Durham University

EXAMINATION PAPER

Examination Session:	Year:	Exam Code:
May/June	2023	MATH42320-WE01

Title:
Statistical Mechanics V

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:	

ED01/2023

SECTION A

Q1 Consider a thermodynamic system whose temperature T and pressure p satisfy the following relations:

$$T(E,V) = \frac{\gamma E}{N k_B} \qquad p(E,V) = \frac{\gamma E}{V}$$

Here E is the internal energy, V the volume, and N the number of particles. γ is a constant. You may take the first law of thermodynamics to be $dE = TdS - pdV$.

(a) Using the relations above, find an expression for the entropy S that is consistent with the above. Is the answer you found for S unique?

(b) Your colleague claims that they have found a system whose temperature and pressure satisfy the relations

$$T = \frac{\gamma E}{N k_B} \qquad p = \frac{\gamma E}{V} - \beta \frac{E^2}{V^2}$$

where β is a non-zero constant. Is this consistent with the laws of thermodynamics? Explain your answer.

Q2 Consider a classical particle moving in one dimension q with the usual free particle Hamiltonian:

$$H(q,p) = \frac{p^2}{2m} \tag{1}$$

For this problem you may need the Poisson bracket $\{A, B\}$ between two functions A, B on phase space: $\{A, B\} = \frac{\partial A}{\partial q}\frac{\partial B}{\partial p} - \frac{\partial A}{\partial p}\frac{\partial B}{\partial q}$. You may also need Liouville's equation: $\frac{\partial \rho}{\partial t} + \{\rho, H\} = 0$.

(a) Compute the Poisson brackets $\{H, p\}$, $\{H, q\}$, and $\{q, p^2\}$.

(b) 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) $\rho_1(q,p) = \mathcal{N}_1 \exp(-\beta_1 H)$

(ii) $\rho_2(q,p) = \mathcal{N}_2 \exp(-\beta_2 p^4)$

(iii) $\rho_3(q,p) = \mathcal{N}_3 \exp(-\beta_3 q^2)$

(c) Show that a probability distribution of the form

$$\rho(q,p) = f(pt - \alpha q)$$

is a solution to Liouville's equation with Hamiltonian (1) for an appropriate choice of the constant α, which you should find. Here $f(x)$ is an arbitrary function of one variable.

Q3 Consider a system of N particles confined inside a volume V. Moreover, the single particle density of states is given by the function $g(E, V, N)$.

(a) Express the partition function $Z(\beta, V, N)$ in terms of the density of states $g(E, V, N)$.

(b) Compute the partition function for the case where,

$$g(E, V, N) = f(V, N)\, E^n\,,$$

when $E > 0$ and zero otherwise. Your final answer should depend on the positive function $f(V, N)$ and the positive integer n.

(c) For the same system as in part (b), compute the mean energy $\langle E \rangle$.

Q4 A quantum system has four single particle states $|E_0, 1\rangle$, $|E_0, 2\rangle$, $|E_1, 1\rangle$ and $|E_1, 2\rangle$, with corresponding single particle energies E_0 and E_1.

(a) List all possible microstates and evaluate the partition function for the system of two identical Fermions which are held at temperature T.

(b) Repeat the same for two identical Bosons.

SECTION B

Q5 Consider a free classical particle moving in two dimensions (q_1, q_2) in a box of size L. The classical Hamiltonian of the particle is the following:

$$H(q_1, q_2, p_1, p_2) = \frac{1}{2m}\left(p_1^2 + p_2^2\right) \qquad (2)$$

where we have $q_i \in [0, L]$ for $i = 1, 2$.

(a) Compute in the microcanonical ensemble the accessible area of phase space $\mathcal{N}(E)$, defined by

$$\mathcal{N}(E) = \int dpdq\delta(H(q,p) - E) \qquad (3)$$

(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 and the pressure as a function of E. (Note: as the particle moves in two dimensions, the pressure should be viewed as the thermodynamic variable conjugate to the area $A = L^2$). Is your answer consistent with expectations from the ideal gas equation of state? Explain your answer.

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

Q6 Consider a particle moving in one dimension undergoing a random walk. At each step in the random walk, the particle takes a step where the displacement s is drawn from a normalized probability distribution with density function $w(s)$, where $w(s)$ is a Gaussian of width a:

$$w(s) = \frac{1}{\sqrt{2\pi}a} \exp\left(-\frac{s^2}{2a^2}\right)$$

(a) Write down the mean $\langle s \rangle$ and variance $\langle s^2 \rangle_c$ for a single step.

(b) Calculate the characteristic function $\tilde{w}(k)$ associated with the PDF for a single step.

(c) After N steps, calculate the mean $\langle X \rangle$ and variance $\langle X^2 \rangle_c$ of the total displacement from the origin X.

(d) Calculate the PDF for the total displacement X after N steps, $p(X)$.

(e) Now consider the modified random walk with the following probability distribution for a single step:

$$w(s) = \frac{1}{\sqrt{2\pi}a} \exp\left(-\frac{(s-\mu)^2}{2a^2}\right)$$

where $\mu \neq 0$ is a new parameter. For this new choice of $w(s)$, find the mean $\langle X \rangle$ and variance $\langle X^2 \rangle_c$ of the total displacement from the origin X after N steps.

Q7 Consider the system of N non-interacting distinguishable classical particles of mass m moving in one dimension. The particles are subject to a simple harmonic oscillator potential of frequency ω as well as a gravitational acceleration g. The resulting potential for the i-th particle with linear coordinate x_i is,

$$V(x_i) = \frac{1}{2}\, m^2 \omega^2\, x_i^2 + mgx_i\,.$$

The system of the particles is held at fixed temperature T.

(a) Write down the full Hamiltonian of the system of N particles.

(b) Compute the partition function of the system Z_N.
Hint: You are given that $\int_{-\infty}^{+\infty} e^{-x^2}\, dx = \sqrt{\pi}$.

(c) Compute the mean energy of the system $\langle E \rangle$ as well as the heat capacity,

$$C_v = \frac{\partial \langle E \rangle}{\partial T}\,.$$

(d) Does the system satisfy the equipartition theorem? Should we expect it to satisfy it and why?

Q8 Consider a gas of $\langle N \rangle$ non-interacting Bosons moving inside a d dimensional container of volume V. The single particle energy is $E = w\, k^b$ where k is the modulus of the d-dimensional wavevector. The constants b and w are positive numbers.

(a) Express the single particle density of states $g(E)$ as a function of the single particle energy E and the volume V_d of the d-dimensional sphere of unit radius.

(b) Write an integral expression for the grand canonical partition function $\mathcal{Z}$ as a function of the temperature T, the chemical potential μ, the constant b and the number of dimensions d.

(c) Use the grand canonical partition function $\mathcal{Z}$ to write an equation relating the density $\langle N \rangle / V$, the fugacity z and the temperature T. Your answer should be also expressible in terms of the function,

$$g_y(z) = \frac{1}{\Gamma(y)} \int_0^{+\infty} \frac{x^{y-1}}{z^{-1}\, e^x - 1}\, dx\,.$$

(d) Given that $g_y(1)$ is finite only when $y > 1$, find the necessary condition for Bose-Einstein condensation to happen.