Physics 140A Winter 2011

Homework 6 due Monday March 7

1. Consider the dispersion relation for elastic waves in a monotomic linear lattice of N atoms with nearest neighbor interactions. (a) Show that the density of modes is:

$$D(\omega) = \frac{2N}{\pi} \frac{1}{(\omega_m^2 - \omega^2)^{1/2}} \tag{1}$$

where ω_m is the maximum frequency.

(b) Sketch $D(\omega)$ versus ω.

(c) Suppose that an optical phonon branch has the form $\omega = \omega_0 - AK^2$ near $K = 0$ in three dimensions. Show that

$$\begin{aligned} D(\omega) &= \frac{L}{(2\pi)^3} \frac{2\pi}{A^{3/2}} (\omega_0^2 - \omega^2)^{1/2} \quad \text{for } \omega < \omega_0 & (2) \\ &= 0 \quad \text{for } \omega > \omega_0 & (3) \end{aligned}$$

2. Consider a layered crystal made up of layers of atoms with rigid coupling between layers so that the motion of the atoms is restricted to the plane of the layer. Show that the phonon heat capacity in the Debye approximation in the low temperature limit is proportional to T^2. (b) Suppose now that the adjacent layers are very weakly bound to each other (as is often the case in real layered structures). What form would you expect the phonon heat capacity to approach at extremely low temperatures? (Try to be quantitative here about what energy scale should set the scale for this crossover).

HW 6 Solutions

Note Title 3/2/2010

① dispersion relation : $\omega = \left(\frac{4C}{M}\right)^{\frac{1}{2}} \sin\left(\frac{Ka}{2}\right)$

(a) $D(\omega) = \frac{L}{\pi} \frac{1}{\frac{d\omega}{dK}}$

$$\frac{d\omega}{dK} = \left(\frac{4C}{M}\right)^{\frac{1}{2}} \frac{a}{2} \cos\left(\frac{Ka}{2}\right)$$

$$= \left(\frac{a}{2}\right)\left(\frac{4C}{M}\right)^{\frac{1}{2}}\left(1 - \sin^2 \frac{Ka}{2}\right)^{\frac{1}{2}}$$

$$= \frac{a}{2}\left(\left(\frac{4C}{M}\right) - \omega^2\right)^{\frac{1}{2}}$$

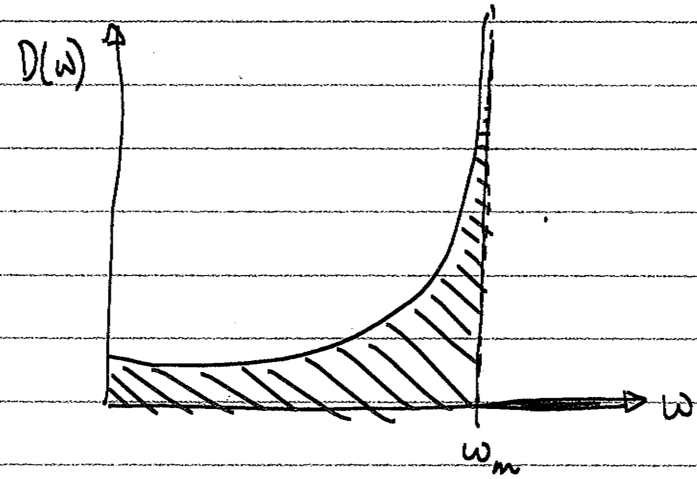
but $\omega_{max} = \omega_m = \left(\frac{4C}{M}\right)^{\frac{1}{2}}$, so

$$\frac{d\omega}{dK} = \frac{a}{2}(\omega_m^2 - \omega^2)^{\frac{1}{2}}$$

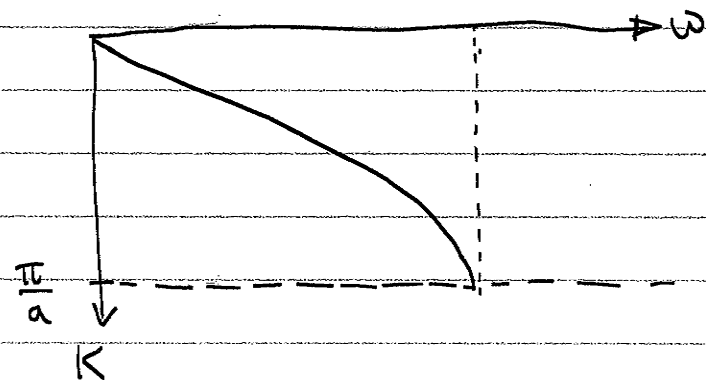
& $D(\omega) = \frac{2L}{\pi a} \frac{1}{(\omega_m^2 - \omega^2)^{\frac{1}{2}}}$ but $L = Na$

$$\Rightarrow \boxed{D(\omega) = \frac{2N}{\pi} \frac{1}{(\omega_m^2 - \omega^2)^{\frac{1}{2}}}}$$

(b)



Density of State



Dispersion

(c) optical branch in 3D: $\omega = \omega_0 - AK^2$

$$D(\omega) = \left(\frac{L}{2\pi}\right)^3 \int \frac{dS_\omega}{|\vec{\nabla}\omega|}$$

$$\vec{\nabla}\omega = -2A(K_x, K_y, K_z) = -2A\vec{K}$$

$$|\vec{\nabla}\omega| = 2AK$$

$$= 2A\left(\frac{\omega_0 - \omega}{A}\right)^{\frac{1}{2}} = 2A^{\frac{1}{2}}(\omega_0 - \omega)^{\frac{1}{2}}$$

now, since $|\vec{\nabla}\omega|$ is independent of angle in K-space,

we can write $D(\omega) = \frac{1}{2}A^{-\frac{1}{2}}(\omega_0-\omega)^{-\frac{1}{2}} \underbrace{\int dS_\omega}_{=4\pi K^2}$

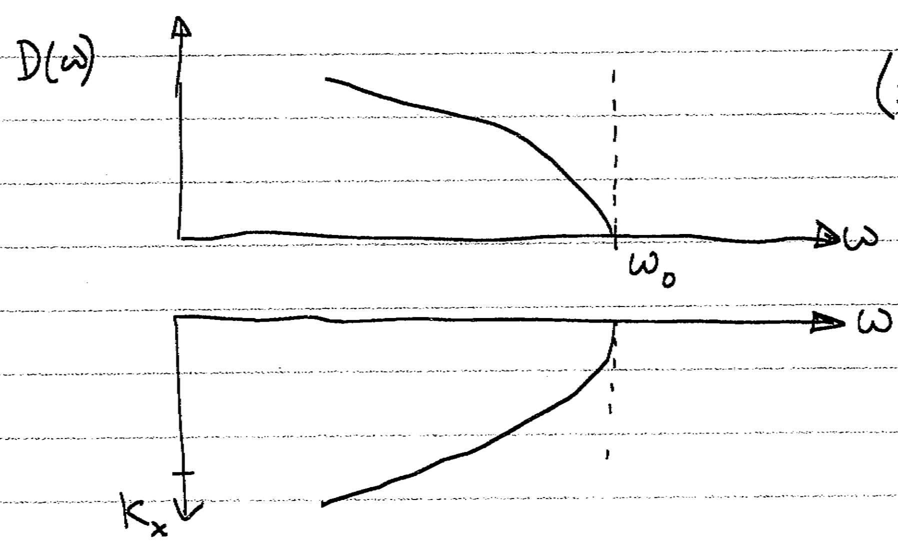
surface area at constant ω

$$S_\omega = 4\pi K^2 = 4\pi\left[\frac{(\omega_0-\omega)}{A}\right]$$

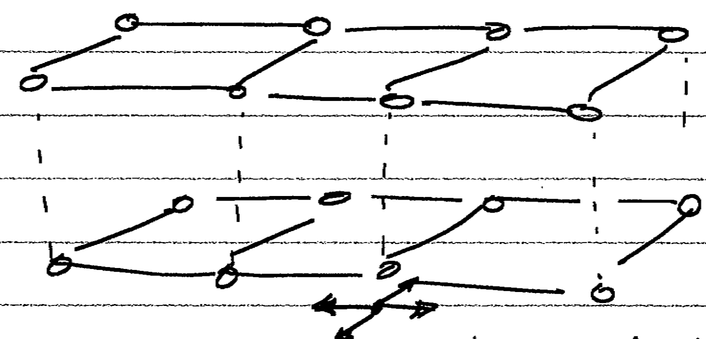
so $D(\omega) = \left(\frac{L}{2\pi}\right)^3 \frac{1}{2} A^{-\frac{3}{2}} (\omega_0-\omega)^{\frac{1}{2}} 4\pi$

$$\Rightarrow \boxed{D(\omega) = \begin{cases} \left(\frac{L}{2\pi}\right)^3 \frac{2\pi}{A^{3/2}} (\omega_0-\omega)^{\frac{1}{2}} & \text{for } \omega < \omega_0 \\ 0 & \text{for } \omega > \omega_0 \end{cases}}$$

(since $\omega_{max} = \omega_0$)



(2)



motion restricted to 2D plane

Debye approximation $\omega = vK$

in 2D, we have one allowed value of K per area $\left(\frac{2\pi}{L}\right)^2$ in $\vec{K}$-space. The total number of modes is then:

$$N = \underbrace{\left(\frac{L}{2\pi}\right)^2}_{\text{density of modes.}} \underbrace{\left(\pi K^2\right)}_{\text{area in } K\text{-space}}$$

or $N = \left(\frac{L}{2\pi}\right)^2 \pi \frac{\omega^2}{v^2}$

$$D(\omega) = \frac{dN}{d\omega} = \left(\frac{A}{4\pi}\right)\frac{2\omega}{v^2} = \left(\frac{A}{2\pi v^2}\right)\omega$$

now, $U = \int_0^{\omega_D} D(\omega)\left(\frac{\hbar\omega}{e^{\hbar\omega\beta} - 1}\right) d\omega$

but we define $x \equiv \hbar\omega\beta = \dfrac{\hbar\omega}{k_B T}$

$$\Rightarrow \quad d\omega = \frac{k_B T}{\hbar}\, dx$$

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

$$U = \frac{A}{2\pi v^2} \int_0^{\omega_D} \frac{\hbar\omega^2}{(e^x - 1)}\, d\omega$$

$$= \frac{A\hbar}{2\pi v^2} \left(\frac{k_B T}{\hbar}\right)^2 \left(\frac{k_B T}{\hbar}\right) \int_0^{x_D} \frac{x^2 dx}{(e^x - 1)^2}$$

for low T, $x \to \infty$, so $\displaystyle\int_0^\infty \frac{x^2 dx}{(e^x - 1)^2} \to$ const.

indep. of T.

$$U = \frac{A k_B^3}{2\pi v^2 \hbar^2} T^3 \cdot (\text{const})$$

$$C_A = \left(\frac{\partial U}{\partial T}\right)_A = \frac{3 A k_B^3}{2\pi v^2 \hbar^2} T^2$$

$\boxed{\text{so we expect } C \propto T^2 \text{ at low T.}}$

if the layers are weakly bound to each other, then

we would say that $\omega^2 = (v_\parallel K_\parallel)^2 + (v_\perp K_\perp)^2$

where $K_\parallel$ lies in the plane & $K_\perp$ lies $\perp$ to the plane.

we then have 2 T-scales, $\theta_{D\parallel}$ & $\theta_{D\perp}$

where $\theta_{D\perp} \ll \theta_{D\parallel}$

we expect $C \propto \left(\frac{T}{\theta_{D\parallel}}\right)^2 \int_0^{x_{D\parallel}} \frac{x^2\,dx}{(e^x-1)^2}$

$$+ \left(\frac{T}{\theta_{D\perp}}\right)^3 \int_0^{x_{D\perp}} \frac{x^3\,dx}{(e^x-1)^2}$$

or $C \propto C_\parallel(T) + C_\perp(T)$

and for $\theta_{D\perp} < T < \theta_{D\parallel}$ we have $C \propto T^2$

but for $T < \theta_{D\perp}$ we have $C \propto T^3$