Variational Nonequilibrium Statistical Mechanics

Wintersemester 2018/19
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UNIVERSITÄT BAYREUTH

Blatt 6 - Hausaufgabe

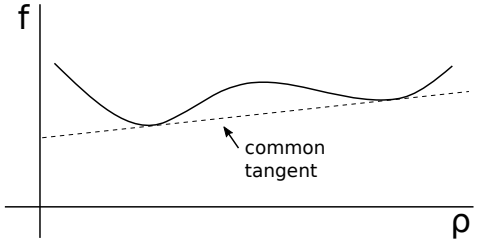
Übung am 7. December 2018

Aufgabe 1: Phase coexistence

A monocomponent system at constant temperature T undergoes a first order phase transition between phases A and B. Demonstrate that:

a) The coexisting points share a common tangent in the $\rho - f$ plane (see figure). Here $\rho = N/V$ is the density and $f = F/V$ is the Helmholtz free energy per unit of volume.

b) How would you calculate the coexistence in the grand ensemble?



c) Show that in a binary mixture at constant temperature T and pressure P, two coexisting phases share a common tangent in the $x - g$ plane. Here $x = N_i/N$ is the composition of one of the species $(i = 1, 2)$, and $g = G/N$ with G the Gibbs free energy.

Aufgabe 2: Ideal gas in the grand ensemble

a) Deduce the equation of state of an ideal gas $PV = Nk_BT$ form the grand canonical partition function.
b) Calculate the fluctuations in the number of particles $(\Delta N)^2 = \langle N^2 \rangle - \langle N \rangle^2$.

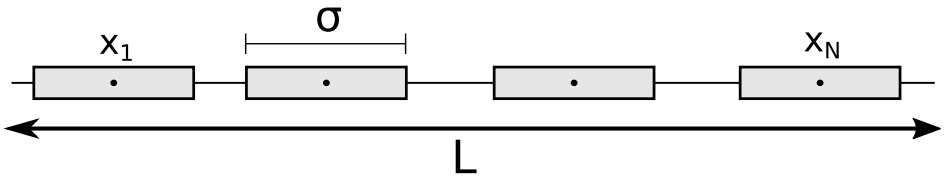
Aufgabe 3: Hard rods

Consider a system of N one dimensional hard rods of length σ confined in a line segment of length L (see figure). The interaction potential $\phi(x)$ between two particles separated by a distance x is infinite if the particles overlap $(x < \sigma)$ and zero otherwise.

a) Calculate the canonical partition function.

b) Show that the pressure is $P = k_BT\rho(1 + \eta/(1 - \eta))$ with $\eta = \sigma\rho$ and $\rho = N/L$.

Hint: Consider the particles are ordered $x_1 < x_2 < \cdots < x_N$ and use the variable change $\zeta_i = x_i - (i - 0.5)\sigma$. The boundary conditions are $x_1 > \sigma/2$ and $x_N < L - \sigma/2$.



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Aufgabe 4: Density profile of hard rods

Calculate the canonical density profile $\rho(x)$ of a system of $N = 2$ one-dimensional hard rods confined in a line segment of length $L > 2\sigma$.