Fermi's Golden Rule

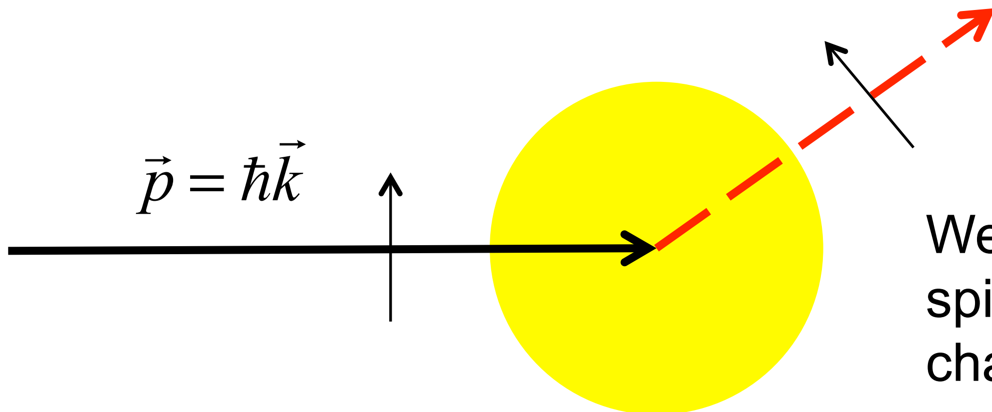
Mark Lundstrom

Electrical and Computer Engineering
Purdue University, West Lafayette, IN USA

8/31/17

Transition rate

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



We will assume that the spin state does not change during the scattering event.

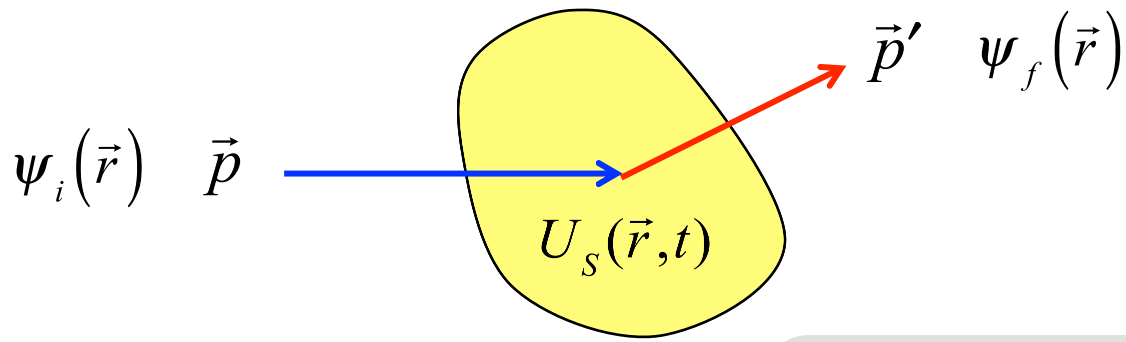
Probability per sec that an electron is scattered from a initial state to one particular final state.

Computed by “Fermi’s Golden Rule”

Outline

1) **Fermi's Golden Rule**
2) Example 1: Static scattering potential
3) Example 2: Delta-function scattering potential
4) Example 3: Oscillating scattering potential
5) Scattering by Acoustic and optical phonons
6) Summary

Fermi's Golden Rule



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

$$H_{\vec{p}',\vec{p}} = \int_{-\infty}^{+\infty} \psi_f^* U_{S0}(\vec{r}) \psi_i d\vec{r}$$

matrix element
(**note the order of the subscripts**)

$E' = E + \Delta E$

$\Delta E = 0$ for a static U_S

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

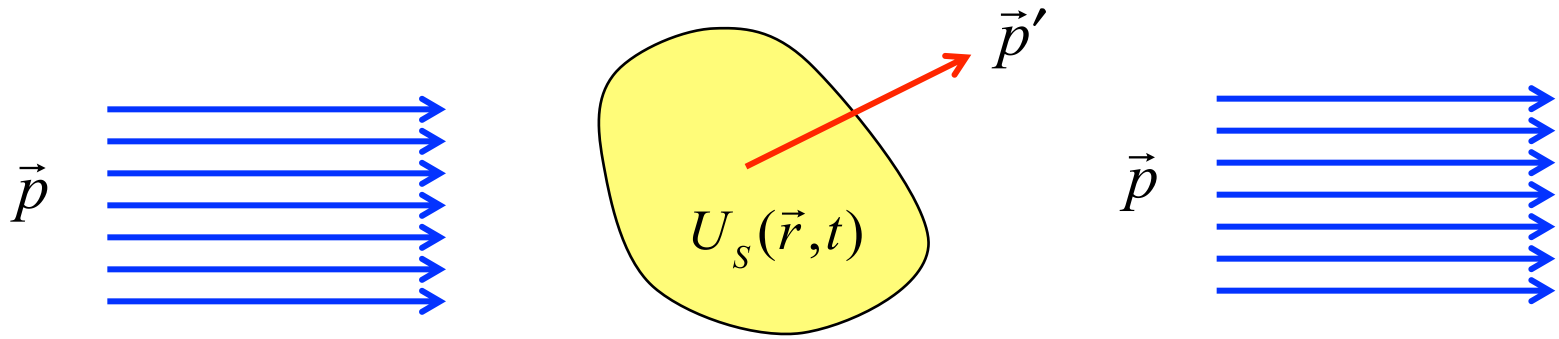
$U_{S0} e^{\pm i\omega t}$

References

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

See also J.H. Davies, *The Physics of Low-Dimensional Systems*, Cambridge Univ. Press, 1998. (Chapter 8, Secs. 8.1 and 8.3.)

FGR: Assumptions



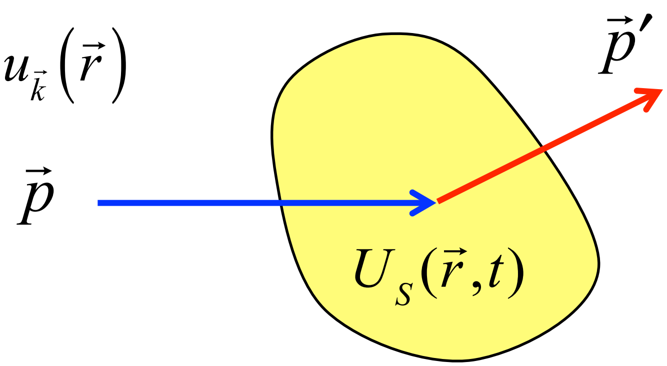
1) Weak scattering (Born approximation)
2) Infrequent scattering: $\Delta E \Delta t \approx \hbar$

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

Energy conservation comes at long times from FGR.

Scattering of **Bloch** waves

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



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

$$H_{\vec{p}',\vec{p}} = \int_{-\infty}^{+\infty} \psi_f^* U_S(\vec{r},t)\psi_i d\vec{r}$$

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

$$H_{\vec{p}',\vec{p}} = I\left(\vec{p},\vec{p}'\right)\frac{1}{\Omega}\int_{-\infty}^{+\infty} e^{-i\vec{p}'\bullet r/\hbar} U_S(\vec{r},t) e^{i\vec{p}\bullet\vec{r}/\hbar} d\vec{r}$$

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

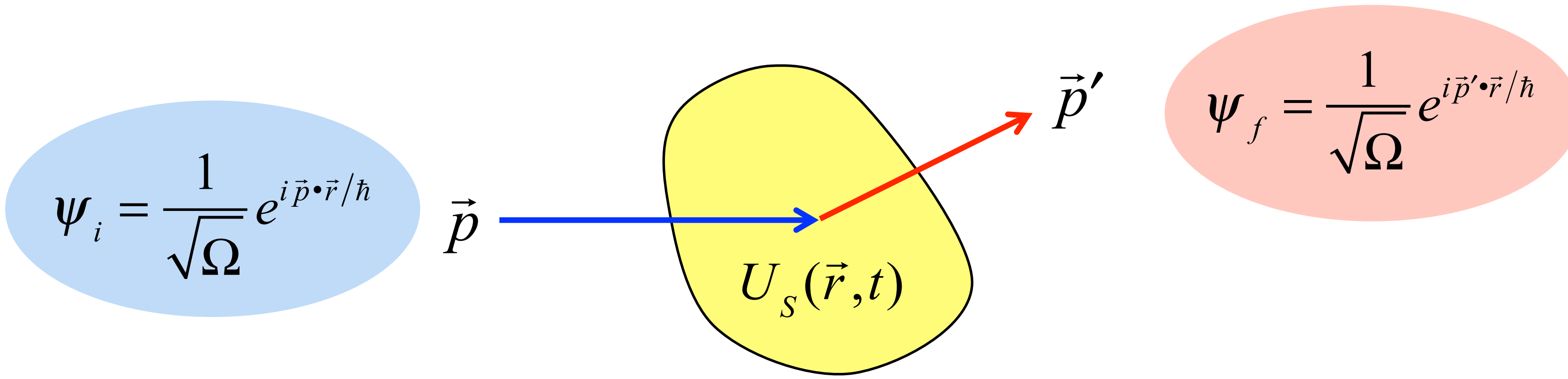
Overlap integrals

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



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

$$H_{\vec{p}',\vec{p}} = \int_{-\infty}^{+\infty} \psi_f^* U_{S0}(\vec{r})\psi_i d\vec{r}$$

$$H_{\vec{p}',\vec{p}} = \frac{1}{\Omega}\int_{-\infty}^{+\infty} e^{-i\vec{p}'\bullet r/\hbar} U_{S0}(\vec{r}) e^{i\vec{p}\bullet\vec{r}/\hbar} d\vec{r}$$

- Identify scattering potential
- Compute the matrix element
- Compute the transition rate
- Compute characteristics times

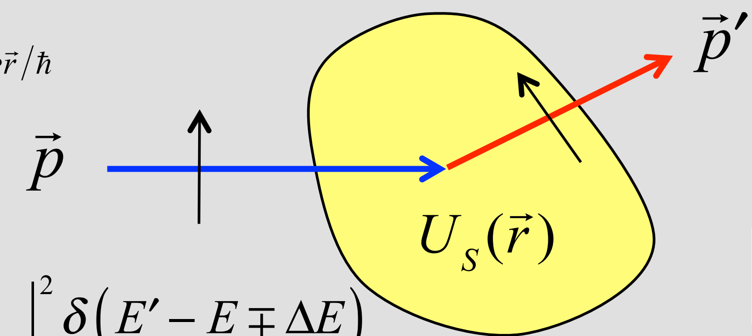
Outline

1) Fermi's Golden Rule
2) **Example 1: Static scattering potential**
3) Example 2: Delta-function scattering potential
4) Example 3: Oscillating scattering potential
5) Scattering by Acoustic and optical phonons
6) Summary

Example 1: Static potential

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

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



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

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

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

short range: neutral impurity

long range: charged impurity

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

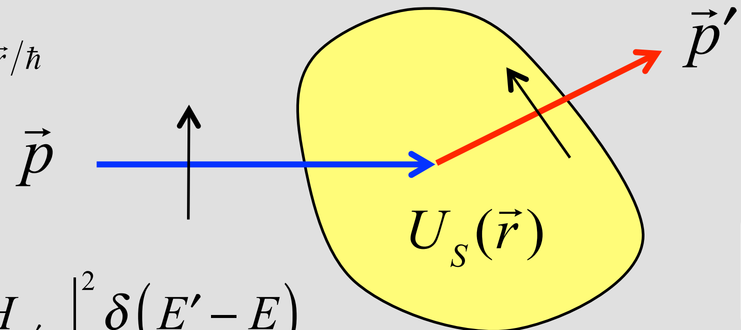
$$\vec{q} = \left(\vec{p} - \vec{p}'\right)/\hbar = \vec{k}' - \vec{k}$$

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

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

Ionized impurity scattering

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

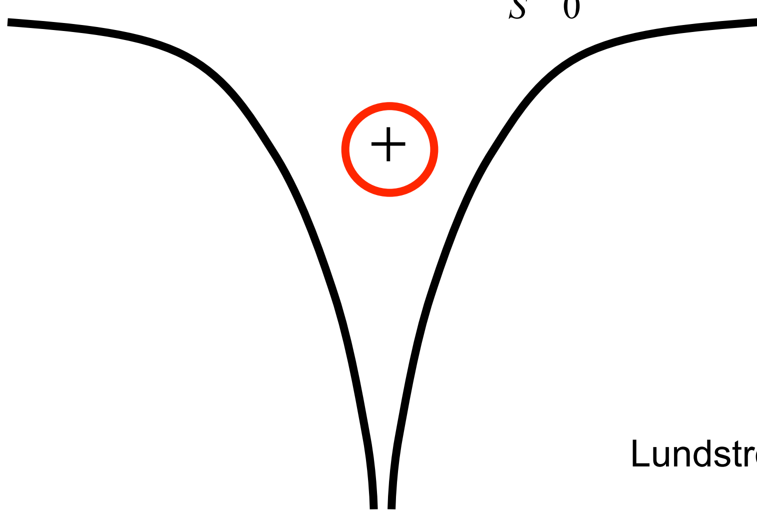


$$\psi_f = \frac{1}{\sqrt{\Omega}} e^{i\vec{p}'\bullet\vec{r}/\hbar}$$

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

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

$$U_S(\vec{r}) = \pm\frac{q^2}{4\pi\kappa_S\varepsilon_0 r}$$



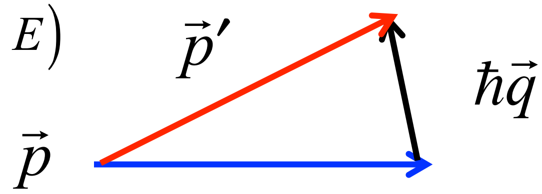
According to FGR, the transition rate is independent of the sign of the scattering potential.

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

Static potential summary

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

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



elastic
anisotropic

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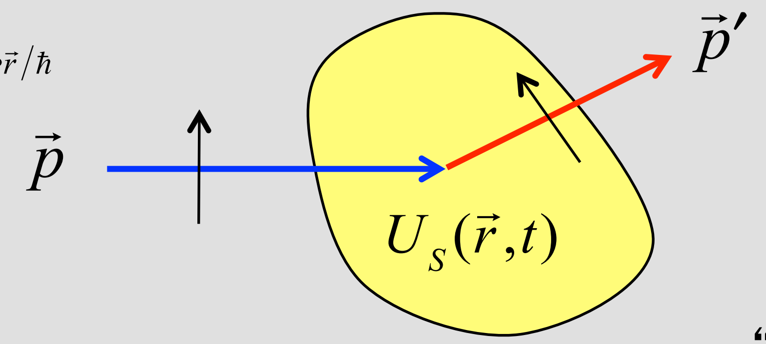
Example 2: Static delta-function potential

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



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

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

"short range potential"

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

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

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

Delta-function potential scattering rate

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

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

(Sum is over only the half of the final states with spin parallel to the initial state.)

$$\frac{1}{\tau(E)} \propto \frac{D(E)}{2}$$

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

Scattering rate summary

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

transition rate

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

out-scattering rate

$$\frac{1}{\tau(E)} \propto \frac{D(E)}{2}$$

result

Example 2: Momentum relaxation

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

$$\frac{1}{\tau_m(\vec{p})} \propto \frac{1}{\Omega}\sum_{\vec{p}',\uparrow}\delta(E'-E)(1-\cos\theta) = \frac{D(E)}{2} - \frac{1}{\Omega}\sum_{\vec{p}',\uparrow}\delta(E'-E)\cos\theta$$

$$\frac{1}{\Omega}\sum_{\vec{p}',\uparrow}\delta(E'-E)\cos\theta = \frac{\Omega}{8\pi^3}\frac{1}{\Omega}\int_0^{2\pi} d\phi\int_0^{\pi}\sin\theta\cos\theta d\theta\int_0^{\infty}\delta(E'-E)\,p^2\,dp = 0$$

$$\frac{1}{\tau_m(\vec{p})} = \frac{1}{\tau(\vec{p})} \propto \frac{D(E)}{2}$$

Elastic, isotropic scattering

Example 2: Summary

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

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

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

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

$$\frac{1}{\tau(E)} \propto D(E)$$

$$\frac{1}{\tau_m(E)} = \frac{1}{\tau(E)}$$ (isotropic)

$$\frac{1}{\tau_E(E)} = 0$$ (elastic)

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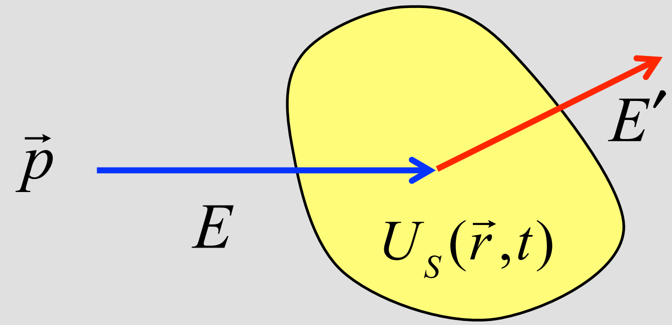
Example 3: Oscillating potential

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



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

$$U_S(\vec{r},t) = \frac{U_q^{a,e}}{\sqrt{\Omega}} e^{\pm i(\vec{q}\bullet\vec{r}-\omega t)}$$

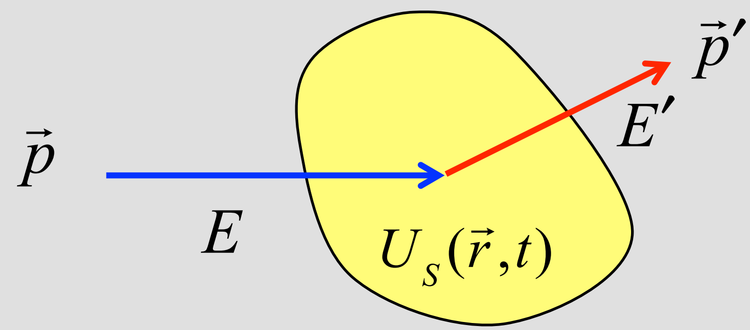
$$S(\vec{p},\vec{p}') = \frac{2\pi}{\hbar}\left|H_{\vec{p}',\vec{p}}\right|^2 \delta\left(E' - E \mp \Delta E\right) \qquad \Delta E = \pm\hbar\omega$$ (energy conservation)

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

$$H_{p',p} = \frac{U_q^{a,e}}{\sqrt{\Omega}}\delta\left(p' - \vec{p} \mp \hbar\vec{q}\right)$$ [(crystal) momentum conservation]

Momentum conservation

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

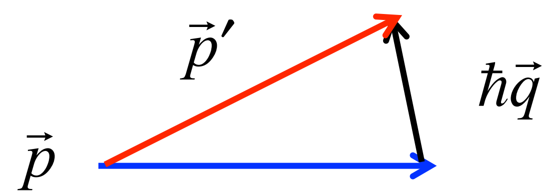


$$\psi_f = \frac{1}{\sqrt{\Omega}} e^{i\vec{p}'\bullet\vec{r}/\hbar}$$

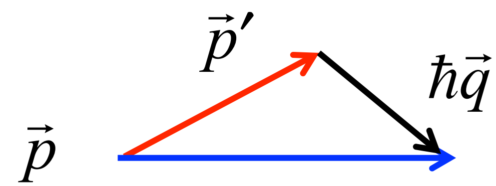
$$U_S(\vec{r},t) = \frac{U_q^{a,e}}{\sqrt{\Omega}} e^{\pm i(\vec{q}\bullet\vec{r}-\omega t)}$$

$$H_{p',p} = \frac{U_q^{a,e}}{\sqrt{\Omega}} \delta(\vec{p}' - \vec{p} \mp \hbar q)$$ (momentum conservation)

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

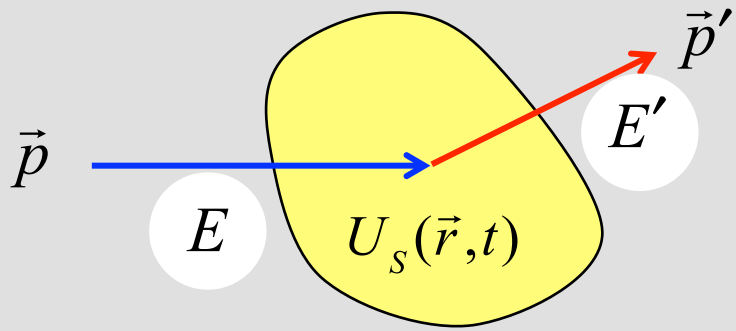


$\vec{p}' = \vec{p} - \hbar\vec{q}$ (EMS)



Energy **and** momentum conservation

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



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

$$U_S(\vec{r},t) = \frac{U_q^{a,e}}{\sqrt{\Omega}} e^{\pm i(\vec{q}\bullet\vec{r}-\omega t)}$$

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

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

Scattering rate

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

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

$$\frac{1}{\tau(\vec{p})} = \sum_{\vec{p}\,'\uparrow} S(\vec{p},\vec{p}\,') = K^{a,e}\frac{1}{\Omega}\sum_{p'\uparrow}\delta\left(E' - E \mp \hbar\omega\right) \qquad \text{(isotropic scattering)}$$

$$\frac{1}{\tau(E)} = K^{a,e}\frac{D_f\left(E \pm \hbar\omega\right)}{2} \propto D_f\left(E \pm \hbar\omega\right)$$

Scattering rate is proportional to the density of final states.

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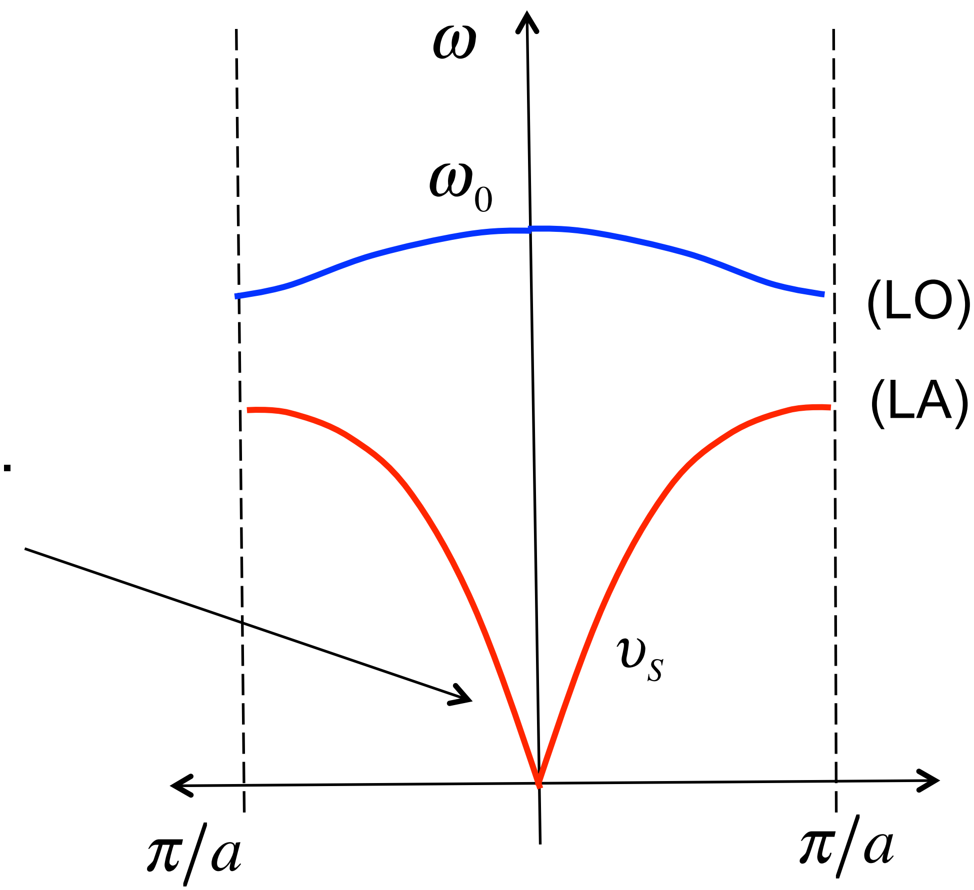
Acoustic phonon scattering

Typical phonons involved in intra-valley acoustic phonon scattering.

$\hbar\omega \approx 0$

(at 300 K)



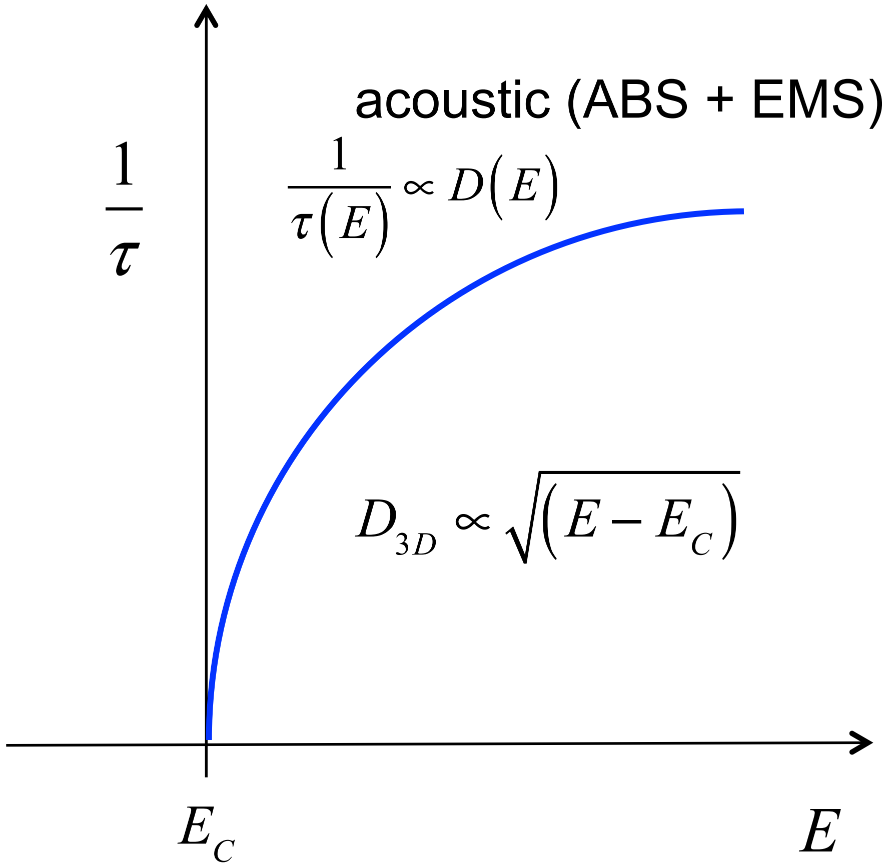
Acoustic phonon scattering

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

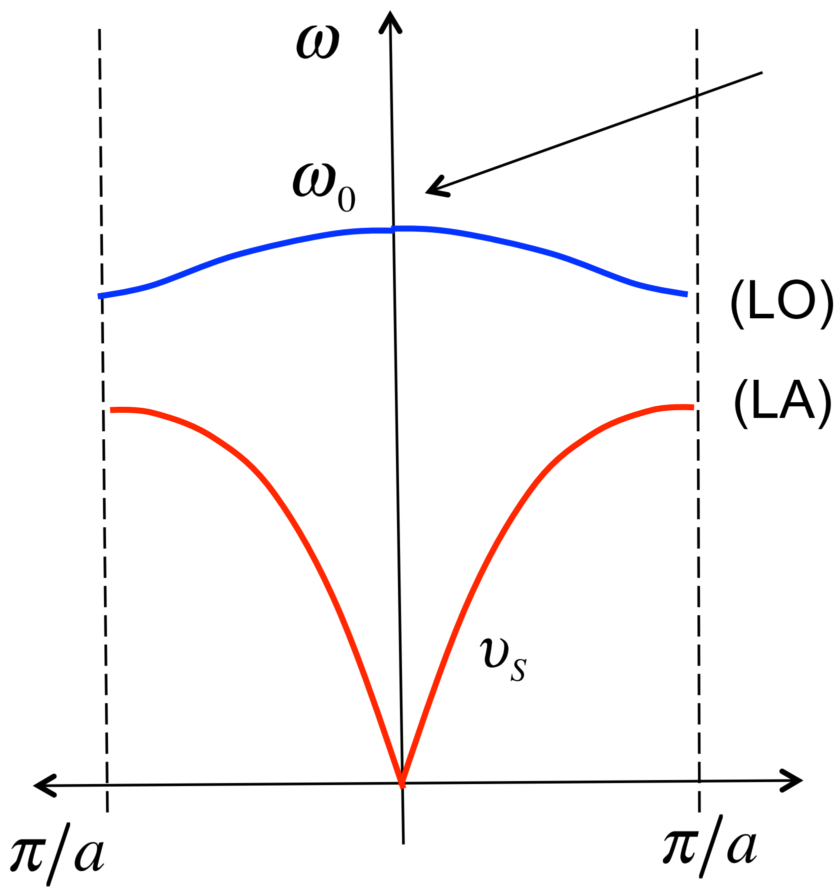
i) Acoustic phonons

$$\hbar\omega << k_B T$$

$$1/\tau_{abs}(E) = 1/\tau_{ems}(E) \propto D(E)/2$$



Optical phonon scattering



Typical phonons involved in intra-valley optical phonon scattering.

$$\hbar\omega \approx k_B T$$

(at 300 K)

Optical phonon scattering

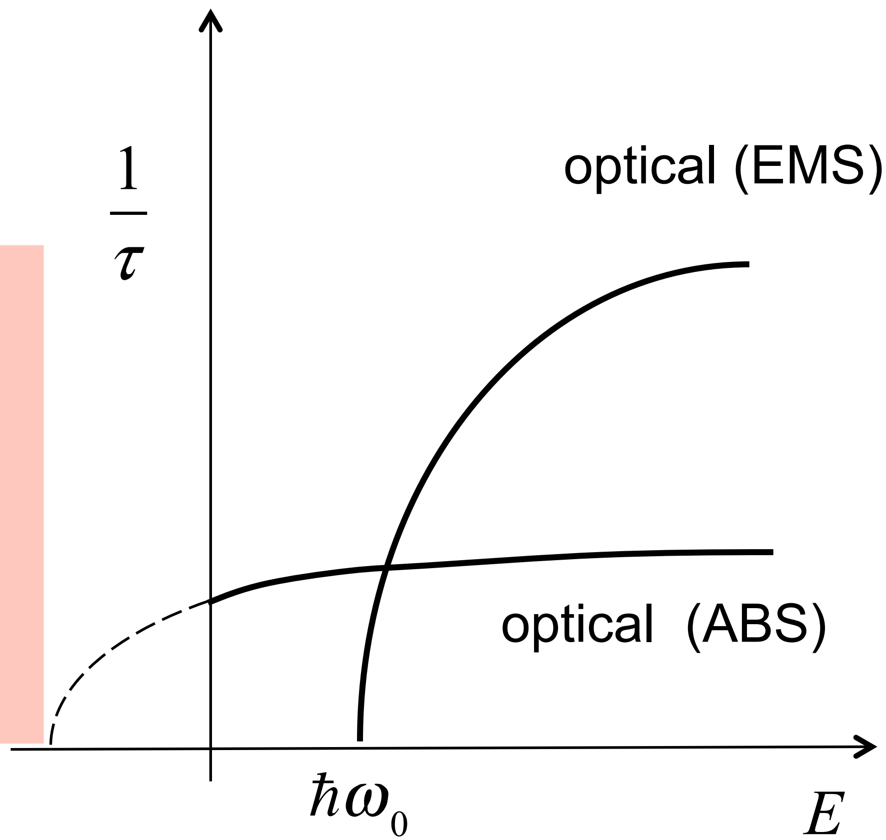
$$\frac{1}{\tau(E)} \propto D_f\left(E \pm \hbar\omega\right)$$

ii) Optical phonons

$$\hbar\omega \approx \hbar\omega_0 > k_B T_L$$

$$1/\tau_{abs}(E) \propto D\left(E + \hbar\omega_0\right)/2$$

$$1/\tau_{ems}(E) \propto D\left(E - \hbar\omega_0\right)/2$$



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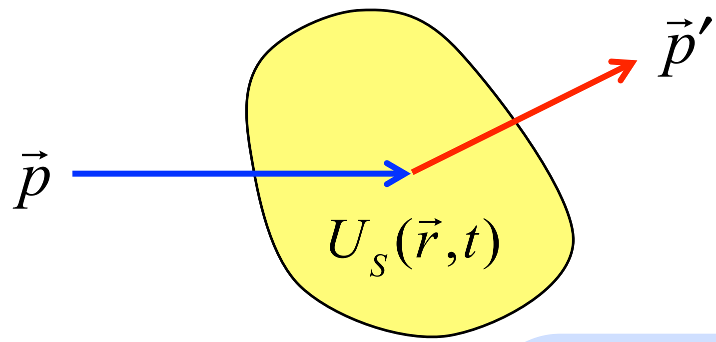
Procedure

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



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

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

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

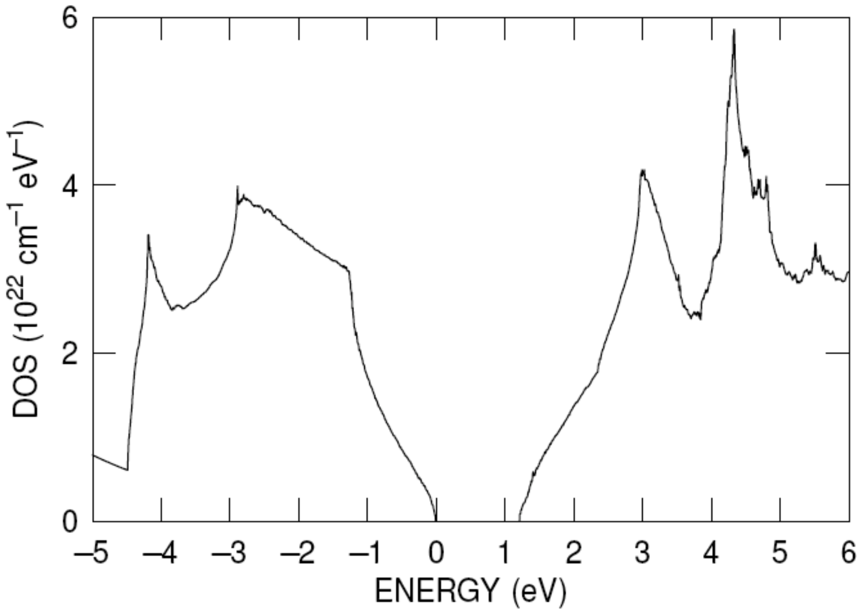
1) Identify the scattering potential

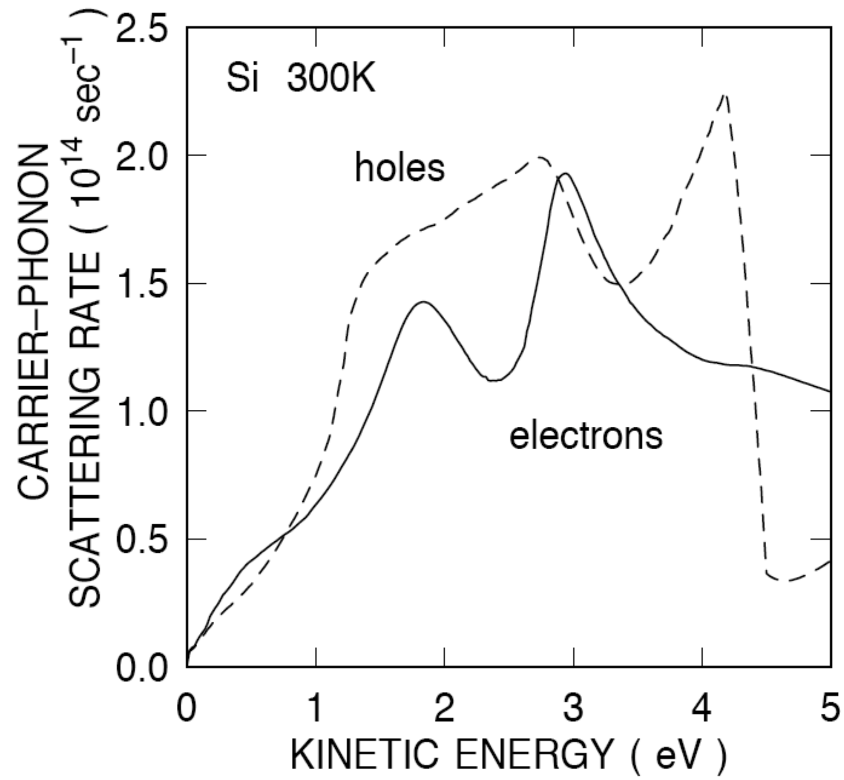
2) Specify the wavefunction (e.g. 1D, 2D, 3D)

3) Compute the matrix element and transition rate.

4) Compute the characteristics times.

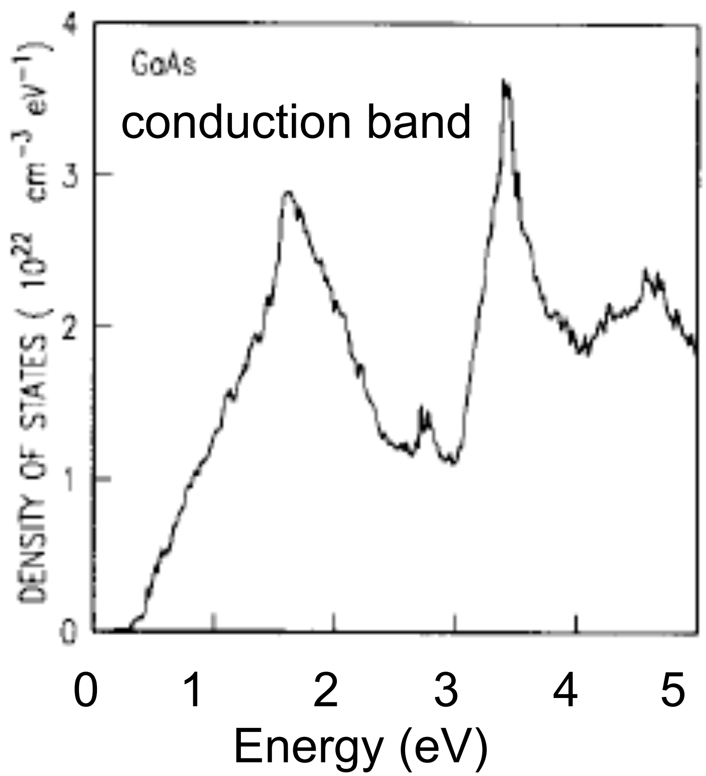
Phonon scattering in Si

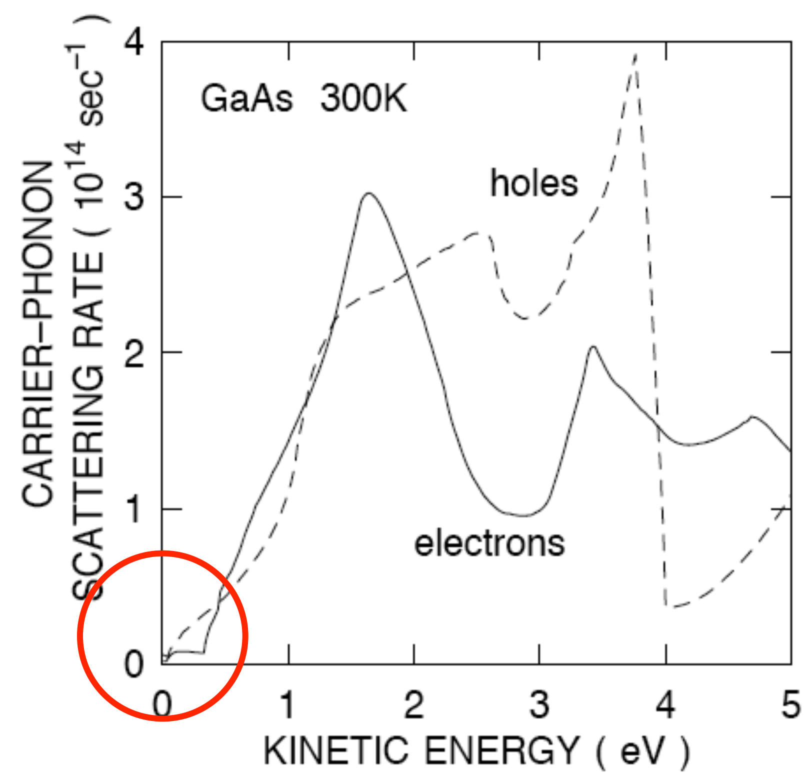




[2] Figures provided by Massimo V. Fischetti, October, 2009.

Phonon scattering 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

In addition to phonons and ionized impurities:

1) Neutral impurity

2) Alloy scattering

3) Surface / edge roughness scattering

4) Plasmon scattering

5) Electron-electron scattering

6) Electron-hole

Summary

1) Characteristic times are derived from the transition rate, $S(p,p')$
2) $S(p,p')$ is obtained from FGR
3) Static potentials of fixed objects lead to elastic scattering
4) Time varying potentials lead to inelastic scattering
5) The scattering rate is proportional to the final DOS
6) Our goal is to understand the general features of scattering in common semiconductors.