LULEÅ TEKNISKA UNIVERSITET Avdelningen för materialvetenskap

Exam in: STATISTICAL PHYSICS AND THERMODYNAMICS 2019-03-30 (F7035T) Suggested solutions

1. The general relation for the specific heat is $C_v = \tau \left(\frac{\partial \sigma}{\partial \tau}\right)_v$

a: in case of the conduction electrons we have $C_v = \gamma \tau$ these two relations combine to give $\gamma \tau = \tau \left(\frac{\partial \sigma}{\partial \tau}\right)_v$ leading to $\frac{\partial \sigma}{\partial \tau} = \gamma = constant$. and hence integrating to $\sigma \propto \tau +$ 'new constant' where the 'new constant' is zero as the the entropy is zero at temperature absolute zero. If the temperature increases from $\tau = 200$ K to 800 K the entropy σ will increase by a factor 4.

b: In the case of the electro magnetic field we have that the energy density is $u \propto \tau^4$ (Stefan-Boltzmann T^4 law) and hence we have for the specific heat $C_v \propto \tau^3$ (Note the similarity to phonons at low temperature the Debye T^3 law). As in a) we arrive at $\frac{\partial \sigma}{\partial \tau} \propto \tau^2$ and hence $\sigma \propto \tau^3$. If the temperature is raised from 500K to 2000K the entropy σ will increase by a factor of $(\frac{2000}{500})^3 = 64$ that is a factor of **64**.

- 2. Use the relation $\frac{1}{\tau} = \frac{\partial \sigma}{\partial E}$. $\sigma = \frac{c^3 A}{4G\hbar} = \frac{c^3 4\pi R_s^2}{4G\hbar} = \frac{c^3 4\pi}{4G\hbar} \frac{4G^2 M^2}{c^4} = \frac{4\pi G E^2}{\hbar c^5}$. Now we can evaluate for the temperature.
 - $\frac{1}{\tau} = \frac{\partial \sigma}{\partial E} = \frac{8\pi GM}{\hbar c^3}$, an alternative route is to use $\tau = \frac{\partial E}{\partial \sigma}$ this will give the same result.

b)
$$U = \frac{3}{2}\tau = 1$$
 eV will give ratio $\frac{18e^{13.6/3^2\tau}}{8e^{13.6/2^2\tau}} = \frac{18}{8}e^{20.4(1/9-1/4)} = \frac{18}{8}e^{-2.833} = 0.1323 \approx 0.13$

3. For a molecule the heat capacity C_v is given by $C_v = (\frac{\partial U}{\partial T})_V$. The partition function is $Z = 1 + 3e^{-\epsilon/\tau}$. The energy is $U = \frac{3\epsilon e^{-\epsilon/\tau}}{Z}$

$$C_v = \left(\frac{\partial U}{\partial \tau}\right)_V = \frac{3\left(\frac{\epsilon}{\tau}\right)^2 e^{\epsilon/\tau}}{(3+e^{\epsilon/\tau})^2} \tag{1}$$

Now let $x = \epsilon / \tau$

$$C_v = \frac{3x^2 e^x}{(3+e^x)^2} \tag{2}$$

Taking the derivative $\frac{\partial C_v}{\partial x}$ we arrive at an equation for the maximum of C_v as $3(2+x) + (2-x)e^x = 0$. The maximum is at about $x \approx 2.845$, which gives $C_v = 1.023$ and using the correct units $C_v = 1.023k_B$.

4. a) The partition sum is given by: $Z = \sum_{n_1=0,n_2=0}^{\infty} e^{-(n_1+n_2+1.0)\hbar\omega/k_BT} = \sum_{n=0}^{\infty} g(n)e^{-(n+1.0)\hbar\omega/k_BT}$, where g(n) is the degeneracy of the energy levels and $n = n_1+n_2$. There are two ways to evaluate this sum. One simple and one more elaborate. Only the simple solution is presented here. The sum for Z can be done as a product of two separate independent geometric sums.

 $Z = \sum_{n_1=0,n_2=0}^{\infty} e^{-(n_1+n_2+1.0)\hbar\omega/k_BT} = \sum_{n_1=0}^{\infty} e^{-(n_1+0.5)\hbar\omega/k_BT} \cdot \sum_{n_2=0}^{\infty} e^{-(n_2+0.5)\hbar\omega/k_BT} = \left(\sum_{n=0}^{\infty} e^{-(n+0.5)\hbar\omega/k_BT}\right)^2 = e^{-\hbar\omega/k_BT} \left(\sum_{n=0}^{\infty} e^{-n\hbar\omega/k_BT}\right)^2 = e^{-\hbar\omega/k_BT} \left(\frac{1}{1-e^{-\hbar\omega/k_BT}}\right)^2 = \text{and we}$ arrive at the following for the partition function Z:

$$Z = \left(\frac{1}{e^{+\hbar\omega/2k_BT} - e^{-\hbar\omega/2k_BT}}\right)^2 = \text{ or } = e^{-\hbar\omega/k_BT} \left(\frac{1}{1 - e^{-\hbar\omega/k_BT}}\right)^2.$$

- b) There is one state of the lower energy and two states with the next higher energy. The probability to find the oscillator in a state of energy is proportional to the Boltzmann factor, we arrive at the following equation. $1e^{-1,0\hbar\omega/k_BT} = 2e^{-2,0\hbar\omega/k_BT}$ and $e^{1\hbar\omega/k_BT} = 2$ which evaluates to $T = \frac{1\hbar\omega}{k_B \ln 2}$ or if you prefer τ , $\tau = \frac{1\hbar\omega}{\ln 2}$, which is equally correct.
- c) The partition sum at this specific temperature is given by: $(k_B T = \tau = \frac{1\hbar\omega}{\ln 2})$ we arrive at the following

$$Z = \left(\frac{1}{e^{+\frac{\ln 2}{2}} - e^{-\frac{\ln 2}{2}}}\right)^2 = \left(\frac{1}{\sqrt{2} - \frac{1}{\sqrt{2}}}\right)^2$$

We continue with the calculation of the probability: (we may choose any of the two energies as their probabilities will be equal at the temperature in question: $(1e^{-1,0\hbar\omega/k_BT} = 2e^{-2,0\hbar\omega/k_BT})$

$$P = e^{-\hbar\omega/k_BT} / \left(\frac{1}{\sqrt{2} - \frac{1}{\sqrt{2}}}\right)^2 = 2^{-1} \left(\sqrt{2} - \frac{1}{\sqrt{2}}\right)^2 = \left(\frac{1}{\sqrt{2}}\right)^2 \left(\sqrt{2} - \frac{1}{\sqrt{2}}\right)^2 = \left(1 - \frac{1}{2}\right)^2 = \frac{1}{4} = 0.25$$

The probability to be in a state of one of these energys is $P = \frac{1}{4} = 0.25$

5. See also problem 10.5 in Kittel and Kroemer **a**: $F = -N_f \epsilon_0 + N_g \tau \left(\ln \frac{N_g}{V n_Q} - 1 \right)$ **b**: $N_g = V n_Q e^{-\epsilon_0/\tau}$ **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.