Homework 5 Solutions

1. (a) The dispersion relation is $\omega = \omega_m |\sin\frac{1}{2}Ka|$. We solve this for K to obtain $K = (2/a)\sin^{-1}(\omega/\omega_m)$, whence $dK/d\omega = (2/a)(\omega_m{}^2 - \omega^2)^{-1/2}$ and, from (15), $D(\omega) = (2L/\pi a)(\omega_m{}^2 - \omega^2)^{-1/2}$. This is singular at $\omega = \omega_m$. (b) The volume of a sphere of radius K in Fourier space is $\Omega = 4\pi K^3/3 = (4\pi/3)[(\omega_0 - \omega)/A]^{3/2}$, and the density of orbitals near ω_0 is $D(\omega) = (L/2\pi)^3 |d\Omega/d\omega| = (L/2\pi)^3 (2\pi/A^{3/2})(\omega_0 - \omega)^{1/2}$, provided $\omega < \omega_0$. It is apparent that $D(\omega)$ vanishes for ω above the minimum ω_0.

2. The potential energy associated with the dilation is $\frac{1}{2}B(\Delta V/V)^2 a^3 \approx \frac{1}{2}k_B T$. This is $\frac{1}{2}k_B T$ and not $\frac{3}{2}k_B T$, because the other degrees of freedom are to be associated with shear distortions of the lattice cell. Thus $<(\Delta V)^2> = 1.5\times10^{-47}; (\Delta V)_{rms} = 4.7\times10^{-24}\,cm^3;$ and $(\Delta V)_{rms}/V = 0.125$. Now $3\Delta a/a \approx \Delta V/V$, whence $(\Delta a)_{rms}/a = 0.04$.

4. (a) The motion is constrained to each layer and is therefore essentially two-dimensional. Consider one plane of area A. There is one allowed value of K per area $(2\pi/L)^2$ in K space, or $(L/2\pi)^2 = A/4\pi^2$ allowed values of K per unit area of K space. The total number of modes with wavevector less than K is, with $\omega = vK$,

$$N = (A/4\pi^2)(\pi K^2) = A\omega^2/4\pi v^2.$$

The density of modes of each polarization type is $D(\omega) = dN/d\omega = A\omega/2\pi v^2$. The thermal average phonon energy for the two polarization types is, for each layer,

$$U = 2\int_0^{\omega_D} D(\omega)\, n(\omega,\tau)\, \hbar\omega\, d\omega = 2\int_0^{\omega_D} \frac{A\omega}{2\pi v^2}\frac{\hbar\omega}{\exp(h\omega/\tau) - 1} d\omega,$$

where ω_D is defined by $N = \int_D^{\omega_D} D(\omega)\, d\omega$. In the regime $\hbar\omega_D >> \tau$, we have

$$U \cong \frac{2A\tau^3}{2\pi v^2\hbar^2}\int_0^\infty \frac{x^2}{e^x - 1} dx.$$

Thus the heat capacity $C = k_B\, \partial U/\partial\tau \propto T^2$.

(b) If the layers are weakly bound together, the system behaves as a linear structure with each plane as a vibrating unit. By induction from the results for 2 and 3 dimensions, we expect $C \propto T$. But this only holds at extremely low temperatures such that $\tau << \hbar\omega_D \approx \hbar v N_{layer}/L$, where N_{layer}/L is the number of layers per unit length.