Physics 551 Lecture #15

Title: Other physical properties of the lattice

A general form of $\mathcal{D}(\omega)$, the density of lattice vibrational modes for a particular frequency, can be stated.

$$\mathcal{D}(\omega) = \frac{V}{(2\pi)^3} \oint \frac{dS_\omega}{v_g} \quad ; \quad S_\omega \text{ is a surfaces of constant } \omega$$
$$v_g \text{ is the group velocity}$$

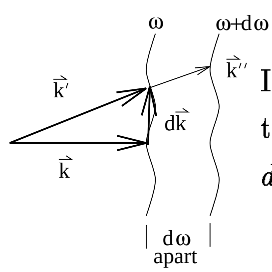
The derivation of this form follows.

The number of modes within a small frequency increment from ω to $\omega + d\omega$ is just the volume of k-space contained/volume for one mode (assuming the density in k-space is isotropic). Hence $d\omega$ must be rewritten in terms of dk since that is the "unit" of momentum space.

$$\begin{aligned} \omega &= F(k_x, k_y, k_z) \\ d\omega &= \frac{\partial \omega}{\partial k_x} dk_y + \frac{\partial \omega}{\partial k_y} dk_y + \frac{\partial \omega}{\partial k_2} dk_z \\ d\omega &= \nabla_k \omega \cdot d\vec{k} \text{ where } \nabla_k \equiv \frac{\partial}{\partial k_x}\hat{i} + \frac{\partial}{\partial k_y}\hat{j} + \frac{\partial}{\partial k_z}\hat{k} \end{aligned}$$

Now $d\omega$ must lie between a $\vec{k}$ and $\vec{k}'$ (or $\vec{k}''$)

Two constant energy contours $d\omega$ apart



If $\vec{k}'$ and $\vec{k}$ lie at the <u>same</u> ω,
then $d\vec{k} = \vec{k}' - \vec{k}$ and $d\omega = 0$
$d\omega = 0 = \nabla_k \omega \cdot d\vec{k}$

but $d\vec{k} \neq 0$ and $\nabla_k \omega \neq 0$, therefore $\nabla_k \omega$ is perpendicular to the constant frequency surface.

With this observation in hand, then

$$d\omega = \nabla_k \omega \cdot d\vec{k} \text{ for } d\omega \neq 0$$

gives $|\nabla_k \omega|$ projected on $d\vec{k}$ or

$$|\nabla_k \omega| d\vec{k}_\perp = d\omega$$

The volume between the two energy surfaces is

$$\oint dk_\perp dS_\omega = \oint \frac{dS_\omega}{|\nabla_k \omega|} d\omega$$

Number of modes in a increment $d\omega$

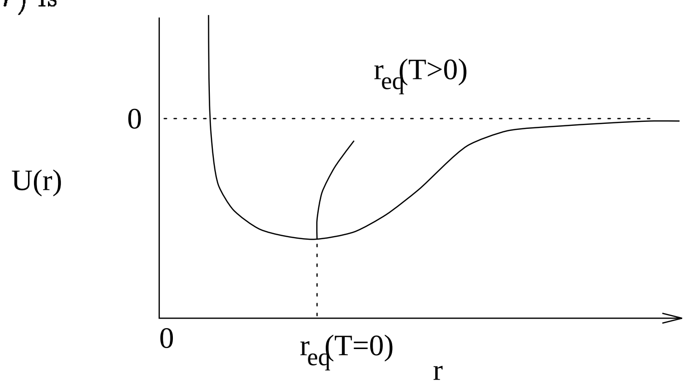
$$\mathcal{D}(\omega) = \frac{\oint \frac{dS_\omega}{|\nabla_k \omega|}}{\frac{(2\pi)^3}{V}} = \frac{V}{(2\pi)^3} \oint \frac{dS_\omega}{|\nabla_k \omega|}$$

$$\text{and } v_g = |\nabla_k \omega|$$

Thermal Expansion:

If the pair interaction potential were truly quadriatic, then there would be no expansion. However,

$U(r)$ is



and so is harmonic only at the bottom of the well. If $T > 0$, then we are obligated to keep higher order terms in the expansion of U(r)

$$U(r) = U(r_{eq}) + \frac{1}{2}\frac{d^2U}{dr^2}|_{r=r_{eq}}(r - r_{eq})^2 + \mathcal{O}(r^3) + \mathcal{O}(r^4) + ...$$

thus we may write

$$x = (r - r_{eq})$$

$$U(x) = U(r) - U(r_{eq}) = cx^2 - gx^3 - fx^4 \text{ and so on}$$

$$< x >= \frac{\int_{-\infty}^{\infty} dx\ x\ exp(-\frac{U(x)}{k_B T})}{\int_{-\infty}^{\infty} dx\ exp(-\frac{U(x)}{k_B T})}$$

Thermal Conductivity

The thermal conductivity is just the diffusion of the phonon gas in the context of kinetic theory.

$j = -\kappa \frac{dT}{dx}$

dT/dx temperature gradient

κ conductivity (Watts cm^{-1} deg^{-1})

j thermal energy crossing a unit area in unit time $= \frac{Q}{At}$

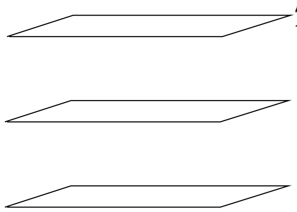
The process of thermal conductivity in normal materials at normal temperature is a result of random processes.

Heat in $\Longrightarrow$ phonons $\Longrightarrow$ transport (Balistic motion and scattering) gives heat out

We will show that for an isotropic material

$$\kappa = \frac{1}{3} C v \ell \qquad \begin{aligned} C &\equiv \text{heat capacity/unit volume} \\ \ell &= \text{mean free path between collisions} \\ v &= \text{average velocity of the "phonon" gas} \end{aligned}$$

Consider a gas of phonons with number density n and temperature gradient dT/dx. Calculate the net energy flow across a plane $\perp$ to the temperature gradient



$T + \ell_x \frac{dT}{dx}$ $\quad (T + \Delta T)$ $\quad c = \frac{C}{N} \equiv$ heat capacity/per phonon

T $\quad \updownarrow$ x-dir

T - $\ell_x \frac{dT}{dx}$ $\quad (T - \Delta T)$

$$\begin{aligned} Q_{down} &= \frac{n}{2} < |v_x| > c(T + \Delta T) \\ Q_{up} &= \frac{n}{2} < |v_x| > c(T - \Delta T) \qquad \Delta T = \ell_x \frac{dT}{dx} \end{aligned}$$

$$Q_{net} = Q_{down} - Q_{up} = n < |v_x| > c\Delta T = nc < |v_x| > \ \ell_x \frac{dT}{dx}$$

Now $\ell_x =< |v_x| > \tau \quad \tau \equiv$ relaxation time (mean time between collisions).

So

$Q_{net} = nc < |v_x|^2 > \ \tau \ \frac{dT}{dx} \qquad \frac{1}{3} < v^2 >=< v_x^2 > \Longrightarrow$ isotropic medium

(Q_{net} is per unit time, unit area)

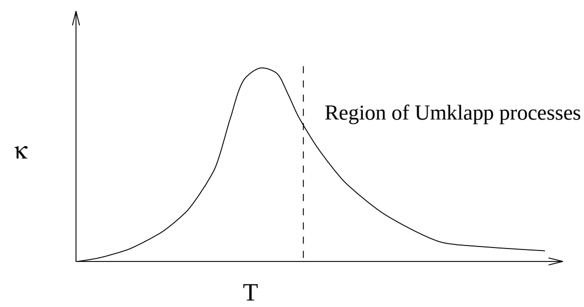
$Q_{net} = \frac{1}{3} \ nc < v^2 > \ \tau \ \frac{dT}{dx}$

$j_u = \kappa \frac{dT}{dx} \qquad$ So $\begin{aligned} \kappa &= \tfrac{1}{3} nc < v^2 > \tau \\ \kappa &= \tfrac{1}{3} C v \ell \quad \text{Thermal conductivity} \end{aligned}$

So what is ℓ (mean free path)?

ℓ is determined by phonon-phonon scattering in the high temperature limits, number of phonons $\propto T$

Thus $\ell \propto 1/T \quad \kappa \propto \frac{1}{T} \quad T \gg 0°\text{K} \qquad \ell \sim 10 - 100\text{Å}$



What are the phonon-phonon processes?

There are two kinds, Normal and Umklapp. As a result of the non-linear response of the crystal, two phonons can combine to form a third phonon (or vice-versa). This process is similar in many ways to the inelastic scattering of a neutron. Phonon 1 interacts with the "static" displacement of phonon 2 (in a moving reference frame) and satisfies the Bragg condition. Thus, phonon 2 is destroyed and phonon 1's energy and momentum are altered. So

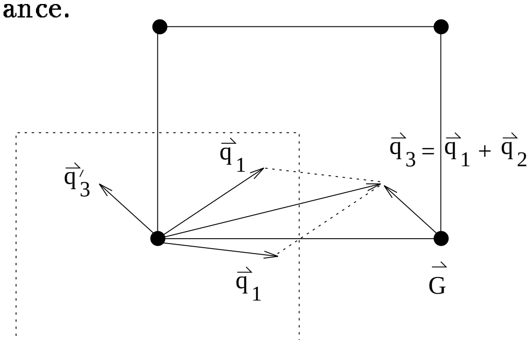
$$\text{phonon 1} + \text{phonon 2} = \text{phonon 3}$$

subject to the constraints of conservation of crystal momentum and conservation of energy.

$$\vec{q}_1 + \vec{q}_2 = \vec{q}_3 \quad \text{and}$$

$$\omega_1 + \omega_2 = \omega_3$$

If $\vec{q}_3$ lies within 1^{st} B.Z., this is denoted a NORMAL process. If $\vec{q}_3$ lies beyond 1^{st} B.Z., ($\vec{q}_1 + \vec{q}_2 = \vec{q}\,'_3 + \vec{G}$), this is called an UMKLAPP process. With an Umklapp process, the direction of energy flow can be changed. This is the origin of thermal resistance.



$\vec{q}_3$ is the same and

$\vec{q}_3 - \vec{G} = \vec{q}\,'_3$

$v_g \equiv$ group velocity is completely changed.