Durham University

EXAMINATION PAPER

Examination Session:	Year:	Exam Code:
May/June	2021	MATH4231-WE01

Title: Statistical Mechanics IV

Time (for guidance only):	3 hours	
Additional Material provided:		
Materials Permitted:		
Calculators Permitted:	Yes	Models Permitted: There is no restriction on the model of calculator which may be used.

Instructions to Candidates:	Credit will be given for your answers to all questions. All questions carry the same marks. Please start each question on a new page. Please write your CIS username at the top of each page. To receive credit, your answers must show your working and explain your reasoning.

Revision:	

Q1 Here we study a generalization of the one-dimensional Ising model. We consider a one dimensional lattice of N sites, at each of which lives a discrete variable σ_i which can take one of q values: $\sigma_i \in \{1, 2, \cdots q\}$. It interacts with its nearest neighbour variables through the Hamiltonian:

$$H_q = -J \sum_{\langle ij \rangle} \delta_{\sigma_i, \sigma_j}$$

where the sum $\langle ij \rangle$ runs over the links of the 1d lattice. As usual the Kronecker delta $\delta_{i,j} = 0$ if $i \neq j$ and $\delta_{i,j} = 1$ if $i = j$. We assume the lattice is periodic, i.e. space is a circle and $\sigma_{i+N} \equiv \sigma_i$.

1.1 How many ground states does the system have at $T = 0$ if $J > 0$?

1.2 Show that, up to a constant shift of the Hamiltonian, this model with $q = 3$ is equivalent to a system with spin variables

$$\boldsymbol{s}_i \in \left\{ (1, 0)\,, \left(-\frac{1}{2}, \frac{\sqrt{3}}{2} \right), \left(-\frac{1}{2}, -\frac{\sqrt{3}}{2} \right) \right\}$$

and Hamiltonian

$$H' = -J' \sum_{\langle ij \rangle} \boldsymbol{s_i} \cdot \boldsymbol{s}_j$$

Determine the relationship between J' and J for this equivalence to hold.

1.3 Construct a mean-field theory for the Hamiltonian

$$H = H' - \boldsymbol{B} \sum_i \boldsymbol{s}_i$$

and compute the partition function Z in the mean-field limit on a 1d lattice with N sites, in terms of $\boldsymbol{B}$ and the average magnetization $\boldsymbol{m} = \frac{1}{N} \sum_i \boldsymbol{s}_i$.

1.4 Compute the self-consistency conditions that determine each component of $\boldsymbol{m}$. (You do not need to solve them).

Q2 Consider a reversible thermodynamic cycle which consists of the following 4 processes:

- AB: adiabatic compression from $A = (V_1, p_1)$ to $B = (V_2, p_2)$.
- BC: volume increase at constant pressure p_2 from $B = (V_2, p_2)$ to $C = (V_3, p_2)$.
- CD: adiabatic expansion from $C = (V_3, p_2)$ to $D = (V_4, p_1)$.
- DA: volume decrease at constant pressure p_1 from $D = (V_4, p_1)$ to $A = (V_1, p_1)$.

Take the working substance of the system to be an ideal gas with the equation of state $pV = Nk_BT$ and internal energy $E = \alpha N k_B T$, with α a constant.

2.1 Draw the cycle in the (p, V) plane. Calculate the work done on the system and the heat absorbed in each of the four processes.

2.2 Let W be the total work done on the system in a cycle and let Q_{BC} be the heat absorbed by the system in the process BC. Compute the efficiency of the engine:

$$\eta = \left| \frac{W}{Q_{BC}} \right|$$

in terms of the temperatures $T_{A/B/C/D}$ of the states A, B, C, and D. Compare your result to that of a Carnot engine and comment on the discrepancy, if any.

2.3 Express your answer for the efficiency in terms of the ratio of pressures p_1/p_2.

2.4 Compute the change in entropy of the system along each of the legs of the cycle.

Q3 In this problem we will consider the following Hamiltonian for a classical particle living in one dimension under the influence of gravity:

$$H(q,p) = \frac{p^2}{2m} + mgq$$

where the motion of the particle q is restricted to $q > 0$, and the constants m, g are both positive.

Parts 3.1 and 3.2 may be attempted in either order.

3.1 (i) Write down Hamilton's equations for the motion of the particle. Consider the initial conditions:

$$q(t=0) = q_0 \qquad p(t=0) = 0$$

where q_0 is a positive constant. Find the solution to the equations of motion satisfying the above initial conditions for $t > 0$ and for $t < t^*$, where t^* is defined as the time when $q(t = t^\star) = 0$.

(ii) Consider the following normalized probability density function for the particle at a time $t = 0$:

$$\rho_a(q,p,t=0) = \delta(q - q_0)\delta(p)$$

Solve for the time evolution of this probability density at later times $\rho_a(q,p,t)$ with $0 < t < t^*$, where t^* is defined as above.

3.2 (i) Draw the contours of constant energy $E = H(q,p)$ in phase space (q,p) for the particle.

(ii) In the microcanonical ensemble, compute the "area" of accessible states $\mathcal{N}(E)$, defined as

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

(iii) Compute the entropy $S(E)$ and the temperature $T(E)$ of this particle in the microcanonical ensemble. (You may take the number of states $\Omega(E) = \mathcal{N}(E)$). Calculate the mean position $\langle q(E) \rangle$ of the particle in the microcanonical ensemble.

Q4 Consider a classical gas of N indistinguishable and non interacting particles which is placed inside a volume V and held at temperature T. The Hamiltonian of a single particle can be written as,

$$H = a\,\left(p_x^2 + p_y^2 + p_z^2\right)^{b/2}\,, \quad a, b > 0\,.$$

4.1 Compute the single particle partition function and from that infer the partition function of the system of N particles.

4.2 Compute the internal energy $\langle E \rangle$ and the pressure P.

4.3 Consider the thermodynamic limit, and compute the chemical potential μ.

Hint: At some point you should find useful the Gamma function defined through $\Gamma(\gamma) = \int_0^{+\infty} x^{\gamma-1} e^{-x}\, dx$.

Q5 You are given a finite temperature system of two identical particles each of which may occupy any of the three energy levels,

$$E_n = n\,\varepsilon, \quad n = 0, 1, 2\,.$$

Moreover, the lowest energy microstate with $E_0 = 0$ is doubly degenerate while the levels for $n = 1, 2$ are non-degenerate. For each of the following cases enumerate the inequivalent configurations, determine the partition function and the average energy.

5.1 The particles obey Fermi statistics

5.2 The particles obey Bose statistics

5.3 The particles are distinguishable

5.4 Without performing any calculation, which of the above systems would have the smallest entropy at zero temperature? Justify your answer.