LULEÅ TEKNISKA UNIVERSITET
Avdelningen för materialvetenskap

Exam in: STATISTICAL PHYSICS AND THERMODYNAMICS 2017-03-24 (F7035T)
Suggested solutions

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1. Separation of phases is treated in the course book chapter 11. A couple of important topics of a good solution are: The treatment of 'entropy of mixing' $\sigma_M = -N[(1-x)\ln(1-x)+x\ln(x)]$. The free energy $f = u-\tau\sigma$ (per atom). The construction of a graph of $\frac{\sigma_M}{N}$ vs x. Figure I of the problem gives a free energy that gives rise to a separation of phases below a certain temperature into two phases of different mixing x. Figure II does not support any phase separation of the mixture.

2. As problem 7.1 in Kittel Kroemer. Start to evaluate the Density of States (DOS). As a system usa a square of side L. The energy of a particle in a 2 dimensional box is given by

$$\epsilon_n = \frac{\hbar^2}{2m}\left(\frac{\pi}{L}\right)^2 (n_x^2 + n_y^2) = \frac{\hbar^2}{2m}\left(\frac{\pi}{L}\right)^2 n^2 \tag{1}$$

The number of electrons N (Fermions) inside a circle of radius n defined in $n^2 = n_x^2 + n_y^2$ is given by (including spin):

$$N = 2\cdot\frac{1}{4}\pi n^2 = \frac{\pi 2mL^2}{2\hbar^2\pi^2}\,\epsilon \quad \text{for all electrons } = 2\cdot\frac{1}{4}\pi n_F^2 \tag{2}$$

differentiating to get DOS

$$D(\epsilon) = \frac{dN}{d\epsilon} = \frac{mL^2}{\hbar^2\pi} \quad \text{(a constant)} \tag{3}$$

3. 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.
$Z = \sum_{n_1=0,n_2=0}^{\infty} e^{-(n_1+n_2+1.0)\hbar\omega/k_BT} = \sum_{n_1=0}^{\infty} e^{-(n_1+0.5)\hbar\omega/k_BT}\cdot\sum_{n_2=0}^{\infty} e^{-(n_2+0.5)\hbar\omega/k_BT} = \left(\sum_{n=0}^{\infty} e^{-(n+0.5)\hbar\omega/k_BT}\right)^2 = e^{-\hbar\omega/k_BT}\left(\sum_{n=0}^{\infty} e^{-n\hbar\omega/k_BT}\right)^2 = e^{-\hbar\omega/k_BT}\left(\frac{1}{1-e^{-\hbar\omega/k_BT}}\right)^2 =$ 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: ($k_BT = \tau = \frac{1\hbar\omega}{\ln 2}$) 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 $P = \frac{1}{4} = 0.25$

4. The equation of state for an ideal gas is $pV = Nk_BT$ and we have to derive the corresponding equation if the particles interact weakly by a van der Waals interaction.

   From the partition function Z the pressure may be derived according to $P = k_BT\left(\frac{\partial \ln Z}{\partial V}\right)_T = \frac{Nk_BT}{V-bN} - \frac{aN^2}{V^2}$ which can be rearranged to $\left(P + \frac{aN^2}{V^2}\right)(V - bN) = Nk_BT$.

   In a similar way the energy can be expressed as a derivative of the logarithm of the partition function with respect to the temperature. The inner energy U is given by $U = k_BT^2\left(\frac{\partial \ln Z}{\partial T}\right)_V = N\left(\frac{3k_BT}{2} - \frac{aN}{V}\right)$

5. There are n empty lattice sites these can be choosen in $\binom{N}{n} = \frac{N!}{n!(N-n)!}$ ways. There are n interstitial sites occupied, these can be choosen in $\binom{N}{n} = \frac{N!}{n!(N-n)!}$ ways. Hence there are in total $W(n) = \binom{N}{n}^2$ ways to form as configuration with n atoms at interstitial sites, all with energy $E = n\epsilon$. The entropy $\sigma = \ln(W(n)) = \ln(\frac{N!}{n!(N-n)!})^2 = 2\ln(\frac{N!}{n!(N-n)!}) \approx 2[N\ln N - n\ln n - (N - n)\ln(N-n)]$ Use def of temperature: $\frac{1}{\tau} = \frac{\partial\sigma}{\partial E} = \frac{\partial\sigma}{\partial n}\frac{dn}{dE} = \frac{1}{\epsilon}2[-\ln n + \ln(N-n) = \frac{2}{\epsilon}\ln\frac{N-n}{n}$. This gives $\frac{n}{N} = \frac{1}{e^{\epsilon/2\tau}+1} \approx e^{-\epsilon/2\tau}$ (if $\epsilon >> \tau$).