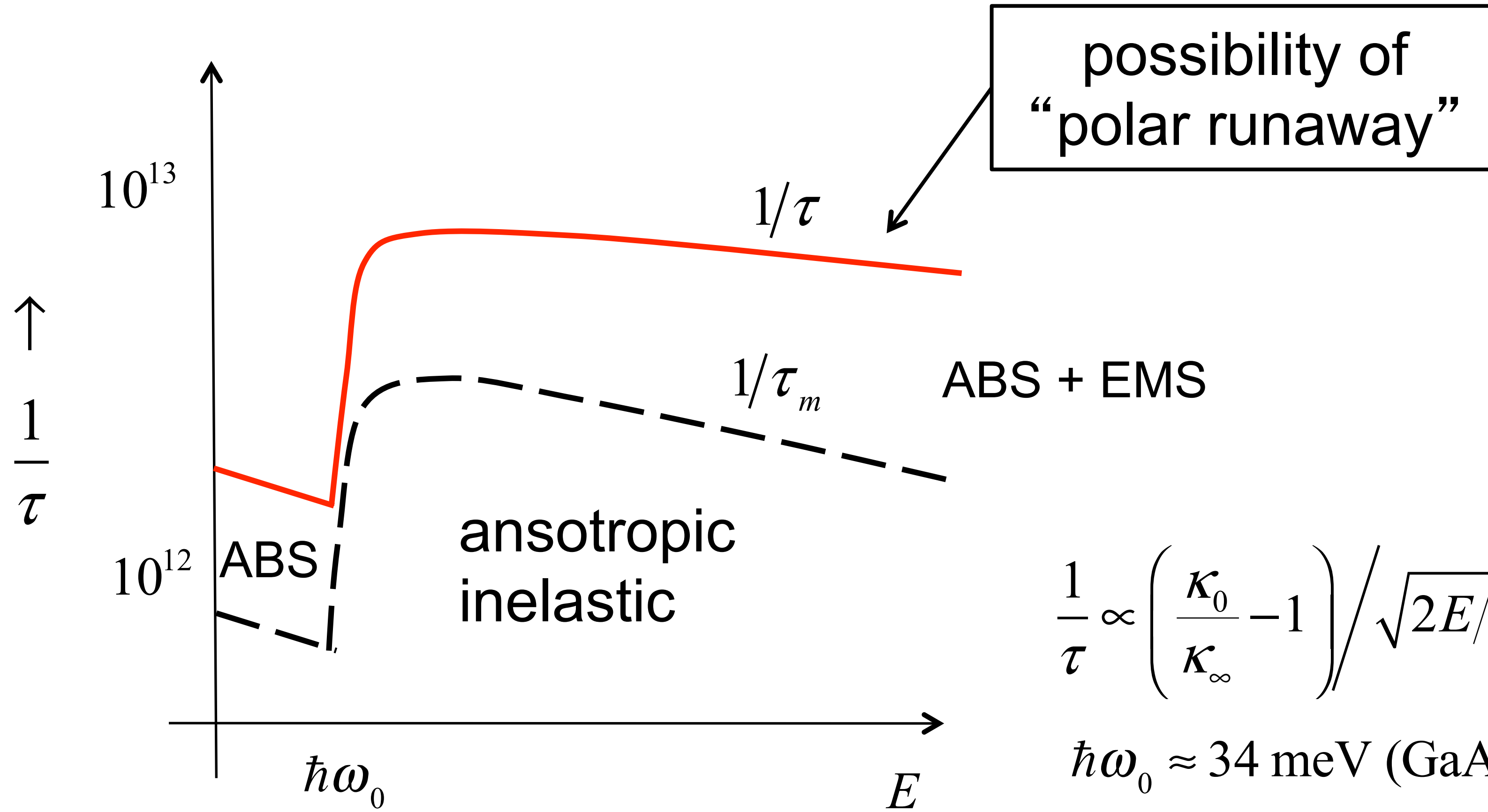
$$N_0 = \frac{1}{e^{\hbar\omega_o/k_B T} - 1}$$

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

isotropic
inelastic

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

POP scattering

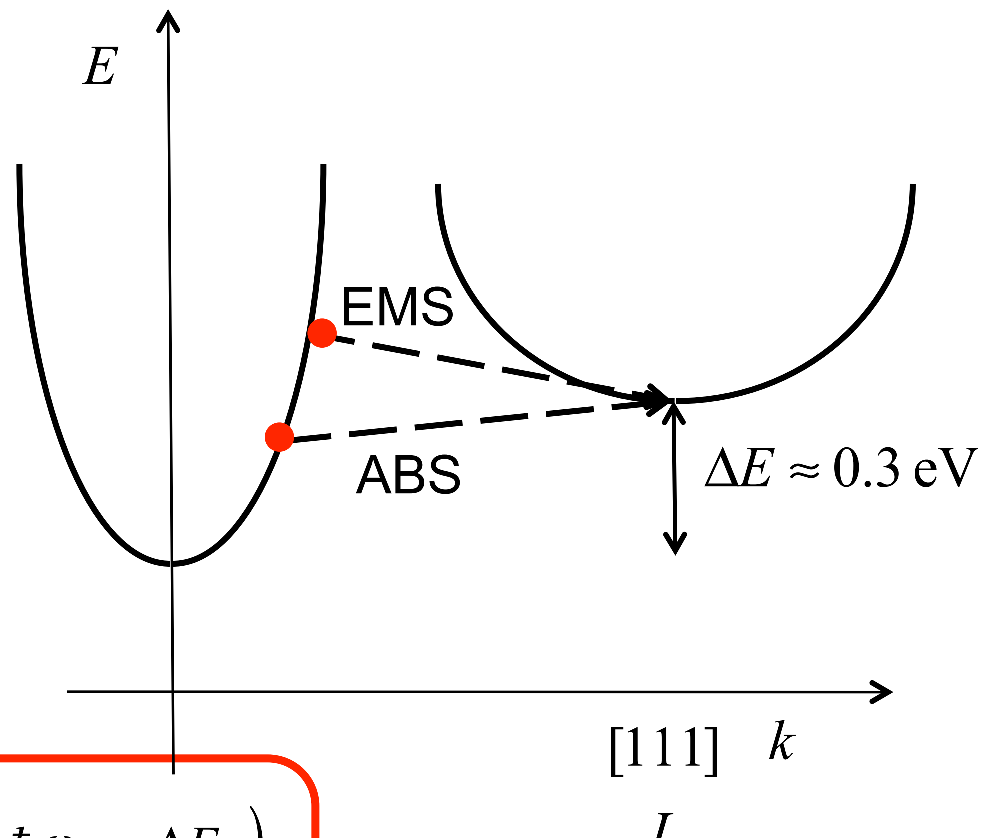


$$\frac{1}{\tau} \propto \left(\frac{\kappa_0}{\kappa_\infty} - 1\right) \bigg/ \sqrt{2E/m^*}$$

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

IV scattering (GaAs)

IV scattering can be treated like ODP scattering

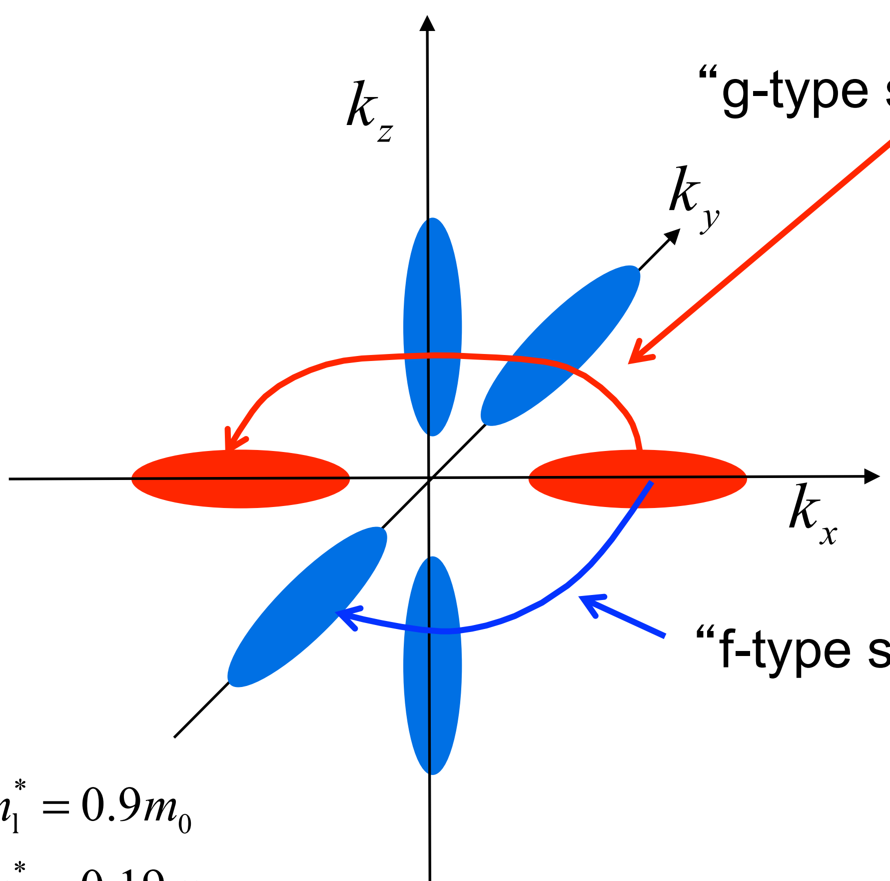


Isotropic: $\dfrac{1}{\tau} = \dfrac{1}{\tau_m}$

Number of final valleys: Z_f

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

equivalent IV scattering (Si)



$m_l^* = 0.9 m_0$

$m_t^* = 0.19 m_0$

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

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

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Scattering rate in common semiconductors

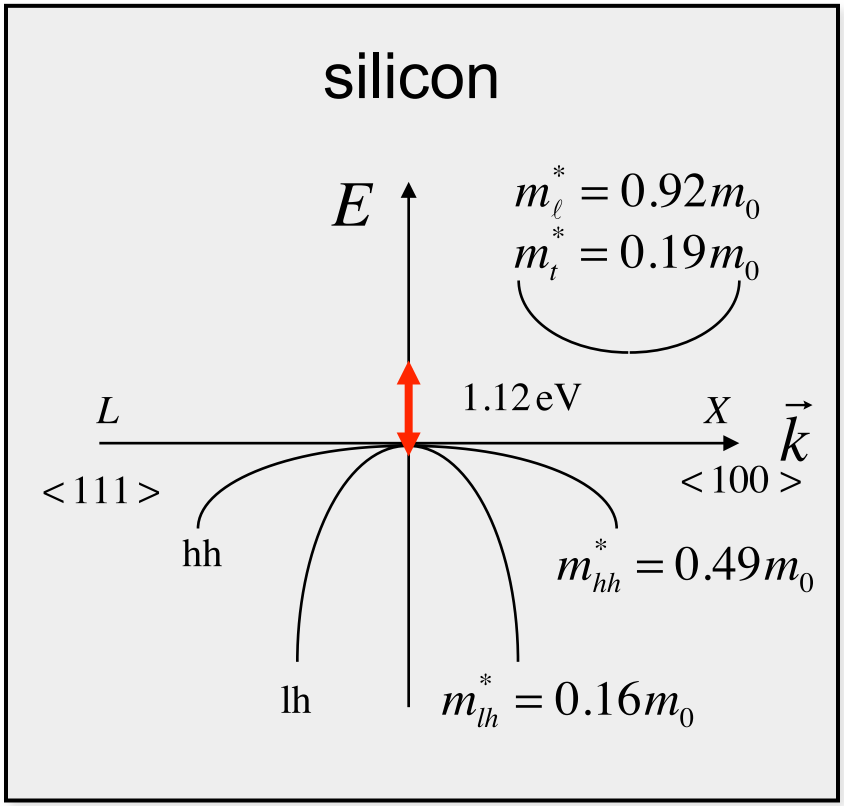
1) What is the total scattering rate vs. energy for common semiconductors?

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

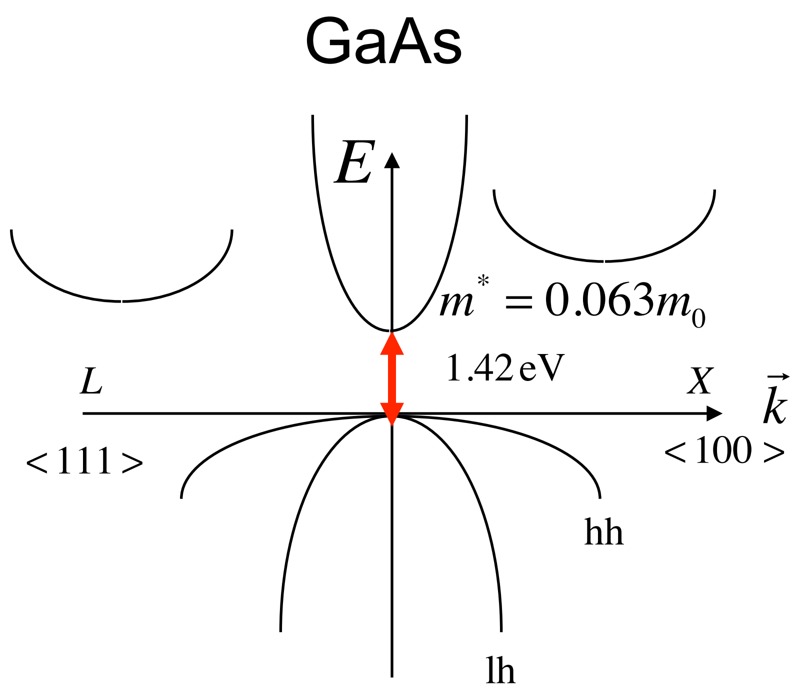
2) How do covalent semicondictors (e.g. Si, Ge) differ from polar semiconductors (e.g. GaAs, InP, InGaAs, ZnSe)?

model bandstructure (for analytical calculations)

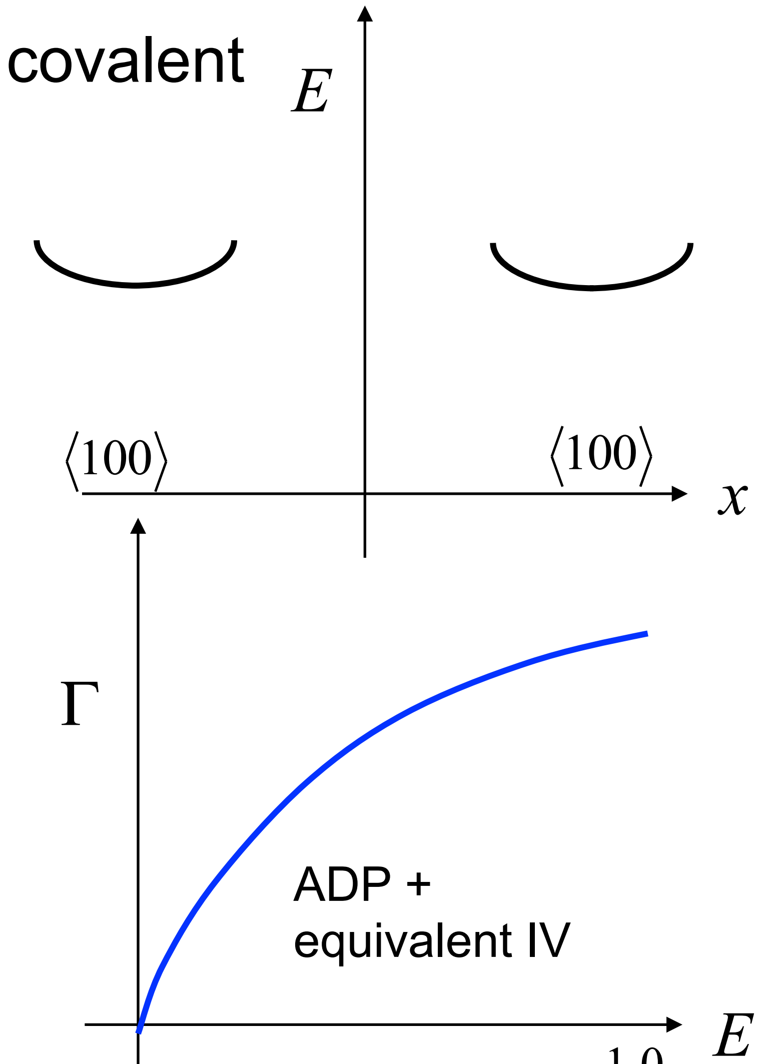
Si, covalent, indirect BG

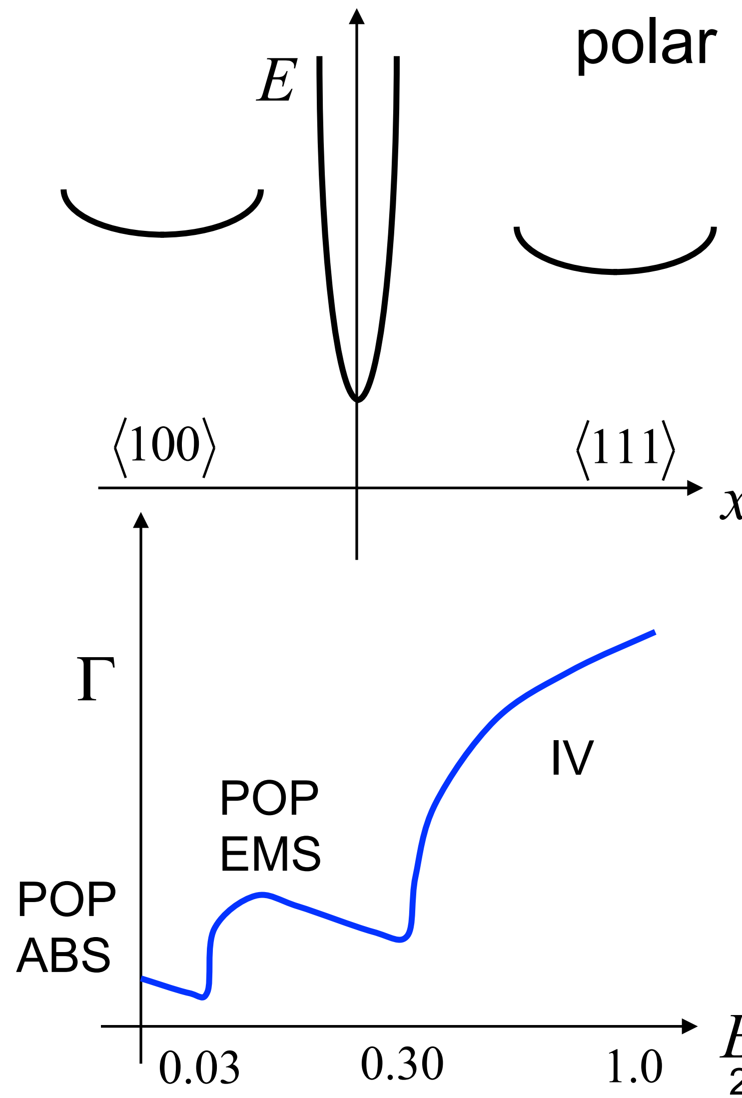


GaAs, polar, direct BG



Covalent vs. polar semiconductors



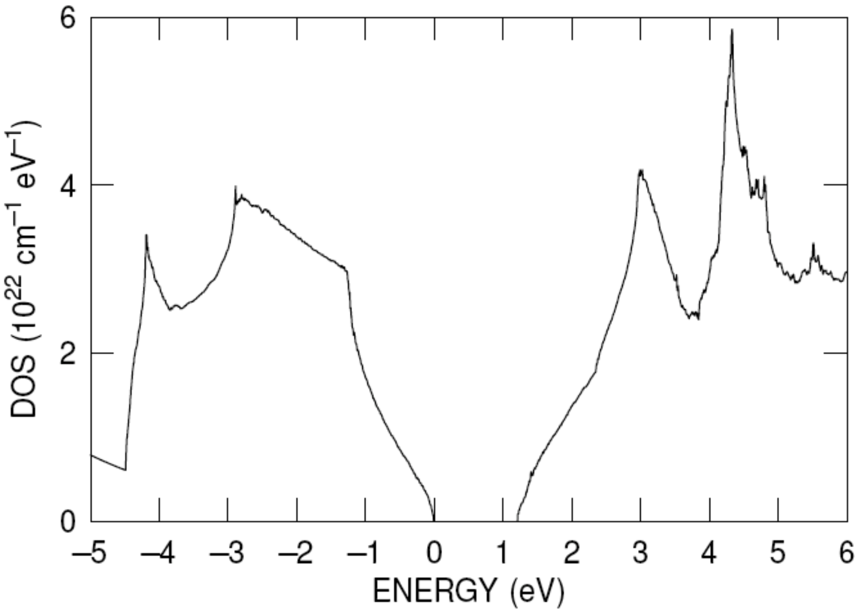


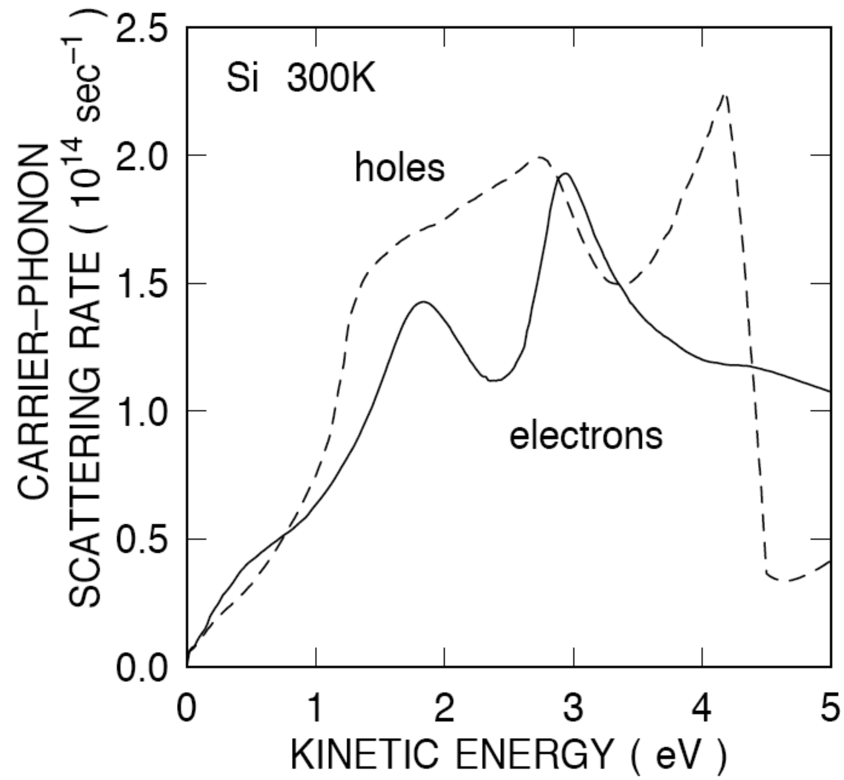
“full band” scattering rates

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

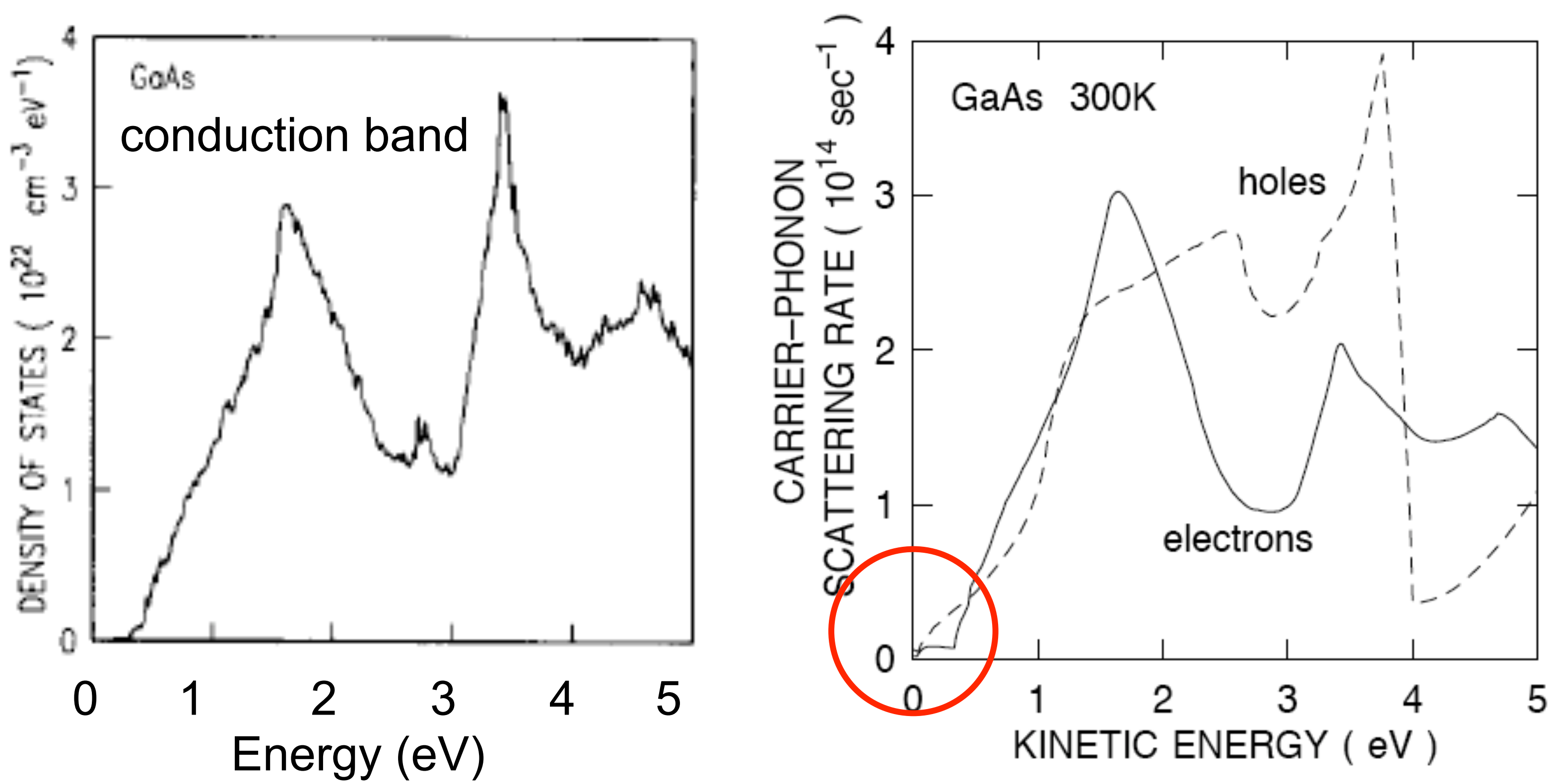
Electrons and holes in Si





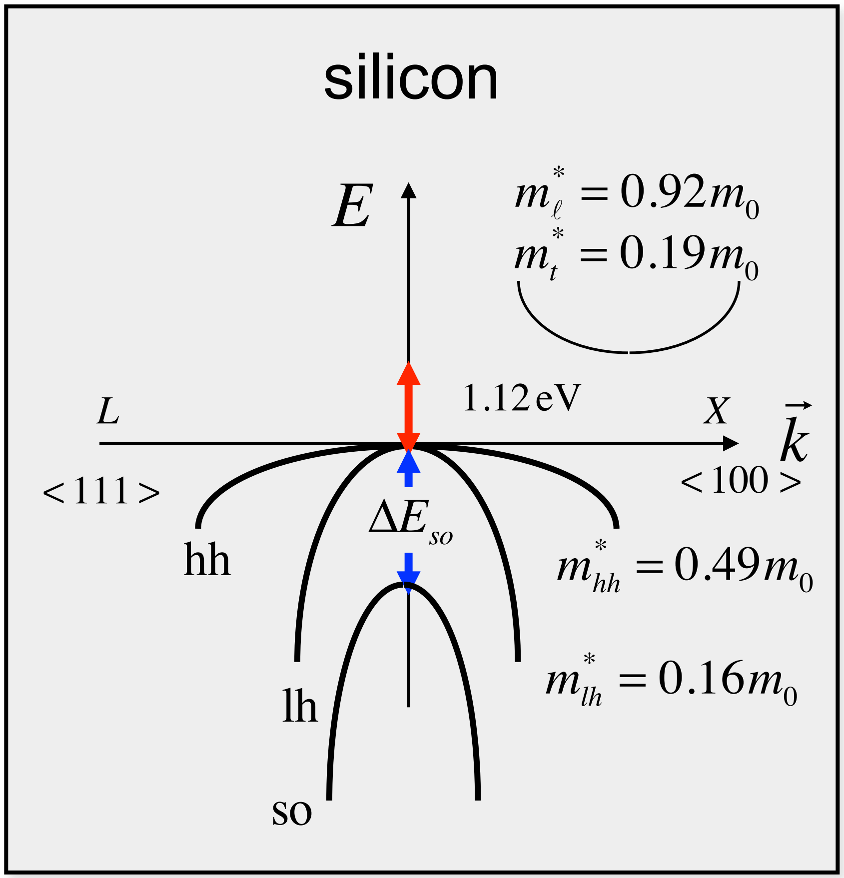
[2] Figures provided by Massimo V. Fischetti, October, 2009.

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.

about holes



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

Intra-band:

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

Inter-band:

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

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

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

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Other scattering mechanisms

1) Neutral impurity

2) Alloy scattering

3) Surface / edge roughness scattering

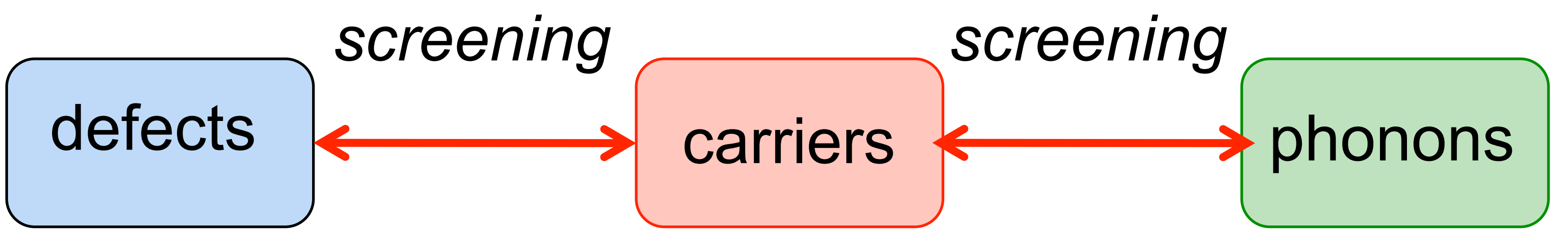
4) Plasmon scattering

5) Electron-electron scattering

6) Electron-hole

7) Crystal defects, etc.

Scattering in semiconductors



- ionized impurities
- neutral impurities
- dislocations
- surface roughness
- alloy

- electron-electron
- electron-plasmon
- electron-hole

- intravalley
  -ADP
  -ODP
  -POP
  -PZ

- intervalley
  -acoustic
  -optical

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 often proportional to the final DOS
4) Static potentials lead to elastic scattering
5) Time varying potentials lead to inelastic scattering
6) The general features of scattering in common semiconductors are readily understood.

Questions?

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