Statistical Mechanics WS 2013/14 Sheet 9

This problem sheet aims a review of topics which have been covered so far. Happy Christmas!

Problem 1 : Characteristic Function and Moments (10 points)

From experiments on a certain random system, the characteristic function $g(k) = \cos(kc)$ was found, where c is a positive real number.

a) (2 points) Derive the corresponding probability density function $w(x)$.

b) (2 points) Calculate $\langle x \rangle$ and $\langle x^2 \rangle$.

c) (3 points) Calculate the m-th moments $\langle x^m \rangle$ using $g(k)$.

d) (3 points) Calculate $\langle x^m \rangle$ using $w(x)$.[Hint for c) and d): $\langle x^m \rangle$ significantly depends on whether m is odd or even]

Problem 2 : Two-State System (10 points)

Consider a system of N identical, non-interacting, and distinguishable molecules which have two energy levels $+\epsilon$ or $-\epsilon$ each.

a) (3 points) Using the microcanonical ensemble, calculate the entropy per molecule $s = S/N$.

b) (3 points) Using the canonical ensemble, calculate the entropy per molecule $s = S/N$.

c) (3 points) Using the grand canonical ensemble, calculate the entropy per molecule $s = S/N$.

d) (1 point) Rewrite the above three results in the thermodynamic limit. What can you see?

Problem 3 : 1D Ising Model (20 points)

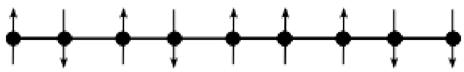

Fig. 1: The one-dimensional spin chain.

Shown in Fig. 1 is a one-dimensional Ising model. It is a system of N quantized spins, located at the points of a one-dimensional lattice. The n-th spin can have two possible values $\sigma_n = \pm 1$. A pair of neighbouring spins has an interaction energy equal to $-V$ if they are parallel and $+V$ if they are antiparallel. Therefore the total energy of any configuration, defined by specifying the values of $\sigma_1, \ldots, \sigma_N$, is

$$H = -V(\sigma_1\sigma_2 + \sigma_2\sigma_3 + \ldots + \sigma_{N-1}\sigma_N) \quad (1)$$

By transforming to new variables, $\zeta_1 = \sigma_1, \zeta_2 = \sigma_2\sigma_1, \zeta_3 = \sigma_3\sigma_2, \ldots, \zeta_N = \sigma_N\sigma_{N-1}$, calculate the average energy and the heat capacity of the system as a function of the temperature.

Problem 4 : Rubber Band (20 points)

1. Consider we have a special kind of rubber band whose equation of state can be approximated simply as

$$\tau = \alpha L T, \quad (2)$$

where τ is the tension(force), α is a constant in units of $[k_B/\text{length}^2]$, L is the length of the rubber band, and T is the temperature. The heat engine using this rubber band has a cycle in the τ-L phase space, as depicted in Fig. 2.

a) (2 points) Find the isothermal process(es) among processes 1-2, 2-3 and 3-1.

b) (2 points) Find the temperatures at each point: T_1, T_2 and T_3.

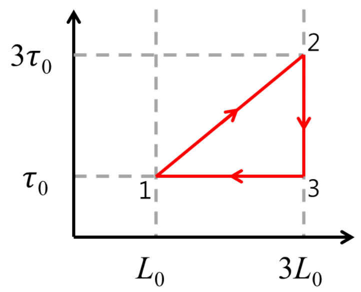

Fig. 2: The heat engine cycle of a rubber band.

c) (2 points) Calculate the total work W. [Hint: Find geometrical meaning of the work from the diagram in Fig. 2.]

d) (2 points) Calculate the heat Q_{12} for the process from point 1 to 2. Is it positive or negative or zero?

e) (2 points) Calculate the efficiency η of this engine which is the ratio of total work W to Q_{12}, i.e., $\eta = \frac{W}{Q_{12}}$.

2. Now consider the rubber band as a three dimensional chain consisting of N sequence of vector segments: $\{\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N\}$, with a unit segmental length L_0. Thus the fully extended length of the rubber chain is denoted by $L_f = NL_0$. Each segmental vector, just like the lattice random walk, is assumed to be one of 6 possible vectors: $\mathbf{r}_i \in \{\pm L_0\hat{\mathbf{x}}, \pm L_0\hat{\mathbf{y}}, \pm L_0\hat{\mathbf{z}}\}$. Suppose that a tension $\boldsymbol{\tau} = \tau\hat{\mathbf{z}}$ applies to this rubber chain, such that the energy ϵ_i for i-th segment is expressed by $\epsilon_i = -\mathbf{r}_i \cdot \boldsymbol{\tau}$ at temperature T.

a) (2 points) Calculate the partition function Z.

b) (2 points) Calculate the average energy $\langle E \rangle$.

c) (2 points) Calculate the average length L of the rubber chain. Use $L = -\frac{\partial \langle E \rangle}{\partial \tau}$.

d) (2 points) Assuming that τ is small, calculate the average length L of the rubber chain. [Hint: Use the Taylor expansion upto the first order of τ.]

e) (2 points) Rewrite the result from d) for τ. You will see that this result leads to Eq. (2). Express the α in Eq. (2) in terms of the above quantities.

Problem 5 : Condition for Equilibrium (20 points)

The first law of thermodynamics states $\Delta U = \Delta Q - p\Delta V$. The second law postulates $\Delta Q \leq T\Delta S$. Starting from these laws show that the conditions for equilibrium are that

a) (10 points) at constant T, V the free energy is minimal ($\Delta F \leq 0$).

b) (10 points) at constant T, p the Gibbs potential is minimal ($\Delta G \leq 0$).