

ECE-656: Fall 2009

Lecture 21: Scattering and FGR

Professor Mark Lundstrom
Electrical and Computer Engineering
Purdue University, West Lafayette, IN USA

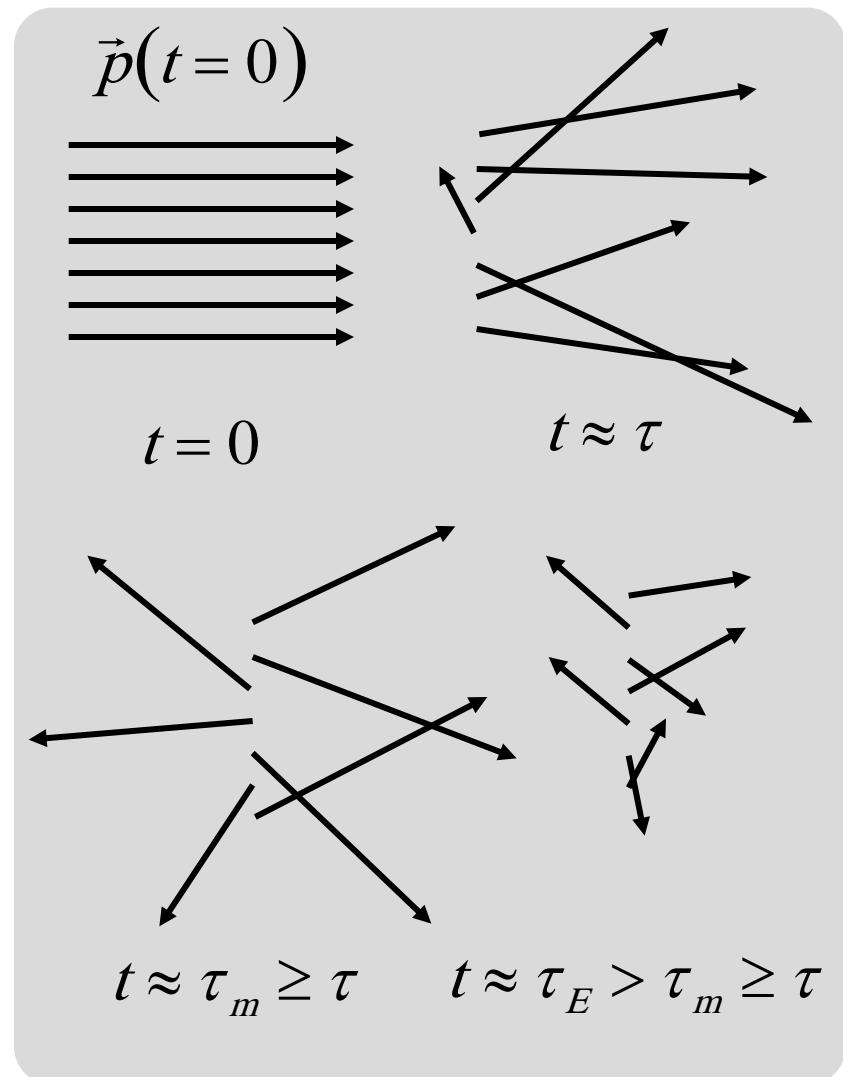
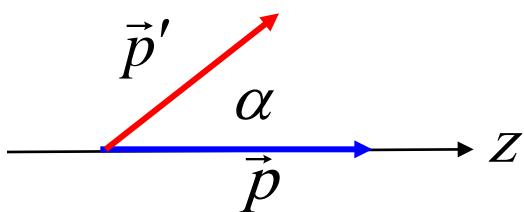
Review: characteristic times

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

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

$$\frac{1}{\tau_m(\vec{p})} = \sum_{\vec{p}', \uparrow} S(\vec{p}, \vec{p}') [1 - (p'/p_0) \cos \alpha]$$

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

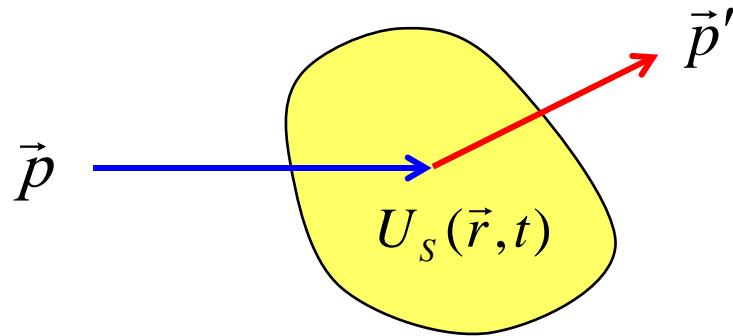


outline

- 1) Fermi's Golden Rule**
- 2) Example: static potential
- 3) Example: oscillating potential
- 4) Discussion
- 5) Summary

(Reference: Chapter 2, Lundstrom)

FGR



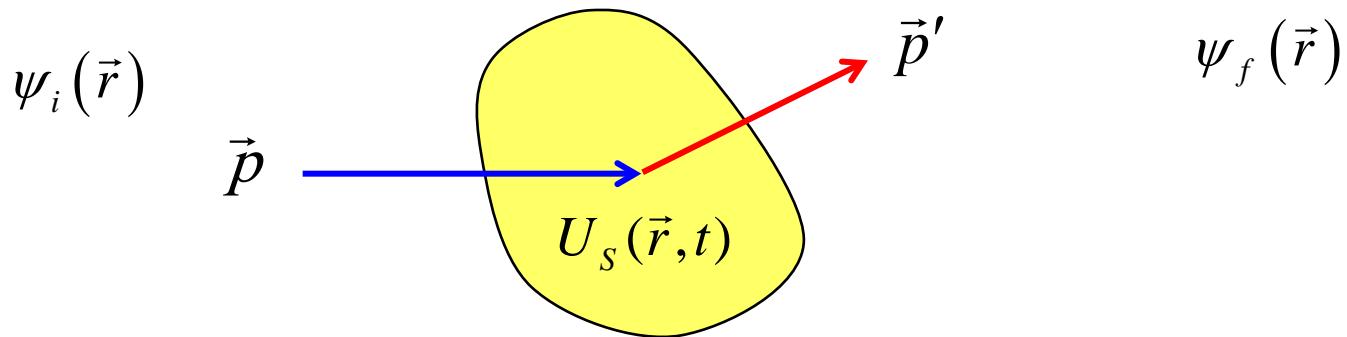
$$S(\vec{p}, \vec{p}') = \frac{2\pi}{\hbar} |H_{p'p}|^2 \delta(E' - E - \Delta E)$$

$$E' = E_0 + \Delta E \quad \Delta E = 0 \text{ for a static } U_s$$

$$\Delta E = \pm \hbar\omega \text{ for an oscillating } U_s$$

(See Sec.1.7 of Lundstrom for a derivation of FGR)

FGR



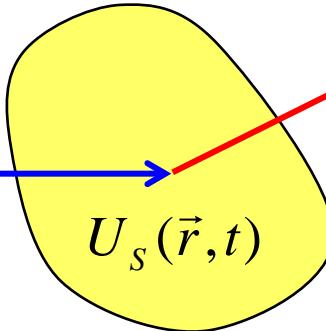
$$S(\vec{p}, \vec{p}') = \frac{2\pi}{\hbar} |H_{\vec{p}', \vec{p}}|^2 \delta(E' - E - \Delta E)$$

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

matrix element
(note the order of
the subscripts)

- 1) Identify the scattering potential
- 2) Specify the wavefunction (e.g.
1D, 2D, 3D)

scattering of Bloch electrons

$$\psi_i = \frac{1}{\sqrt{\Omega}} e^{i \vec{p} \cdot \vec{r} / \hbar} \times u_{\vec{k}}(\vec{r})$$


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

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

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

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

$$I(\vec{k}, \vec{k}') = \int_{\text{unit cell}} u_{\vec{k}'}^*(\vec{r}) u_{\vec{k}}(\vec{r}) d\vec{r} \quad I(\vec{k}, \vec{k}') \approx 1 \quad (\text{parabolic bands})$$

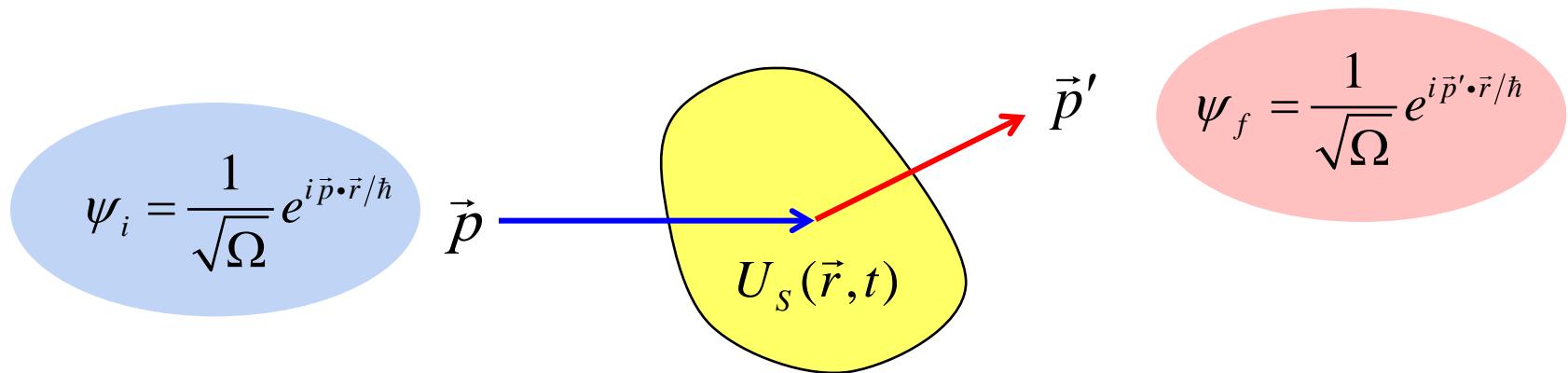
overlap integrals

B.K. Ridley, *Quantum Processes in Semiconductors*, 4th Ed., pp. 82-86, Cambridge, 1997

B.K. Ridley, *Electrons and Phonons in Semiconductor Multilayers*, pp. 60-63, Cambridge, 1997

D.K. Ferry, *Semiconductors*, pp. 214, 461-464, Macmillan, 1991

scattering of plane waves

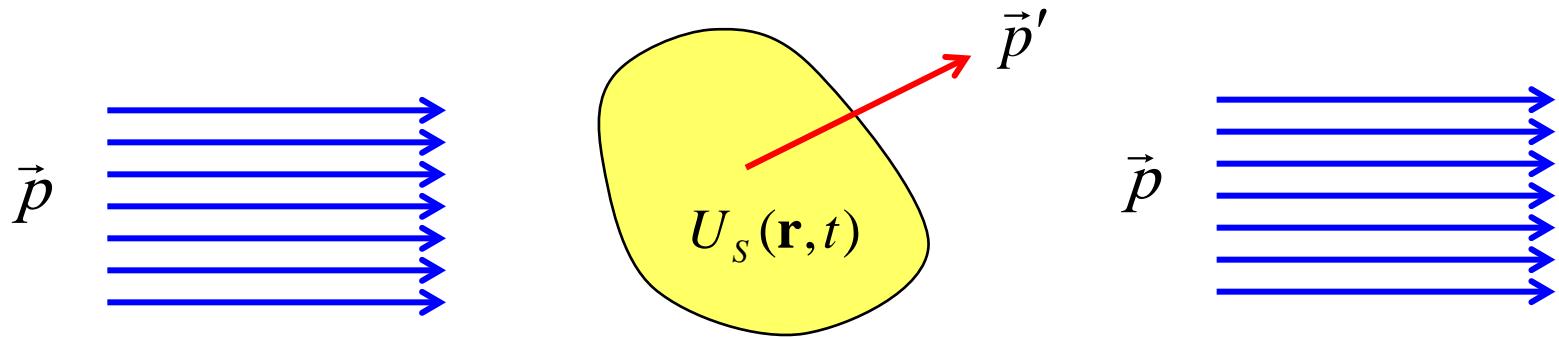


$$S(\vec{p}, \vec{p}') = \frac{2\pi}{\hbar} \left| H_{\vec{p}', \vec{p}} \right|^2 \delta(E' - E - \Delta E)$$

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

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

FGR: assumptions



- 1) Weak scattering
- 2) Infrequent scattering: $\Delta E \Delta t \approx \hbar$

Need a long time between scattering events so that the energy is sharply defined (“collisional broadening”).

outline

- 1) Fermi's Golden Rule
- 2) Example: static potential**
- 3) Example: oscillating potential
- 4) Discussion
- 5) Summary

(Reference: Chapter 2, Lundstrom)

FGR: static scattering potential

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

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

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

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

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

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

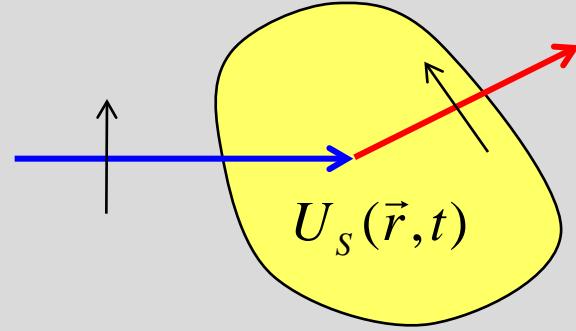
$$H_{\vec{p}', \vec{p}} = U_s(\vec{q})$$

The matrix element is the Fourier transform of the scattering potential.

short range: neutral impurity
long range: charged impurity

$$\vec{q} = (\vec{p} - \vec{p}') / \hbar = \vec{k}' - \vec{k}$$

FGR: delta-function example

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


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

$$U_s(\vec{r}) = C \delta(0)$$

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

“short range potential”

$$H_{p', p} = \frac{1}{\Omega} \int_{-\infty}^{+\infty} e^{-i \vec{p}' \cdot \vec{r} / \hbar} C \delta(0) e^{i \vec{p} \cdot \vec{r} / \hbar} d\vec{r} = \frac{C}{\Omega}$$

$$S(\vec{p}, \vec{p}') = \frac{2\pi}{\hbar} \frac{C^2}{\Omega^2} \delta(E' - E) = K \frac{1}{\Omega} \delta(E' - E)$$

scattering rate

$$S(\vec{p}, \vec{p}') = K \frac{1}{\Omega} \delta(E' - E)$$

$$\frac{1}{\tau(\vec{p})} = \sum_{\vec{p}'\uparrow} S(\vec{p}, \vec{p}') = K \frac{1}{\Omega} \sum_{\vec{p}'\uparrow} \delta(E' - E)$$

$$\frac{1}{\Omega} \sum_{\vec{p}'\uparrow} \delta(E' - E) = \frac{D_{3D}(E)}{2}$$

$$\frac{1}{\Omega} \delta(E' - E) = \frac{m^* \sqrt{2m^* E}}{2\pi^2 \hbar^3}$$

(for parabolic energy bands)

$$\frac{1}{\tau(\vec{p})} \propto D_f(E)$$

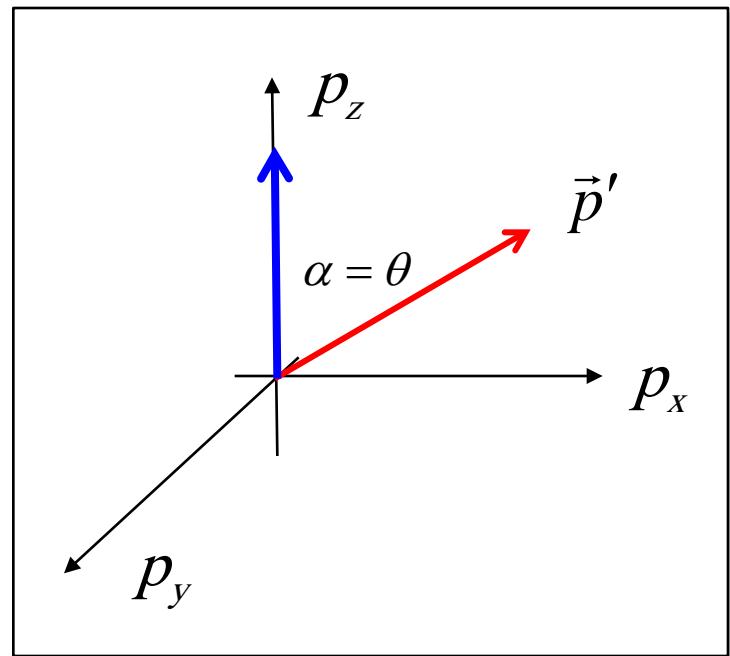
For an incident electron with energy, E , the scattering rate is proportional to the density of final states at energy, E (1D, 2D, 3D)

momentum relaxation rate

$$S(\vec{p}, \vec{p}') = K \frac{1}{\Omega} \delta(E' - E)$$

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

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



momentum relaxation

$$\frac{1}{\tau_m(\vec{p})} = K \frac{1}{\Omega} \sum_{\vec{p}',\uparrow} \delta(E' - E) (1 - \cos \alpha) \quad [\alpha = \theta \text{ in our coordinate system}]$$

$$\frac{1}{\Omega} \delta(E' - E) = \frac{1}{\Omega} \frac{\Omega}{(2\pi)^3 \hbar^3} \int_0^{2\pi} d\phi \int_0^\pi (1 - \cos \theta) \sin \theta d\theta \int_0^\infty p'^2 d' \delta(E' - E)$$

$$\begin{aligned} \text{extra term} &= \int_0^\pi (-\cos \theta) \sin \theta d\theta \\ &= \left. \frac{\cos^2}{2} \right|_0^\pi \\ &= 0 \end{aligned}$$

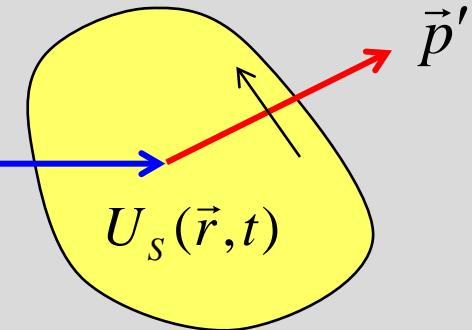
$$\frac{1}{\tau_m(\vec{p})} = \frac{1}{\tau(\vec{p})}$$

isotropic

energy relaxation

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

$$\vec{p}$$



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

$$U_s(\vec{r}, t) = C \delta(0)$$

$$S(\vec{p}, \vec{p}') = K \frac{1}{\Omega} \delta(E' - E)$$

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

$$\frac{1}{\tau_E(\vec{p})} = 0$$

static potential summary

A chalkboard with a mathematical equation written on it. The equation is:

$$\frac{1}{\tau} = \sum_{\vec{P}} S_{\vec{P}, \vec{P}'} (1 - f(\vec{P}))$$

The equation is divided by a horizontal line. The left side of the equation is $\frac{1}{\tau}$. The right side is a sum over \vec{P} of $S_{\vec{P}, \vec{P}'}$ times $(1 - f(\vec{P}))$.

$\epsilon_E(P)$

outline

- 1) Fermi's Golden Rule
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(Reference: Chapter 2, Lundstrom)

example: oscillating potential

The diagram shows a yellow elliptical region representing a potential well $U_s(\vec{r}, t)$. A blue arrow labeled \vec{p} points along the horizontal axis, and a red arrow labeled E' points along the vertical axis. A red arrow labeled \vec{p}' originates from the center of the ellipse.

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

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

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

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

$$H_{\vec{p}', \vec{p}} = \frac{1}{\Omega} \int_{-\infty}^{+\infty} e^{-i \vec{p}' \cdot \vec{r} / \hbar} \left(\frac{U_{\beta}^{a,e}}{\sqrt{\Omega}} e^{\pm i \vec{\beta} \cdot \vec{r}} \right) e^{i \vec{p} \cdot \vec{r} / \hbar} d\vec{r} = U_{\beta}^{a,e} \frac{1}{\Omega^{3/2}} \int_{-\infty}^{+\infty} e^{i (\vec{p} - \vec{p}' \pm \hbar \vec{\beta}) \cdot \vec{r} / \hbar} d\vec{r}$$

$$H_{\vec{p}', \vec{p}} = \frac{U_{\beta}^{a,e}}{\sqrt{\Omega}} \delta_{\vec{p}', \vec{p} \pm \hbar \vec{\beta}}$$

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momentum conservation

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

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

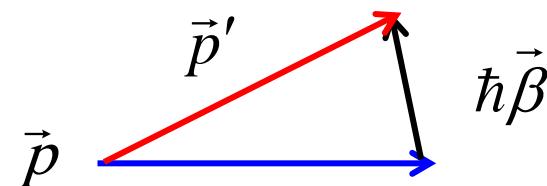
$$U_s(\vec{r}, t) \quad E$$

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

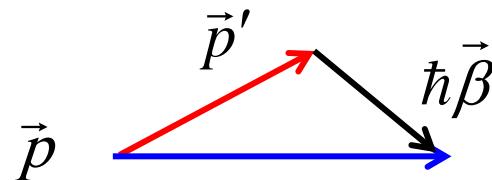
$$H_{p', p} = \frac{U_{\beta}^{a,e}}{\sqrt{\Omega}} \delta_{\vec{p}', \vec{p} \pm \hbar \vec{\beta}}$$

(momentum conservation)

$$\vec{p}' = \vec{p} + \hbar \vec{\beta} \quad (\text{ABS})$$



$$\vec{p}' = \vec{p} - \hbar \vec{\beta} \quad (\text{EMS})$$



energy-momentum conservation

The diagram illustrates a particle interaction. A yellow oval represents a system with a potential $U_s(\vec{r}, t)$. A blue arrow labeled \vec{p} enters from the left, and a red arrow labeled \vec{p}' exits to the right. Two pink circles, each labeled E , represent energy reservoirs. One circle is on the left, and the other is on the right, near the exit point.

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

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

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

$$S(\vec{p}, \vec{p}') = \frac{2\pi}{\hbar} \left| H_{p', p} \right|^2 \delta(E' - E + \Delta E) \quad H_{p', p} = \frac{U_{\beta}}{\sqrt{\Omega}} \delta_{\vec{p}', \vec{p} \pm \hbar \vec{\beta}}$$

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

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

energy-momentum conservation

The diagram illustrates the interaction between two particles. A yellow oval represents a system with position \vec{r} and time t , containing a function $U_s(\vec{r}, t)$. A blue arrow labeled \vec{p} represents the initial momentum of a particle, which is scattered by the system into a red arrow labeled \vec{p}' . Two red circles, each labeled E , represent the initial and final energies of the particle.

$$\psi_i = \frac{1}{\sqrt{\Omega}} e^{i \vec{p} \cdot \vec{r} / \hbar} \quad \vec{p}$$
$$\psi_f = \frac{1}{\sqrt{\Omega}} e^{i \vec{p}' \cdot \vec{r} / \hbar}$$
$$U_s(\vec{r}, t) = \frac{U_{\beta}^{a,e}}{\sqrt{\Omega}} e^{\pm i(\vec{\beta} \cdot \vec{r} - \omega t)}$$

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

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

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

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

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

ABS

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EMS

scattering rate

Assume (for now) that for any transition from E_i to E_f , we can find a vibration that conserves momentum.

$$S(\vec{p}, \vec{p}') = \frac{2\pi}{\hbar} \frac{|U_{\beta}^{a,e}|^2}{\Omega} \delta(E' - E \mp \hbar\omega) \quad \begin{cases} \text{ABS} \\ \text{EMS} \end{cases}$$

$$\frac{1}{\tau(\vec{p})} = \sum_{\vec{p}' \uparrow} S(\vec{p}, \vec{p}') = K \frac{1}{\Omega} \sum_{p' \uparrow} \delta(E' - E \mp \hbar\omega)$$

$$\frac{1}{\tau(\vec{p})} = K \frac{D_f(E \pm \hbar\omega)}{2} \propto D_f(E \pm \hbar\omega)$$

Scattering rate is proportional to the density of final states.

momentum relaxation: oscillating potential

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

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

energy relaxation: oscillating potential

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

$$\frac{1}{\tau_E(\vec{p})} = \sum_{p'\uparrow} S(\vec{p}, \vec{p}') \frac{\Delta E}{E} = \frac{\hbar\omega}{E} \sum_{p'\uparrow} S(\vec{p}, \vec{p}') = \left(\frac{\hbar\omega}{E} \right) \frac{1}{\tau(\vec{p})}$$

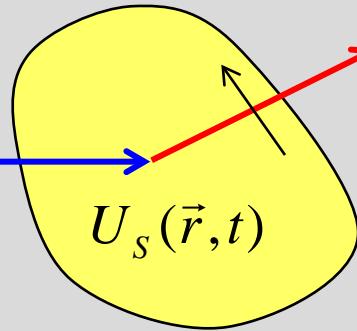
$$\frac{1}{\tau_E(\vec{p})} < \frac{1}{\tau_m(\vec{p})} = \frac{1}{\tau(\vec{p})}$$

$$\tau_E(\vec{p}) > \tau_m(\vec{p}) = \tau(\vec{p})$$

oscillating potential summary

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

$$\vec{p}$$



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

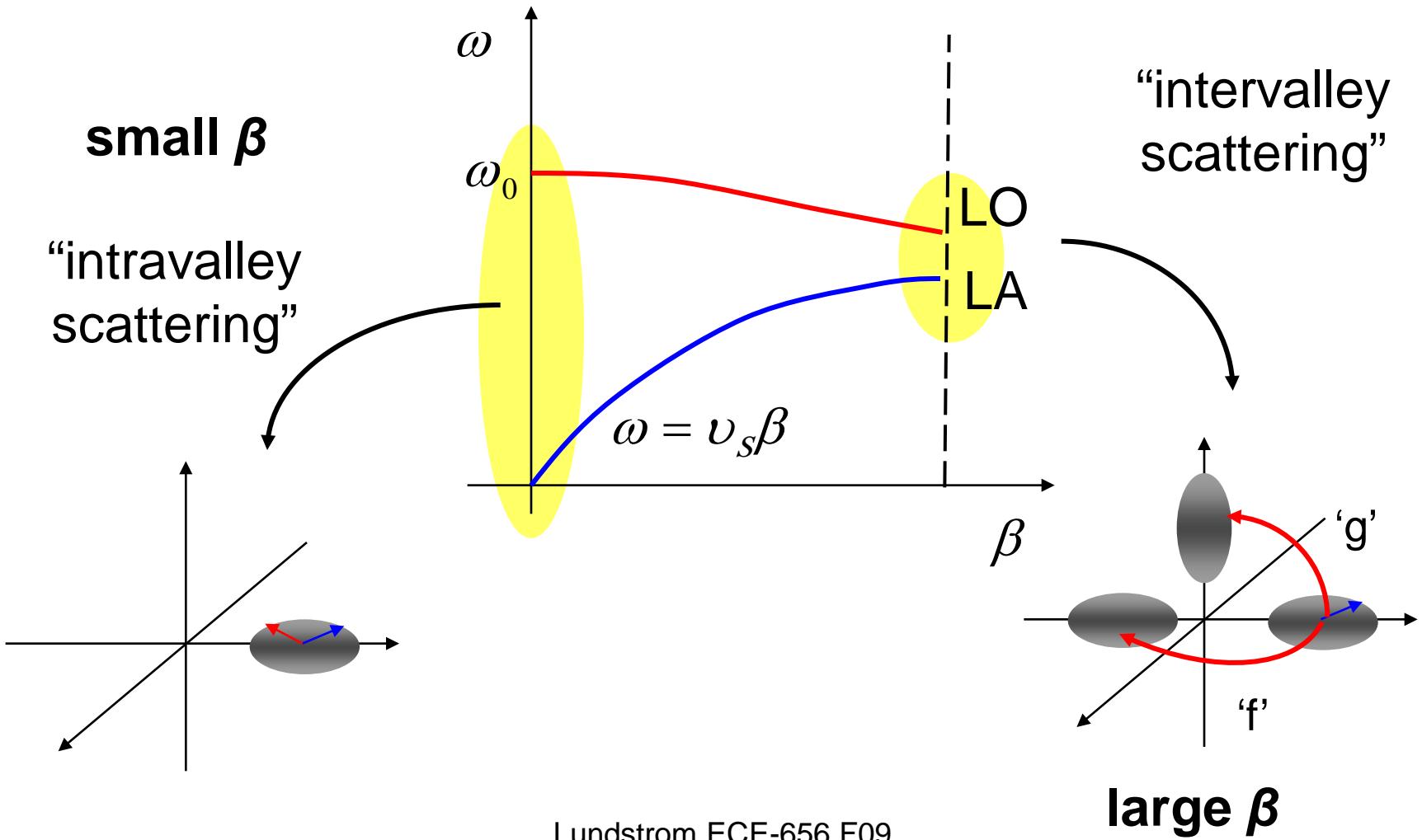
$$U_s(\vec{r}, t) = \frac{U_{\beta}^{a,e}}{\sqrt{\Omega}} e^{\pm i(\vec{\beta} \cdot \vec{r} - \omega t)}$$

$$\frac{1}{\tau(\vec{p})} \sim \frac{D_f(E \pm \hbar\omega)}{2}$$

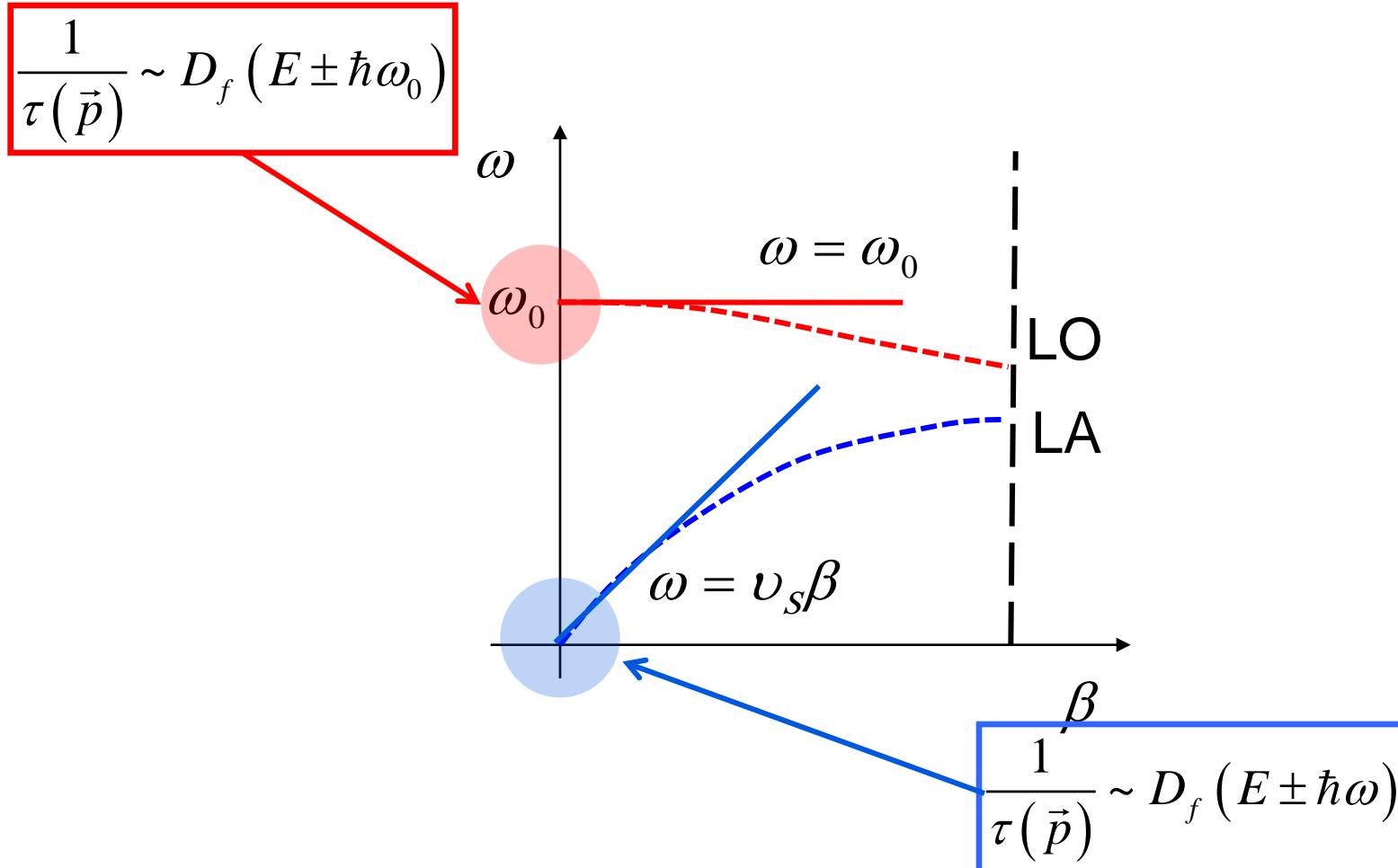
$$\frac{1}{\tau_m(\vec{p})} = \frac{1}{\tau(\vec{p})} \quad (\text{isotropic})$$

$$\frac{1}{\tau_E(\vec{p})} = \frac{\hbar\omega}{E} \frac{1}{\tau(\vec{p})} \quad (\text{inelastic})$$

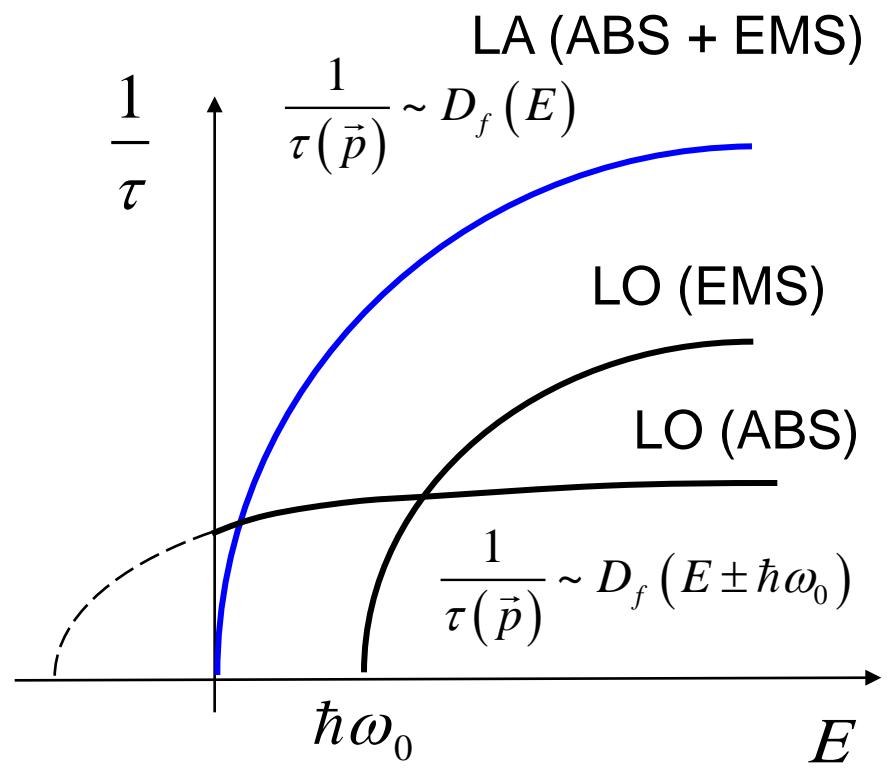
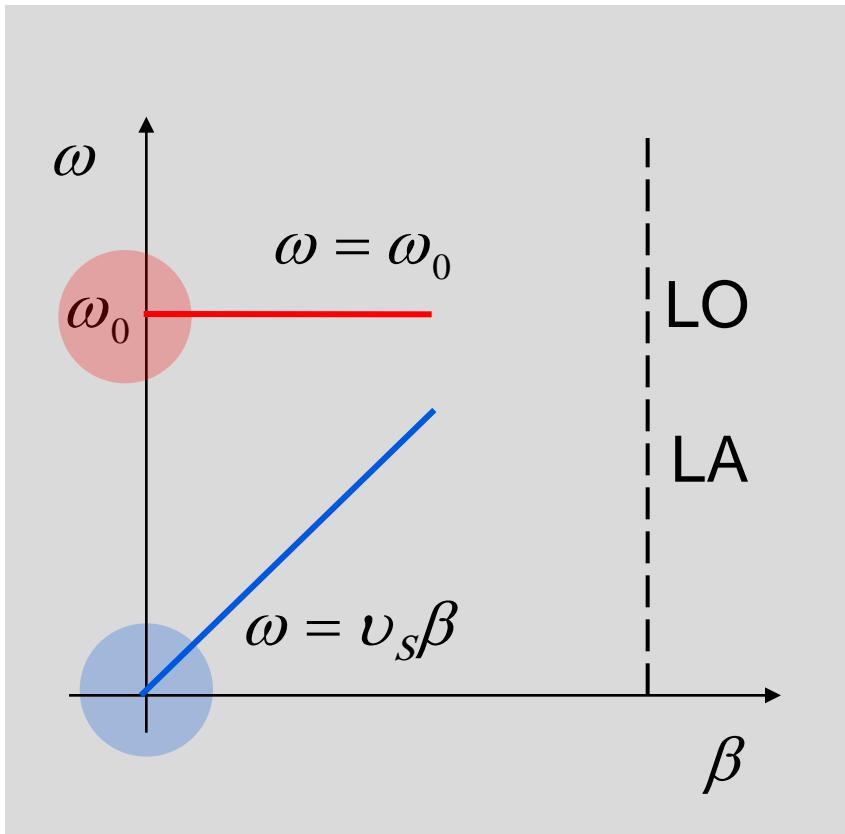
an aside on phonon scattering



phonon scattering



intravalley phonon scattering



outline

- 1) Fermi's Golden Rule
- 2) Example: static potential
- 3) Example: oscillating potential
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constraints on scattering

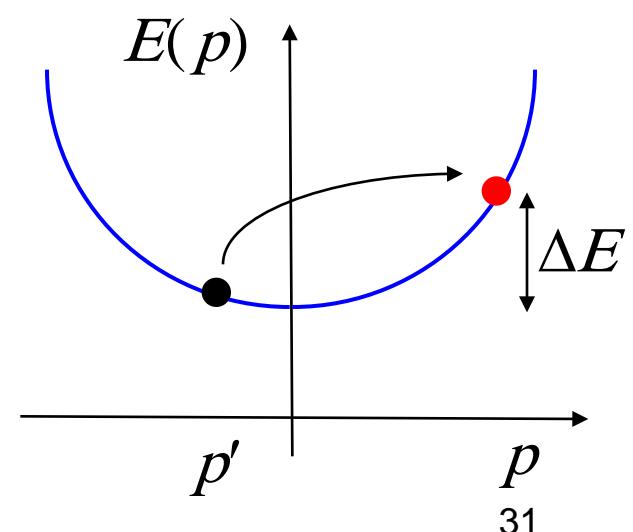
$$\hat{C}f = \sum_{p'} S(\vec{p}', \vec{p}) f(p') [1 - f(p)] - S(\vec{p}, \vec{p}') f(p) [1 - f(p')]$$

in equilibrium:

$$\hat{C}f_0 = 0 = S(\vec{p}', \vec{p}) f_0(p') [1 - f_0(p)] - S(\vec{p}, \vec{p}') f_0(p) [1 - f_0(p')]$$

$$\frac{S(\vec{p}', \vec{p})}{S(\vec{p}, \vec{p}')} = \frac{f_0(p) [1 - f_0(p')]}{f_0(p') [1 - f_0(p)]} = e^{-\Delta E / k_B T}$$

$$\Delta E = E(p) - E(p')$$



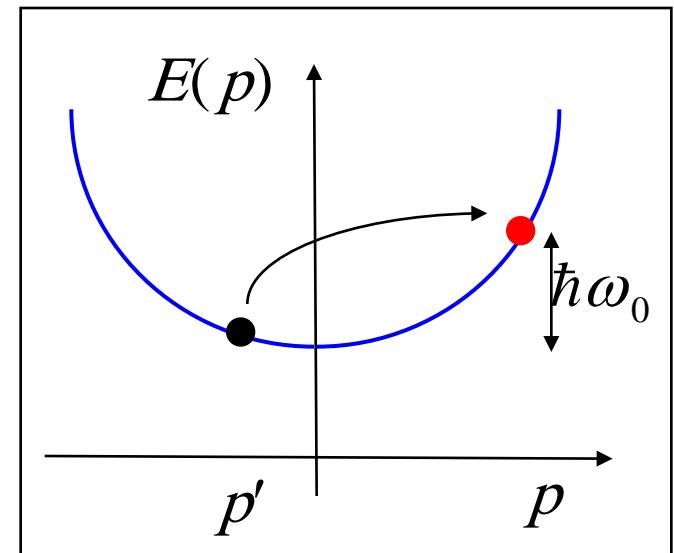
constraints on scattering

$$\frac{S(\vec{p}', \vec{p})}{S(\vec{p}, \vec{p}')} = e^{-\Delta E/k_B T} \quad \Delta E = E(p) - E(p')$$

1) elastic scattering: $\Delta E = 0 \quad S(\vec{p}, \vec{p}') = S(\vec{p}', \vec{p})$

2) phonon scattering: $\Delta E = \hbar\omega_0$

$$\frac{S^{ABS}(\vec{p}', \vec{p})}{S^{EMS}(\vec{p}, \vec{p}')} = e^{-\hbar\omega_0/k_B T}$$



constraints on phonon scattering

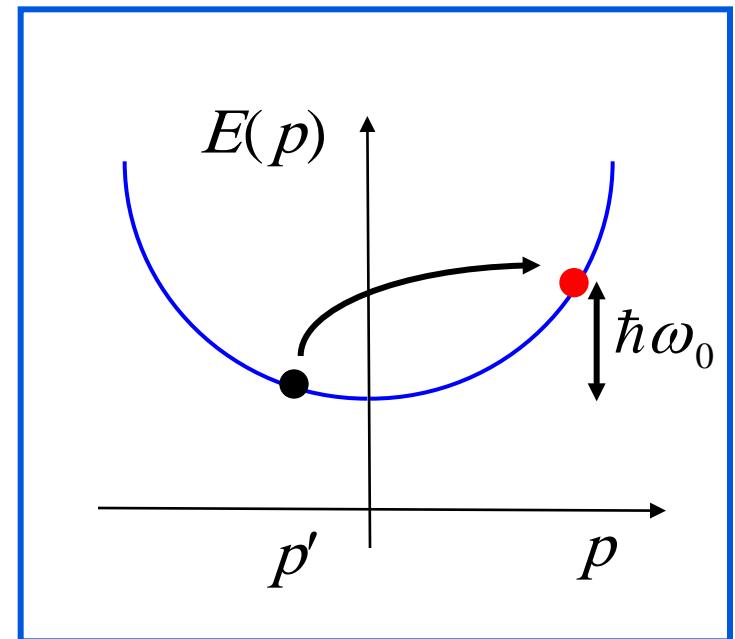
$$\frac{S^{ABS}(\vec{p}', \vec{p})}{S^{EMS}(\vec{p}, \vec{p}')} = e^{-\hbar\omega_0/k_B T} \quad S^{ABS}(\vec{p}', \vec{p}) \approx N_\omega \quad S^{EMS}(\vec{p}, \vec{p}') \approx e^{\hbar\omega_0/k_B T} N_\omega$$

$$N_\omega = \frac{1}{e^{\hbar\omega/k_B T} - 1}$$

$$e^{\hbar\omega/k_B T} N_\omega = \frac{e^{\hbar\omega/k_B T}}{e^{\hbar\omega/k_B T} - 1} = N_\omega + 1$$

$$S^{ABS}(\vec{p}', \vec{p}) \sim N_\omega$$

$$S^{EMS}(\vec{p}, \vec{p}') \sim N_\omega + 1$$



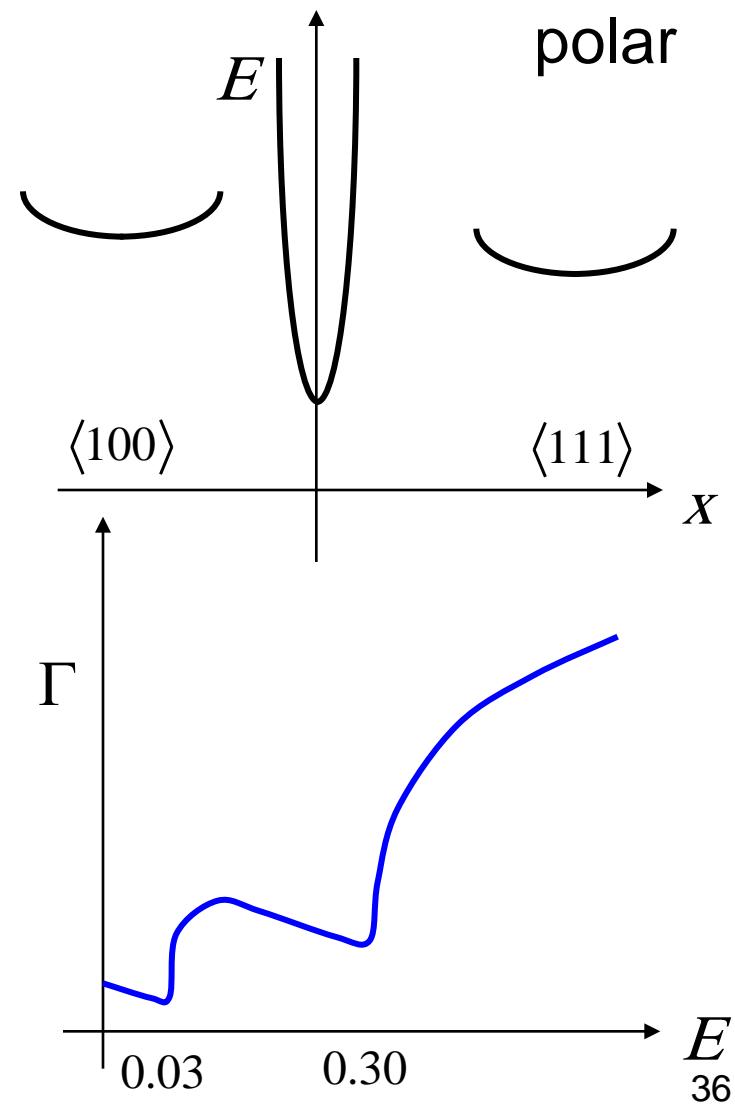
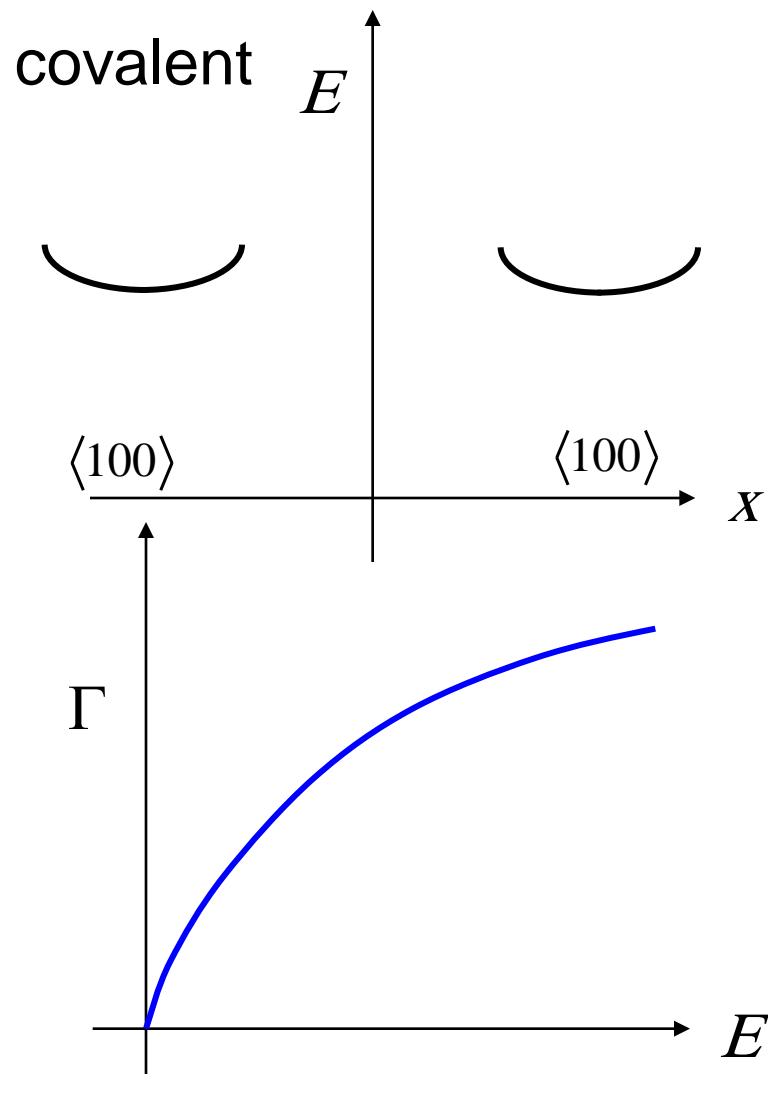
outline

- 1) Fermi's Golden Rule
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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 proportional to the final DOS
- 4) Static potentials lead to elastic scattering
- 5) Time varying potentials lead to inelastic scattering
- 6) General features of scattering in common semiconductors can now be understood (almost)

covalent vs. polar semiconductors



questions

- 1) Fermi's Golden Rule
- 2) Example: static potential
- 3) Example: oscillating potential
- 4) Discussion
- 5) Summary

