PH641, FINAL, June 9, 2009

Note: always indicate what you try to do, even if you are not able to finish the actual work.

Problem 1: An electron has three possible orbitals, given by a quantum number m that can be $-1, 0, +1$. The energy of the orbital is $\epsilon_m = -mB$. Give an expression that allows you to find $\mu(T, V, N)$ for this system. If the average number of particles in state $m = 0$ is n_0, find μ as a function of n_0. Find n_1 and n_{-1} as a function of B and n_0. Write an equation that allows you to find n_0 as a function of B and N.

Electrons are Fermions. This problem focusses on orbitals, and hence we need to use the Fermi-Dirac distribution function:

$$f_{FD}(\epsilon; T, \mu) = \frac{1}{e^{\beta(\epsilon-\mu)} + 1}$$

We have for the average numbers of particles

$$n_m = f_{FD}(-mB; T, \mu)$$

and

$$N = \sum_m n_m = \sum_m f_{FD}(-mB; T, \mu)$$

This equation can be inverted to find $\mu(N, T, V)$. There is no explicit volume, but assume that the volume is hidden in the parameter B.

The expression for n_0 is

$$n_0 = \frac{1}{e^{-\beta\mu} + 1}$$

since the orbital has energy zero. This can be inverted to get

$$\mu = k_B T \log(\frac{n_0}{1 - n_0})$$

Next we consider $n_{\pm 1}$:

$$n_{\pm 1} = \frac{1}{e^{\beta(\mp B - \mu)} + 1}$$

$$n_{\pm 1} = \frac{1}{e^{\mp\beta B}\frac{1-n_0}{n_0} + 1} = \frac{n_0}{(1-n_0)e^{\mp\beta B} + n_0}$$

Since we have $N = \sum_m n_m$ we get

$$\frac{n_0}{(1-n_0)e^{-\beta B} + n_0} + n_0 + \frac{n_0}{(1-n_0)e^{+\beta B} + n_0} = N$$

which can be solved to find $n_0(T, B, N)$

Problem 2: Consider a wire of length L. Treat this as a one dimensional system. The frequency of the lattice vibrations (phonons) in this wire is given by $\omega = v_s|k|$, where v_s is the speed of sound in the wire. The wave vector k is quantized according to $k = n\frac{\pi}{L}$, with $n = 0, \pm1, \pm2, \cdots$. Find the one-phonon partition function for this system. Use the formulas $\mathcal{Z}(T, L, N) = \frac{1}{N!}\mathcal{Z}_1^N(T, L)$ and $\log(N!) \approx N\log(N) - N$ to find the Helmholtz free energy for the system. Calculate the stress τ, which is the equivalent of pressure for this one-dimensional system.

We have

$$\mathcal{Z}_1(T, L) = \sum_{n=-\infty}^{\infty} e^{-\beta\hbar v_s|n|\frac{\pi}{L}}$$

$$\mathcal{Z}_1(T, L) = 2\sum_{n=0}^{\infty} e^{-\beta\hbar v_s n\frac{\pi}{L}} - 1$$

$$\mathcal{Z}_1(T, L) = 2\frac{1}{1 - e^{-\beta\hbar v_s\frac{\pi}{L}}} - 1$$

$$\mathcal{Z}_1(T, L) = \frac{1 + e^{-\beta\hbar v_s\frac{\pi}{L}}}{1 - e^{-\beta\hbar v_s\frac{\pi}{L}}} = \coth\left(\frac{\pi\hbar v_s}{2Lk_BT}\right)$$

The Helmholtz free energy is

$$F(T, L, N) = -k_BT\log\left(\frac{1}{N!}\mathcal{Z}_1^N(T, L)\right)$$

$$F(T, L, N) = -Nk_BT\log\left(\frac{\mathcal{Z}_1}{N}\right) - Nk_BT$$

The internal stress is given by:

$$\tau = -\left(\frac{\partial F}{\partial L}\right)_{T,N} = Nk_BT\frac{1}{\mathcal{Z}_1}\left(\frac{\partial \mathcal{Z}_1}{\partial L}\right)_{T,N}$$

$$\tau = Nk_BT\tanh(\frac{\pi\hbar v_s}{2Lk_BT})\frac{-1}{\sinh^2(\frac{\pi\hbar v_s}{2Lk_BT})}\frac{-\pi\hbar v_s}{2L^2k_BT}$$

$$\tau = Nk_BT\frac{1}{\cosh(\frac{\pi\hbar v_s}{2Lk_BT})\sinh(\frac{\pi\hbar v_s}{2Lk_BT})}\frac{\pi\hbar v_s}{2L^2k_BT}$$

$$\tau = \frac{Nk_BT}{L}\frac{1}{\sinh(\frac{\pi\hbar v_s}{Lk_BT})}\frac{\pi\hbar v_s}{Lk_BT}$$

If the length and temperature are very large, the last part goes to one, and we have

$$\tau \approx \frac{Nk_BT}{L}$$

as expected.

Problem 3: The multiplicity function for the states of a single particle as a function of energy is given by $g_1(\epsilon)$. Consider a system of two particles with combined energy E. The multiplicity function for the combined system is $g_2(E)$. Find an expression for g_2 in terms of g_1. Generalize this result for N particles. Construct an argument why we have $S(E,N) \approx Nk_B\log g_1(\frac{E}{N})$.

If one of the two particles has energy ϵ, the other one has energy $E-\epsilon$. All energy distributions are possible, and we get

$$g_2(E) = \int g_1(\epsilon)g_1(E-\epsilon)d\epsilon$$

If the particles are identical, we need to divide by a factor two.

This can be written in the form:

$$g_2(E) = \int g_1(\epsilon_1)g_1(\epsilon_2)\delta(E-\epsilon_1-\epsilon_2)d\epsilon_1 d\epsilon_2$$

For N particles we have:

$$g_N(E) = \int g_1(\epsilon_1) \cdots g_1(\epsilon_N) \delta(E - \epsilon_1 - \cdots - \epsilon_N) d\epsilon_1 \cdots d\epsilon_N$$

and for identical particles we need to divide by $N!$.

If we think of the particles as identical systems in equilibrium, the maximum number of possibilities occurs when all particles have the same energy. This means

$$g_N(E) \approx \left[g_1(\frac{E}{N}) \right]^N$$

where we divide by $N!$ for identical particles. Since $S = k_B \log(g_N)$ we get

$$S \approx N k_B \log(g_1(\frac{E}{N}))$$

with an additional factor $-k_B \log(N!)$ for identical particles.