LULEÅ TEKNISKA UNIVERSITET
Avdelningen för materialvetenskap

Exam in: Statistical Physics and Thermodynamics 2012-03-23 (F7035T)
Suggested solutions

---

1. There are several routes to make this calculation, three of them are presented here.

   First route The heat capacity is given by $C = \frac{\partial U_{total}}{\partial \tau}$, where $U_{total} = N \cdot U$. The energy is given by $U = \langle \epsilon \rangle = \tau^2 \frac{\partial \ln Z}{\partial \tau}$. The calculation will follow the line from Z we get U and from U we get C. The energies are given by $0, \epsilon, 2\epsilon, ..., S\epsilon$, where the ground state is not degenerated and the other states all have degeneracy 2. From this information the partition function is constructed. The partition function is:

$$Z = \sum_{states} e^{-\epsilon_{state}/\tau} = 1 + \sum_{n=1}^{S} 2 \cdot e^{-n\epsilon/\tau} = -1 + \sum_{n=0}^{S} 2 \cdot e^{-n\epsilon/\tau} = -1 + 2\frac{1 - e^{-(S+1)\epsilon/\tau}}{1 - e^{-\epsilon/\tau}} \tag{1}$$

   In the limit $S\epsilon/\tau >> 1$, ($\tau = k_B T$) the last reduces to

$$Z \approx -1 + 2\frac{1}{1 - e^{-\epsilon/\tau}} = \frac{1 + e^{-\epsilon/\tau}}{1 - e^{-\epsilon/\tau}} \tag{2}$$

   Now we turn to the energy:

$$U = \tau^2 \frac{\partial \ln Z}{\partial \tau} = ... = \frac{2\epsilon}{e^{\epsilon/\tau} - e^{-\epsilon/\tau}} \tag{3}$$

   For the heat capacity we have

$$C = \frac{\partial U_{total}}{\partial \tau} = \frac{\partial}{\partial \tau}\left(\frac{2\epsilon}{e^{\epsilon/\tau} - e^{-\epsilon/\tau}}\right) = 2(\frac{\epsilon}{\tau})^2 \frac{e^{\epsilon/\tau} + e^{-\epsilon/\tau}}{(e^{\epsilon/\tau} - e^{-\epsilon/\tau})^2} \tag{4}$$

   and hence for the total heat capacity

$$C_{total} = 2N(\frac{\epsilon}{\tau})^2 \frac{e^{\epsilon/\tau} + e^{-\epsilon/\tau}}{(e^{\epsilon/\tau} - e^{-\epsilon/\tau})^2} \tag{5}$$

   In the limit $S\epsilon/\tau >> 1$ ie $\tau \to 0$

$$C_{total} \to 2N(\frac{\epsilon}{\tau})^2 \frac{e^{\epsilon/\tau}}{(e^{\epsilon/\tau})^2} = 2N(\frac{\epsilon}{\tau})^2 e^{-\epsilon/\tau} \tag{6}$$

   The contribution to the heat capacity at low temperatures is

$$C = 2N(\frac{\epsilon}{\tau})^2 e^{-\epsilon/\tau} \tag{7}$$

   The pricipal shape of the heat capacity is seen in Figure 1.

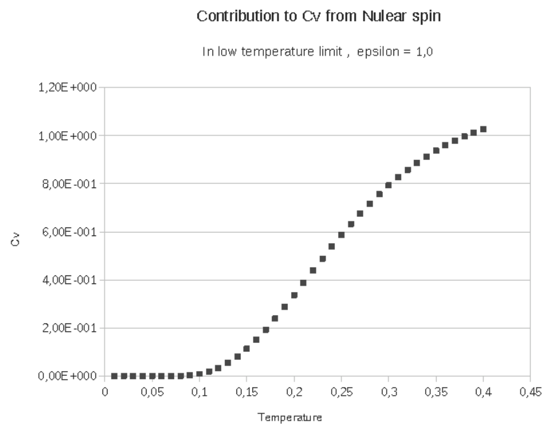

Figure 1: A principal figure showing the heat capacity in the low temperature limit. The choice for the energy $\epsilon = 1.0$ in eq. 7.

Second route The partition function can also be written as:

$$Z = \sum_{states} e^{-\epsilon_{state}/\tau} = 1 + \sum_{n=1}^{S} 2 \cdot e^{-n\epsilon/\tau} \approx 1 + 2 \cdot e^{-\epsilon/\tau} \tag{8}$$

Now we turn to the energy:

$$U = \tau^2 \frac{\partial \ln Z}{\partial \tau} = ... = \frac{2\epsilon}{e^{\epsilon/\tau} + 2} \tag{9}$$

For the heat capacity we have

$$C = \frac{\partial U_{total}}{\partial \tau} = \frac{\partial}{\partial \tau}\left(\frac{2\epsilon}{e^{\epsilon/\tau} + 2}\right) = 2(\frac{\epsilon}{\tau})^2 \frac{e^{\epsilon/\tau}}{(e^{\epsilon/\tau} + 2)^2} \approx 2(\frac{\epsilon}{\tau})^2 e^{-\epsilon/\tau} \tag{10}$$

Third route This problem can also be solved by a route over $F = -\tau \ln(Z)$ and then $\sigma = -(\frac{\partial F}{\partial \tau})_{V,N}$ and at last $C_V = \tau(\frac{\partial \sigma}{\partial \tau})_V$.

The partition function can also be written as:

$$Z = \sum_{states} e^{-\epsilon_{state}/\tau} = 1 + \sum_{n=1}^{S} 2 \cdot e^{-n\epsilon/\tau} \approx 1 + 2 \cdot e^{-\epsilon/\tau} \tag{11}$$

Now we turn to the Free energy and making use of the approximasion $\ln(1+x) = x - \frac{x^2}{2} + \frac{x^3}{3} - ...$ the free energy is

$$F = -\tau \ln(1 + 2 \cdot e^{-\epsilon/\tau}) \approx -2\tau \cdot e^{-\epsilon/\tau} \tag{12}$$

Now we calculate the entropy:

$$\sigma = -(\frac{\partial F}{\partial \tau})_{V,N} = -\frac{\partial}{\partial \tau}(-2\tau \cdot e^{-\epsilon/\tau}) = 2e^{-\epsilon/\tau}(1 + \frac{\epsilon}{\tau}) \tag{13}$$

For the heat capacity we have

$$C_V = \tau(\frac{\partial\sigma}{\partial\tau})_V = \tau\frac{\partial}{\partial\tau}\left(2e^{-\epsilon/\tau}(1+\frac{\epsilon}{\tau})\right) = 2\tau e^{-\epsilon/\tau}(\frac{\epsilon}{\tau^2}(1+\frac{\epsilon}{\tau}) - \frac{\epsilon}{\tau^2}) = 2(\frac{\epsilon}{\tau})^2 e^{-\epsilon/\tau} \tag{14}$$

As we can see all three routes, though apparently different, produce the same result for the heat capacity in the limit of small temperatures.

2. This problem is about comparing Boltzmann factors taking degeneracy into acount.

   a) The energy $2,5\hbar\omega$ implies that one of quantum numbers is one while the other two are zero. The direction of the excitation can be choosen in three different ways, ie the excited state has a threefold degeneracy. We get the following equation for the probabillitys: $e^{-1,5\hbar\omega/k_BT} = 3e^{-2,5\hbar\omega/k_BT}$ leading to $e^{\hbar\omega/k_BT} = 3$ and solving for T gives $T = \frac{\hbar\omega}{k_B \ln 3}$

   b) The partition function is given by: $Z = \sum_{n_1=0,n_2=0,n_3=0}^{\infty} e^{-(n_1+n_2+n_3+\frac{3}{2})\ \hbar\omega/k_BT} = \sum_{n=0}^{\infty} g(n)e^{-(n+\frac{3}{2})\ \hbar\omega/k_BT}$, where $g(n)$ is the degeneracy of the energy levels. $g(0) = 1, g(1) = 3, g(2) = 6(=1+2+3), g(3) = 10(=1+2+3+4), g(4) = 15(=1+2+3+4+5)$ and so on. Z may be calculated in different ways. One is by noting that it can be calculated as three separate one dimensional oscillators and then multiplying these three independent results to form the three dimensional result. Another way is to determine $g(n)$ this is done in the following geometrical way, for each n the values for n_x, n_y and n_x form a triangle with sides of equal length $n+1$. Say $n=4$ the n_x, n_y and n_x will run from 0 to 4 with the constraint $n_x + n_y + n_x = 4$ this is a triangle with side length 5 $(n+1)$. Now $g(n)$ is simply the number of integer coordinate sites on this triangle. On a triangle with n there are $n+1$ rows and the row with the least sites has just 1 site and the one with the most has $n+1$ giving an average of sites per row $(n+2)/2$. Hence we arrive at the desired result $g(n) = (n+1)(n+2)/2$ and is just the average value times the number of terms. The partition sum consists of three geometrical sums. $g(n) = \frac{n^2}{2} + \frac{3n}{2} + 1$. The three sums are given by: $1 + x + x^2 + x^3 + x^4 ... = \frac{1}{1-x}$ and $x + 2x^2 + 3x^3 + 4x^4 .. = \frac{x}{(1-x)^2}$ and $x + 2^2x^2 + 3^2x^3 + 4^2x^4 .. = \frac{x(1+x)}{(1-x)^3}$ (you can take the derivative of the first one to arrive at the desired result) and hence:

$$Z = e^{-\frac{3\hbar\omega}{2\tau}}\left(\frac{1}{1-e^{-\frac{\hbar\omega}{\tau}}} + \frac{3}{2}\frac{e^{-\frac{\hbar\omega}{\tau}}}{(1-e^{-\frac{\hbar\omega}{\tau}})^2} + \frac{1}{2}\frac{e^{-\frac{\hbar\omega}{\tau}}(1+e^{-\frac{\hbar\omega}{\tau}})}{(1-e^{-\frac{\hbar\omega}{\tau}})^3}\right)$$

   With $\tau = \frac{\hbar\omega}{\ln 3}$ we arrive at:

$$Z = \left(\frac{1}{3}\right)^{\frac{3}{2}}\left(\frac{1}{1-\frac{1}{3}} + \frac{3}{2}\frac{\frac{1}{3}}{(1-\frac{1}{3})^2} + \frac{1}{2}\frac{\frac{1}{3}(1+\frac{1}{3})}{(1-\frac{1}{3})^3}\right) = \left(\frac{1}{3}\right)^{\frac{3}{2}} \cdot 3.375 = 0.649519052$$

   The Boltzmann factor of the ground state is $\left(\frac{1}{3}\right)^{\frac{3}{2}}$ and the probabillity for the system to be in the ground state is $1/3.375 = 0.296296...$

3. The proton has 2 possible spin directions - and + with energys $-Bm_\mu$ and $+Bm_\mu$. The partition function for a proton in the magnetic field B is

$$Z = e^{Bm_\mu/\tau} + e^{-Bm_\mu/\tau}.$$

The probabillity for a proton to be in the - direction (or state) is given by

$$P(-Bm_\mu) = \frac{e^{Bm_\mu/\tau}}{e^{Bm_\mu/\tau} + e^{-Bm_\mu/\tau}}.$$

and similar for the + direction. As there are N protons the number of protons in the - direction will be $N_- = NP(-Bm_\mu)$ and in the + direction $N_+ = NP(+Bm_\mu)$. The absorbed power is proportional to the difference in the number of protons in the + state to the number in the - state, Power $\propto N_+ - N_- = N(P(+Bm_\mu) - P(-Bm_\mu))$.

$$N_- - N_+ = N\frac{e^{Bm_\mu/\tau} - e^{-Bm_\mu/\tau}}{e^{Bm_\mu/\tau} + e^{-Bm_\mu/\tau}} = N\tanh(Bm_\mu/\tau)$$

In the high temperature limit ($Bm_\mu << \tau$) we have

$$N_- - N_+ = N\tanh(Bm_\mu/\tau) \approx N\frac{Bm_\mu}{\tau}$$

4. See also problem 10.5 in Kittel and Kroemer **a:** $F = -N_f\epsilon_0 + N_g\tau\left(\ln\frac{N_g}{Vn_Q} - 1\right)$ **b:** $N_g = Vn_Qe^{-\epsilon_0/\tau}$ **c:** Make a figure of $\ln p$ as a function of $1/T$. The slope of the straight line is $-\frac{\epsilon_0}{k_B}$ which gives an energy $\epsilon_0 = 0.53$eV.

5. The distribution inside the box is: $P(v) = 4\pi(\frac{M}{2\pi\tau})^{3/2}v^2e^{-Mv^2/2\tau}$ in the exiting beam from the oven the distribution is $\propto vP(v)$ (sid 395 CK). The most probable velocity is given by the maximum of $\propto vP(v)$. $\frac{\mathrm{d}}{\mathrm{d}v}(v^3e^{-Mv^2/2\tau} = ... = e^{-Mv^2/2\tau}(3v^2 - v^4M/\tau) = 0$. Which gives the most probable velocity $v_{ms} = \sqrt{\frac{3\tau}{M}}$. The time for the drum to rotate half a turn is the same as the it takes for a Sodium (Na) with the v_{ms} to travel through the drum the distance d, denote this time as $t_{1/2}$. The equation to solve is $t_{1/2} \cdot v_{ms} = d$. For the angular velocity $\omega = \frac{2\pi}{2t_{1/2}} = \frac{\pi}{d}\sqrt{\frac{3\tau}{M}} = \frac{\pi}{d}\sqrt{\frac{3k_BT}{M}} = \frac{\pi}{0.10}\sqrt{\frac{3\cdot1.3807\cdot10^{-23}\cdot573.1}{22.9898\cdot1.661\cdot10^{-27}}} = 24769.826 \approx 2.48\cdot10^4$rad/s (=3942.2402 revolutions per second)