CHAPTER 5

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 $(\Delta a)_{rms}/a = 0.04$.

3. (a) $<R^2> = (\hbar/2\rho V)\Sigma\omega^{-1}$, where from (20) for a Debye spectrum $\Sigma\omega^{-1} = \int d\omega\, D(\omega)\omega^{-1} = 3V\omega_D{}^2/4\pi^3 v^3$, whence $<R^2> = 3\hbar\omega_D{}^2/8\pi^2\rho v^3$. (b) In one dimension from (15) we have $D(\omega) = L/\pi v$, whence $\int d\omega\, D(\omega)\,\omega^{-1}$ diverges at the lower limit. The mean square strain in one dimension is $<(\partial R/\partial x)^2> = \frac{1}{2}\Sigma K^2 u_0{}^2 = (\hbar/2MNv)\Sigma K = (\hbar/2MNv)(K_D{}^2/2) = \hbar\omega_D{}^2/4MNv^3.$

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.

5. (a) From the Planck distribution $< n > + \frac{1}{2} = \frac{1}{2}(e^x + 1)/(e^x - 1) = \frac{1}{2} \coth(x/2)$, where $x = \hbar\omega/k_B T$. The partition function $Z = e^{-x/2} \, \Sigma \, e^{-sx} = e^{-x/2}/(1 - e^{-x}) = [2 \sinh(x/2)]^{-1}$ and the free energy is $F = k_B T \log Z = k_B T \log[2 \sinh(x/2)]$. (b) With $\omega(\Delta) = \omega(0)(1 - \gamma\Delta)$, the condition $\partial F/\partial\Delta = 0$ becomes $B\Delta = \gamma\Sigma \, \frac{1}{2} \hbar\omega \coth(\hbar\omega/2k_B T)$ on direct differentiation. The energy $< n > \hbar\omega$ is just the term to the right of the summation symbol, so that $B\Delta = \gamma U(T)$. (c) By definition of γ, we have $\delta\omega/\omega = -\gamma\delta V/V$, or $d \log \omega = -\delta \, d \log V$. But $\theta \propto \omega_D$, whence $d \log \theta = -\gamma \, d \log V$.