

## Week 5 Summary:

### Scattering in a Nutshell

Professor Mark Lundstrom  
Electrical and Computer Engineering  
Purdue University, West Lafayette, IN USA  
DLR-103 and EE-334C / 765-494-3515  
lundstro at purdue.edu



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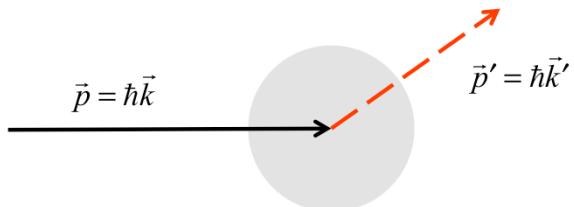
## topics

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- 1) Transition rates, FGR, and characteristic times
- 2) Charged impurity scattering
- 3) Phonon scattering
- 4) Scattering in common semiconductors
- 5) Scattering in reduced dimensions

## transition rate

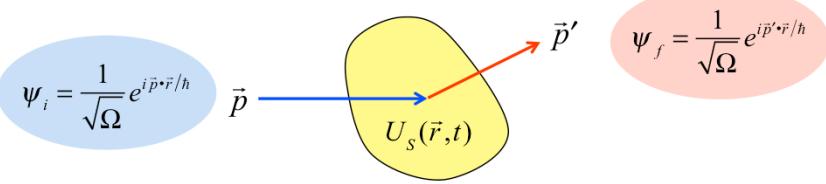
$$S(\vec{p}, \vec{p}') = S(\vec{p} \rightarrow \vec{p}')$$



Probability per sec that an electron is scattered from a initial state to one particular final state.

Computed by “Fermi’s Golden Rule”

## scattering of plane waves



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

$$H_{\vec{p}', \vec{p}} = \frac{1}{\Omega} \int_{-\infty}^{+\infty} e^{-i\vec{p}' \cdot \vec{r}/\hbar} U_s(\vec{r}) e^{i\vec{p} \cdot \vec{r}/\hbar} d\vec{r} \quad \vec{p}' = \vec{p} \pm \hbar\vec{\beta}$$

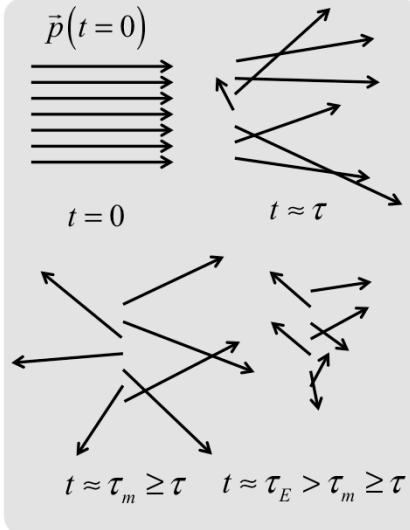
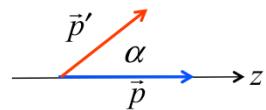
## characteristic times

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

$(\tau, \text{single particle lifetime})$

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

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



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## general observations

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

Isotropic scattering behaves this way.  $\frac{1}{\tau(E_i)} = \frac{1}{\tau_m(E_i)}$

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

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

## II scattering summary

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

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

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

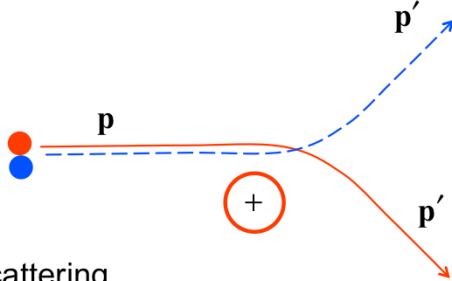
2)  $S(\vec{p}, \vec{p}') \sim q^4$

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

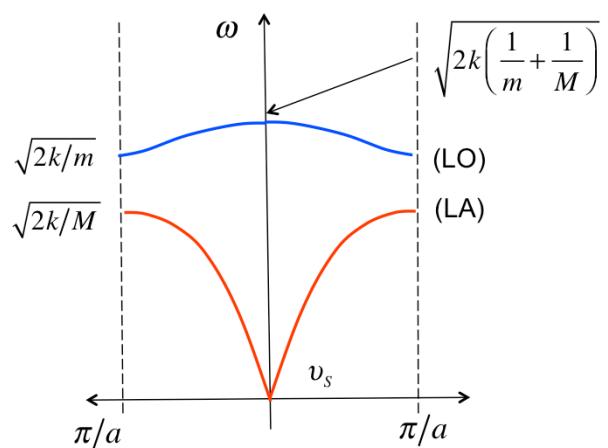
4) favors small angle scattering

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

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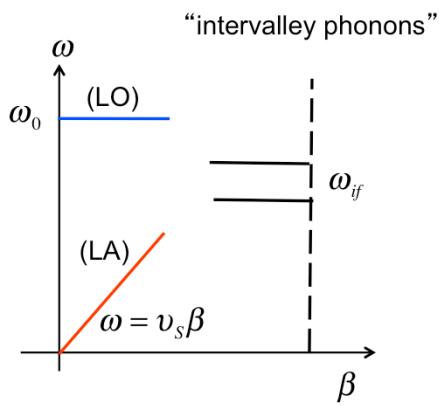
## phonon dispersion



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## simplified phonon dispersion

- 1) Longitudinal modes couple most strongly with electrons.
- 2) **Intravalley** scattering requires small  $\beta$ .
- 3) **Intervalley** requires  $\beta$  near the Brillouin zone boundary.



## energy and momentum conservation

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

$$E \quad U_s(\vec{r}, t) \quad E' \quad \vec{p}' \quad \psi_f = \frac{1}{\sqrt{\Omega}} e^{i \vec{p}' \cdot \vec{r} / \hbar}$$

$$U_s(\vec{r}, t) = \frac{U_{\beta}^{a,e}}{\sqrt{\Omega}} e^{\pm i(\vec{\beta} \cdot \vec{r} - \omega t)}$$

$$S(\vec{p}, \vec{p}') = \frac{2\pi}{\hbar} \frac{|U_{\beta}^{a,e}|^2}{\Omega} \delta(E' - E \mp \hbar\omega) \delta_{\vec{p}', \vec{p} \pm \hbar\vec{\beta}}$$

$$E' = E + \hbar\omega$$

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

ABS

$$E' = E - \hbar\omega$$

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

EMS

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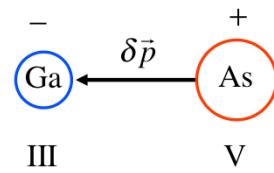
## acoustic deformation potential (ADP) scattering

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$$U_s = \delta E_c = D_c \frac{\delta a}{a} = D_c \frac{\partial u_\beta}{\partial x} \quad u_\beta(x, t) = A_\beta e^{\pm i(\beta z - \omega t)}$$

$$U_s = D_A \frac{\partial u_\beta}{\partial x} = \pm i\beta D_A u_\beta = K_\beta u_\beta \quad |K_\beta|^2 = \beta^2 D_A^2$$

## optical phonons in polar semiconductors



$$U_s = K_\beta u_\beta$$

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$$u_\beta(x, t) = A_\beta e^{\pm i(\beta z - \omega t)}$$

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

***small angle scattering dominates***

“polar optical phonon scattering”

## electron-phonon scattering potentials

$$u_\beta(\vec{r}, t) = A_\beta e^{\pm i(\vec{\beta} \cdot \vec{r} - \omega_\beta t)} \quad U_s = K_\beta u_\beta$$

ADP       $|K_\beta|^2 = \beta^2 D_A^2$

ODP       $|K_\beta|^2 = D_0^2$

PZ       $|K_\beta|^2 = (qe_{PZ}/\kappa_s \epsilon_0)^2$

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

## transition rate for phonon scattering

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

$$U_s(\vec{r}) = K_\beta u_\beta \quad u_\beta(\vec{r}) = A_\beta e^{\pm i\vec{\beta} \cdot \vec{r}} \quad |H_{p',p}|^2 = |K_\beta|^2 |A_\beta|^2 \delta_{\vec{p}', \vec{p} \pm \hbar\vec{\beta}}$$

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

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

## energy-momentum conservation

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

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

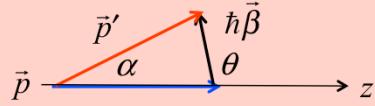
$$\delta_{\vec{p}', \vec{p} \pm \hbar\vec{\beta}} \delta(E' - E \mp \hbar\omega_\beta) \rightarrow \frac{1}{\hbar v \beta} \delta\left(\pm \cos \theta + \frac{\hbar \beta}{2p} \mp \frac{\omega_\beta}{v \beta}\right)$$

## final answer: transition rate

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

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

$$C_\beta = \frac{\pi}{\hbar\rho v \omega \beta} |K_\beta|^2 \quad N_\omega = \frac{1}{e^{\hbar\omega/k_B T} - 1}$$



## general expression for the phonon scattering rate

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

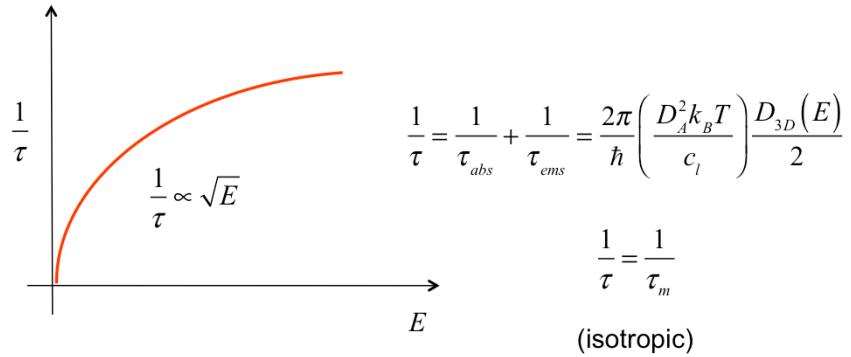
Integration of the delta function simply restricts  $\beta$  to those values that satisfy energy and momentum conservation.

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

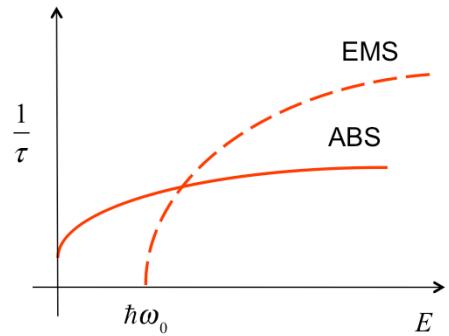
$$\frac{1}{\tau} = \frac{1}{4\pi^2} \int_{\beta_{\min}}^{\beta_{\max}} C_\beta \left( N_\omega + \frac{1}{2} \mp \frac{1}{2} \right) \beta^2 d\beta$$

$$C_\beta = \frac{\pi}{\hbar \rho v \omega \beta} |K_\beta|^2 \quad N_\omega = \frac{1}{e^{\hbar \omega / k_B T} - 1}$$

## acoustic phonon scattering



## optical deformation potential scattering



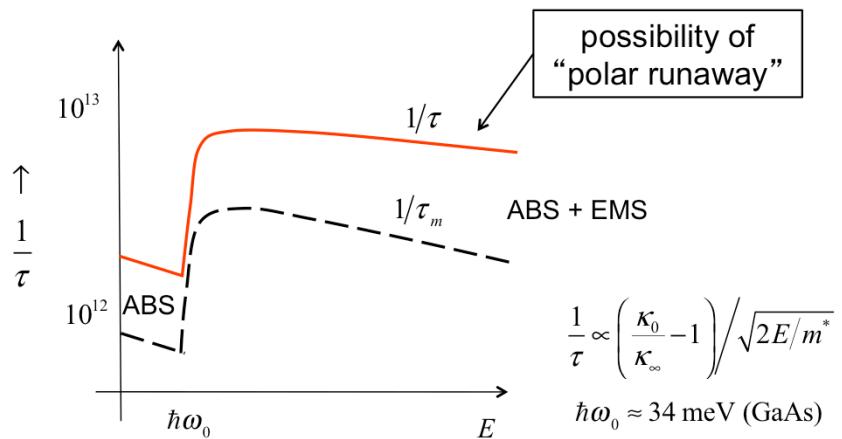
$$\frac{1}{\tau} = \frac{1}{\tau_m} = \frac{2\pi}{\hbar} \left( \frac{\hbar D_o^2}{2\rho\omega_0} \right) \left( N_0 + \frac{1}{2} \mp \frac{1}{2} \right) \frac{D_{3D}(E \pm \hbar\omega_0)}{2}$$

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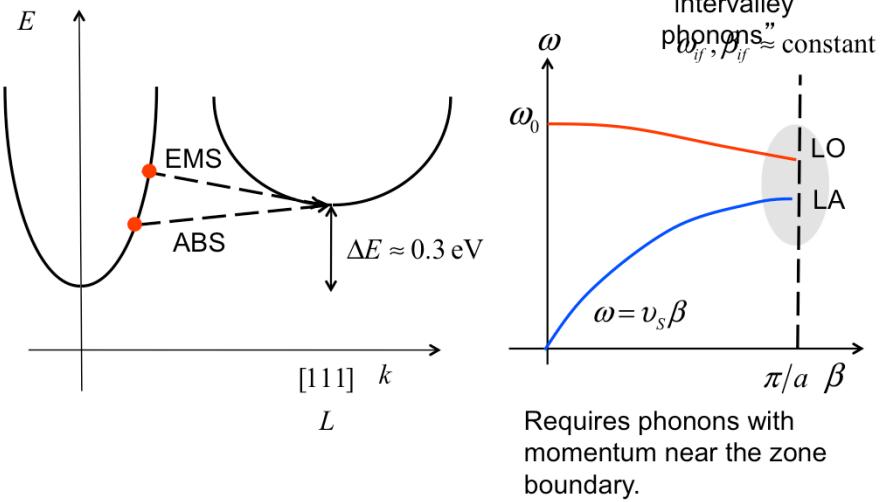
$$\frac{1}{\tau_{abs}} \neq \frac{1}{\tau_{ems}}$$

$$N_0 = \frac{1}{e^{\hbar\omega_0/k_B T_L} - 1}$$

## POP scattering



## IV scattering (GaAs)



## IV scattering (GaAs)

Postulate:

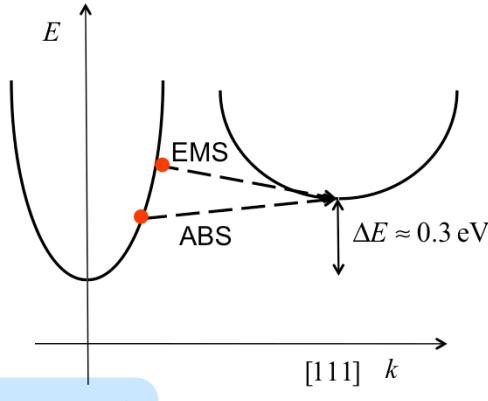
$$U_S = D_{if} u_\beta$$

Then IV scattering looks like ODP scattering

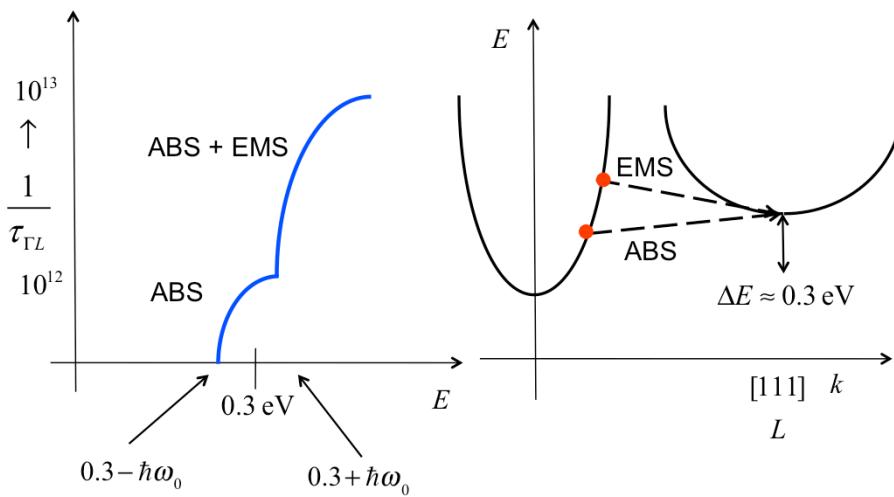
$$\text{Isotropic: } \frac{1}{\tau} = \frac{1}{\tau_m}$$

Number of final valleys:  $Z_f$

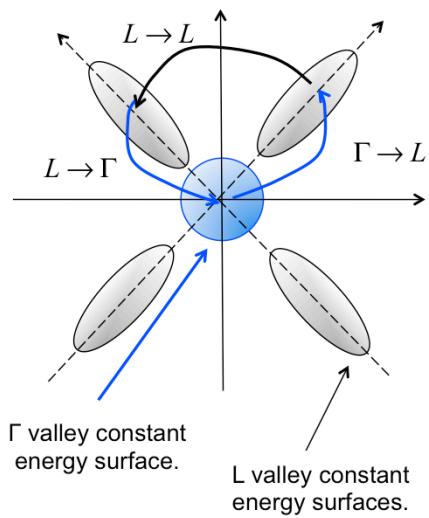
$$\frac{1}{\tau} = \frac{2\pi}{\hbar} \left( \frac{\hbar D_{if}^2 Z_f}{2\rho\omega_{if}} \right) \left( N_{if} + \frac{1}{2} \mp \frac{1}{2} \right) \frac{D_f (E \pm \hbar\omega_{if} - \Delta E_{fi})}{2}$$



## IV scattering (GaAs)



## L-L and L- $\Gamma$ IV scattering (GaAs)



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

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

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

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

Compare rates:

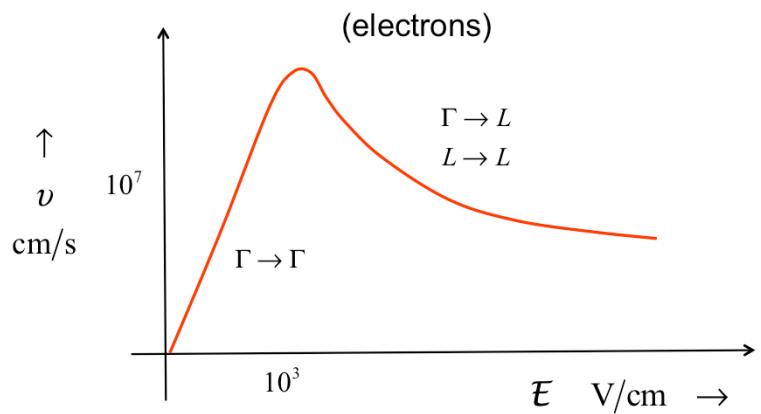
$1/\tau_{\Gamma \rightarrow \Gamma}$  (POP)

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

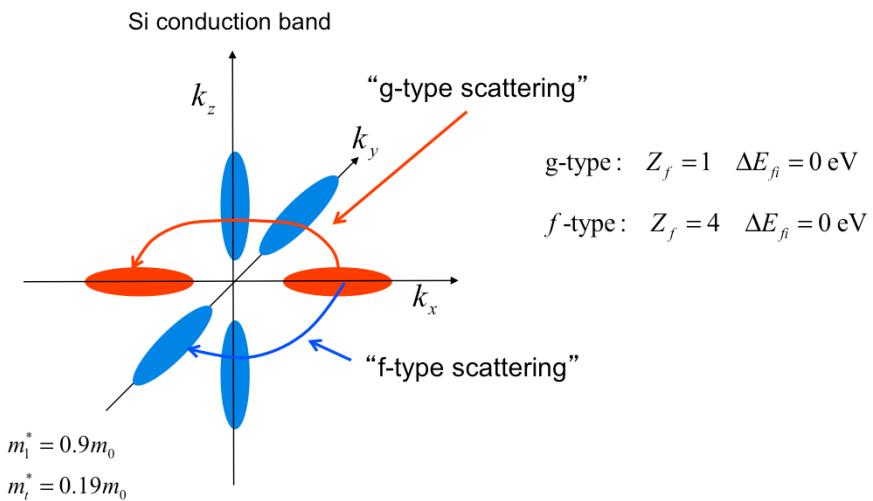
$1/\tau_{L \rightarrow L}$

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

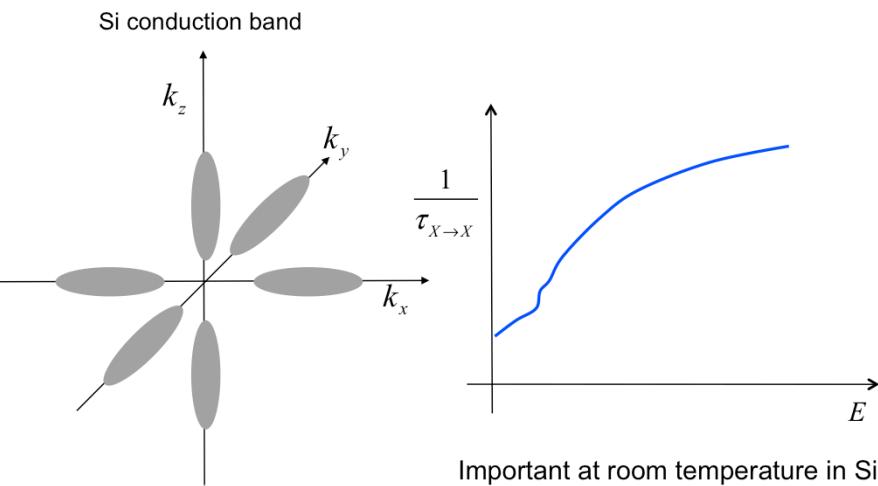
## velocity vs. electric field: GaAs



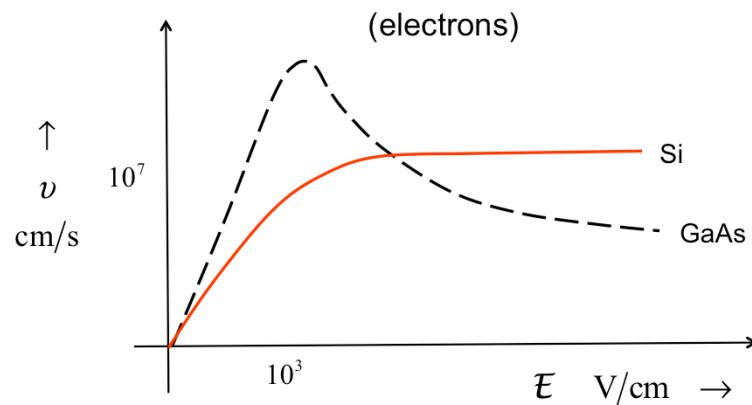
## equivalent IV scattering (Si)



## equivalent IV scattering (Si)



## velocity vs. electric field: Si



## scattering rate in common semiconductors

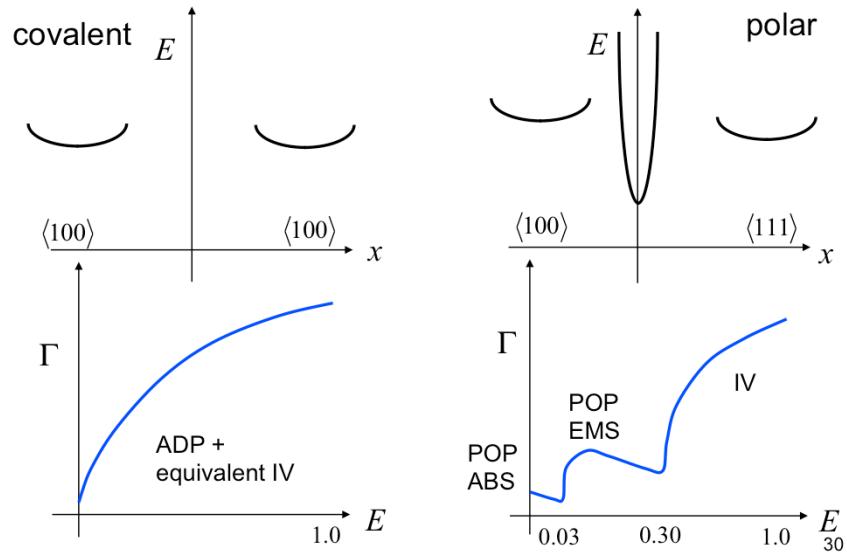
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- 1) What is the total scattering rate vs. energy for common semiconductors?

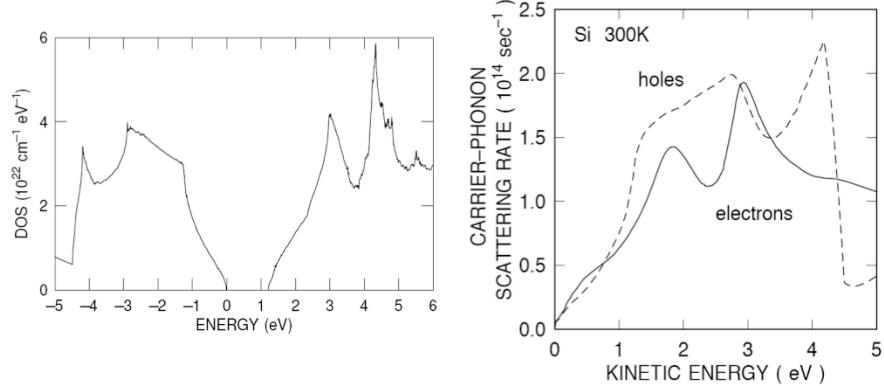
$$\Gamma = \sum_i \frac{1}{\tau_i}$$

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

## covalent vs. polar semiconductors

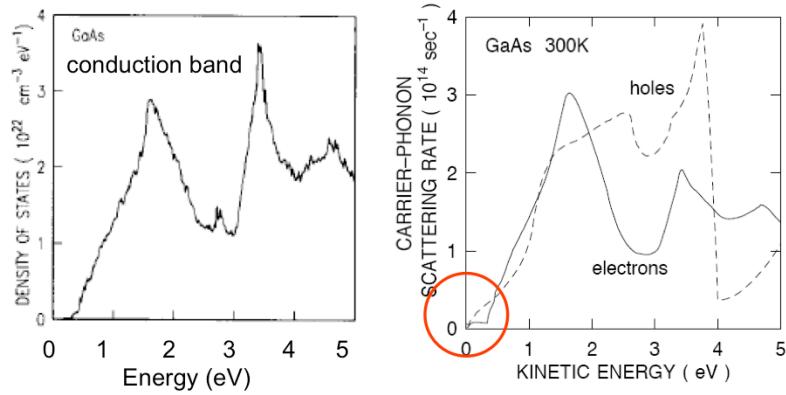


## electrons and holes in Si



[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.

## other scattering mechanisms

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- 1) Neutral impurity
- 2) Alloy scattering
- 3) Surface / edge roughness scattering
- 4) Plasmon scattering
- 5) Electron-electron scattering
- 6) Electron-hole

## scattering in semiconductors



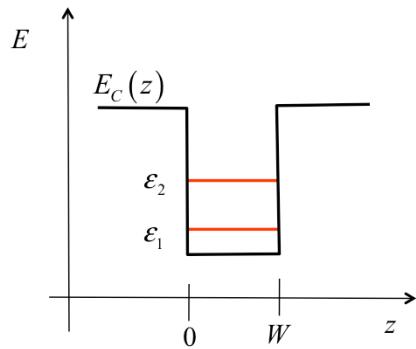
- ionized impurities
  - neutral impurities
  - dislocations
  - surface roughness
  - alloy
- electron-electron
  - electron-plasmon
  - electron-hole
- intravalley
    - ADP
    - ODP
    - POP
    - PZ
  - intervalley
    - acoustic
    - optical

## summary

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- 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 proportional to the final DOS
- 4) Static potentials lead to elastic scattering
- 5) Time varying potentials lead to inelastic scattering
- 6) We can understand the general features of scattering in common semiconductors.

## quantum confined carriers



$$\psi_n(x, y, z) = F_n(z) \frac{1}{\sqrt{A}} e^{i \vec{k}_\parallel \cdot \vec{r}}$$

For an infinite well:

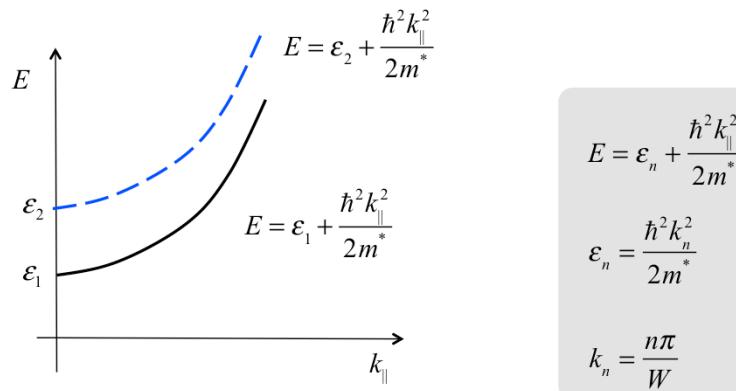
$$F_n(z) = \sqrt{\frac{2}{W}} \sin k_n z$$

$$k_n = \frac{n\pi}{W}$$

Electrons are free to move in the x-y plane

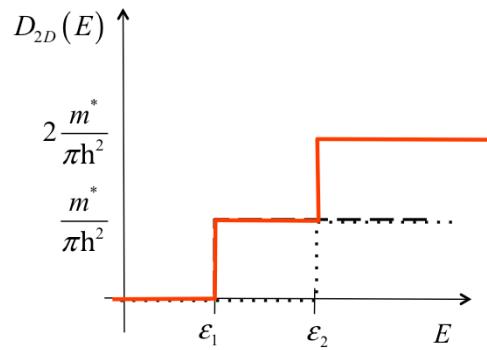
Note that  $p_z = \hbar k_z$  is quantized.

## quantum confined carriers



Electrons are free to move in the x-y plane

## quantum confined carriers



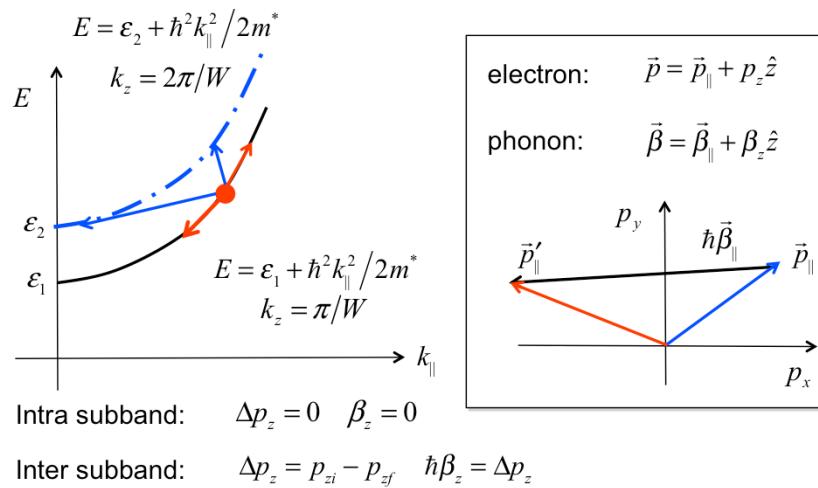
$$E = \epsilon_n + \frac{\hbar^2 k_{\perp}^2}{2m^*}$$

$$\epsilon_n = \frac{\hbar^2 n^2 \pi^2}{2m^* W^2}$$

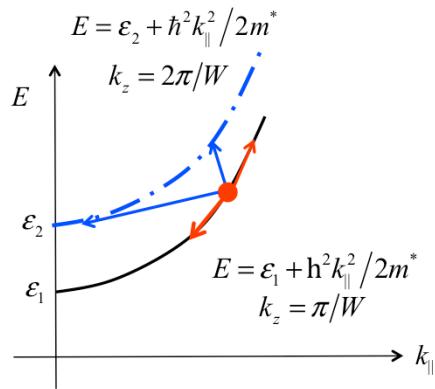
$$D_{2D}(E) = \frac{m^*}{\pi \hbar^2} \sum_{n=1}^{\infty} \Theta(E - \epsilon_n)$$

(A valley degeneracy of 1 is assumed.)

## momentum conservation approximation



## MCA



$$\Delta p_z \Delta z \geq \hbar$$

Momentum does not need to be strictly conserved!

Recall that for short times, energy is not strictly conserved.

Momentum and energy conservation result from FGR in the appropriate limits.

## what changes from 3D?

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

$$|H_{p', p}|^2 = \frac{1}{\Omega} U_{ac} \sum_{\beta} \underbrace{\left| \int_{-\infty}^{+\infty} \psi_f^*(e^{\pm i\vec{\beta} \cdot \vec{r}}) \psi_i d\vec{r} \right|^2}_{\delta_{\vec{p}', \vec{p} \pm \hbar\vec{\beta}}}$$

$$U_{ac} = \frac{D_A^2 k_B T_L}{2c_l}$$

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

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

(For 3D electrons and 3D phonons)

Now assume 2D electrons and 3D phonons.

## 2D electrons and 3D phonons

2D electrons:

$$\psi_{i,n}(\vec{r},z) = F_n(z) \frac{1}{\sqrt{A}} e^{i\vec{k}_\parallel \cdot \vec{r}} \quad \psi_{f,n'}(\vec{r},z) = F_{n'}(z) \frac{1}{\sqrt{A}} e^{i\vec{k}'_\parallel \cdot \vec{r}}$$

3D phonons:

$$u_\beta(\vec{r}) = A_\beta e^{\pm i\vec{\beta} \cdot \vec{r}} = A_\beta \left( e^{\pm i\vec{\beta}_\parallel \cdot \vec{r}} e^{\pm i\beta_z z} \right)$$

$$|H_{p',p}|^2 = \frac{1}{\Omega} U_{ac} \sum_{\vec{\beta}} \left| \int_{-\infty}^{+\infty} \psi_f^*(e^{\pm i\vec{\beta} \cdot \vec{r}}) \psi_i d\vec{r} \right|^2$$

## 2D scattering rate

$$S(\vec{p}, \vec{p}') = \frac{2\pi}{\hbar} \frac{U_{ac}}{A} \delta_{\vec{p}'_\parallel, \vec{p}_\parallel \pm \hbar \vec{\beta}_\parallel} |F_{n', n}|^2 \delta(E' - E \mp \hbar\omega) \quad U_{ac} = \frac{D_A^2 k_B T_L}{2c_l}$$

$$\frac{1}{\tau} = \frac{1}{\tau_m} = \sum_{\vec{p}'_\parallel} S(\vec{p}_\parallel, \vec{p}'_\parallel) \quad |F_{n', n}|^2 = \frac{1}{2W} (2 + \delta_{n, n'})$$

(infinite barrier well)

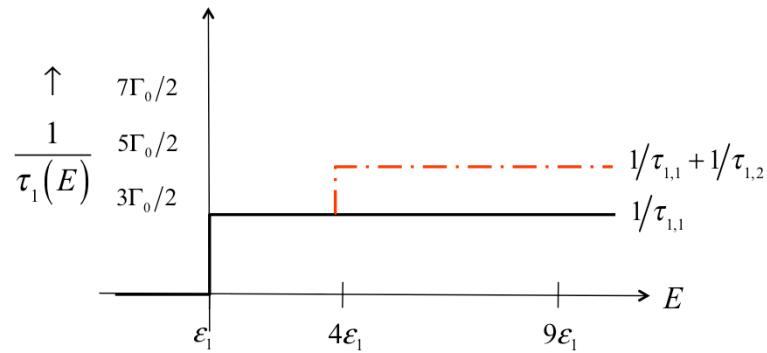
$$\frac{1}{\tau} = \frac{2\pi}{\hbar} U_{ac} \frac{D_{2D}(E)}{2} \frac{(2 + \delta_{n, n'})}{2W}$$

$$\tau \propto E^0$$

$$s = 0$$

## 2D scattering rate vs. energy

$$\frac{1}{\tau_{n,n'}} = \frac{2\pi}{\hbar} U_{ac} \frac{D_{2D}(E)}{2} \frac{(2 + \delta_{n,n'})}{2W} = \Gamma_0 \frac{(2 + \delta_{n,n'})}{2}$$



## topics

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