PHY304: Statistical Mechanics

Assignment 5

February 13, 2025

1. A thermalized ideal gas particle is suddenly confined to a one-dimension trap. The corresponding mixed state is described by an initial density function $\rho(q, p, t = 0) = \delta(q) f(p)$, where $f(p) = \exp(-p^2/2mk_BT)/\sqrt{2\pi mk_BT}$.

   (a) Starting from Liouville's equation, derive $\rho(q, p, t)$ and sketch it in the (q, p) plane.

   (b) Derive the expressions for the averages $\langle q^2 \rangle$ and $\langle p^2 \rangle$ at $t > 0$.

2. Consider an ensemble of N particles, where each particle can be treated as a 3-dimensional isotropic simple harmonic oscillator. The Hamiltonian for this system is given by

$$H = \sum_{i=1}^{3N} \frac{1}{2m} p_i^2 + \frac{m\omega^2}{2} q_i^2$$

   (a) Show that the Liouville's theorem holds for this system.

   (b) How does the phase-space volume for the system evolves in time?

   (c) If the initial distribution of q_i and p_i's for each particle is normal, i.e.,

$$\rho(q_i, p_i, t = 0) = \frac{1}{2\pi} \exp\left[-\frac{1}{2}\left(p_i^2 + m\omega^2 q_i^2\right)\right],$$

   what will be the distribution $\rho(q_i, p_i, t)$ at time t?

3. One of the foundational assumptions of Liouville's theorem is that the system obeys the conservation of energy. Consider again the system of N particles each in a 3-dimensional isotropic harmonic potential, the Hamiltonian for which is given in the previous problem. This time, we add the condition that each particle experiences a frictional force given by $-\gamma p_i$, where $\gamma > 0$ is friction coefficient.

   Show that for this system, the infinitesimal phase-space volume is no longer constant, and thus the phase-space density is not conserved.

4. Consider N harmonic oscillators with coordinates and momenta $\{q_i, p_i\}$, and subject to a Hamiltonian

$$\mathcal{H}(\{q_i, p_i\}) = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \frac{1}{2} m\omega^2 q_i^2 .$$

   (a) Calculate the entropy S, as a function of the total energy E.

   (b) Calculate the energy E, and heat capacity C, as functions of temperature T, and N.

   (c) Find the joint probability density $P(p, q)$ for a single oscillator. Hence calculate the mean kinetic energy, and mean potential energy for each oscillator.

5. A paramagnet in one dimension can be modelled as a linear chain of $N + 1$ spins. Each spin interacts with its neighbours in such a way that the energy is $U = n\epsilon$ where n is the number of domain walls separating regions of up spins from down as shown by a vertical line in the representation below.

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   How many ways can n domain walls be arranged? Calculate the entropy, $S(U)$, and hence show that the energy is related to the temperature as

$$U = \frac{N\epsilon}{\exp(\epsilon/kT) + 1} .$$

   Sketch the energy and the heat capacity as a function of temperature, paying particular attention to the asymptotic behaviour for low and for high temperatures.