Exercises in Statistical Mechanics

Based on course by Doron Cohen, has to be proofed
Department of Physics, Ben-Gurion University, Beer-Sheva 84105, Israel

This exercises pool is intended for a graduate course in "statistical mechanics". Some of the problems are original, while other were assembled from various undocumented sources. In particular some problems originate from exams that were written by B. Horovitz (BGU), S. Fishman (Technion), and D. Cohen (BGU).

[Exercise 5021]

virial/equi theorems

An equipartition type relation is obtained in the following way:
Consider N particles with coordinates $\vec{q}_i$, and conjugate momenta $\vec{p}_i$ (with $i = 1, ..., N$), and subject to a Hamiltonian $\mathcal{H}(\vec{p}_i, \vec{q}_i)$.

(a) Write down the expression for the classical canonic partition function $Z[\mathcal{H}]$ and show that it is invariant under the rescaling $\vec{q}_i \to \lambda\vec{q}_i$ and $\vec{p}_i \to \vec{p}_i/\lambda$ of a pair of conjugate variables, i.e. $Z[\mathcal{H}_\lambda]$ is independent of λ, where $\mathcal{H}_\lambda$ is the Hamiltonian obtained after the above rescaling.

(b) Now assume a Hamiltonian of the form $\mathcal{H} = \sum_i \frac{(\vec{p}_i)^2}{2m} + V(\{\vec{q}_i\})$. Use the result that $Z[\mathcal{H}_\lambda]$ is independent of λ to prove the virial relation

$$\left\langle \frac{(\vec{p}_1)^2}{m} \right\rangle = \left\langle \frac{\partial V}{\partial \vec{q}_1} \cdot \vec{q}_1 \right\rangle$$

where the brackets denote thermal averages.

(c) Show that classical equipartition, $\langle x_i \frac{\partial \mathcal{H}}{\partial x_j} \rangle = \delta_{ij} k_B T$, also yields the result (b). Give an example of a quantum system where classical equipartition fails.

(d) Quantum mechanical version: Write down the expression for the quantum partition function. Show that it is also invariant under the rescalings $\vec{q}_i \to \lambda\vec{q}_i$ and $\vec{p}_i \to \vec{p}_i/\lambda$ where $\vec{p}_i$ and $\vec{q}_i$ are now quantum mechanical operators. (Hint: Use Schrödinger's equation and $\vec{p}_i = -i\hbar\partial/\partial\vec{q}_i$.) Show that the result in (b) is valid also in the quantum case.