Exam: Statistical Mechanics 2016/17, ICFP Master (first year)

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Introduction

Some general information:

- Starting time: 9:00 AM, finishing time: 12:00 PM (noon)
- External material is not allowed (no books, scripts, calculators, computers, etc.). Use only paper provided by ENS.
- Don't forget to write your name onto the cover sheet.
- Please transfer your answers from the green scratch paper (brouillon) to the white exam paper.
- Please leave the scratch paper at your desk.
- Do not forget to sign the register ("feuilles d'émargement").

I. THE GAS-AND-PISTON MODEL

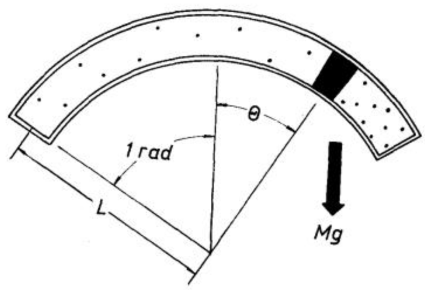

FIG. 1: The gas-and-piston model, consisting of an airtight circular container of radius L permitting heat exchange with the exterior, and a moveable gas-tight piston acted on by the gravitational force Mg. The angular position of the piston is described through the variable θ which satisfies $-1 < \theta < 1$. The piston has surface area S that satisfies $S \ll L^2$. An ideal gas of N molecules fills the left compartment, and likewise an ideal gas of N molecules fills the compartment to the right. The gravitational pull on the molecules is neglected. The mass M of the piston is proportional to N.

Consider the simple statistical-mechanical model of Fig. 1 (gas-and-piston model), which consists of an airtight circular container of radius L allowing heat exchange, and a moveable gas-tight piston acted on by the gravitational force Mg. The position of the piston is described through the angular variable θ which satisfies $-1 < \theta < 1$. The piston has surface area S that satisfies $S \ll L^2$. An ideal gas of N molecules fills the left compartment, and likewise an ideal gas of N molecules fills the compartment to the right. The mass M of the piston is proportional to N. We neglect the gravitational pull on the molecules.

- In general terms, sketch the behavior of this system for fixed, but large N, in the limit of infinite temperatures, as well as in the limit of zero temperature.
- Write down the partition function $Z_N(T)$ of this system as an integral over piston position AND coordinates of the $2N$ gas particles. NB: Use an analogy to what we did for the partition function of a system of N particles in one dimension:

$$Z_N(T) = \frac{1}{N!} \int dx_1 \dots dx_N \exp\left[-\beta V(x_1, \dots, x_N)\right] \quad (1)$$

  (i.e., do not worry about thermal quantum wavelengths, etc.)
- Use the fact that the molecules in the compartments can be treated as ideal to integrate out the molecular positions, that is, write the partition function $Z_N(T)$ of the gas-and-piston

model as an integral over the piston position θ only. Can you determine the free energy $F_N(T)$ without approximation for general N?

- The partition function and the free energy, as written, do not take into account the particle velocities or the piston velocity. Is this an approximation, i.e., are the partition function and the free energy correct only in the limit of small velocities?

II. GAS-AND-PISTON MODEL AND CONSTRAINED FREE ENERGIES

We now describe the gas-and-piston model of Fig. 1 through a fixed value of the angle θ, that is, through a constrained partition function $Z_N(\theta, T)$, and an associated constrained free energy $F_N(\theta, T)$ (NB with $Z_N(\theta, T) = \exp[-\beta F_N(\theta, T)]$) for which the position of the piston is fixed. In other words, $Z_N(\theta, T)$ is the partition function $Z_N(T)$ under the condition (constraint) that the piston position equals θ.

- State the conditions on $F_N(\theta, T)$ that follow from the basic symmetry requirements of this problem. Sketch the two possible functional forms of $F_N(\theta, T)$ that are compatible with this symmetry.
- Compute $F_N(\theta, T)$ for small θ up to the order θ^4.
- A famous theory analyzes general phase transitions in terms of constrained free energies. What is the name of this theory, and what is its principal insight (that can also be applied to the gas-and-piston model)?
- Compute the phase transition temperature T_c predicted by the constrained free energy in the case of the gas-and-piston model, if we suppose that the true value of θ, $\theta_{\min}$, minimizes the constrained free energy $F(\theta, T)$. What is the value of $\theta_{\min}$ for $T \gtrsim T_c$ and for $T \lesssim T_c$? Is the free energy $F_N(\theta_{\min}, T)$ analytic for all temperatures?
- The analysis in terms of the constrained free energy, is it exact at finite N for the gas-and-piston model? Is it exact in the limit of infinite N?
- Explain whether the analogous famous constrained theory for the Ising model in the thermodynamic limit is qualitatively correct for the one-dimensional Ising model. Further state whether it is qualitatively correct for the two-dimensional Ising model. Is it qualitatively correct for the Ising model in high dimensions?

III. GAS-AND-PISTON MODEL AND MECHANICAL STABILITY

We now study the gas-and-piston model, in the constrained formulation, from the point of view of mechanical stability. This means that we suppose that if the piston in Fig. 1 is pushed to the right, the volume of the right compartment is decreased, and its pressure increased. An analogous analysis applies to the left compartment. This then creates a force.

- In the following, suppose that the temperature in both compartments equals the outside temperature T. Write down the restoring force on the piston at (fixed) angle θ as a function of this temperature. Take into account the gravitational force on the piston. Use the ideal-gas law $PV = NkT$ for describing each of the two gas volumes and neglect the gravitational effects on gas molecules.

- Show that at the critical temperature T_c, the restoring force (for small displacements of θ around 0) vanishes.

IV. CRITICAL SLOWING DOWN

At a second-order critical point, the dynamics undergoes what is called critical slowing down. Critical slowing down can also be observed in the gas-and-piston model:

- For temperatures slightly above T_c, show that the relationship between the restoring force and the (fixed) angle θ defines a harmonic oscillator. To do so, use the isothermal hypothesis: suppose that even for a moving piston the temperatures in both compartments equals the outside temperature T. Neglect friction and damping effects and keep the previous approach (Gravitational force on the piston only, ideal-gas law $PV = NkT$ for describing each of the two gas volumes with the same temperature everywhere).

- For temperatures slightly above T_c, compute the harmonic-oscillator angular frequency ω corresponding to this motion. Describe the $T \to T_c^+$ limit of $\omega(T)$.

- The isothermal hypothesis states that the temperature in the two compartments is the same as the outside temperature even if the piston moves. Discuss why this hypothesis is justified for $T \to T_C^+$ (Hint: The walls of the gas-and-piston model permit heat exchange).

V. ORDER PARAMETERS AND CORRELATION FUNCTIONS

In many systems in statistical physics, the order parameter of a phase transition (which in the gas-and-piston model is represented by the angular variable θ) is intimately related to the expectation value of a correlation functions in the limit of infinite distances.

- Explain this relationship between order parameter and correlation function for the case of the Ising model. Make sure to explain this relation in one dimension and in higher dimensions.
- Explain what becomes of the relationship between order parameter and correlation functions in the limit of infinite distances for the XY-model, or for similar lattice models described by Kosterlitz-Thouless theory.
- In a liquid-gas transition (described by the van-der Waals theory):
  - Is there an order parameter that describes the transition?
  - If such an order parameter exists, is is related to a correlation function in the limit of infinite distances?