LULEÅ TEKNISKA UNIVERSITET
Avdelningen för materialvetenskap

Exam in: STATISTICAL PHYSICS AND THERMODYNAMICS 2012-05-18 (F7035T)
Suggested solutions

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1. 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 $U = k_BT^2\left(\frac{\partial \ln Z}{\partial T}\right)_V = N\left(\frac{3k_BT}{2} - \frac{aN}{V}\right)$

2. From the energy $\epsilon(j) = j(j+1)\epsilon_0$ and degeneration $g(j) = 2j+1$ we arrive at the partition function $Z_R(\tau) = \sum e^{-\epsilon_i/\tau} = \sum_{j=0}^{\infty}(2j+1)e^{-j(j+1)\epsilon_0/\tau}$. The high temperature limit $\tau >> \epsilon_0$ this becomes $Z_R(\tau) \approx \int_0^{\infty}(2j+1)e^{-j(j+1)\epsilon_0/\tau}\ \mathrm{d}j$, a change of variables ($j(j+1) = x^2$ and $\mathrm{d}j(2j+1) = 2x\ \mathrm{d}x$), $= \int_0^{\infty} 2xe^{-x^2\epsilon_0/\tau}\ \mathrm{d}x = [-\frac{\tau}{\epsilon_0}e^{-x^2\epsilon_0/\tau}]_0^{\infty} = \frac{\tau}{\epsilon_0}$

   The specific heat C_v, (high temperature) The Free energy $F = -\tau \ln Z_R \approx = -\tau \ln \frac{\tau}{\epsilon_0}$, entropy $\sigma = -\frac{\partial F}{\partial \tau} \approx \ln \frac{\tau}{\epsilon_0} + 1$, and $C_v = \tau\frac{\partial \sigma}{\partial \tau} \approx 1$. ie. $C_v = 1k_B$ per molecule in the high temperature limit.

   For low temperatures, $\tau << \epsilon_0$ we get $Z_R(\tau) \approx 1 + 3e^{-2\epsilon_0/\tau}$ and $F = -\tau\ln(1 + 3e^{-2\epsilon_0/\tau})$ and $\sigma = -\frac{\partial F}{\partial \tau} = \ln(1 + 3e^{-2\epsilon_0/\tau}) + \tau\frac{1}{1+3e^{-2\epsilon_0/\tau}} \cdot \frac{6\epsilon_0}{\tau^2}e^{-2\epsilon_0/\tau}$. This leads to $C_v = \tau\frac{\partial \sigma}{\partial \tau} = ... = \frac{18\epsilon_0^2e^{-2\epsilon_0/\tau}}{\tau^2(1+3e^{-2\epsilon_0/\tau})}\left[1 - \frac{e^{-2\epsilon_0/\tau}}{1+3e^{-2\epsilon_0/\tau}}\right]$ approximate $\frac{1}{1+x} \approx 1-x$ as x is small this gives $C_v \approx \frac{18\epsilon_0^2e^{-2\epsilon_0/\tau}}{\tau^2}(1 - 3e^{-2\epsilon_0/\tau})(1 - e^{-2\epsilon_0/\tau}(1 - 3e^{-2\epsilon_0/\tau})) \approx \frac{18\epsilon_0^2e^{-2\epsilon_0/\tau}}{\tau^2}$. Answer $\tau >> \epsilon_0 : C_v = 1$, and $Z_R(\tau) = \frac{\tau}{\epsilon_0}$ and for $\tau << \epsilon_0 : C_v = \frac{18\epsilon_0^2e^{-2\epsilon_0/\tau}}{\tau^2}$, and $Z_R(\tau) = 1 + 3e^{-2\epsilon_0/\tau}$

3. As only the difference is of interest we can put the energy of the ground state to zero and the excited state to ϵ. The partition sum becomes: $Z = 1 + 2e^{-\epsilon/\tau}$ and hence the energy will be $U =< \epsilon >= \frac{0+2\epsilon e^{-\epsilon/\tau}}{1+2e^{-\epsilon/\tau}} = \frac{2\epsilon}{2+e^{\epsilon/\tau}} = \frac{2\epsilon}{2+e^{\epsilon/k_BT}}$ an alternative rout is to take the derivative of Z which gives $U = \tau^2\frac{\partial \ln Z}{\partial \tau} = \tau^2\frac{1}{Z}2e^{-\epsilon/\tau}\frac{\epsilon}{\tau^2} = \frac{2\epsilon}{2+e^{\epsilon/\tau}} = \frac{2\epsilon}{2+e^{\epsilon/k_BT}}$. Finally we arrive at C_v by a derivative of U with respect to τ $C_v = \frac{\partial U}{\partial \tau} = \frac{2\epsilon^2e^{\epsilon/\tau}/\tau^2}{(2+e^{\epsilon/\tau})^2}$. This can be written as $\frac{2x^2e^x}{(2+e^x)^2}$ where $x = \epsilon/\tau$. To find the maximum take the derivative with respect to x. $\frac{(2x+x^2)e^x}{3+e^x)^2} - \frac{2x^2e^{2x}}{(3+e^x)^3} = 0$ which gives the condition $(x-2)(e^x-2) = 8$. This may be solved graphically or by a pocket calculator. The solution is $x \approx 2.655$ ie. $\epsilon = x\ \tau = x\ k_B\ T = 2.655 \cdot 1.3807 \cdot 10^{-23} \cdot 450 = 1.650 \cdot 10^{-20}$J $= 0.103$eV.

4. Here Claypeyrons equation will be used : $\frac{dp}{dT} = \frac{q}{T\Delta v} = -\frac{3.689 \cdot 10^9}{T}$ ($\Delta v = v_{\text{liquid}} - v_{\text{is}} = \frac{1}{999.8} - \frac{1}{916.8} = -9.0550 \cdot 10^{-5}$ m^3/kg, $q = 334 \cdot 10^3$ J/kg). This gives for small changes of temperature: $\Delta T = -\frac{T\Delta p}{3.689 \cdot 10^9} = -0.0666 \approx -0.07$K, ie a lowering of the freezing point by 0.07K.

5. In a 3D Ising model on a cubic lattice each spin has 6 nearest neighbours, and in a Mean Field assumption these 6 nearest neighbours will have the magnitude $< m >$ and the spin we perform our calculation on will take the following values $s_i = \pm 1$.. This gives $Z = \sum_i e^{-\epsilon_i/\tau} = e^{+6m/\tau} + e^{-6m/\tau}$ and the magnetisation will be $< m >= \frac{+1e^{+6m/\tau} - 1e^{-6m/\tau}}{e^{+6m/\tau} + e^{-6m/\tau}} = \tanh(\frac{6m}{\tau})$. As m s small we may approximate $\tanh x \approx x - x^3/3$. This gives $m = \frac{6m}{\tau} - (\frac{6m}{\tau})^3 \frac{1}{3}$ the equation $m^2 = \frac{3\tau^2}{216}(6-\tau)$ a solution close to $m = 0$ as is $\tau \approx \tau_c$: $m^2 = \frac{3\tau_c^2}{216}(6-\tau)$ and $m = \frac{\sqrt{3}\tau_c}{\sqrt{216}} \sqrt{(6-\tau)}$ and we arrive at the exponent $\beta = \frac{1}{2}$.