Acoustic Phonon Scattering

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Introductory Notes

We will calculate scattering rates:

The governing equation is:

$$S(\vec{k},\vec{k}') = \frac{2\pi}{\hbar}|V_{kk}|^2 \delta(E_{k'} - E_k \pm \hbar\omega)$$

matrix element of perturbation

long time limit leads to energy conservation…no collisional broadening

Two cases for Matrix element:

(a) δ -function perturbation for which the matrix element is constant.

(b) Matrix element is a function of the momentum transfer of the system.

(a) Constant Matrix element:

$$S(\vec{k},\vec{k}') = \frac{2\pi}{\hbar}|V_0|^2 \delta(E_{k'} - E_k \pm \hbar\omega_0)$$

The total scattering rate out of a state $\vec{k}$ is given by:

$$\frac{1}{\tau(\vec{k})} = \sum_{\vec{k}',\uparrow} S(\vec{k},\vec{k}') = \frac{2\pi|V_0|^2}{\hbar}\frac{\Omega}{(2\pi)^3}\int_0^{2\pi} d\varphi \int_{-1}^{1} d(\cos\theta)\int_0^{\infty} k'^2 dk' \delta(E_{k'} - E_k \pm \hbar\omega_0)$$

(nondegenerate semiconductor: state at p' is empty)

Assuming parabolic energy bands and doing the integration:

$$\frac{1}{\tau(\vec{k})} = \frac{2\pi|V_0|^2}{\hbar}\frac{1}{2} g_c(E_k \mp \hbar\omega_0)$$

- Description of the acoustic phonon scattering in the *elastic* and *equipartition* approximation.
- The more final states are available the higher the scattering rates…..*makes sense*.
- Only those final states with spin *parallel* to the incident electron's are available.

(b) Momentum dependent matrix element:

Used in general description of phonon scattering and given by:

$$S(\vec{k},\vec{k}') = \frac{2\pi}{\hbar}\left|M(\vec{k},\vec{k})\right|^2 \delta(E_{k'} - E_k \pm \hbar\omega_0)\delta(\vec{k}' - \vec{k} \pm \vec{q})$$

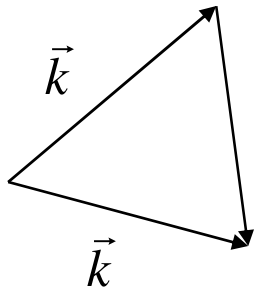
Long time limit leads to energy conservation.

Momentum is always conserved.

To establish a relation between E and q :

$$E_{k'} - E_k \pm \hbar\omega_0 = \frac{\hbar^2}{2m^*}k'^2 - \frac{\hbar^2}{2m^*}k^2 \pm \hbar\omega_0$$

$$= \frac{\hbar^2 kq}{2m^*}\left[\frac{q}{2k} \mp \cos\theta \pm \frac{m^*\omega_0}{\hbar kq}\right]$$



$$\vec{k}' = \vec{k} + \vec{q}$$

Using the following relationship:

$$\delta[ax] = \frac{1}{|a|}\delta(x)$$

We arrive at the general expression:

$$S(\vec{k},\vec{k}') = \frac{2\pi}{\hbar}\left|M(\vec{k},\vec{k})\right|^2 \frac{m^*}{\hbar^2 kq}\delta\left(\frac{q}{2k} \mp \cos\theta \pm \frac{m^*\omega_0}{\hbar kq}\right)$$

We can integrate the expression in terms of the momentum transfer $\vec{q}$ in the scattering process. After doing the integration:

$$\frac{1}{\tau(\vec{k})} = \frac{m^*\Omega}{2\pi\hbar^3 k}\int_{q_{\min}}^{q_{\max}} q\left|M(\vec{k},\vec{k})\right|^2 dq$$

Where the limits of the integration are obtained from setting the argument of the δ function to zero, *i.e.*

$$\frac{q}{2k} \mp \cos\theta \pm \frac{m^*\omega_0}{\hbar kq} = 0$$

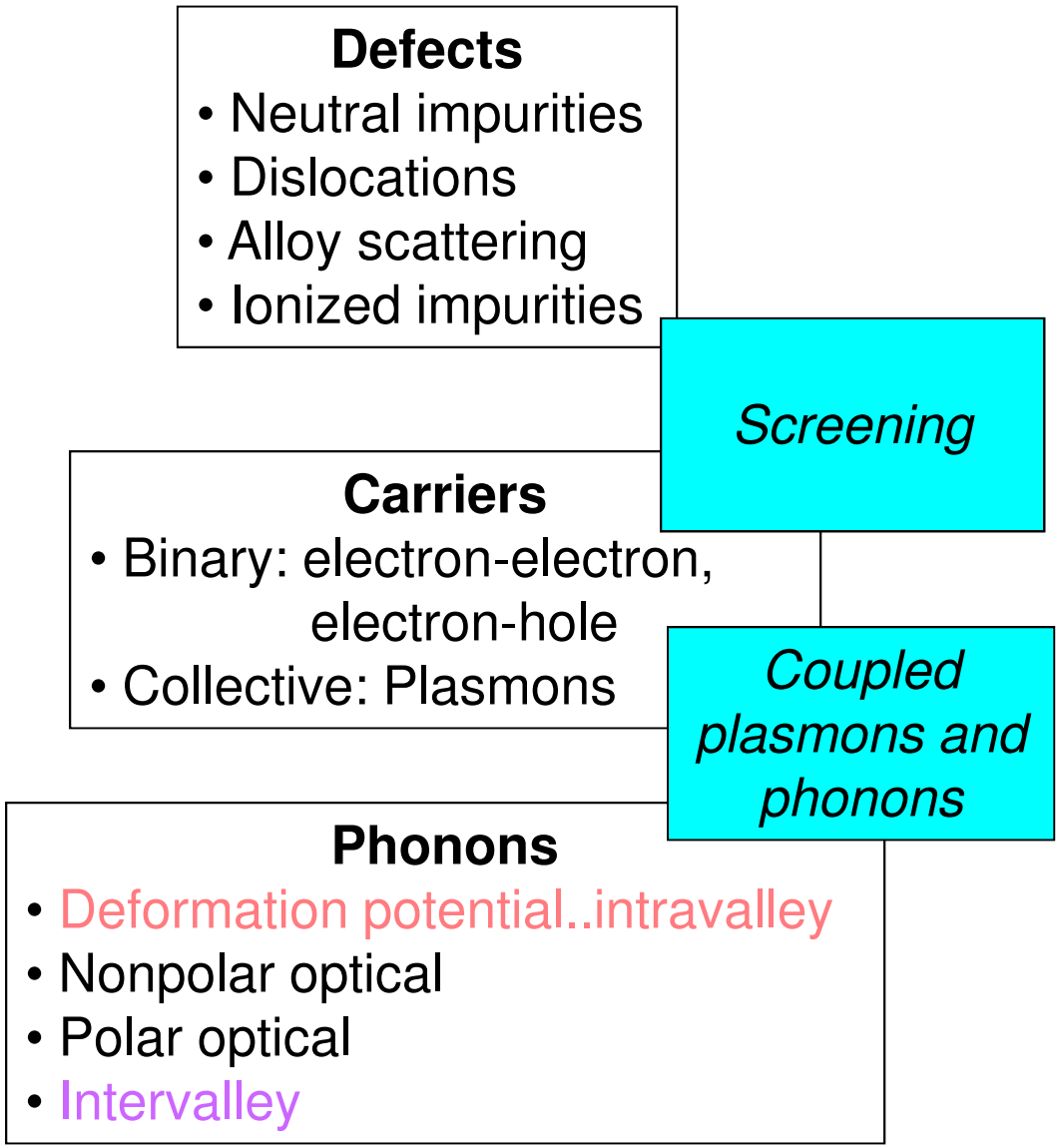
Common scattering mechanisms in semiconductors:

Our goal is to study *electron* scattering in common semiconductors. *Hole* scattering is complicated:

- ✓ There exist *degenerate* heavy and light hole bands with their warped constant energy surfaces.
- ✓ For energetic carriers, *overlap integrals* need to be considered and even a detailed, numerical description of band structure is needed.

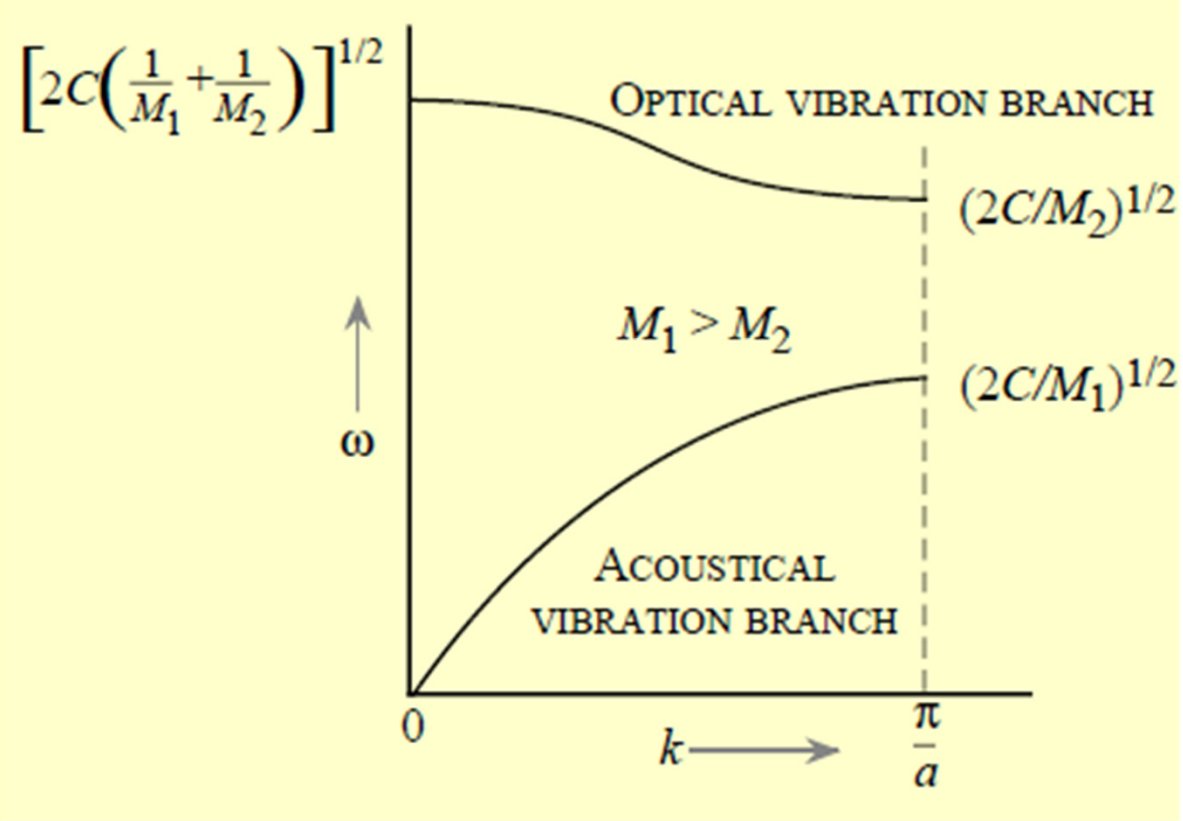
The total scattering rate:

$$\Gamma(k) = \sum_i \frac{1}{\tau_i(k)}$$


Defects
• Neutral impurities
• Dislocations
• Alloy scattering
• Ionized impurities
Screening
Carriers
• Binary: electron-electron, electron-hole
• Collective: Plasmons
Coupled plasmons and phonons
Phonons
• Deformation potential..intravalley
• Nonpolar optical
• Polar optical
• Intervalley

Description of Acoustic Deformation Potential Scattering

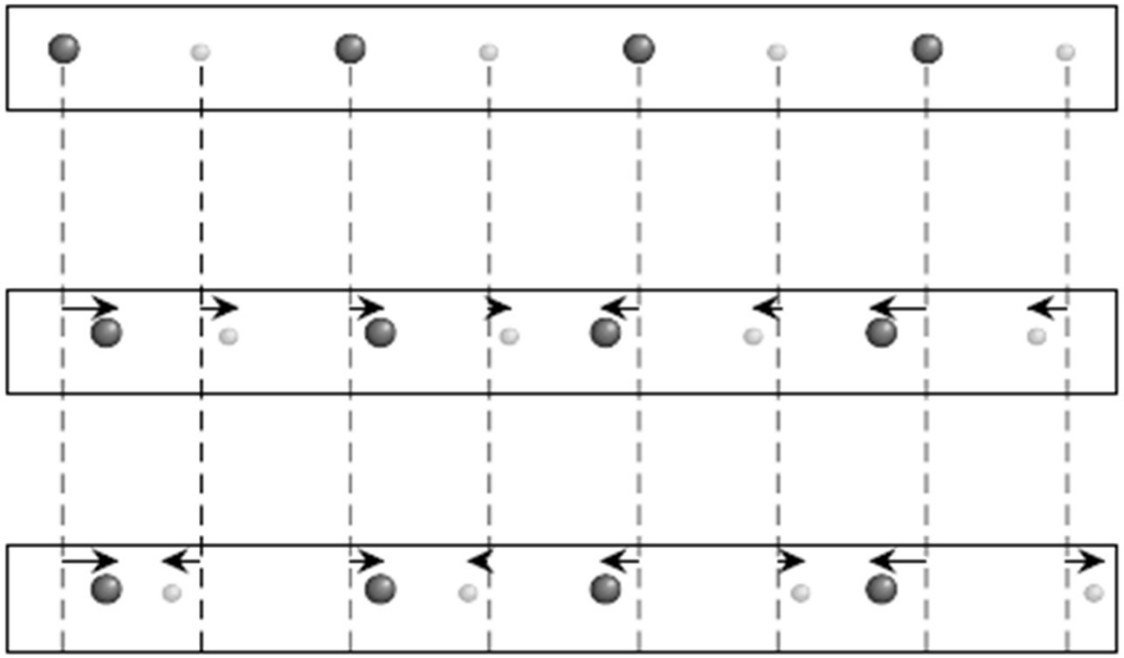
Solutions for a simple diatomic lattice model



Near $k = 0$

$$\omega^2 \approx 2C\left(\frac{1}{M_1}+\frac{1}{M_2}\right) \qquad \text{Optical branch}$$

$$\omega^2 \approx \frac{C/2}{M_1+M_2}\,k^2a^2 \qquad \text{Acoustic branch}$$

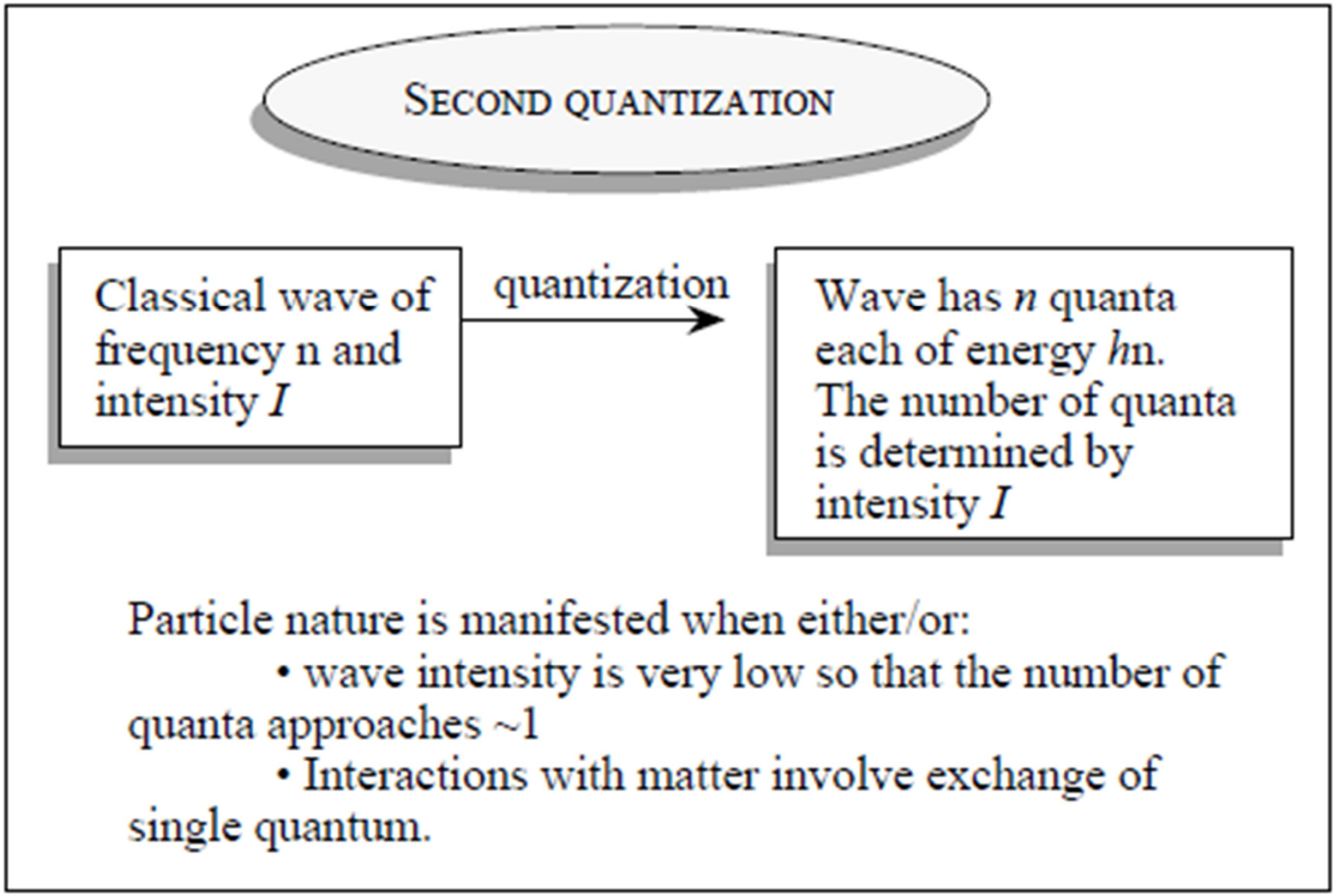


(a)

EQUILIBRIUM POSITIONS OF ATOMS

ACOUSTICAL VIBRATION: The two atoms on the unit cell vibrate along the same direction

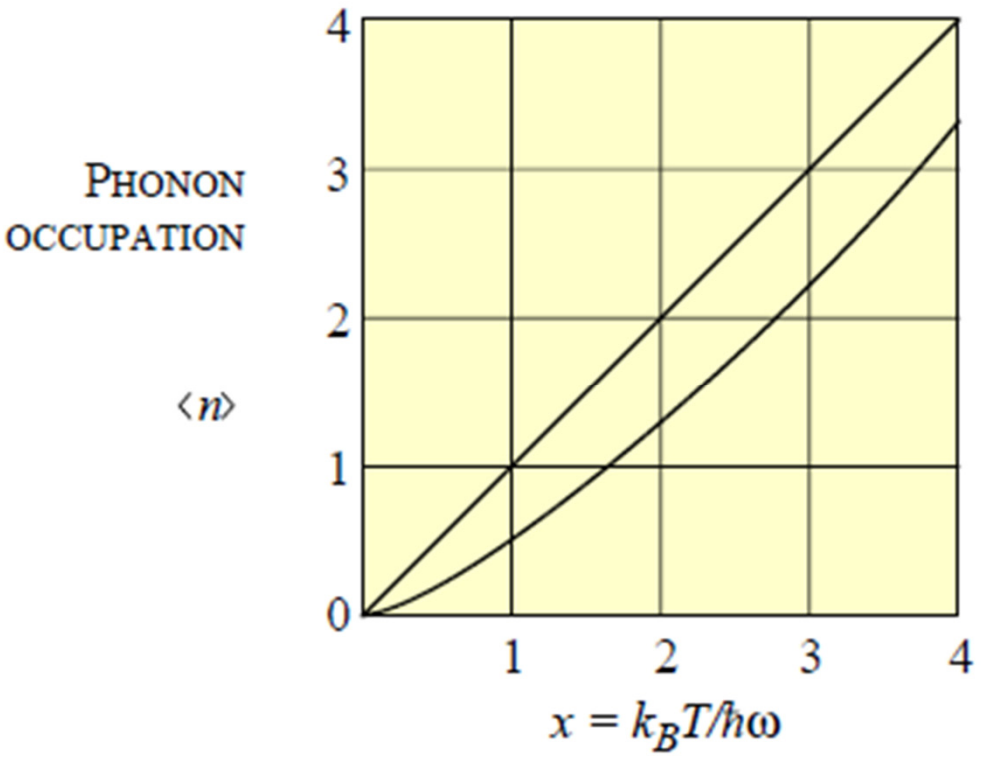
OPTICAL VIBRATION: The two atoms on the unit cell vibrate in opposing motion.



A conceptual picture of second quantization.

Bose Einstein statistics

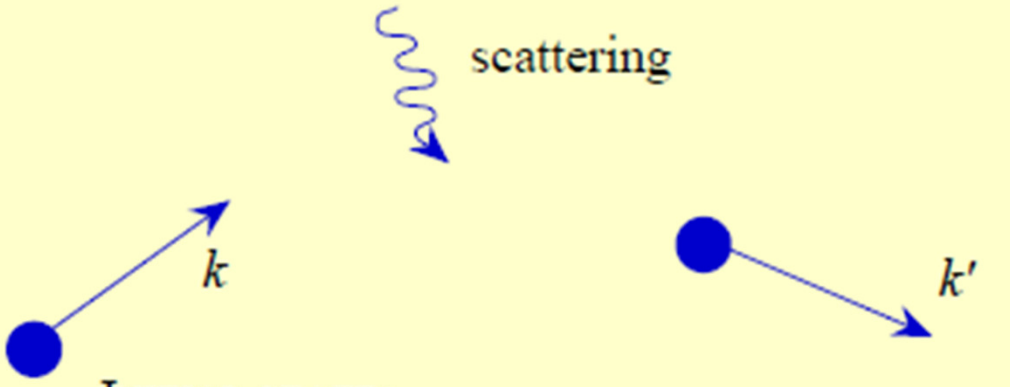
$$\langle n(\omega)\rangle = \frac{1}{\exp\left(\frac{\hbar\omega}{k_B T}\right) - 1}$$



$$\hbar\omega \ll k_B T$$

$$\langle n\rangle \sim \frac{k_B T}{\hbar\omega}$$

SCATTERING PROBLEM



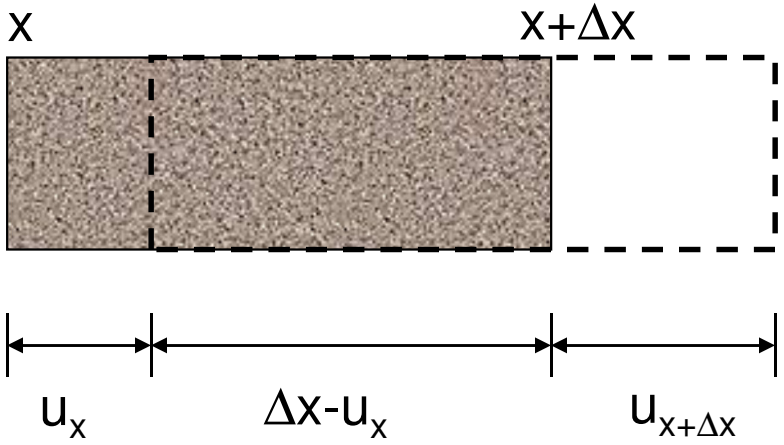
INITIAL STATE:
electron: k
phonons: $|n_{qb}\rangle$

FINAL STATE:
electron: k'
phonons: $|n'_{qb}\rangle$

ABSORPTION OF PHONON: $n' = n - 1$

EMISSION OF PHONONS: $n' = n + 1$

Strain Tensor…a concept:



Fractional change in length:

$$\frac{\partial u_x}{\partial x} = s(x) = \varepsilon_{xx}$$

New length becomes,

$$\Delta x' = \Delta x + \varepsilon_{xx}\Delta x = (1+\varepsilon_{xx})\Delta x$$

Extending this concept for a volume, one gets the volume dilation:

$$\frac{\delta V}{V} \approx \varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz} = \frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial x} + \frac{\partial u_z}{\partial x} = \nabla \cdot \vec{u} = \Delta$$

Deformation potential scattering: Intravalley

- long wavelength phonons are considered. Vibrations of the solid resemble those of an elastic continuum.
- The essential concept due to Bardeen and Shockley: For a *solid* continuum.

$$\delta E_n(\vec{k}) = \sum_{\alpha\beta} \Xi_{\alpha\beta} S_{\alpha\beta}$$

where $\Xi_{\alpha\beta}$ is the deformation potential tensor.

- The above concept is verified by a simple example:

Fermi level expression (low Temp): $E_F = \left(\frac{3\pi^2 N}{V}\right)^{2/3} \frac{\hbar}{2m^*}$

For a change in volume by an amount δV:

$$\delta E_F = -\frac{2}{3} E_F \frac{\delta V}{V} = -\frac{2}{3} E_F \Delta = c\Delta$$

The deformation potential is now expressed in terms of phonon coordinates with the position as a *continuous variable* rather and from an *atomic* point of view:

$$\Delta = \nabla \cdot \vec{u}$$

$$= \sum_{q,\nu} \sqrt{\frac{\hbar}{2mN\,\omega_{q\nu}}}\,\vec{q}\cdot\vec{e}_{q\nu}\left[\hat{a}_{\vec{q},\nu}\,e^{i\vec{q}.\vec{r}} - \hat{a}^{+}_{\vec{q},\nu}\,e^{-i\vec{q}.\vec{r}}\right]$$

Now, we would interpret δE_F as the deformation potential electron-Phonon interaction. This leads to:

$$H_{ep,dp} = c\Delta = \Xi_{ac}\nabla_r \cdot \vec{u}$$

Recast:

Let H_{ep} be the electron-phonon interaction. To describe the interaction one needs to evaluate the matrix element of the form:

$$M_{fi} = \sum_{q\nu} \left\langle \psi_f \left| \hat{u}_{q\nu}(\vec{R},t) H_{q\nu}(\vec{r}) \right| \psi_i \right\rangle$$

Ion displacement at $\vec{R}$ location In the crystal

Electronic component of the electron-phonon interaction

Substituting the values leads to:

$$M_{fi} = \sum_{q\nu} \frac{1}{V} \int d\vec{r} u_{n'k'}{}^{*} e^{-i\vec{k}'\cdot\vec{r}} H_{q\nu}(\vec{r}) u_{nk} e^{i\vec{k}\cdot\vec{r}}$$

$$\cdot \prod_{q_i b_i} \prod_{q_j b_j} \sqrt{\frac{\hbar}{2mn\omega_{q\nu}}} \left\langle Q_{q_j b_j} n_{q_j b_j} \left| \hat{a}_{q\nu} e^{i\vec{q}\cdot\vec{R}} + \hat{a}_{q\nu}{}^{+} e^{-i\vec{q}\cdot\vec{R}} \right| Q_{q_i b_i} n_{q_i b_i} \right\rangle$$

The integration over the phonon coordinates leads to the condition That $q = q_j = q_i$ and $\nu = b_i = b_j$, which leaves only one term in the double product. Since the number of phonons in a given mode of lattice vibrations is not necessarily conserved, we have that, in general,

$$\left\langle n'_{q\nu} \left| \hat{a}_{q\nu} e^{i\vec{q}\cdot\vec{R}} + \hat{a}_{q\nu}{}^{+} e^{-i\vec{q}\cdot\vec{R}} \right| n_{q\nu} \right\rangle$$

$$= e^{i\vec{q}\cdot\vec{R}} \left\langle n'_{q\nu} \left| \hat{a}_{q\nu} \right| n_{q\nu} \right\rangle + e^{-i\vec{q}\cdot\vec{R}} \left\langle n'_{q\nu} \left| \hat{a}_{q\nu}{}^{+} \right| n_{q\nu} \right\rangle$$

$$= e^{i\vec{q}\cdot\vec{R}} \sqrt{n_{q\nu}}\, \delta_{n_{q\nu'}, n_{q\nu}-1} + e^{-i\vec{q}\cdot\vec{R}} \sqrt{n_{q\nu}+1}\, \delta_{n_{q\nu'}, n_{q\nu}+1}$$

# of phonons in final state

# of phonons in initial state

$n'_{q\nu} = n_{q\nu} - 1$

ABSORPTION

$n'_{q\nu} = n_{q\nu} + 1$

EMISSION

After the integration over the phonon coordinates, the expression simplifies to:

$$M_{fi} = \sum_{q\nu} \begin{bmatrix} (n_{q\nu})^{1/2} \\ (n_{q\nu}+1)^{1/2} \end{bmatrix} \sqrt{\frac{\hbar}{2mn\omega_{q\nu}}} \frac{1}{V} \int_V d\vec{r} u_{n'k'}^{*} e^{i(\vec{k}-\vec{k}')\cdot\vec{r}} H_{q\nu}(\vec{r}) e^{\pm i\vec{q}\cdot\vec{R}} u_{nk}$$

Because of the periodic properties of the Bloch function and of the integration, the integral over the crystal can be factored into an integral over a unit cell, and a sum over all unit cells. This is achieved by using:

$$\vec{r} = \vec{R} + \vec{r}'$$

Lattice vector
(location of unit cell)

Vector within
the unit cell

Therefore:

$$\frac{1}{V}\int_V d\vec{r} u_{n'k'}^{*} e^{i(\vec{k}-\vec{k}')\cdot\vec{r}} H_{q\nu}(\vec{r}) e^{\pm i\vec{q}\cdot\vec{R}} u_{nk}$$

$$= \frac{1}{V}\sum_R \int_\Omega d\vec{r}' u_{n'k'}^{*}(\vec{r}'+\vec{R}) e^{i(\vec{k}-\vec{k}')\cdot(\vec{r}+\vec{R})} e^{\pm i\vec{q}\cdot\vec{R}} H_{q\nu}(\vec{r}'+\vec{R}) u_{nk}(\vec{r}'+\vec{R})$$

$$= \frac{1}{V}\sum_R e^{i(\vec{k}-\vec{k}'\pm\vec{q})\cdot\vec{R}} \int_\Omega d\vec{r}' u_{n'k'}^{*}(\vec{r}') e^{i(\vec{k}-\vec{k}')\cdot\vec{r}'} H_{q\nu}(\vec{r}') u_{nk}(\vec{r}')$$

$$= \frac{N}{V}\delta_{\vec{k}-\vec{k}'\pm\vec{q},\vec{G}} \int_\Omega d\vec{r}' u_{n'k'}^{*}(\vec{r}') e^{i(\vec{k}-\vec{k}')\cdot\vec{r}'} H_{q\nu}(\vec{r}') u_{nk}(\vec{r}')$$

$$= \delta_{\vec{k}-\vec{k}'\pm\vec{q},\vec{G}} \frac{1}{\Omega}\int_\Omega d\vec{r}' u_{n'k'}^{*}(\vec{r}') e^{i(\vec{k}-\vec{k}')\cdot\vec{r}'} H_{q\nu}(\vec{r}') u_{nk}(\vec{r}')$$

$$C_{q\nu} I_{nn'}(\vec{k},\vec{k}')$$

$$I_{nn'}(\vec{k},\vec{k}') = \int_\Omega d\vec{r}' \psi_{n'k'}^{*}(\vec{r}') \psi_{nk}(\vec{r}')$$

$$C_{q\nu} I_{nn'}(\vec{k},\vec{k}') = \int_\Omega d\vec{r}' \psi_{n'k'}^{*}(\vec{r}') H_{q\nu}(\vec{r}') \psi_{nk}(\vec{r}')$$

So *comparing* this equation for the previously derived expression For M_{fi}:

$$C_{q\nu} = \Xi_{ac}\vec{q}\cdot\vec{e}_{q\nu} = \Xi_{ac}q \quad \text{,when } \vec{e}_{q\nu} \parallel \vec{q} \qquad \text{(longitudinal)}$$

$$= 0 \quad \text{,when } \vec{e}_{q\nu} \perp \vec{q} \qquad \text{(transverse)}$$

This last result suggests that only *Longitudinal acoustic waves* with polarization direction along the direction of propagation couple to the carriers in a spherically-symmetric band.

So the matrix element for scattering (ignoring non-parabolicity):

$$\left|M(\vec{k},\vec{k}')\right|^2 = \frac{\hbar\Xi_{ac}{}^2}{2\rho V\omega_q} q^2\left(n_q + \frac{1}{2} \mp \frac{1}{2}\right)\delta(\vec{k}' - \vec{k} \pm \vec{q})$$

where, $n_q = \dfrac{1}{e^{\hbar\omega_q / k_B T} - 1}$ is the number of phonons in state $\vec{q}$

So the total scattering rate is given by:

$$\frac{1}{\tau(\vec{k})} = \frac{m^* V}{2\pi\hbar^3 k} \int_{q_{\min}}^{q_{\max}} q \left| M(\vec{k}, \vec{q}) \right|^2 dq$$

To evaluate the limits we once again use:

$$\frac{q}{2k} \mp \cos\theta \pm \frac{m^* \omega_0}{\hbar k q} = 0$$

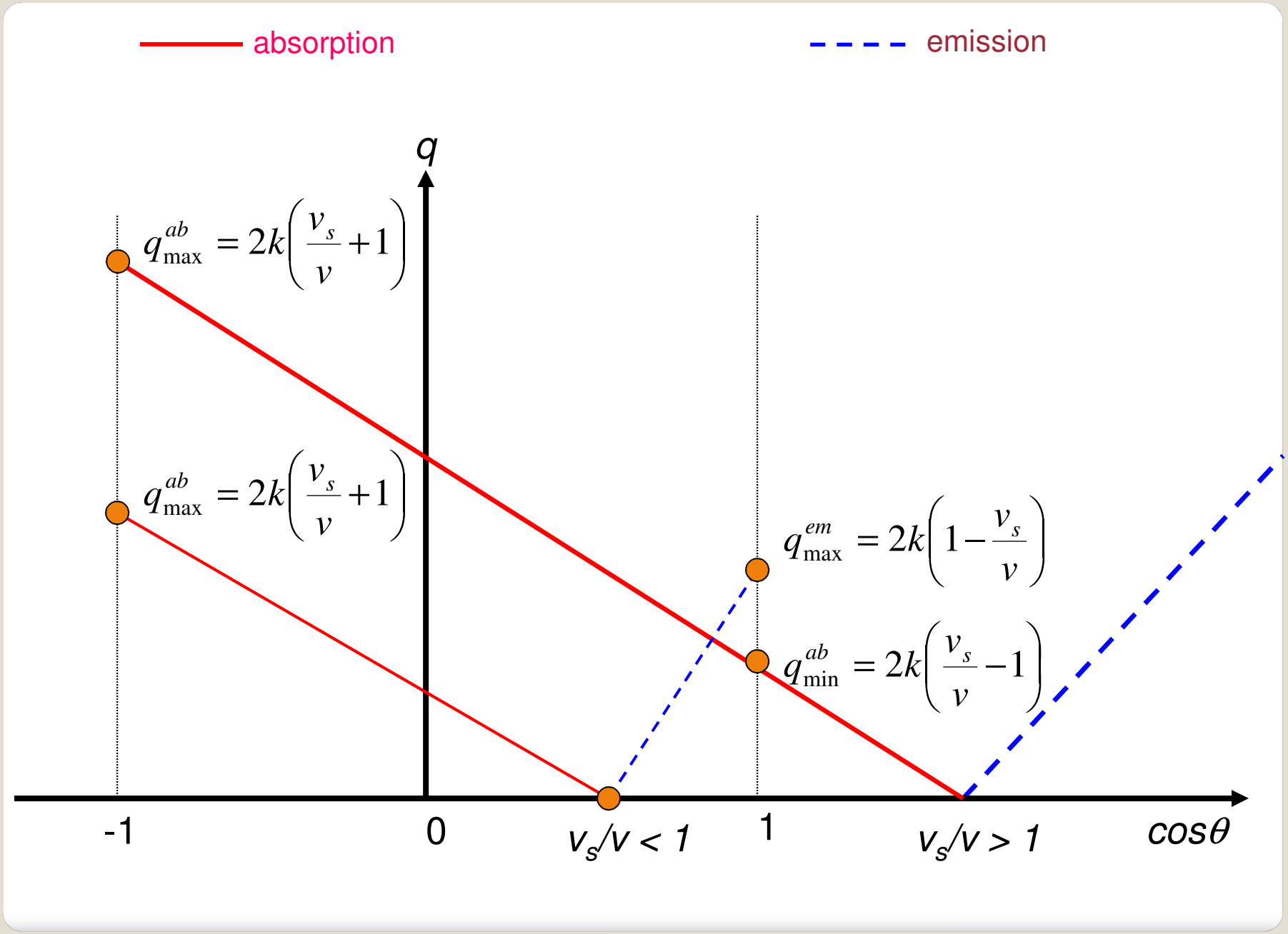
$$\Rightarrow \cos\theta = \frac{m^* \omega_0}{\hbar k q} \mp \frac{q}{2k}$$

Utilizing the fact that we are considering long wavelength phonons (in acoustic limit):

$$\omega_q = v_s q$$

$$q^{abs} = 2k\left(\frac{v_s}{v} - \cos\theta\right)$$

$$q^{em} = 2k\left(\cos\theta - \frac{v_s}{v}\right)$$


absorption
emission
q
$q^{ab}_{\max} = 2k\left(\frac{v_s}{v}+1\right)$
$q^{ab}_{\max} = 2k\left(\frac{v_s}{v}+1\right)$
$q^{em}_{\max} = 2k\left(1-\frac{v_s}{v}\right)$
$q^{ab}_{\min} = 2k\left(\frac{v_s}{v}-1\right)$
-1
0
$v_s/v < 1$
1
$v_s/v > 1$
cosθ

Few observations:

- For emission process, $cos\theta$ is between 0 and 1, which means that an electron can only emit a phonon in the forward direction.

- For $v_s/v > 1$, $q^{em}_{\max}$ and $q^{em}_{\min}$ do not exist.

  This observation suggest that an electron must travel with a velocity in excess of the sound velocity v_s to be able to emit a phonon. This is known as *CERENKOV* condition.

- At room temperature the average electron velocity is on the order of 10^7 cm/s whereas the sound wave is on the order of 10^5 cm/s. Therefore $v_s/v << 1$ and for both the absorption and the emission processes: $0 \le q \le 2k$, which means that limits for integration of both the processes are the same.

  The maximum phonon energy involved in this case is:

$$\hbar\omega_q^{\max} = \hbar v_s 2k \approx 1meV$$

  This energy is much smaller than the thermal energy of the electron ($3/2k_BT \sim 40$ *meV*), which suggests that scattering by acoustic (long wavelength) phonons can be considered as elastic.

- The number of phonons in a given mode *q* is given by:

$$n_q = \frac{1}{e^{\hbar\omega_q / k_B T} - 1} \geq 1, \qquad \text{for} \quad \hbar\omega_q << k_B T \approx 25meV$$

Since $n_q >> 1$, we also have that $n_q \sim n_q + 1$, *i. e.* the matrix elements squared for absorption and emission processes are (aside from the δ-function) the same. This is known as EQUIPARTITION approximation.

For elastic scattering, we have seen that the limits of integration for the absorption and the emission processes are also same. So considering matrix element for absorption only:

$$\left|M(\vec{k},\vec{q})\right|^2 = \frac{\hbar \Xi_{ac}{}^2}{2\rho V \omega_q} q^2 \left(n_q\right)$$

$$= \frac{\Xi_{ac}{}^2 k_B T}{2\rho V \omega v_s{}^2}$$

The total scattering rate out of some initial state $\vec{k}$ is a sum of absorption and emission rates that are nearly equal for equipartition
Which gives:

$$\frac{1}{\tau(\vec{k})} = 2\frac{m^* V}{2\pi\hbar^3 k}\int_0^{2k} q\,\frac{\Xi_{ac}{}^2 k_B T}{2\rho V \omega v_s{}^2}\,dq$$

$$= \frac{m^* \Xi_{ac}{}^2 k_B T}{\pi\hbar^3 \rho v_s{}^2}\sqrt{\frac{2m^* E_k}{\hbar^2}}$$

From the definition of density of states:

$$\frac{1}{\tau(\vec{k})} = \frac{2\pi}{\hbar}\frac{\Xi_{ac}{}^2 k_B T}{\rho V v_s{}^2}\frac{1}{2}g_c(E_k)$$

$$= \frac{1}{\tau_0}E_k{}^{1/2}$$

$$\Rightarrow \tau_{ac}(\vec{k}) = \tau_0 E_k{}^{-1/2}$$