Physics 112 Problem Set 7
Holzapfel, Section 102

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1. (a) Defining the absolute activity $\lambda = \exp(\mu/\tau)$, the Gibbs sum is

$$\mathcal{Z} = \sum_{ASN} \exp\left(\frac{N\mu - \epsilon}{\tau}\right) = 1 + \lambda \exp(-\epsilon/\tau) + \lambda^2 \exp(-2\epsilon/\tau).$$

Then the average occupancy is

$$\langle N \rangle = \lambda \frac{d}{d\lambda}(\log \mathcal{Z}) = \frac{\lambda \exp(-\epsilon/\tau) + 2\lambda^2 \exp(-2\epsilon/\tau)}{\mathcal{Z}}.$$

(b) Now, since the state with energy ϵ is doubly degenerate, the Gibbs sum is

$$\mathcal{Z} = 1 + 2\lambda \exp(-\epsilon/\tau) + \lambda^2 \exp(-2\epsilon/\tau).$$

Thus

$$\langle N \rangle = \lambda \frac{d}{d\lambda}(\log \mathcal{Z}) = \frac{2\lambda \exp(-\epsilon/\tau) + 2\lambda^2 \exp(-2\epsilon/\tau)}{\mathcal{Z}}.$$

2. For a single particle, $N = 1$, so we will calculate the partition function Z, from which we can calculate the mean energy $\langle U \rangle$.

$$Z = \sum_s \exp(-\epsilon_s/\tau) = \sum_s \exp(-p_s c/\tau).$$

To convert the sum to an integral, we need an expression for the density of states in momentum space (this is valid since we are in the high-energy limit, $pc \gg Mc^2$)

$$D(p)\ dp = \frac{1}{8} 4\pi p^2 dp = \frac{1}{2}\pi p^2\ dp$$

where the factor of $1/8$ comes from integrating over the positive portion of p-space (note that we've assumed spherical symmetry). Then the partition function becomes

$$Z = \frac{\pi}{2} \int_0^\infty p^2 \exp(-pc/\tau) dp = \frac{\pi\tau^3}{2c^3} \int_0^\infty x^2 \exp(-x) dx = \frac{\pi\tau^3}{c^3}.$$

Then the average energy is

$$\langle U \rangle = \tau^2 \frac{\partial \log Z}{\partial \tau} = \tau^2 \frac{c^3}{\pi \tau^3} \frac{3\pi \tau^2}{c^3} = 3\tau.$$

3. (a) The pressure of an individual state with energy ϵ_s is $-(\partial \epsilon_s / \partial V)_N$, so the expected pressure, averaging over all states and normalizing by the partition function, is

$$p = -\frac{1}{Z} \sum_s \left(\frac{\partial \epsilon_s}{\partial V} \right)_N \exp(-\epsilon_s / \tau).$$

(b) For an ideal gas,

$$\epsilon_s = \frac{\hbar^2}{2M} \left(\frac{\pi n}{V^{1/3}} \right)^2$$

so

$$\left(\frac{\partial \epsilon_s}{\partial V} \right)_N = -\frac{2}{3} \frac{\hbar^2}{2M} \frac{(\pi n)^2}{V^{5/3}} = -\frac{2}{3} \frac{\epsilon_s}{V}.$$

(c) Using the result from (a), the pressure is

$$p = \frac{2}{3V} \frac{1}{Z} \sum_s \epsilon_s \exp(-\epsilon_s / \tau) = \frac{2U}{3V}.$$

(d) We know that at $T = 0$, the internal energy is $U = 3N\epsilon_F / 5$, where ϵ_F is the Fermi energy (Kittel 7.10). So $p = 2n\epsilon_F / 5$ at $T = 0$. Also, $\epsilon_F = (\hbar^2 / 2m)(3\pi^2 n)^{2/3}$ (Kittel 7.7).

With $n = 8 \times 10^{22}$ cm^{-3} and $m_e = 9.11 \times 10^{-31}$ kg, this evaluates to $p = 3.4 \times 10^5$ atm.

4. (a) The total number of atoms is the sum of the average number of atoms in each orbital, so, defining $\lambda = \exp(\mu / \tau)$

$$N = \lambda \sum_s \exp(-\epsilon_s / \tau)$$

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For the states with lower internal energy, ϵ_s is the same as for an ideal monatomic gas with one internal energy state, so $\sum_s \exp(-\epsilon_s / \tau) = Z_1 = V n_Q$. For the states with greater internal energy, $\epsilon_{s'} = \epsilon_s + \Delta$, so

$$\sum_s \exp \left(\frac{-\epsilon_s - \Delta}{\tau} \right) = \exp(-\Delta / \tau) Z_1 = \exp(-\Delta / \tau) V n_Q.$$

Then

$$N = \lambda V n_Q (1 + \exp(-\Delta / \tau))$$

so

$$\lambda = \frac{n}{n_Q} \frac{1}{1 + \exp(-\Delta / \tau)}$$

and

$$\mu = \tau \log\left(\frac{n}{n_Q}\right) - \tau \log\left(1 + \exp\left(\frac{-\Delta}{\tau}\right)\right).$$

(b) The partition function for a single atom is

$$Z_1 = \sum_s \exp(-\epsilon_s/\tau)$$

so by the same logic as in (a)

$$Z_1 = V n_Q (1 + \exp(-\Delta/\tau)).$$

Then for N atoms,

$$Z = \frac{Z_1^N}{N!} = \frac{(V n_Q)^N}{N!}\left(1 + \exp\left(\frac{-\Delta}{\tau}\right)\right)^N.$$

Thus

$$F = -\tau \log Z = -\tau N \log(V n_Q) + \tau N \log N - \tau N - \tau N \log(1 + \exp(-\Delta/\tau))$$
$$F = \tau N(\log(n/n_Q) - 1) - \tau N \log(1 + \exp(-\Delta/\tau))$$
$$F = F_{ideal} - \tau N \log(1 + \exp(-\Delta/\tau))$$

where F_{ideal} is the free energy for the ideal gas with one internal energy state.

(c) The entropy is given by

$$\sigma = -\left(\frac{\partial F}{\partial \tau}\right)_V$$

and recall that the entropy for an ideal gas with one internal energy state is given by $\sigma_{ideal} = N(\log(n_Q/n) + 5/2)$. Thus

$$\sigma = N\left(\log\left(\frac{n_Q}{n} + \frac{5}{2}\right)\right) + N\log\left(1 + \exp\left(\frac{-\Delta}{\tau}\right)\right) + N\tau \frac{\exp(-\Delta/\tau)}{1 + \exp(-\Delta/\tau)}\frac{\Delta}{\tau^2}$$
$$\sigma = N\left(\log\left(\frac{n_Q}{n} + \frac{5}{2}\right)\right) + N\log\left(1 + \exp\left(\frac{-\Delta}{\tau}\right)\right) + \frac{N\Delta}{\tau}\frac{1}{1 + \exp(\Delta/\tau)}.$$

(d) The pressure is the same as for an ideal gas with one internal energy state,

$$p = -\left(\frac{\partial F}{\partial V}\right)_\tau = \frac{N\tau}{V},$$

since we have not introduced any new terms with volume dependence.

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(e) The heat capacity at constant pressure is

$$C_p = \tau \left(\frac{\partial \sigma}{\partial T} \right)_p = k_B \tau \left(\frac{\partial \sigma}{\partial \tau} \right)_p$$

$$C_p = k_B \tau N \frac{\partial}{\partial \tau} \left(\log(n_Q) - \log(n) \right) + N k_b \tau \frac{\Delta}{\tau^2} \frac{\exp(-\Delta/\tau)}{1 + \exp(-\Delta/\tau)}$$

$$- N k_B \tau \frac{\Delta}{\tau^2} \frac{1}{1 + \exp(\Delta/\tau)} + N k_B \tau \frac{\Delta}{\tau} \frac{\Delta}{\tau^2} \frac{\exp(\Delta/\tau)}{(1 + \exp(\Delta/\tau))^2}$$

$$C_p = N k_B \tau \left(\frac{3}{2\tau} - \frac{\partial}{\partial \tau} \log \left(\frac{p}{\tau} \right) \right) + N k_B \frac{\Delta^2}{\tau^2} \frac{\exp(\Delta/\tau)}{(1 + \exp(\Delta/\tau))^2}$$

$$C_p = \frac{5}{2} N k_B + N k_B \frac{\Delta^2}{\tau^2} \frac{\exp(\Delta/\tau)}{(1 + \exp(\Delta/\tau))^2}.$$

5. (a) Starting from $N = \lambda \sum_s \exp(-\epsilon_s/\tau)$, we know that in the classical limit, we can approximte the sum with an integral. Each momentum state dp takes up a de Broglie wavelength of h/dp, and thus occupies an area of $(h/dp)^2$. Thus the density of states is $D(p)dp = A(dp)^2/h^2$, and assuming momentum space is circularly symmetric, $(dp)^2 = 2\pi p dp$. Also, $p^2 = 2mE$ implies $2p dp = 2m dE$, so

$$D(E)dE = \frac{2\pi A m}{h^2} dE.$$

then

$$N = \lambda \sum_s \exp(-\epsilon_s/\tau) = \lambda \frac{2\pi A m}{h^2} \int_0^\infty \exp(-\epsilon/\tau)d\epsilon = \lambda \frac{2\pi A m}{h^2} \tau.$$

Since $\lambda = \exp(\mu/\tau)$, this means

$$\mu = \tau \log \left(\frac{N h^2}{2\pi A m \tau} \right).$$

(b) We know that each degree of freedom in an atom of three-dimensional ideal gas carries $\tau/2$ energy, for a total energy of $U = 3N\tau/2$. By analogy, for a two-dimensional gas, $U = N\tau$.

(c) The entropy can be calculated from the free energy. From (a), the partition function is

$$Z_1 = \frac{2\pi A m \tau}{h^2}$$

and $Z = Z_1^N/N!$, so

$$F = -\tau \log Z = -N\tau \log \left(\frac{2\pi A m \tau}{h^2} \right) + N\tau \log N - N\tau$$

$$F = -N\tau \left(\log \left(\frac{2\pi A m \tau}{N h^2} \right) + 1 \right).$$

Thus

$$\sigma = -\left(\frac{\partial F}{\partial \tau}\right)_V = N\left(\log\left(\frac{2\pi Am\tau}{Nh^2}\right) + 1\right) + N\tau\frac{1}{\tau} = N\left(\log\left(\frac{2\pi Am\tau}{Nh^2}\right) + 2\right).$$

6. (a) Since both electrons and holes have degeneracy 2, and the energy gap is E_g, the equilibrium condition $\mu_e + \mu_h = 0$ implies $\log(n_e/2n_{Q,e}) + \log(n_h/2n_{Q,h}\exp(-E_g/\tau)) = 0$, or

$$n_e n_h = (2n_{Q,e})(2n_{Q,h})\exp(-E_g/\tau)$$

$$n_e n_h = 4(m_e m_h)^{3/2}\left(\frac{\tau}{2\pi\hbar^2}\right)^3 \exp(-E_g/\tau).$$

In equilibrium, the density of holes and electrons needs to be equal (or more phonons would be produced), so $n_e = n_h$, and

$$n_e = 2\left(\frac{\tau\sqrt{m_e m_h}}{2\pi\hbar^2}\right)^{3/2}\exp(-E_g/2\tau).$$

(b) The chemical potential $\mu_e = \tau\log(n_e/2n_{Q,e})$, so

$$\mu_e = \tau\log 2 + \frac{3}{2}\tau\log\left(\frac{\tau}{2\pi\hbar^2}\right) + \frac{3}{2}\tau\log(\sqrt{m_e m_h}) - \frac{E_g}{2} - \tau\log 2 - \frac{3}{2}\tau\log\left(\frac{m_e\tau}{2\pi\hbar^2}\right)$$

$$\mu_e = \frac{3}{4}\tau\log\left(\frac{m_h}{m_e}\right) - \frac{E_g}{2}.$$

(c) The equilibrium condition reflects just the chemical potential due to the free electrons, since the electrons from donor atoms are not part of the "gas," so $\log((n'_e - n_d)/2n_{Q,e}) + \log(n'_h/2n_{Q,h}\exp(-E_g/\tau)) = 0$, or

$$(n'_e - n_d)n'_h = (2n_{Q,e})(2n_{Q,h})\exp(-E_g/\tau) = n_e^2.$$

Since $n'_e = n'_h$ in equilibrium (which reflects that all electrons can interact with the holes),

$$n'^2_e - n_d n'_e - n_e^2 = 0$$

$$n_e = \frac{n_d + \sqrt{n_d^2 + 4n_e^2}}{2}$$

$$n_e = \frac{n_d}{2} + \sqrt{\frac{n_d^2}{4} + n_e^2}.$$