ECE-656: Fall 2009

Lecture 21: Scattering and FGR

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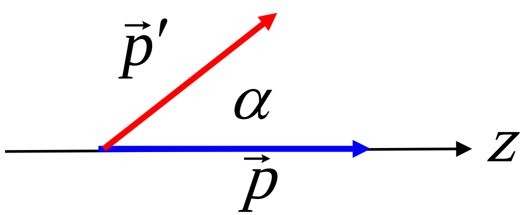
Review: characteristic times

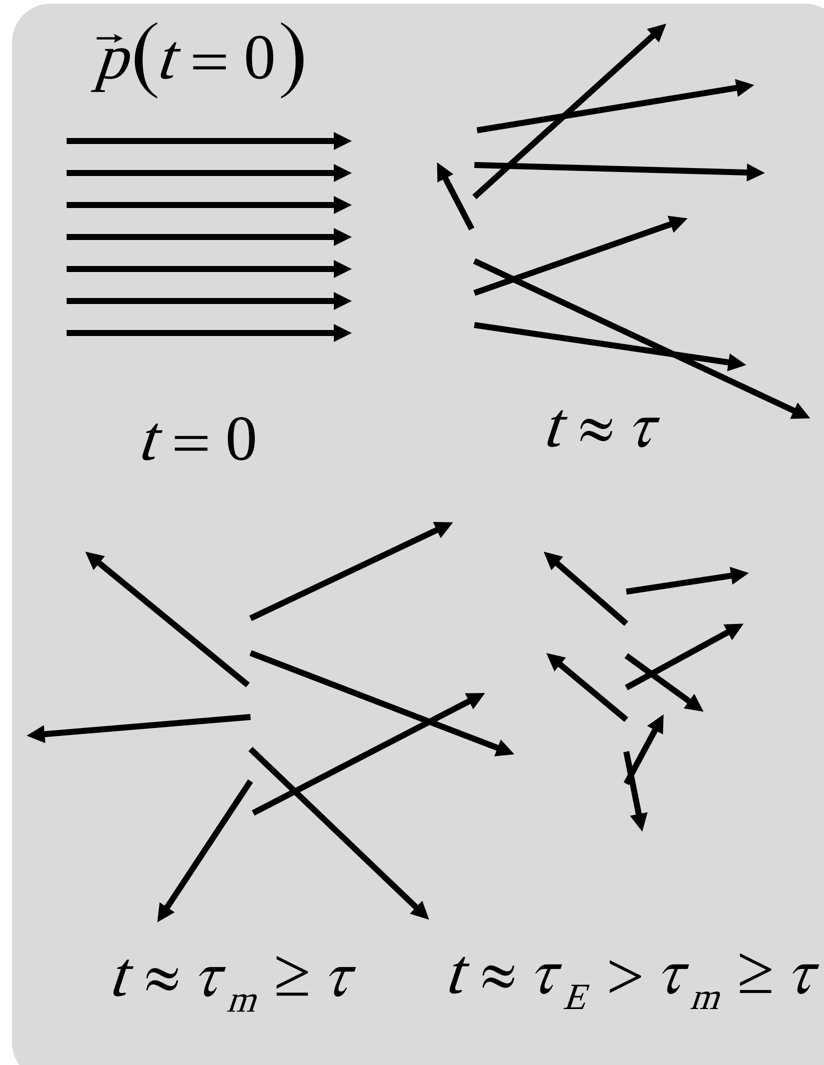
$$\frac{1}{\tau(\vec{p})} == \sum_{\vec{p}',\uparrow} S(\vec{p},\vec{p}')$$

(τ, single particle lifetime)

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

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



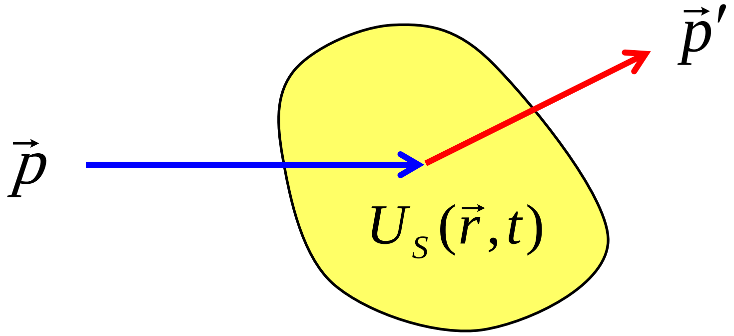


outline

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

(Reference: Chapter 2, Lundstrom)

FGR



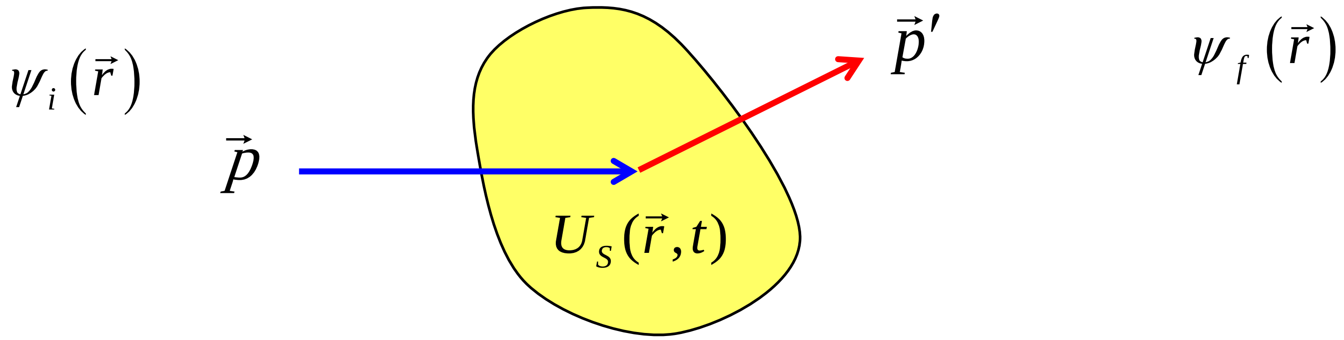
$$S\left(\vec{p},\vec{p}'\right) = \frac{2\pi}{\hbar}\left|H_{p'p}\right|^2 \delta\left(E' - E - \Delta E\right)$$

$E' = E_0 + \Delta E$ $\quad$ $\Delta E = 0$ for a static U_S

$\Delta E = \pm\hbar\omega$ for an oscillating U_S

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

FGR



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

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

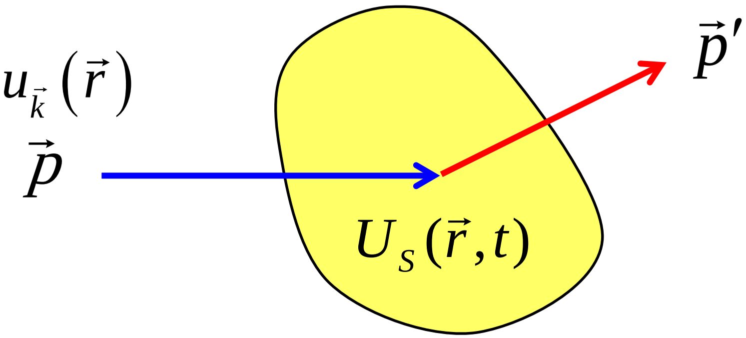
matrix element (note the order of the subscripts)

1) Identifiy the scattering potential

2) Specify the wavefunction (e.g. 1D, 2D, 3D)

scattering of Bloch electrons

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



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

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

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

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

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

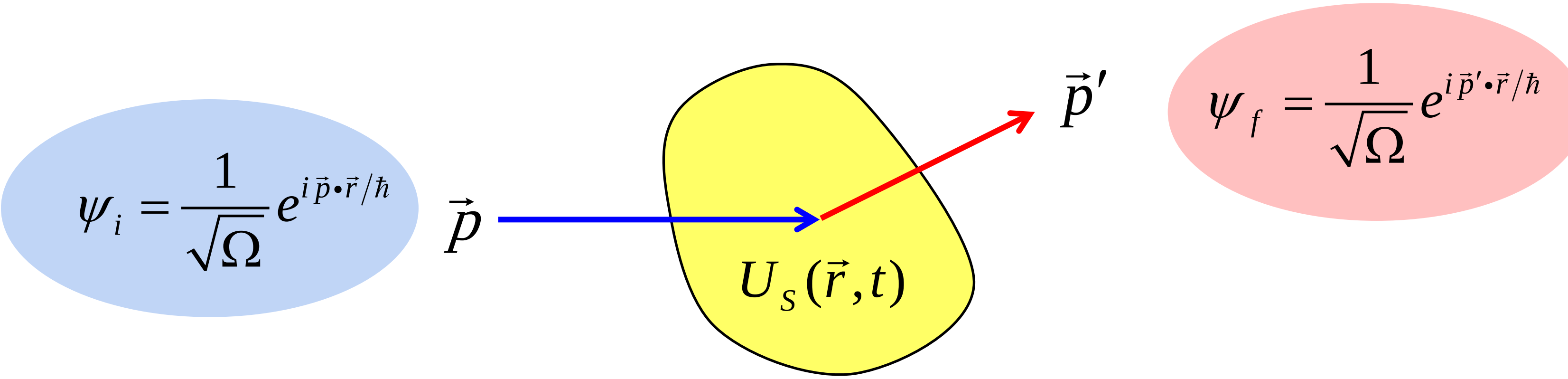
overlap integrals

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

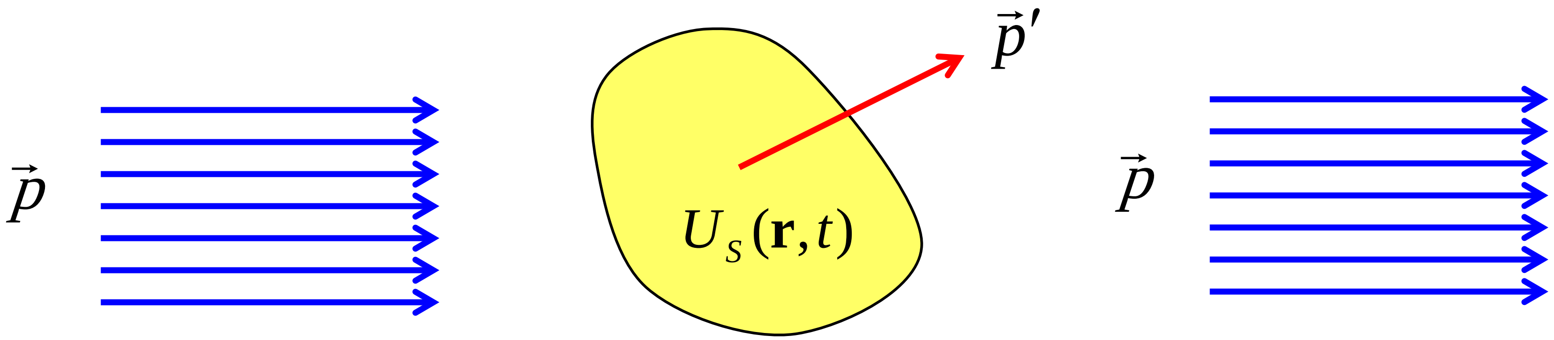


$$S(\vec{p},\vec{\mathbf{p}}') = \frac{2\pi}{\hbar} \left|H_{\vec{p}',\vec{p}}\right|^2 \delta\left(E' - E - \Delta E\right)$$

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

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

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 shaoprpy defined (“collisional broadening”).

outline

1) Fermi's Golden Rule

2) Example: static potential

3) Example: oscillating potential

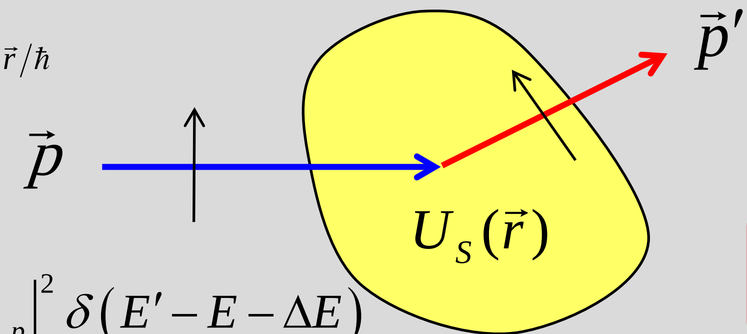
4) Discussion

5) Summary

(Reference: Chapter 2, Lundstrom)

FGR: static scattering potential

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



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

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

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

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

short range: neutral impurity
long range: charged impurity

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

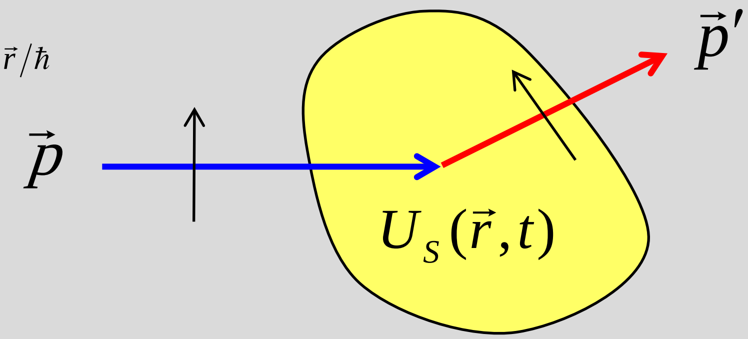
$$\vec{q} = \left(\vec{p} - \vec{p}'\right)/\hbar = \vec{k}' - \vec{k}$$

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

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

FGR: delta-function example

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



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

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

"short range potential"

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

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

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

scattering rate

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

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

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

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

(for parabolic energy bands)

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

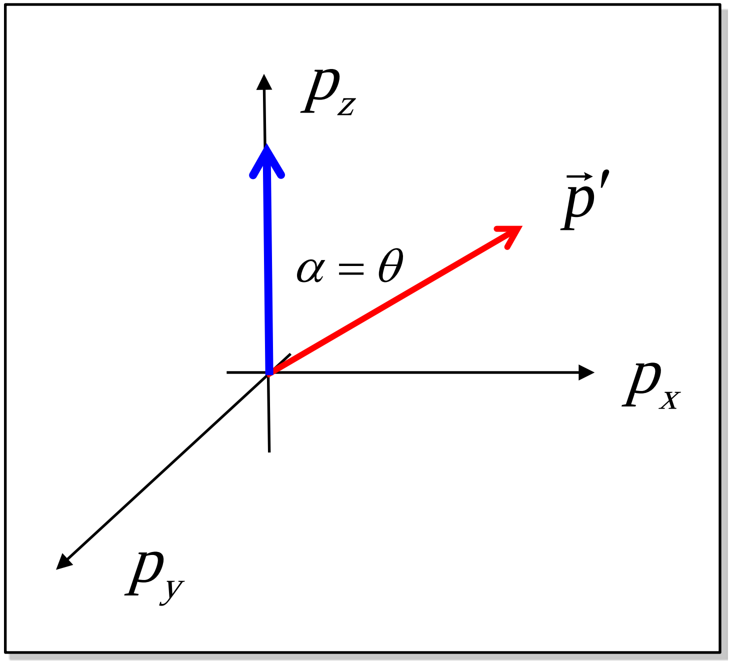
For an incident electron with energy, *E*, the scattering rate is proportional to the density of final states at energy, *E* (1D, 2D, 3D)

momentum relaxation rate

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

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

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



momentum relaxation

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

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

$$\text{extra term} = \int_0^{\pi}(-\cos\theta)\sin\theta\, d\theta$$

$$= \left.\frac{\cos^2}{2}\right|_0^{\pi}$$

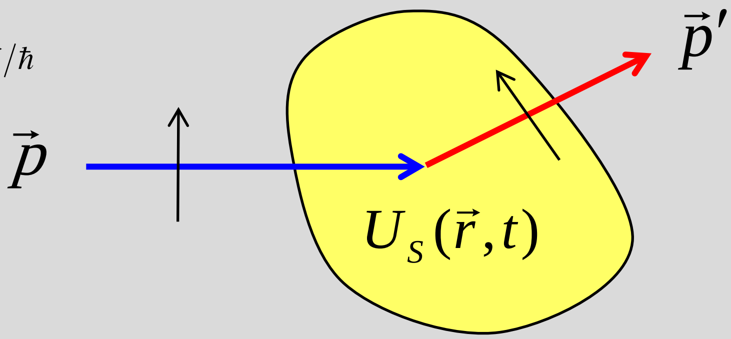
$$= 0$$

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

isotropic

energy relaxation

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



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

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

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

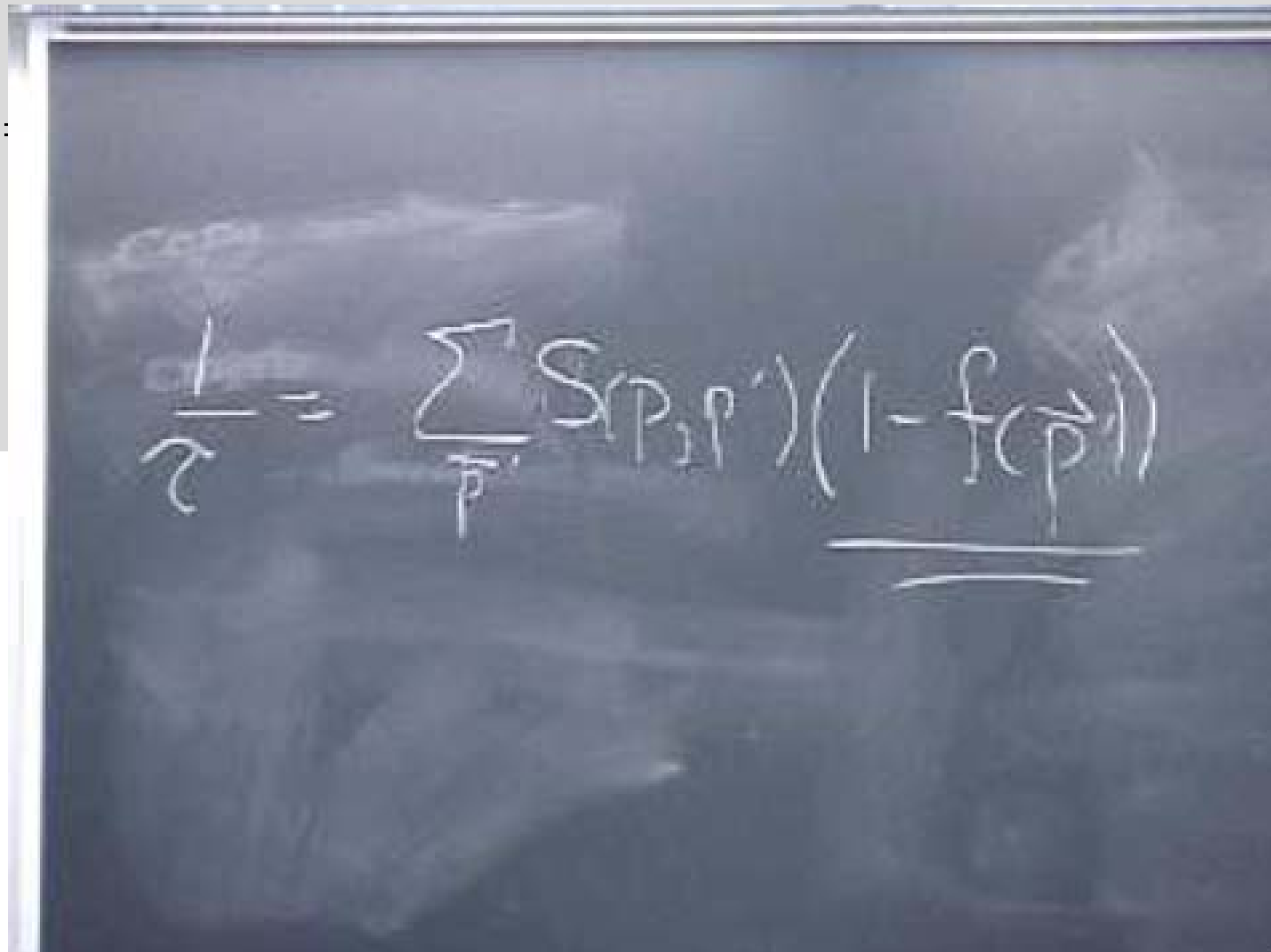
$$\frac{1}{\tau_E(\vec{p})} = \sum_{\mathbf{p}',\uparrow} S(\vec{p},\vec{p}')\frac{\Delta E}{E}$$

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

static potential summary

$\psi_i =$ … $i\vec{p}'\bullet\vec{r}/\hbar$

… $\delta(0)$



… $_E(p)$

outline

1) Fermi's Golden Rule

2) Example: static potential

3) **Example: oscillating potential**

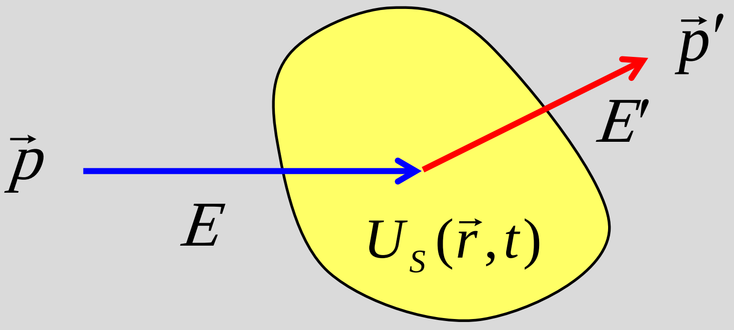
4) Discussion

5) Summary

(Reference: Chapter 2, Lundstrom)

example: oscillating potential

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



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

$$U_S(\vec{r},t) = \frac{U_\beta^{a,e}}{\sqrt{\Omega}} e^{\pm i\left(\vec{\beta}\bullet\vec{r}-\omega t\right)}$$

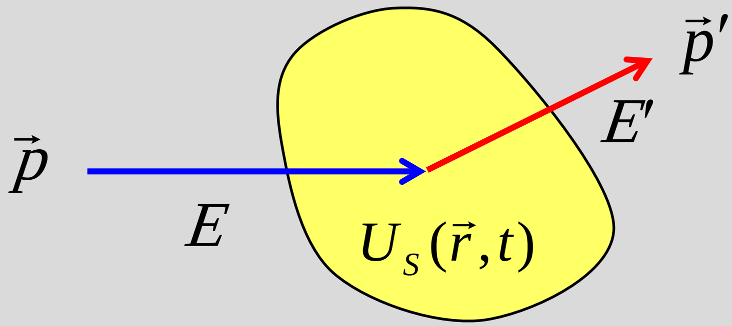
$$S(\vec{p},\vec{p}\,') = \frac{2\pi}{\hbar}\left|H_{\vec{p}\,',\vec{p}}\right|^2 \delta\left(E'-E-\Delta E\right) \qquad \Delta E = \pm\hbar\omega$$

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

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

momentum conservation

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



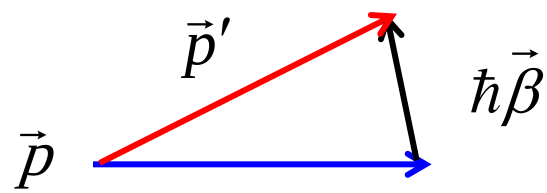
$$\psi_f = \frac{1}{\sqrt{\Omega}} e^{i\vec{p}\,'\bullet\vec{r}/\hbar}$$

$$U_S(\vec{r},t) = \frac{U_\beta^{a,e}}{\sqrt{\Omega}} e^{\pm i\left(\vec{\beta}\bullet\vec{r}-\omega t\right)}$$

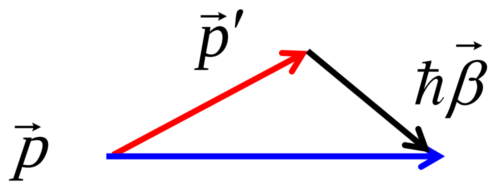
$$H_{p',p} = \frac{U_\beta^{a,e}}{\sqrt{\Omega}} \delta_{\vec{p}\,',\vec{p}\pm\hbar\vec{\beta}}$$

(momentum conservation)

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

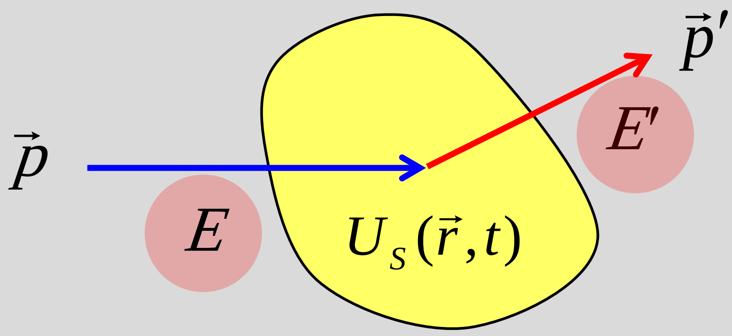


$\vec{p}\,' = \vec{p} - \hbar\vec{\beta}$ (EMS)



energy-momentum conservation

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



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

$$U_S\left(\vec{r},t\right) = \frac{U_\beta^{a,e}}{\sqrt{\Omega}} e^{\pm i\left(\vec{\beta}\bullet\vec{r}-\omega t\right)}$$

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

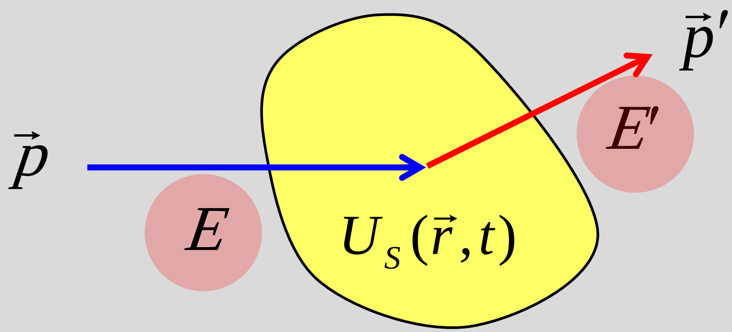
$$H_{p',p} = \frac{U_\beta}{\sqrt{\Omega}}\delta_{\vec{p}\,',\vec{p}\pm\hbar\vec{\beta}}$$

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

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

energy-momentum conservation

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



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

$$U_S(\vec{r},t) = \frac{U_\beta^{a,e}}{\sqrt{\Omega}} e^{\pm i\left(\vec{\beta}\bullet\vec{r}-\omega t\right)}$$

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

$E' = E + \hbar\omega$	$E' = E - \hbar\omega$
$\vec{p}\,' = \vec{p} + \hbar\vec{\beta}$	$\vec{p}\,' = \vec{p} - \hbar\vec{\beta}$
ABS	EMS

scattering rate

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

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

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

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

Scattering rate is proportional to the density of final states.

momentum relaxation: oscillating potential

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

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

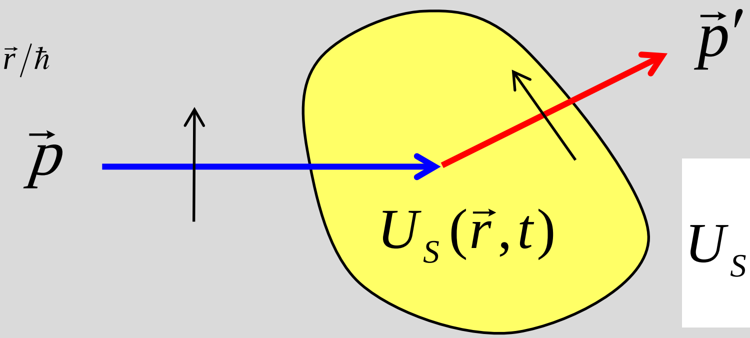
$$\frac{1}{\tau_E(\vec{p})} = \sum_{p'\uparrow} S(\vec{p},\vec{p}\,')\frac{\Delta E}{E} = \frac{\hbar\omega}{E}\sum_{p'\uparrow} S(\vec{p},\vec{p}\,') = \left(\frac{\hbar\omega}{E}\right)\frac{1}{\tau(\vec{p})}$$

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

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

oscillating potential summary

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



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

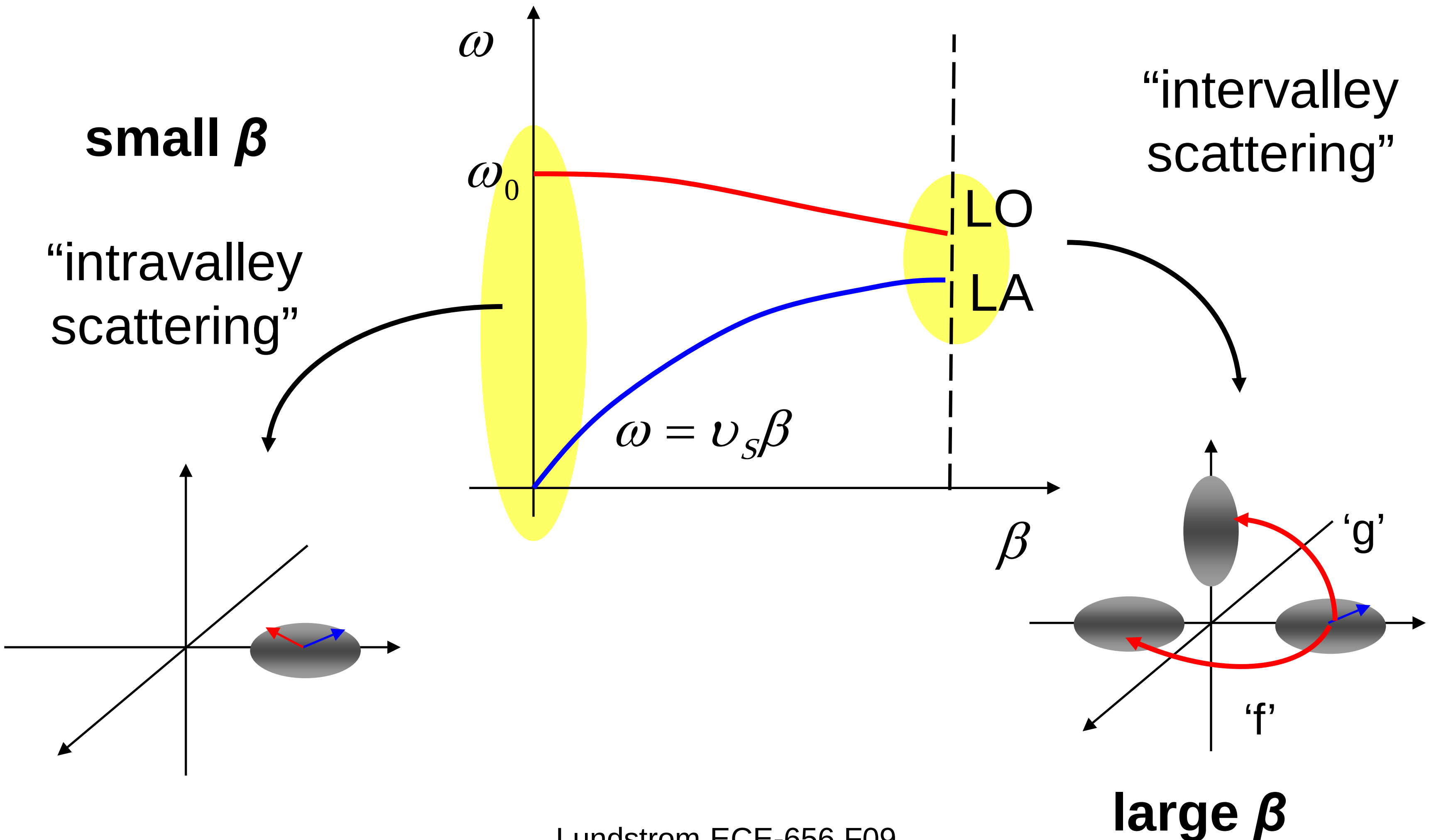
$$U_S\left(\vec{r},t\right) = \frac{U_\beta^{a,e}}{\sqrt{\Omega}} e^{\pm i\left(\vec{\beta}\bullet\vec{r}-\omega t\right)}$$

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

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

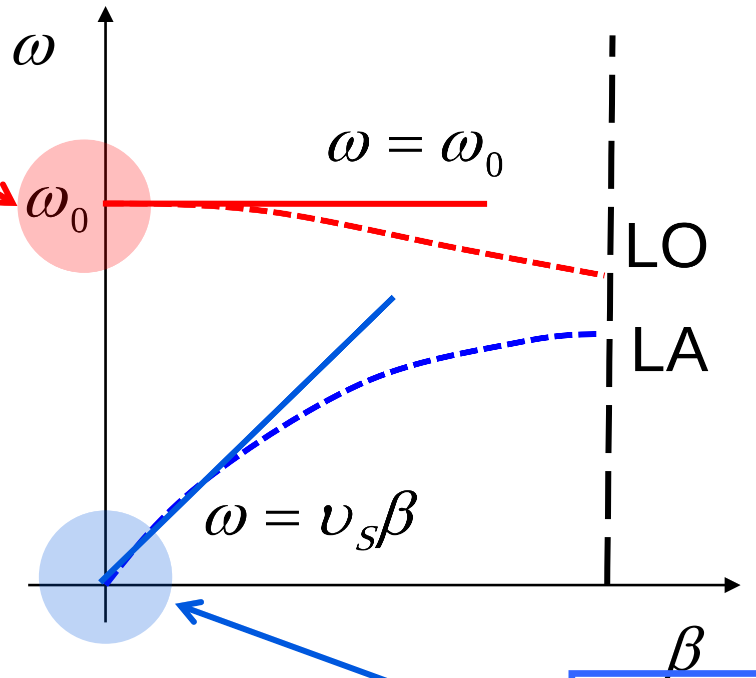
$$\frac{1}{\tau_E\left(\vec{p}\right)} = \frac{\hbar\omega}{E}\frac{1}{\tau\left(\vec{p}\right)}$$ (inelastic)

an aside on phonon scattering



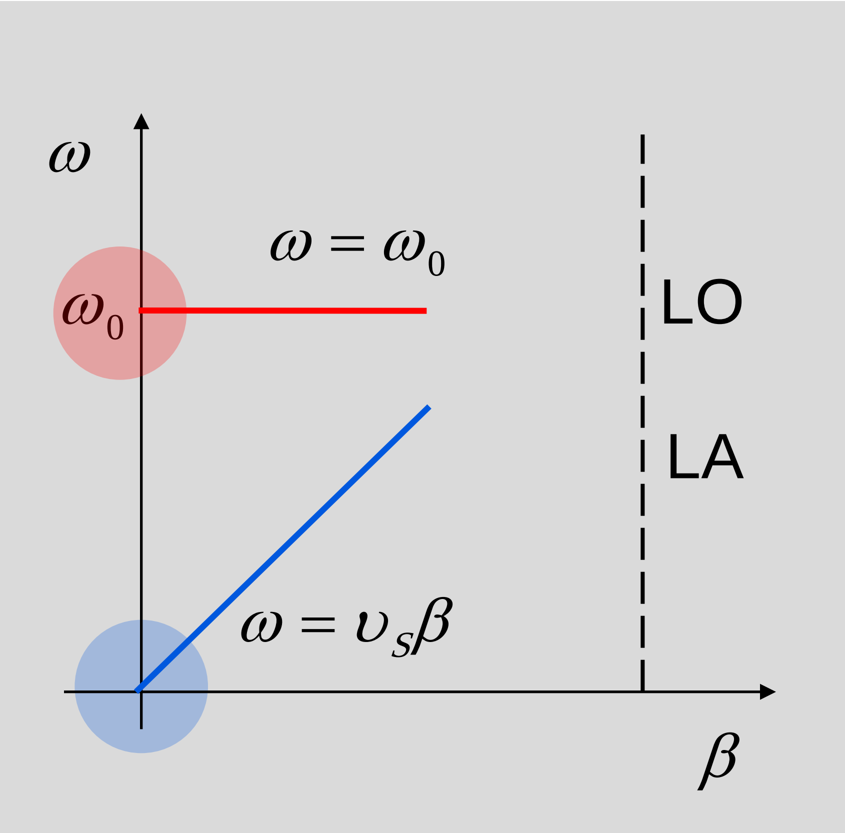
phonon scattering

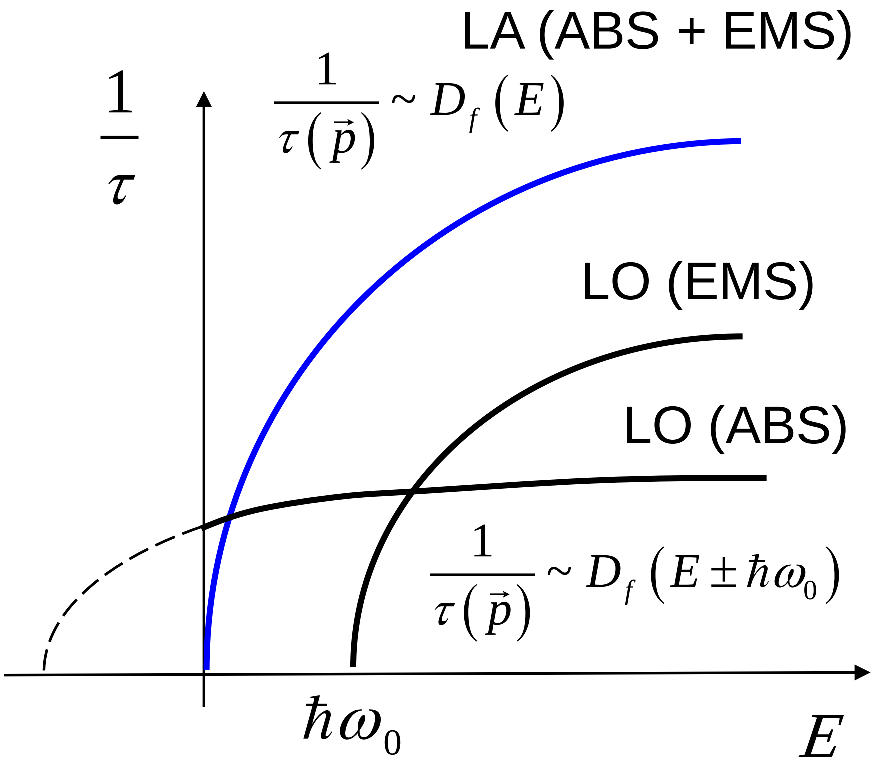
$$\frac{1}{\tau(\vec{p})} \sim D_f\left(E \pm \hbar\omega_0\right)$$



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

intravalley phonon scattering





outline

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

constraints on scattering

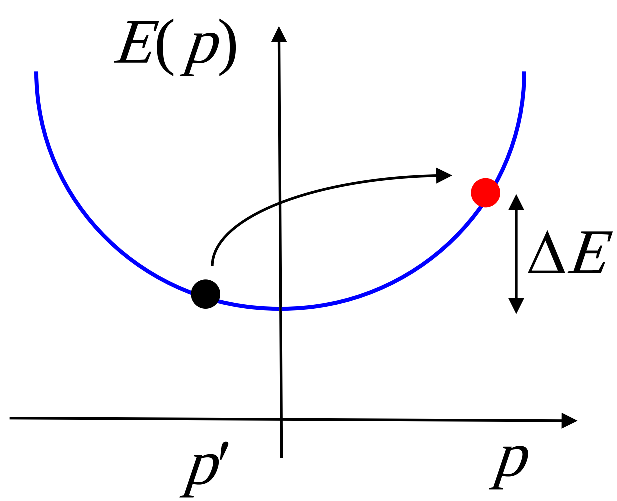
$$\hat{C}f = \sum_{p'} S(\vec{p}', \vec{p}) f(p')\left[1 - f(p)\right] - S(\vec{p}, \vec{p}') f(p)\left[1 - f(p')\right]$$

in equilibrium:

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

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

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



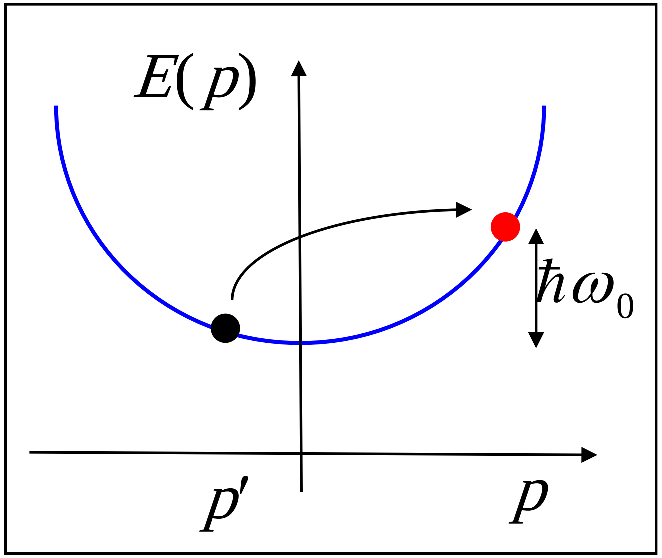
constraints on scattering

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

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

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

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



constraints on phonon scattering

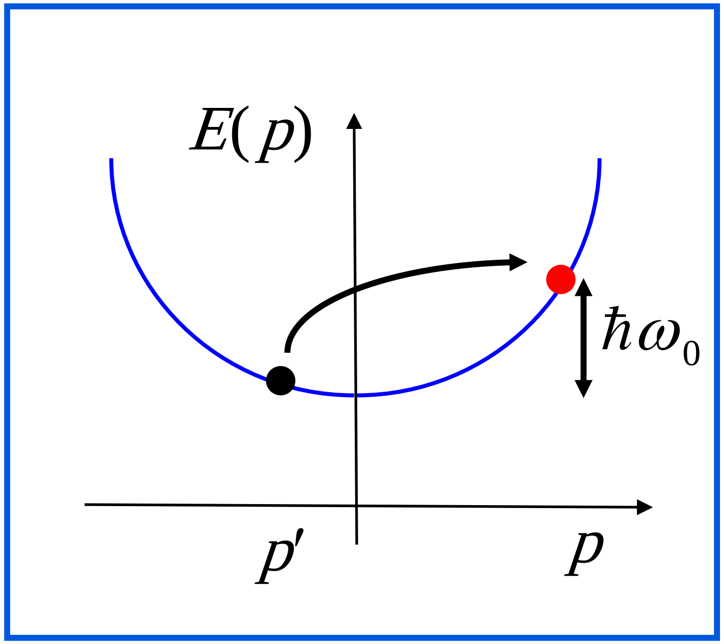
$$\frac{S^{ABS}\left(\vec{p}', \vec{p}\right)}{S^{EMS}\left(\vec{p}, \vec{p}'\right)} = e^{-\hbar\omega_0/k_B T} \quad S^{ABS}\left(\vec{p}', \vec{p}\right) \approx N_\omega \quad S^{EMS}\left(\vec{p}, \vec{p}'\right) \approx e^{\hbar\omega_0/k_B T} N_\omega$$

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

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

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

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



outline

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

summary

1) Characteristic times are derived from the transition rate, $S(p,p')$

2) $S(p,p')$ is obtained from Fermi's Golden Rule

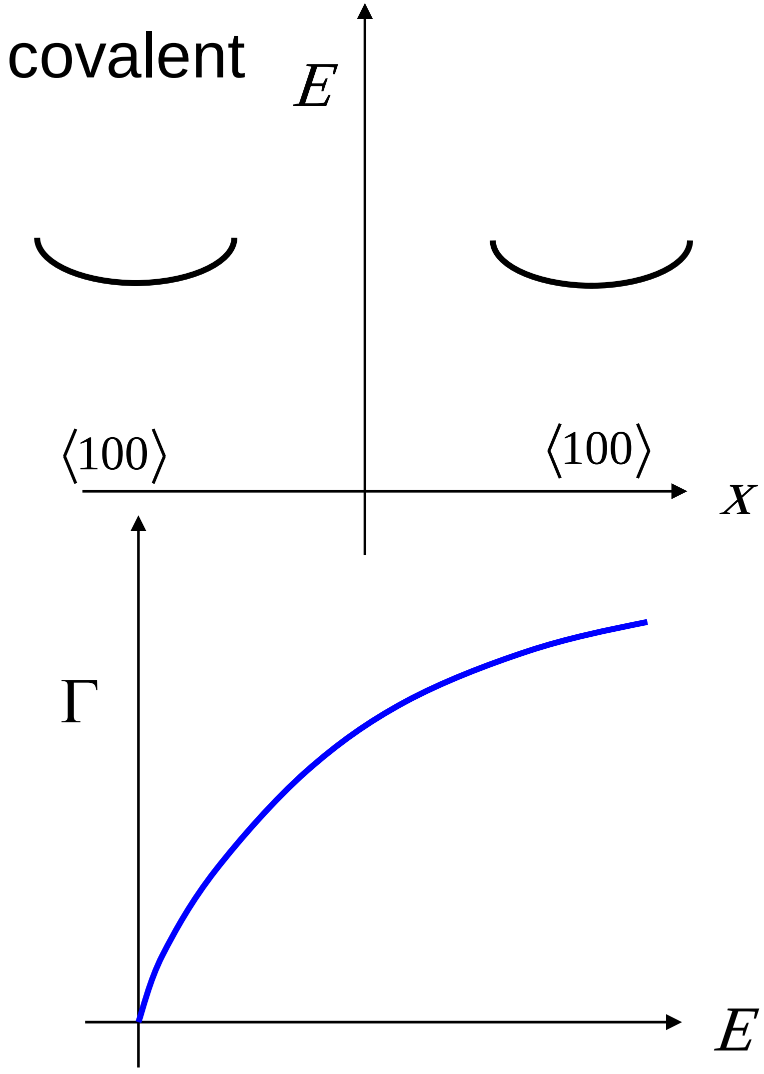
3) The scattering rate is proportional to the final DOS

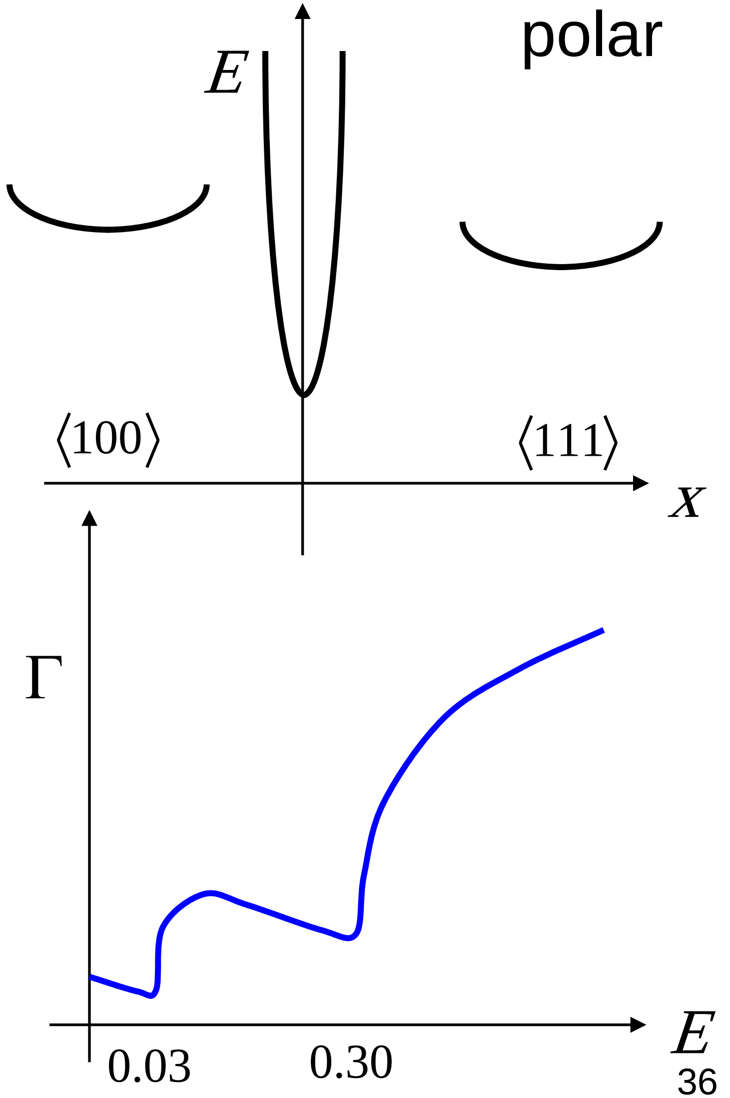
4) Static potentials lead to elastic scattering

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