Exam — Session 1

Duration: 2 h.

Documents, cell phones, computers, tablets, pocket calculators, etc., are not allowed.
The text contains 4 pages in total, and the 2 exercices are independent from each other.

1 One-dimensional gas of hard rods (Tonks gas)

Let us consider a simple one-dimensional model for a classical fluid, composed of N hard rods of length ℓ and mass m (see Fig. 1). The rods are confined along a one-dimensional space of length L and are maintained at a fixed temperature T (canonical ensemble). The rods interact through a two-body hard-wall potential $V(x)$. We denote by x_i the position of the middle of the ith rod ($i = 1, \ldots, N$).

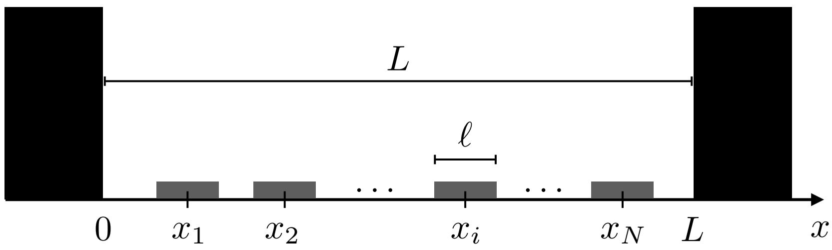

Figure 1: Sketch of a one-dimensional gas of N hard rods confined along a one-dimensional space of length L by two walls (in black).

(a) Are the rods distinguishable or indistinguishable? Very briefly justify your answer.

(b) Show that in the (semi-)classical, dilute limit, the canonical partition function of the system takes the form

$$Z = \left(\frac{2\pi m k_{\mathrm{B}} T}{h^2}\right)^{N/2} I_N(L),$$

with k_{B} and h the Boltzmann and Planck constants, respectively, and where the integral $I_N(L)$ is defined as

$$I_N(L) = \int_{\ell/2}^{L-(N-1)\ell-\ell/2} \mathrm{d}x_1 \ldots \int_{x_{i-1}+\ell}^{L-(N-i)\ell-\ell/2} \mathrm{d}x_i \ldots \int_{x_{N-1}+\ell}^{L-\ell/2} \mathrm{d}x_N. \tag{1.1}$$

We remind the reader that $\int_{-\infty}^{+\infty} \mathrm{d}u \exp(-u^2) = \pi^{1/2}$.

(c) By performing the change of variables

$$y_i = x_i + (N-i)\,\ell + \frac{\ell}{2} \qquad (i = 1, \ldots, N)$$

in Eq. (1.1), show that

$$I_N(L) = \frac{(L - N\ell)^N}{N!}.$$

(d) Deduce from your answers to the previous questions the equation of state of the system, *i.e.*, the pressure P as a function of the parameters of the problem. Sketch the isothermal curves P as a function of the system size L for various temperatures. Does the system showcase a phase transition?

(e) The virial expansion of the equation of state is given by

$$\beta P = \sum_{n=1}^{\infty} B_n(T) \rho^n,$$

where $\beta = 1/k_{\mathrm{B}}T$, $\rho = N/L$ is the density, and

$$B_2\left(T\right) = \frac{1}{2} \int \mathrm{d}x \left[1 - \mathrm{e}^{-\beta V(x)}\right].$$

Calculate in two different ways the second virial coefficient $B_2(T)$ and check the consistency of your results.

(f) For the one-dimensional system at hand, the isothermal compressibility is defined as

$$\chi_T = -\frac{1}{L} \left(\frac{\partial L}{\partial P}\right)_T.$$

Calculate χ_T and comment on your result.

2 The Blume–Capel model

The Blume–Capel model describes a magnetic material with some nonmagnetic vacancies. Let us consider a lattice [we denote by $N(\gg 1)$ the number of lattice sites and by z the number of nearest neighbors] of spins S_i that can take the values -1, 0, and $+1$. A spin 0 corresponds to a vacancy (nonmagnetic impurity or empty site) and spins $+1$ or -1 correspond to the two different orientations of the magnetic species. We assume that the Hamiltonian of the system in presence of a homogeneous magnetic field h is given by

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} S_i S_j + \Delta \sum_{i=1}^{N} S_i^2 - h \sum_{i=1}^{N} S_i, \tag{2.1}$$

where $J > 0$ is the exchange interaction and where Δ is a constant that can be either negative or positive. In the Hamiltonian above, $\langle i,j \rangle$ denotes a summation over nearest neighbors.

2.1 General discussion

(a) Justify that $-\Delta$ is the energy of creation of a vacancy. In which case ($\Delta > 0$ or $\Delta < 0$) is it favorable to create a vacancy?

(b) At $T = 0$ and $h = 0$, calculate the energy of the system in the three different states $S_i = +1$, $S_i = -1$, and $S_i = 0$ ($\forall i = 1, \ldots, N$). Which state(s) is (are) selected at $T = 0$, depending on the value of Δ with respect to $zJ/2$?

(c) Which limit of Δ corresponds to the usual two-state Ising model?

2.2 Mean-field approximation

We now aim at performing a mean-field approximation (MFA). We write $S_i = m + \delta S_i$, where $m = \langle S_i \rangle$ is the average magnetization and δS_i the fluctuations of the spin S_i around m.

(a) Define the spin-spin correlation function C_{ij}. What is the value of C_{ij} in the MFA?

(b) Show that within the MFA, it is possible to write the Hamiltonian (2.1) as

$$\mathcal{H} \simeq \frac{1}{2} N z J m^2 - (h + zJm) \sum_{i=1}^{N} S_i + \Delta \sum_{i=1}^{N} S_i^2.$$

(c) Calculate the free energy F within the MFA.

(d) Demonstrate that the average value $m = \langle S_i \rangle$ is given by the expression

$$m = -\frac{1}{N}\frac{\partial F}{\partial h}.$$

Deduce that, within the MFA, the magnetization obeys the self-consistent equation (SCE)

$$m = \frac{2\sinh\left(\beta[h + zJm]\right)}{\exp\left(\beta\Delta\right) + 2\cosh\left(\beta[h + zJm]\right)}.$$

From now on, we consider the case of vanishing magnetic field, $h = 0$.

(e) In the case $\Delta \to -\infty$, discuss the solutions of the SCE.

(f) In the general case, show that $m = 0$ is a solution of the SCE.

(g) We now aim at discussing graphically the solutions of the SCE. We define $t = k_{\mathrm{B}}T/zJ$ and $\delta = \Delta/zJ$.

(i) Express the SCE in term of the function

$$f(m) = \frac{2\sinh\left(m/t\right)}{\exp\left(\delta/t\right) + 2\cosh\left(m/t\right)}.$$

(ii) What is the value of $f(0)$?

(iii) What are the limits of $f(m)$ when $m \to \pm\infty$?

(iv) Calculate

$$\left.\frac{\mathrm{d}f}{\mathrm{d}m}\right|_{m=0}$$

and discuss graphically the number of solutions to the SCE. Show that there is a critical reduced temperature t_{c} defined by the equation

$$t_{\mathrm{c}} = \frac{2}{2 + \exp\left(\delta/t_{\mathrm{c}}\right)}.$$

(v) On next page in Fig. 2 (colored lines) is plotted the function

$$g(t,\delta) = \frac{2}{2 + \exp\left(\delta/t\right)} \tag{2.2}$$

as a function of t for different values δ_i of δ. Which δ_i's are positive and which of them are negative? Sort by ascending order the δ_i's.

(vi) Plot the curve $g(t,\delta)$ for the value of δ corresponding to the Ising model and give the corresponding t_{c}.

(vii) Using your previous discussion and question 2.1(b), sketch the general behavior of t_{c} as a function of δ.

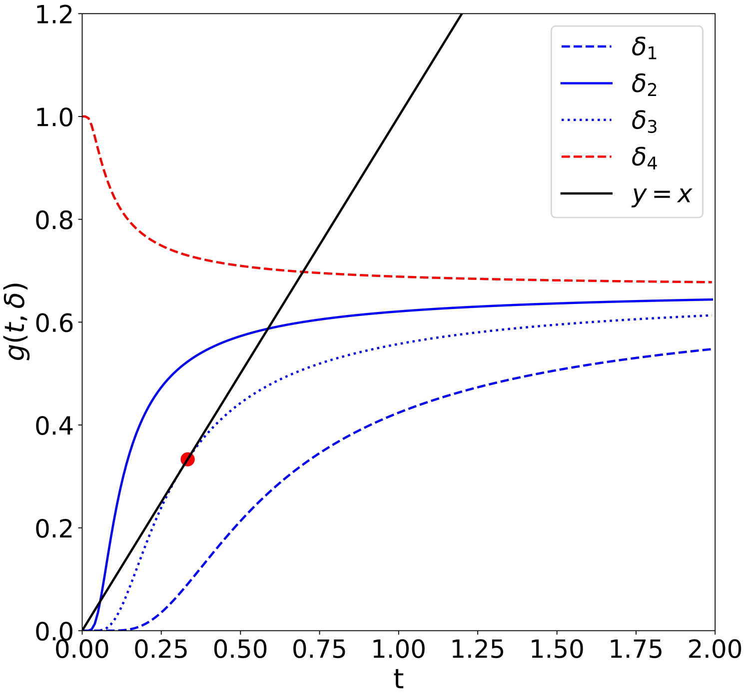

Figure 2: Colored lines: Plot of $g(t, \delta)$ as defined in Eq. (2.2) as a function of t for different values δ_i of δ. Black solid line: t.