

Exam

Statistical Mechanics

22 November 2023, 2pm



Velocity distribution [4 pts]

We consider a system of N classical particles in equilibrium at a temperature T in two dimensions.

- a) Derive the speed distribution $v = |\vec{v}|$ of a particle (with $\vec{v} = (v_x, v_y)$).
- b) Calculate the following averages $\langle v^2 \rangle$ and $\langle v^4 \rangle$.
- c) Find the most probable value of the speed v^*
- d) Calculate the probability that the kinetic energy of a particle is larger than $k_B T$.

Ideal Gas [3 pts]

Calculate the chemical potential of an ideal gas in the canonical ensemble $\mu(N, V, T) = \partial F / \partial N|_{V, T}$. Obtain the same relation in the grand canonical ensemble.

Anharmonic oscillator [2 pts]

We consider a set of N non-interacting particles with mass m at a temperature T and subject to the following potential

$$\Phi(x, y, z) = \frac{K}{2} (x^2 + y^2) + \frac{K'}{4} z^4$$

Find the total (kinetic plus potential) energy for this system.

Interacting system [6 pts]

Let us consider a system of N interacting particles in a volume V and at a temperature T . The system is described by a Hamiltonian

$$\mathcal{H} = \sum_{i=1}^N \frac{\vec{p}_i^2}{2m} + \sum_{i < j} \phi(|\vec{q}_i - \vec{q}_j|)$$

with $\phi(r)$ a pair potential. One can show that the average energy of the system can be written as

$$E = \langle \mathcal{H} \rangle = \frac{3Nk_B T}{2} + \frac{N^2}{2V} \int d\vec{\rho} g(\rho) \phi(\rho) \quad (1)$$

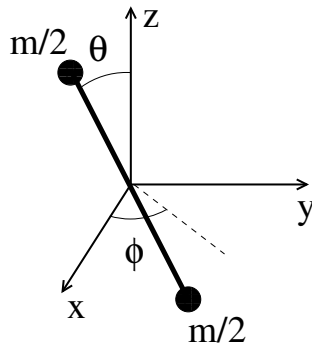


Figure 1:

where $g(\rho)$ is the radial distribution function which is related to the pair correlation function $n^{(2)}(\vec{r}, \vec{\rho})$ as

$$n^{(2)}(\vec{r}, \vec{\rho}) = \left\langle \sum_{i \neq j} \delta(\vec{r} - \vec{q}_i) \delta(\vec{r} + \vec{\rho} - \vec{q}_j) \right\rangle = n^2 g(\rho)$$

The last equality is valid if the system is translation invariant and isotropic. At low densities $g(\rho)$ is approximated with the probability to find two particles at distance ρ neglecting the effects of all other particles (as done when deriving the virial expansion). Use this approximation and (1) to get the specific heat per particle for:

- A hard sphere gas. Argue that the obtained specific heat is actually exact.
- A square well potential defined as

$$\phi(r) = \begin{cases} +\infty & 0 < r < \sigma \\ -\varepsilon & \sigma < r < 2\sigma \\ 0 & r > 2\sigma \end{cases} \quad (2)$$

Optional: Prove Eq. (1).

Rigid Rotor [5 pts]

We consider a simple model of a gas of N molecules in equilibrium at temperature T and volume V . A molecule consists of two equal masses $m/2$ separated by a fixed distance R . A configuration of the molecule is given by the center of mass position \vec{Q} and the two polar angles θ and ϕ which identify the orientation of the molecule with respect to the cartesian axes (see Fig. 1). The conjugated momenta are \vec{P} , p_θ and p_ϕ .

The Hamiltonian for one molecule is given by:

$$\mathcal{H}_1 = \frac{\vec{P}^2}{2m} + \frac{p_\theta^2}{2I} + \frac{p_\phi^2}{2I \sin^2 \theta}$$

where $I = mR^2/4$ is the moment of inertia.

To obtain the canonical single molecule partition function $Z_1(V, T)$ one needs to integrate over the center of mass position and momentum and also over $dp_\theta d\theta dp_\phi d\phi$.

- Obtain the average internal energy E of the system from the calculation of $Z_1(V, T)$
- Obtain E via the equipartition theorem and show that the result matches that of a).
- Calculate the pressure of the gas of molecules.