EXAMINATION PAPER

Examination Session:	Year:	Exam Code:
May/June	2024	MATH4231-WE01

Title:
Statistical Mechanics IV

Time:	3 hours	
Additional Material provided:		
Materials Permitted:		
Calculators Permitted:	No	Models Permitted: Use of electronic calculators is forbidden.

Instructions to Candidates:	Answer all questions. Section A is worth 40% and Section B is worth 60%. Within each section, all questions carry equal marks. Students must use the mathematics specific answer book.

Revision:	

ED01/2024

SECTION A

Q1 Consider a thermodynamic system with pressure p, volume V, and temperature T, with the following internal energy E and equation of state:

$$E(T) = \alpha T^2\,, \quad pV = \beta T\,.$$

Here α and β are constants.

Suppose we run a reversible cycle using this system that involves four processes, carried out in order:

(i) Expansion from volume V_0 to volume V_1 at constant pressure p_1.

(ii) A decrease of pressure from p_1 to p_0 at constant volume V_1.

(iii) Compression from volume V_1 to volume V_0 at constant pressure p_0.

(iv) An increase of pressure from p_0 to p_1 at constant volume V_0.

For this cycle, the 1st law takes the form $dE = TdS - pdV$.

(a) Compute the change in energy, the work, and the heat for each of the four processes. Do any of these four processes represent an adiabatic process?

(b) What is the total change in entropy around the entire cycle?

Q2 In this problem we will consider the following Hamiltonian for a particle living in two dimensions (q_1, q_2) with the following potential:

$$H(q_i, p_i) = \frac{1}{2m}(p_1^2 + p_2^2) + \frac{1}{2}m\omega_1^2 q_1^2 + \frac{1}{2}m\omega_2^2 q_2^2\,.$$

Here the range of q_1 and q_2 is unbounded. Recall that the surface area of a unit 3-sphere (which is the boundary of a 4-dimensional unit ball) is given by $\Omega_4 = 2\pi^2$.

(a) In the microcanonical ensemble, compute the "area" of accessible states $\mathcal{N}(E)$ in the full phase space $\mathcal{P}$, defined as

$$\mathcal{N}(E) = \int_{\mathcal{P}} d\mu\,\delta(H(q,p) - E)$$

(b) Compute in the microcanonical ensemble the entropy $S(E) = k_B \log \Omega(E)$, where $\Omega(E) = \frac{\mathcal{N}}{\mathcal{N}_0}$, and as usual we take $\mathcal{N}_0 = \frac{h^2}{E}$, with h a constant.

(c) Compute in the microcanonical ensemble the temperature as a function of E.

(d) Compute the unconditional probability distribution $\rho_{\text{unc}}(p_1)$ of p_1 in the microcanonical ensemble. You do not need to normalize it correctly: in this problem we are only asking for the p_1 dependence.

Q3 A quantum system has a single particle state $|E_0\rangle$ that has $E_0 = 0$, and n states $|E_1, i = 1 \ldots n\rangle$, that have corresponding single particle energies $\varepsilon > 0$.

(a) Draw a figure to list the possible microstates for the case in which the system has two indistinguishable Fermions, and for the case in which it has two indistinguishable Bosons, indicating the degeneracies for each.

(b) Evaluate the partition function for each case when the system is held at temperature T.

(c) Determine the entropy for the system in each case in the approximation that $k_B T \ll \varepsilon$, and comment on the difference between the Fermionic and Bosonic systems in this limit.

Q4 Consider a quantum system with discrete states $|n\rangle$, and neglect any possible dependence on the volume in the following discussion. Define the following statistical ensembles, by specifying which quantities are kept fixed and writing down the appropriate discrete probability distributions $p(|n\rangle)$:

(a) Microcanonical ensemble.

(b) Canonical ensemble.

(c) Grand canonical ensemble.

SECTION B

Q5 Consider a 2-dimensional system with Hamiltonian:

$$\mathcal{H}(q_1, q_2, p_1, p_2) = \frac{p_1^2}{2m} + \frac{p_2^2}{2mq_1^2}\,, \tag{1}$$

where q_1 and q_2 are bounded: $q_1 \in [0, R]$, $q_2 \in [0, 2\pi]$. Note the factor of q_1^2 in the denominator of the second term of the Hamiltonian. Recall also that the Poisson bracket is defined as $\{A, B\} = \sum_i \frac{\partial A}{\partial q_i}\frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i}\frac{\partial B}{\partial q_i}$, and Liouville's equation is given by $\frac{\partial \rho}{\partial t} + \{\rho, \mathcal{H}\} = 0$.

(a) Write down Hamilton's equations for this system.

(b) Suppose that a particle has initial conditions $q_1(\text{t=0}) = a$, $q_2(\text{t} = 0) = b$, $p_1(\text{t} = 0) = c$, $p_2(\text{t=0}) = 0$, with $a, b, c > 0$. Using Hamilton's equations, determine the equation of motion of the particle. At what time t does it reach the boundary at $q_1 = R$?

(c) Compute the Poisson brackets $\{\mathcal{H}, p_1\}$, $\{\mathcal{H}, p_2\}$.

(d) We now study probability distributions $\rho(q, p; t)$ that evolve according to Hamiltonian evolution with Hamiltonian (1). Which of the following probability distributions are time-independent solutions to Liouville's equation? Briefly explain your reasoning:

(i) $\rho_1(q_i, p_i) = \mathcal{N}_1 \exp(-\mathcal{H})$

(ii) $\rho_2(q_i, p_i) = \mathcal{N}_2 \exp(-\mathcal{H} + p_1)$

(iii) $\rho_3(q_i, p_i) = \mathcal{N}_3 \exp(-\mathcal{H} + p_2)$

Q6 Consider a particle moving in one dimension undergoing a random walk. At each time step, the particle then takes a combined step s_{comb}, which is the sum of a random step s and a deterministic step $s_{\text{det}} = b$:

$$s_{\text{comb}} = s + s_{\text{det}} = s + b.$$

Here, the random displacement s is drawn from a normalized probability distribution with density function $w(s)$, where $w(s)$ is a uniform distribution of width $2a$ centered at zero:

$$w(s) = \begin{cases} \mathcal{M} & -a < s < a \\ 0 & \text{otherwise} \end{cases}.$$

(a) Calculate the constant $\mathcal{M}$ in terms of the width a, assuming that $w(s)$ is a properly normalized probability distribution.

(b) Calculate the mean $\langle s \rangle$ and the variance $\langle s^2 \rangle_c$ associated with the PDF $w(s)$.

(c) Calculate the characteristic function $\tilde{w}(k)$ associated with the PDF $w(s)$.

(d) After N steps, calculate the mean $\langle X \rangle$ and the variance $\langle X^2 \rangle_c$ associated with the total displacement $X = \sum_{i=1}^{N} s_{\text{comb}}^{(i)}$, where $s_{\text{comb}}^{(i)} = s^{(i)} + b$ is the ith combined step of the particle.

Q7 (a) The simple harmonic oscillator (SHO) in one dimension is given by the classical Hamiltonian

$$H = \frac{p^2}{2m} + \frac{m}{2}\omega^2 x^2 \ ,$$

which when quantised yields discrete energy levels

$$E_n = \hbar\omega(n + \frac{1}{2}), \qquad (n \in \mathbb{Z}^+).$$

Derive the canonical partition function at temperature T for the harmonic oscillator, and hence the mean energy $\langle E \rangle$ for a single SHO. Comment on how your answer for $\langle E \rangle$ relates to the equipartition theorem at high T.

(b) Now consider a simplified model of graphite, in which each carbon atom acts as a harmonic oscillator, oscillating with frequency ω within the layer and frequency ω' perpendicular to it. The oscillations in the three directions are independent, such that the expression for the energy of each carbon atom is

$$H = \frac{p_x^2 + p_y^2 + p_z^2}{2m} + \frac{m}{2}(\omega^2 x^2 + \omega^2 y^2 + \omega'^2 z^2) \ ,$$

where the x, y coordinates are in the plane and the z coordinate is perpendicular. The oscillations within the layer are much slower than the perpendicular oscillations, such that at temperature T we have $\hbar\omega \ll T$ and $\hbar\omega' \gg T$.

(i) Given the temperature conditions some of the dimensions may be treated classically. Use your result to part (a) to identify which dimension(s) these are.

(ii) Determine the canonical partition function treating these dimension(s) classically and the other(s) in full as in part (a).

(iii) From your answer determine $\langle E \rangle$.

(iv) Determine the specific heat, and discuss with reference to part (a), its behaviour when T drops below $\hbar\omega$ and tends to zero.

Q8 An interesting model for superconductors is a system in which electrons (which recall are fermions) with chemical potential μ and energy ε can either sit in an almost full 'valence band' with negative energies, or jump to an almost empty conduction band that has energies greater than ε_0 (leaving behind a 'hole' in the valence band), such that overall they have following continuous energy spectrum:

$$g(\varepsilon) \;=\; \begin{cases} A(\varepsilon - \varepsilon_0)^{1/2} & \varepsilon_0 < \varepsilon < \infty \\ A|\varepsilon|^{1/2} & -\infty < \varepsilon < 0 \end{cases}$$

where A is a constant. There are no states with $0 < \varepsilon < \varepsilon_0$. We will refer to the states with positive energy in the conduction band as 'particles', while the unnoccupied states they leave behind we call 'holes'.

(a) Show that when in equilibrium at temperature T, the probability p_{particle} of finding a particular state of energy $\varepsilon = \mu + \alpha$ occupied by a particle is equal to the probability p_{hole} of finding a state of energy $\mu - \alpha$ being *un*occupied, where α is a positive constant.

(b) Obtain explicit integral expressions for the mean number of particles and the mean number of holes.

(c) Given the physical set-up, we expect the mean number of particles $\langle N_{\text{particle}} \rangle$ to be equal to the mean number of holes $\langle N_{\text{hole}} \rangle$. Use this fact and your answer to part (b) to find an equation for the chemical potential μ which is valid at all temperatures.

(d) Use your result to find an equation for $\langle N_{\text{particle}} \rangle$ at low temperatures.