Statistical Physics (PH312)
HW #1, Fall 2018

due : Oct 4, 2018

Note that you SHOULD show the details of your work.

1. Consider an entropy defined by the density function $\rho(p, q, t)$ in the phase space Γ as

$$S(t) = -\int dpdq\, \rho(p, q, t) \ln \rho(p, q, t).$$

(a) Show that if $\rho(p, q, t)$ satisfies the Liouville's equation with a Hamiltonian $\mathcal{H}$, $dS/dt = 0$.
(b) Using the Lagrange multipliers method, find the density function ρ_{max} that maximizes the entropy defined above, subject to the constraint of fixed average energy, $\langle \mathcal{H} \rangle = \int dpdq\, \rho(p, q)\mathcal{H}(p, q) = E$.
(c) Show that ρ_{max} is stationary, i.e., $\partial \rho_{max}/\partial t = 0$.

2. (a) Show that the phase space volume element $d\Gamma = \prod_{i=1}^{3N} dp_i dq_i$ remains invariant under a canoncial transformation of the generalized coordiantes (p, q) to any other set of (P, Q).
(b) Also, show explicitly that the phase space volume element of a single particle remains the same under transformation from the Cartesian coordiantes (x, y, z, p_x, p_y, p_z) to the spherical coordinates $(r, \theta, \phi, p_r, p_\theta, p_\phi)$.
(c) Since we do not have a factor $\sin\theta$ in $d\Gamma$, the result of (b) seems to be inconsistent with the intuitive notion of equal weight for equal solid angles. Show that if we average out any physical quantity (its dependence on the conjugate angular momenta comes only through the kinetic energy, then we recover $\sin\theta$ as a result of integration.

3. Show that the entropies defined in different ways as below are equivalent to one another:

$$\begin{aligned} S(E) &= k \ln \Gamma(E) \\ S(E) &= k \ln g(E) \\ S(E) &= k \ln \Sigma(E) \end{aligned}$$

where $\Gamma(E)$ denotes the volume in the phase space occupied by the microcanonical ensemble, $\Sigma(E)$ denotes the volume enclosed by the energy surface of energy E, and $g(E) = \partial\Sigma(E)/\partial E$.

4. Consider a microcanonical ensemble of total energy E of a system with indistinguishable N particles confined in an one-dimensional box, the Hamiltonian of which is given by

$$\mathcal{H} = \sum_{i=1}^{N} (c|p_i| + U(q_i))$$

where $U(q_i) = 0$ for $0 \geq q_i \geq L$ and $U(q_i) = \infty$ otherwise.
(a) Calculate the phase space volume $\Gamma(E, L, N)$.
(b) Calculate the entropy $S(E, L, N)$.
(c) Calculate the pressure P. Note that P is the pressure, while p_i denotes the momentum of ith particle.
(d) Calculate the heat capacities C_L and C_p.
(e) Find the probability $p(p_1)$ of a particle having momentum p_1.

5. (a) For the canonical ensemble, show that

$$\left(\frac{\partial \langle E \rangle}{\partial V}\right)_{N,\beta} + \beta \left(\frac{\partial \langle p \rangle}{\partial \beta}\right)_{N,V} = -\langle p \rangle.$$

(b) From the thermodynamics, show that

$$\left(\frac{\partial E}{\partial V}\right)_{N,T} - T \left(\frac{\partial p}{\partial T}\right)_{N,V} = -p.$$

(c) Is it possible that $\beta \propto T$? If not, explain why.

6. Consider an ideal gas consisting of N rodlike molecules, each having a moment of inertia I and a constant electric dipole moment μ. The Hamiltonian of an individual particle is given by

$$\mathcal{H} = \frac{p^2}{2m} + \frac{1}{2I}\left(p_\theta^2 + \frac{p_\phi^2}{\sin^2\theta}\right) - \mu E \cos\theta$$

The particles are placed in an external electric field of strength E. θ and ϕ are the polar and azimuthal angles, and p_θ and p_ϕ are their conjugate momenta.
(a) Compute the partition function.
(b) Calculate the average electric polarization $P = \langle \mu \cos\theta \rangle$ per particle.
(c) What is the polarizability, $\chi_T = \lim_{E\to 0} \partial P / \partial E$?
(d) Calculate the average rotational energy per particle. What are the high and low temperature limits?
(e) Obtain the dielectric constant of the gas.

7. Consider an ideal gas of N noninteracting particles in a d-dimensional box of volume V. The Hamiltonian has only the kinetic energy as

$$\mathcal{H} = \sum_{i=1}^{N} a \, |\mathbf{p}_i|^s$$

where $\mathbf{p}_i$ is the momentum of ith particle.
(a) Calculate the partition function $Z(T, V, N)$ and the Helmholtz free energy.
(b) Calculate the pressure and the internal energy.
(c) Now suppose that you have a classical gas of N noninteracting diatomic molecules. The Hamiltonian for a single particle is given by

$$\mathcal{H}_i = \frac{1}{2m}\left(\left|\mathbf{p}_i^{(1)}\right|^s + \left|\mathbf{p}_i^{(2)}\right|^s\right) + \frac{1}{2}K \left|\mathbf{q}_i^{(1)} - \mathbf{q}_i^{(2)}\right|^t$$

where $\mathbf{p}_i^{(1)}, \mathbf{p}_i^{(2)}, \mathbf{q}_i^{(1)}, \mathbf{q}_i^{(2)}$ are the momenta and coordinates of the two atoms in a diatomic molecule. Calculate the mean distance $\langle \left|\mathbf{q}_i^{(1)} - \mathbf{q}_i^{(2)}\right|^t \rangle$.
(d) Calculate $\gamma = C_P/C_V$ for the diatomic gas.