Statistical Physics I - PHYS 663 - *Spring 2018*

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Homework

HW

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due *2018-05-10*

> Substitution HW
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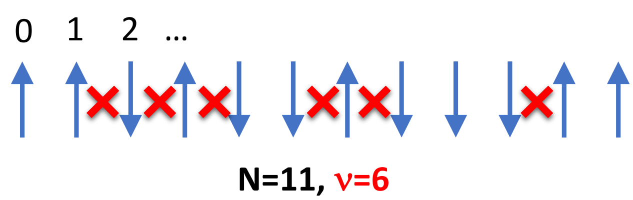
> Problems on this sheet can replace regular HW problems with comparable point values.

I. ONE-DIMENSIONAL ISING MODEL WITH INTERACTION *[(2+2+4+4) PTS]*

Here we consider a system with *interacting* degrees of freedom. $N+1$ Ising spins $S_i = \pm 1$, $i = 0, 1, 2, \ldots, N$, are arranged in a line. The energy of a microstate is given by the Hamiltonian

$$\mathcal{H}(\{S\}) = -J \sum_{i=1}^{N} S_i S_{i-1} \,.$$



a) To determine the number of microstates, it is useful to find out how many states have the same energy. The system's energy can be expressed through the number of broken bonds ν (a broken bond is a pair of neighboring spins with anti-parallel spins, see sketch). Calculate the possible energies E_ν and the corresponding number of microstates. What is the partition function $Z^{(mc)}(E_\nu)$?

b) Using the results from a), calculate the canonical partition function:

$$Z^{(c)}(\beta) = \sum_{\{S\}} e^{-\beta \mathcal{H}(\{S\})} = \sum_{\nu} Z^{(\mathrm{mc})}(E_\nu) e^{-\beta E_\nu}$$

c) Calculate and sketch the average energy, heat capacity, and Gibbs entropy as function of temperature for $N \to \infty$ (canonical ensemble).

d) Find a relation between heat capacity C and square energy deviations $\Delta E^2 = \left\langle (\mathcal{H} - \langle \mathcal{H} \rangle)^2 \right\rangle$ and justify that fluctuations $\Delta E/N$ vanish in the thermodynamic limit $N \to \infty$.

II. ISING SPIN SYSTEM IN MAGNETIC FIELD *[(2+2+4+4) PTS]*

In a classical Ising spin system with N spins, each spin can be in one of two states: $S = \pm 1$. We consider such a system of non-interacting spins in an external magnetic field H. The energy of a single spin i has the value $E_i = \mu H S_i = \epsilon_0 S_i$. The macrostates are defined by the total energy $E = M\epsilon_0$ for $M = -N, \ldots, N$. Calculate:

a) the number of microstates in a macrostate,

b) the entropy $S_B(E)$,

c) the temperature $T(E)$ for $N \gg 1$, and

d) energy and entropy as function of temperature.

III. IDEAL GAS OF RELATIVISTIC PARTICLES *[4+3 PTS]*

We consider an ideal gas of N non-interacting relativistic particles in a volume $V = L^3$ in 3 dimensions. These particles follow the Boltzmann statistics. The energy of a particle i is proportional to its momentum, i.e., $\epsilon_i = c|\mathbf{p}_i|$.

a) Calculate $E(\beta)$ and the heat capacity C of the gas.

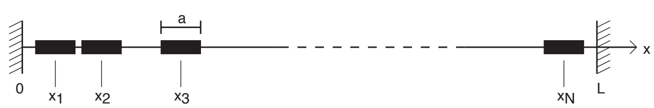
a) Calculate $S_B(\beta)$.

IV. GAS OF EXTENDED PARTICLES *[(5+2) PTS]*

We consider N classical rods of length a in a one-dimensional "volume" of length $L \geq Na$. The interaction potential of two neighboring particles at their center of mass coordinates x_i and x_j shall be

$$\Phi(x_i - x_j) = \begin{cases} \infty & |x_i - x_j| \leq a \\ 0 & \text{sonst} \end{cases}$$

Therefore the particles cannot permeate each other or interchange positions.



a) Calculate the equation of state $p(T, L, N)$ of the system.

b) Obtain the equation of state in the thermodynamic limit ($N, L \to \infty$ and $n = N/L = \text{const.}$).

V. TWO-COMPONENT GAS *[(3+5) PTS]*

Here we consider a gas consisting of two types of particles, which only differ in their mass (e.g. two isotopes of one element). N_1 particles have the mass m_1 and N_2 particles mass m_2. All particles should be considered classical and non-interacting, i.e.,

$$\mathcal{H}(\vec{X}) = \sum_{i=1}^{N_1} \frac{p_i^2}{2m_1} + \sum_{i=N_1+1}^{N_1+N_2} \frac{p_i^2}{2m_2}.$$

The gas has temperature T and is enclosed in volume V.

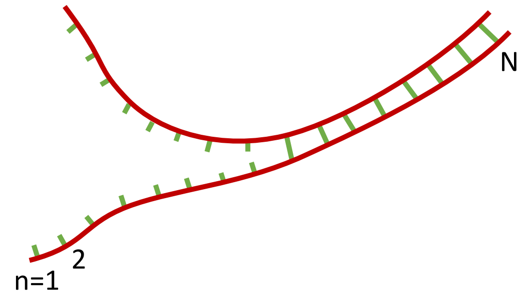
a) Calculate the Helmholtz free energy $F(T, V, N_1, N_2)$. Verify the homogeneity relation $F(T, \lambda V, \lambda N_1, \lambda N_2) = \lambda F(T, V, N_1, N_2)$.

b) Calculate from that the Gibbs free energy $G(T, p, N_1, N_2)$ via Legendre transformation. What is the homogeneity relation for G?

c) From the homogeneity relation for G derive the Gibbs-Duhem relation $G(T, p, N_1, N_2) = \mu_1 N_1 + \mu_2 N_2$.

VI. MOLECULAR ZIPPER *[(4+6) PTS]*

As a (strongly) simplified model for a DNA double helix molecule, we consider a "molecular zipper": two linear molecule strands, which are linked by N connectors. These connectors can open when heated, but only sequentially starting from the beginning of the strands. Breaking one connection cost a finite energy $\epsilon > 0$ and connector $n+1$ can only open if link n is already broken (open). Connection N shall always be closed.



a) Calculate the canonical partition function $Z^{(c)}$ of this system.

b) Calculate the average number of open links $\langle n \rangle$ as function of $x \equiv e^{-\beta\epsilon}$ and sketch $\langle n \rangle / N$ as function of x. Discuss the result.