Heat capacity of chain lattice. (a) Consider a dielectric crystal made up of chains of atoms, with rigid coupling between chains so that the motion of the atoms is restricted to the line of the chain. Show that the phonon heat capacity in the Debye approximation in the low temperature limit is proportional to T. (b) Suppose instead, as in many chain structures, that adjacent chains are very weakly bound to each other. What form would you expect the phonon heat capacity to approach at extremely low temperature?

(a)

$$\text{For 1-D system, volume per state} = \frac{2\pi}{L} \qquad \text{(L = length of sample)}$$

$$\text{Length of an infinitesimal segment in k-space} = dk$$

$$\text{Number of states in line segment} = \frac{dk}{\frac{2\pi}{L}} = \frac{Ldk}{2\pi}$$

$$\therefore \quad D(\omega)d\omega = \frac{Ldk}{2\pi}$$

$$\Rightarrow D(\omega) = \frac{L}{2\pi}\frac{dk}{d\omega} = \frac{L}{2\pi v} \qquad \text{(Debye's approximation } \omega = vk\text{)}$$

$$U = \int \frac{1}{\exp[\frac{\hbar\omega}{k_B T}] - 1} \hbar\omega D(\omega)\, d\omega$$

Since it is a 1 - D system, there are only one acoustic branches and apply Debye's applroximation to define Debye frequency ω_D as

$$N = \int_0^{\omega_D} D(\omega)d\omega \Rightarrow N = \int_0^{\omega_D} \frac{L}{2\pi v} d\omega \Rightarrow N = \frac{L\omega_D}{2\pi v} \Rightarrow \omega_D = \frac{2\pi N v}{L}$$

$$U = \int_0^{\omega_D} \frac{1}{\exp[\frac{\hbar\omega}{k_B T}] - 1} \hbar\omega D(\omega)d\omega = \int_0^{\omega_D} \frac{1}{\exp[\frac{\hbar\omega}{k_B T}] - 1} \hbar\omega \frac{L}{2\pi v} d\omega$$

$$= \frac{L\hbar}{2\pi v} \int_0^{\omega_D} \frac{\omega}{\exp[\frac{\hbar\omega}{k_B T}] - 1} d\omega$$

Substitution $x = \frac{\hbar\omega}{k_B T} \Rightarrow \omega = \frac{k_B T x}{\hbar}$

As $T \to 0$

$$U = \frac{L\hbar}{2\pi v} \left(\frac{k_B T}{\hbar}\right)^2 \int_0^{\infty} \frac{x}{e^x - 1} dx \Rightarrow U \propto T$$

$$\Rightarrow C = \frac{\partial U}{\partial T} \propto T$$

Hence $C \propto T^d$, where d is the dimension of the system..

(b) Assume the lines are in the z-direction. We can approximate the coupling between planes with very stiff springs along the x- and y- directions (i.e. large spring constant C_x and C_y). As a result, v is large in x- and y-directions and the equal energy surface is like a Frisbee lying in the k_x-k_y plane.

At high temperature, the Frisbee is chopped off by the first Brillouin zone and looks like two parallel planes in the k_x-k_y direction. This geometry is equivalent to that of 1-D system, with the energy of these planes depends on k_z only. As temperature is lowered so that :

$$k_B T \ll \hbar\omega_{D_x} = \hbar\,(v_x K_x) = \hbar\frac{v_x 2\pi}{a_x}$$

(where a_x = separation between the lines in x - direction.)

Then the Frisbee will shrink to the size within the first Brillouin zone. Now it looks like a disk lying in k_x-k_y plane and the k_x and k_y-dimension will play a dominant role because it has more states then k_z-direction. This corresponds to that of a two dimensional system at very low temperature, i.e. $C \propto T^2$.