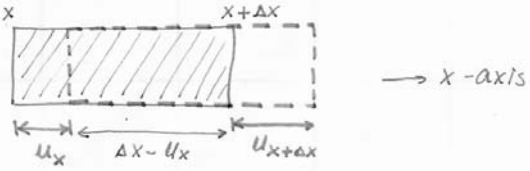
Strain tensor

- Consider an element of a homogeneous, isotropic elastic substance of length Δx. In the absence of strain, this element extends from x to $x+\Delta x$.



In the presence of stress, an elastic strain is produced, the equilibrium position of the left-hand end of the element ~~dis~~ being displaced a distance u_x along the x-axis, and the right-hand end of the element being displaced $u_{x+\Delta x}$. The length of the element changes by:

$$\Delta x' = \Delta x - u_x + u_{x+\Delta x} = \Delta x + u_{x+\Delta x} - u_x$$

or: $$\frac{\Delta x' - \Delta x}{\Delta x} = \frac{u_{x+\Delta x} - u_x}{\Delta x} \rightarrow \frac{\partial u}{\partial x} = s(x) = \epsilon_{xx}$$ → fractional change in length

The strain $s(x)$ is defined as the elastic extension of the element per unit length. The length of the element now becomes:

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

- One can generalize the above result in 3D case, in which ϵ_{ij} is a strain TENSOR. If in the undeformed crystal we have unit vectors $\vec{a}, \vec{b}, \vec{c}$ along the principal axes, by a small deformation these vectors will be displaced. The displaced unit vectors are called $\vec{a}', \vec{b}', \vec{c}'$ and can be calculated as:

$$\vec{a}' = (1+\epsilon_{xx})\vec{a} + \epsilon_{xy}\vec{b} + \epsilon_{xz}\vec{c}$$
$$\vec{b}' = \epsilon_{yx}\vec{a} + (1+\epsilon_{yy})\vec{b} + \epsilon_{yz}\vec{c}$$
$$\vec{c}' = \epsilon_{zx}\vec{a} + \epsilon_{zy}\vec{b} + (\epsilon_{zz}+1)\vec{c}$$

The volume of a cube having unit vectors $\vec{a}, \vec{b}, \vec{c}$ ($V=1$) is now changed by the deformation to:

$$1+\delta V = \vec{a}' \cdot [\vec{b}' \times \vec{c}'] \approx 1 + \epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz}$$

i.e. the volume dilatation is given by:

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

ELECTRON - PHONON INTERACTION

In the following, we will describe the matrix elements for:
- deformation potential interaction
- non-polar optical phonons
- polar optical phonon scattering
- intervalley scattering

(A) DEFORMATION POTENTIAL INTERACTION - INTRAVALLEY

→ The problem of determining effective potentials in the calculation of the deformation potential electron-phonon matrix elements is quite complicated. In the limit of long-wavelength phonons, however, accurate results can be obtained. In this case, vibrations of the solid resemble those of an elastic continuum, and their effects can be described in a manner related to the theory of elasticity.

→ The essential concept due to Bardeen and Shockley is that, if the solid is subject to a strain S_{ij} (tensor) that is a slowly varying function of position, there will be a change in energy of each electronic state that is proportional to the strain. Therefore, the change in energy of a state of wavevector $\vec{k}$ and band n is:

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

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

→ The above expression can be easily derived for the case when the strains are dilatations (expansions and contractions of the volume). Let us consider free electrons at low temperature for which:

$$N = \frac{V}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2} \int_0^{E_F} \sqrt{E}\, dE = \frac{V}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2} \frac{2}{3} E_F^{3/2}$$

$$N = \frac{V}{3\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2} E_F^{3/2} \Rightarrow E_F = \left(\frac{3\pi^2 N}{V}\right)^{2/3} \frac{\hbar}{2m^*}$$

Consider now a change in volume containing N electrons by an amount δV. The change in Fermi energy is:

$$\delta E_F = -(3\pi^2 N)^{2/3} \frac{\hbar}{2m^*} \frac{2}{3} V^{-5/3} \delta V = -\frac{2}{3}\left(\frac{3\pi^2 N}{V}\right)^{2/3} \frac{\hbar}{2m^*} \frac{\delta V}{V}$$

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

where $\Delta = \delta V / V$ is the dilatation.

→ The deformation potential interaction is now expressed in terms of the phonon coordinates. Let $\vec{u}_i$ be the displacement vector for an element of volume located at $\vec{R}_i$. The dilatation is then simply given by:

$$\Delta = \nabla \cdot \vec{u}_i \quad \text{(see side notes)}$$

We now interpret $\vec{u}_i$ as an atomic displacement vector, i.e.

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

Treating $\vec{R}_i = \vec{r}$ as a continuous variable gives:

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

→ Interpreting now δE_F as the deformation potential electron-phonon interaction leads to:

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

Comparing (i.e. using this into the expression for H_{fi}) with the expression for H_{fi} leads to:

$$C_{q\nu} = \underset{ac}{\vec{\Xi}_q} \cdot \vec{e}_{q\nu} = \begin{cases} \Xi_{ac}\, q, & \text{when } \vec{e}_{q\nu} \parallel \vec{q} \quad \text{(Longitudinal modes)} \\ 0, & \text{when } \vec{e}_{q\nu} \perp \vec{q} \quad \text{(transverse modes)} \end{cases}$$

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.

→ The matrix element squared for scattering between some initial state $\vec{k}$ and some final state $\vec{k}'$ is, thus, equal to (ignore non-parabolicity):

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

(↦ absorption; ↳ emission)

where:

$$n_q = \frac{1}{e^{\hbar\omega_q/k_BT} - 1} \quad \text{is the number of phonons in a state } \vec{q}.$$

→ The total scattering rate out of some initial state $\vec{k}$ is then given by:

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

where the limits of integration are obtained from the zero's of the δ-function that represents the energy conservation in the system:

$$\frac{q}{2k} \pm \cos\theta \mp \frac{m^* w_q}{\hbar k q} = 0 \qquad \text{(top sign absorption, bottom emission).}$$

or:

$$\mp \frac{q}{2k} + \cos\theta - \frac{m^* w_q}{\hbar k q} = 0 \Rightarrow \boxed{\cos\theta = \frac{m^* w_q}{\hbar k q} \mp \frac{q}{2k}} \quad (*)$$

Equation (*) relates the magnitude q of the phonon wavevector to its angle θ.

(a) Absorption process: $\cos\theta = \frac{m^* w_q}{\hbar k q} - \frac{q}{2k} \Rightarrow q^{abs} = 2k\left[\frac{m^* w_q}{\hbar k q} - \cos\theta\right]$

(b) Emission process: $\cos\theta = \frac{m^* w_q}{\hbar k q} + \frac{q}{2k} \Rightarrow q^{em} = 2k\left(\cos\theta - \frac{m^* w_q}{\hbar k q}\right)$

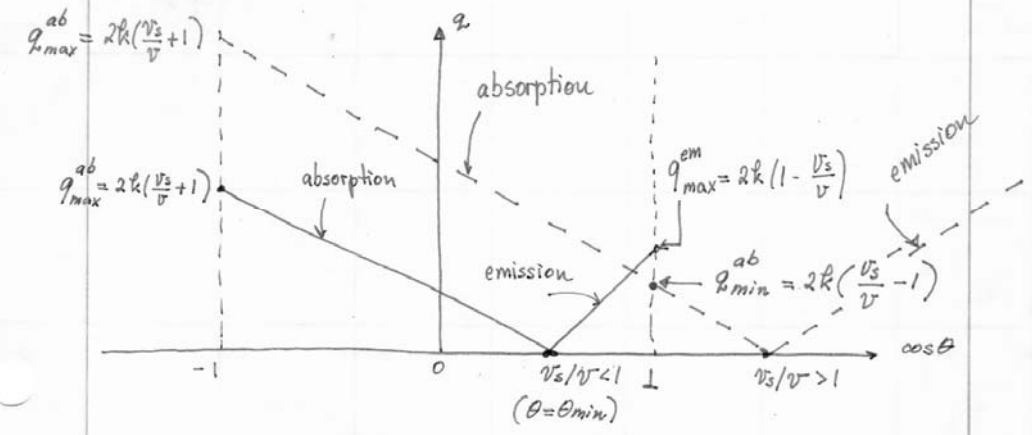
→ For long-wavelength phonons, for which we have evaluated C_{qv}, we have:

$$w_q = v_s q \qquad (v_s \text{ is the sound velocity})$$

which leads to: $q^{abs} = 2k\left(\frac{m^* v_s}{\hbar k} - \cos\theta\right) = 2k\left(\frac{v_s}{v} - \cos\theta\right)$

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

The variation of the phonon wavevector with $\cos\theta$ is shown diagramatically in the figure below:



In the figure shown on the previous page, we have considered two distinct cases: $v_s/v < 1$ and $v_s/v > 1$ ($v = \hbar k/m^*$ is electron velocity)

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

- $v_s/v < 1 \Rightarrow \begin{cases} q^{abs}_{max} = 2k\left(\frac{v_s}{v} + 1\right), & \theta = \pi \\ q^{abs}_{min} = 2k \cdot 0 = 0 & \text{for } \theta = \theta_{min} \end{cases}$

- $v_s/v > 1 \Rightarrow \begin{cases} q^{abs}_{max} = 2k\left(\frac{v_s}{v} + 1\right), & \theta = \pi \\ q^{abs}_{min} = 2k\left(\frac{v_s}{v} - 1\right), & \theta = 0 \end{cases}$

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

- $v_s/v < 1 \Rightarrow \begin{cases} q^{em}_{max} = 2k\left(1 - \frac{v_s}{v}\right), & \theta = 0 \\ q^{em}_{min} = 0 & \theta = \theta_{min} \end{cases}$

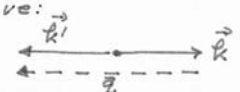
  Note that for the emission process, $\cos\theta$ is between 0 and 1, which means that an electron can only emit a phonon in the forward direction.

- $v_s/v > 0 \Rightarrow q^{em}_{max}, q^{em}_{min}$ does not exist.

  This observation suggests 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.

→ The average electron group velocity at $T = 300\,K$ is on the order of 10^7 cm/s, whereas the sound velocity is on the order of 10^5 cm/s. Therefore $v_s/v \to 0$ and for both the absorption and the emission process we have:

$$0 \leq q \leq 2k$$



The maximum phonon energies involved in either the absorption or the emission process are:

$$\hbar\omega_q^{max} \cong \hbar v_s q_{max} \approx \hbar v_s 2k \approx 1\,meV.$$

This energy is much smaller than the thermal energy of the electron, which suggests that scattering by acoustic (long-wavelength) phonons can be considered as an elastic process.

Note : thermal energy of electron $\cong \frac{3}{2} k_B T \approx 40\,meV.$

→ The number of phonons in a mode q is:

$$n_q = \frac{1}{e^{\hbar\omega_q/k_BT} - 1} \approx \frac{1}{1 + \frac{\hbar\omega_q}{k_BT} - 1} \approx \frac{k_BT}{\hbar\omega_q} \gg 1$$

↑ for $\hbar\omega_q \ll k_BT \approx 25\,meV$

Since $n_q \gg 1$, we also have that $n_q \approx n_q + 1$, 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, the limits of integration for the absorption and emission processes are also the same. Consider matrix element for absorption only:

$$|H(\vec{k},\vec{q})|^2 = \frac{\hbar\,\Xi_{ac}^2\,q^2}{2\rho V \omega_q}(n_q) \longrightarrow \frac{\hbar\,\Xi_{ac}^2\,q^{\not 2}}{2\rho V v_s q\!\!\!/} \frac{k_BT}{\hbar v_s q\!\!\!/} = \frac{\Xi_{ac}^2 k_BT}{2\rho V v_s^2}$$

elastic and equipartition approximation

→ 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

$$\frac{1}{\tau(\vec{k})} = 2 \frac{m^* V}{2\pi\hbar^3 k} \int_0^{2k} q \frac{\Xi_{ac}^2 k_BT}{\rho V v_s^2} dq = \frac{m^* \Xi_{ac}^2 k_BT}{2\pi\hbar^3 k \rho v_s^2} \underbrace{\int_0^{2k} q\,dq}_{\frac{1}{2}q^2\Big|_0^{2k} = \frac{4k^2}{2} = 2k^2}$$

↑ absorption + emission

$$\frac{1}{\tau(\vec{k})} = \frac{m^* \Xi_{ac}^2 k_BT}{\pi\hbar^3 \rho v_s^2} k = \frac{m^* \Xi_{ac}^2 k_BT}{\pi\hbar^3 \rho v_s^2} \sqrt{\frac{2m^* E_K}{\hbar^2}}$$

If we define $\frac{1}{2} g_c(E_K) = \frac{V}{4\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\sqrt{E_K}$ as density of states per unit energy of a given spin:

$$\sqrt{E_K} = \frac{4\pi^2}{V} \frac{\hbar^3}{2m^*\sqrt{2m^*}} \frac{1}{2} g_c(E_K)$$

or:

$$\frac{1}{\tau(k)} = \frac{m^* \Xi_{ac}^2 k_BT}{\pi\hbar^3 \rho v_s^2} \frac{\sqrt{2m^*}}{\hbar} \frac{A\pi^2}{V} \frac{\hbar^3}{\rho m^* \sqrt{2m^*}} \frac{1}{2} g_c(E_K) =$$

$$= \frac{2\pi}{\hbar} \underbrace{\frac{\Xi_{ac}^2 k_BT}{\rho V v_s^2}}_{\text{matrix element squared (absorption + emission)}} \frac{1}{2} g_c(E_K) \quad \Rightarrow \quad \frac{1}{\tau(k)} = \frac{1}{\tau_0} E_K^{1/2} \Rightarrow \tau_{ac}(k) = \tau_0 E_K^{-1/2}$$