



SPECIMEN 2

MODULE CODE: MATH327

MODULE TITLE: More Is Different: Statistical Mechanics, Thermodynamics, and All That

TIME ALLOWED: Two Hours

| | Additional information |
|-----------------------------|--|
| Calculators allowed? | Only calculators deemed acceptable and affixed with an official holographic sticker by the Department of Mathematical Sciences |
| Student permitted materials | Writing materials |
| Provided materials | Answer booklet Question paper |

Instructions for examination:

- This paper has **5** questions.
- Full marks will be awarded for complete solutions to **all** questions.
- Write your answers in the booklet provided.
- Additional answer booklets may be requested from invigilators.
- A formula sheet is provided at the back of this paper.

At the end of the examination:

- Use the ties provided to join answer booklets together (if you used more than one).
- **Leave all exam materials, including this question paper, in the examination room.**

1. Consider a board game in which each player moves their piece according to the spins of a fair wheel that randomly picks numbers 1, 2, \dots , 10. Suppose there are 120 positions to reach the finish line, and in each round all players who have not yet finished spin the wheel to get a number and move their piece forward that number of positions.

(a) What is the minimum number of rounds in which any player can possibly reach the finish line? What is the probability of reaching the finish line in this number of rounds?

[3 marks]

(b) What is the maximum number of rounds in which any player can possibly reach the finish line? What is the probability that a player needs this number of rounds to reach the finish line?

[3 marks]

(c) Using the central limit theorem and the integral

$$\frac{1}{\sqrt{\pi}} \int_U^{\infty} e^{-u^2} du = 0.9773 \quad \text{for} \quad U \approx -1.41487,$$

how many rounds would a player need to have reached the finish line with at least 97.73% probability? Answers may be expressed in either symbolic or numerical form.

[12 marks]

2. Consider a system of N distinguishable spins in a magnetic field of strength $H > 0$. Let n_+ of the spins be parallel to the magnetic field, each contributing energy $-H$ to the internal energy E . The remaining $n_- = N - n_+$ spins are anti-parallel to the magnetic field and each contribute energy H .

(a) What is the internal energy E in terms of N , H , n_+ and n_- ? What are its minimum value (E_{\min}) and maximum value (E_{\max})? Describe the micro-states corresponding to E_{\min} and E_{\max} .

[3 marks]

(b) Suppose the internal energy is fixed to E_{\min} . What is the entropy? What is the entropy if the internal energy is fixed to E_{\max} ?

[3 marks]

(c) What is the entropy if the internal energy is fixed to $E = 0$, in terms of N , H , n_+ and n_- ?

[3 marks]

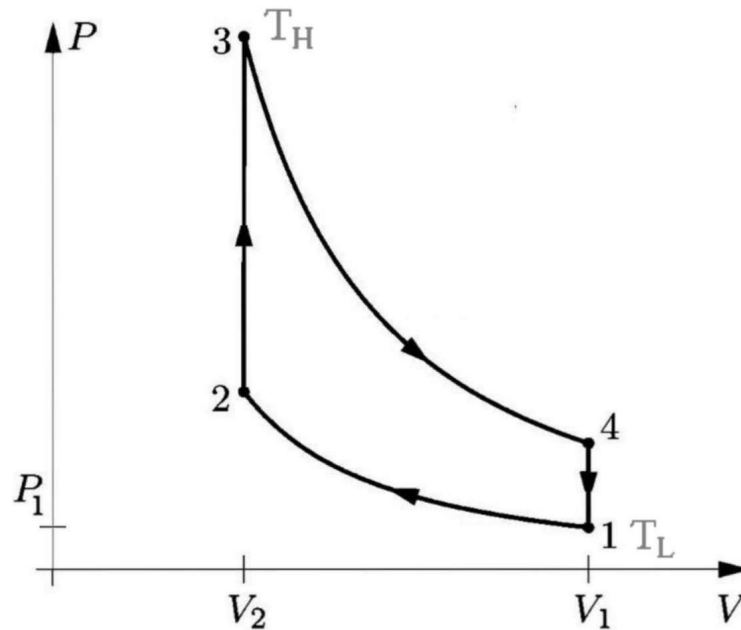
(d) Now let the internal energy fluctuate while fixing the temperature $T = 1/\beta$. Derive the average internal energy $\langle E \rangle$ in terms of N , H , n_+ and n_- .

[8 marks]

(e) Use your result from part (d) to compute the heat capacity c_v of this spin system. What are its high- and low-temperature limits, $\lim_{T \rightarrow \infty} c_v$ and $\lim_{T \rightarrow 0} c_v$?

[4 marks]

3. An ideal gas in a container can access two different thermal reservoirs: a hot reservoir with high temperature T_H and a cold reservoir with low temperature $T_L < T_H$. The system carries out the thermodynamic cycle illustrated by the PV diagram below, where the processes $1 \rightarrow 2$ and $3 \rightarrow 4$ are both adiabatic. Five quantities are given as inputs: The pressure P_1 at point 1; The volume V_1 at points 1 and 4; The volume $V_2 < V_1$ at points 2 and 3; The temperature T_L at point 1; The temperature T_H at point 3.



- (a) Calculate the temperatures $\{T_2, T_4\}$ and pressures $\{P_2, P_3, P_4\}$ in terms of the input quantities.
[5 marks]
- (b) In each stage of the cycle, does the system do work on its surroundings, do the surroundings do work on the system, or is no work done? Explain your choice with clear reasoning.
[3 marks]
- (c) Calculate the net work W_{done} done by the system on its surroundings, in terms of the input quantities.
[5 marks]
- (d) In each stage of the cycle, does heat flow into the gas from the hot reservoir, out of the gas into the cold reservoir, or is no heat exchanged? Explain your choice with clear reasoning.
[3 marks]
- (e) Show that the efficiency of the cycle is $\eta = \frac{W_{\text{done}}}{Q_{\text{in}}} = 1 - \left(\frac{V_2}{V_1}\right)^{2/3}$.
[6 marks]

4. Consider a classical gas of N distinguishable particles in a volume $V = L^3$, with temperature $T = 1/\beta$. The canonical partition function for a single particle is

$$Z_1 = \left(\frac{L}{2\pi\hbar} \right)^3 \int e^{-E/T} d^3p.$$

Each particle moves non-relativistically with energy

$$E_n = \frac{p_n^2}{2m},$$

where $p_n^2 = (p_x^2 + p_y^2 + p_z^2)_n$ is the inner product of the n th particle's momentum $\vec{p}_n = (p_x, p_y, p_z)_n$. All particles have the same mass m .

- (a) Show that the Helmholtz free energy of the gas can be written as $F = -NT \log \left(\frac{V}{\lambda^3} \right)$ and derive an expression for $\lambda(T)$. [4 marks]
- (b) What is the internal energy $\langle E \rangle$ of the gas? [4 marks]
- (c) What is the heat capacity c_v of the gas? [2 marks]
- (d) What is the entropy S of the gas? [4 marks]
- (e) Would the entropy increase, decrease, or stay the same if the N particles were indistinguishable? Explain your choice with clear reasoning. [3 marks]
- (f) Sticking with distinguishable particles, compute the pressure of the gas in terms of N , T and V . [4 marks]

5. Consider the Ising model with N spins and no external magnetic field, for which the canonical partition function at temperature $T = 1/\beta$ is

$$Z(\beta, N) = \sum_{\{s_n\}} \exp[-\beta E(s_n)] \quad \text{with} \quad E(s_n) = - \sum_{(ij)} s_i s_j .$$

Here $s_i \in \{-1, +1\}$ and $\sum_{(ij)}$ sums over nearest neighbours in a lattice.

- (a) Recall the Kronecker delta $\delta_{s_i, s_j} = 1$ for $s_i = s_j$ and vanishes for $s_i \neq s_j$. Considering a single term in the sum over nearest neighbours, show

$$s_i s_j = A \delta_{s_i, s_j} + B$$

by computing the constants A and B .

[4 marks]

- (b) Considering the general expression (with constant J and C)

$$E(s_n) = - \sum_{(ij)} [J \delta_{s_i, s_j} + C] ,$$

show that any expectation value $\langle f(s_n) \rangle$ is independent of C .

[6 marks]

The results of parts (a) and (b) allow us to generalize to systems with

$$Z(\beta, N) = \sum_{\{\sigma_n\}} \exp[-\beta E(\sigma_n)] \quad \text{and} \quad E(\sigma_n) = -J \sum_{(ij)} \delta_{\sigma_i, \sigma_j} ,$$

where each spin variable $\sigma_i \in \{1, 2, \dots, q\}$ now has $q \geq 2$ possible states.

- (c) For $N = 100$ such spins σ_i on a 10×10 square lattice with periodic boundary conditions, how many configurations of spins appear in the sum $\sum_{\{\sigma_n\}}$ defining the partition function?

[2 marks]

- (d) How many interaction terms $\delta_{\sigma_i, \sigma_j}$ appear in the sum $\sum_{(ij)}$ defining the energy for each two-dimensional spin configuration?

[2 marks]

- (e) In the limit $T \rightarrow 0$, with $J > 0$, how many degenerate ground states are there? Describe them.

[4 marks]

FORMULA SHEET

(a) **Binomial coefficient:** $\binom{N}{k} = \frac{N!}{k!(N-k)!}$.

(b) **Stirling's formula:** $\log(N!) = N \log N - N + \mathcal{O}(\log N)$.

(c) **Central Limit Theorem:** A stochastic process with mean μ and variance σ^2 is independently repeated N times with events $x_1 \dots x_N$. For $N \gg 1$, the probability distribution for

$$s = \sum_{i=1}^N x_i \quad \text{is given by} \quad p(s) \approx \frac{1}{\sqrt{2\pi N\sigma^2}} \exp\left\{-\frac{(s - N\mu)^2}{2N\sigma^2}\right\}.$$

(d) The **entropy** for a statistical ensemble with micro-states ω_i , $i = 1, \dots, M$ and corresponding probabilities p_i is

$$S = -\sum_{i=1}^M p_i \log p_i.$$

(e) **Expectation values** for countable and continuous probability spaces:

$$\langle f(X) \rangle = \sum_{X \in A} f(X) P(X), \quad \langle f(x) \rangle = \int f(x) p(x) dx$$

(f) The **micro-canonical ensemble** has $p_i = 1/M$ in thermodynamic equilibrium, with temperature $\frac{1}{T} = \left. \frac{\partial S}{\partial E} \right|_N$ and chemical potential $\mu = -T \left. \frac{\partial S}{\partial N} \right|_E$.

(g) **Canonical ensemble** with temperature T , where E_i is the internal energy of the i th micro-state:

- Partition function Z :

$$p_i = \frac{1}{Z} \exp\left[-\frac{E_i}{T}\right], \quad Z = \sum_{i=1}^M \exp\left[-\frac{E_i}{T}\right].$$

- Helmholtz free energy:

$$F = -T \log Z.$$

- Entropy S , internal energy $\langle E \rangle$, and heat capacity c_v :

$$S = -\frac{\partial F}{\partial T}, \quad \langle E \rangle = -T^2 \frac{\partial}{\partial T} \left(\frac{F}{T} \right), \quad c_v = \left. \frac{\partial \langle E \rangle}{\partial T} \right|_V.$$

- Pressure (if the micro-states depend on the volume V):

$$P = -\left. \frac{\partial \langle E \rangle}{\partial V} \right|_S.$$

(h) **Grand-canonical ensemble** with temperature T and chemical potential μ , where N_i is the particle number of the i th micro-state:

- Partition function Z_g :

$$p_i = \frac{1}{Z_g} \exp \left[-\frac{E_i - \mu N_i}{T} \right], \quad Z_g = \sum_{i=1}^M \exp \left[-\frac{E_i - \mu N_i}{T} \right].$$

- Grand-canonical potential:

$$\Phi = -T \log Z_g.$$

- Entropy S , particle number $\langle N \rangle$ and internal energy $\langle E \rangle$:

$$S = -\frac{\partial \Phi}{\partial T}, \quad \langle N \rangle = -\frac{\partial \Phi}{\partial \mu}, \quad \langle E \rangle = -T^2 \frac{\partial}{\partial T} \left(\frac{\Phi}{T} \right) + \mu \langle N \rangle.$$

(i) **Ideal gas of indistinguishable particles** with mass m and temperature T in volume V :

- If $E(\vec{p}^2)$ is the energy–momentum relation, the canonical partition function for N indistinguishable particles is

$$Z(T) = \frac{1}{N!} \left(\frac{V}{(2\pi\hbar)^3} \int \exp [-E(\vec{p}^2)/T] d^3p \right)^N.$$

- Equation of state and internal energy for a classical ideal gas:

$$PV = NT \quad \langle E \rangle = \frac{3}{2} NT$$

- Condition of constant entropy for a classical ideal gas:

$$VT^{3/2} = \text{constant}.$$

- Change of internal energy for a classical ideal gas, in terms of heat and work:

$$d\langle E \rangle = T dS - P dV = Q + W$$

(j) **Some definite integrals:**

$$\int_{-\infty}^{\infty} e^{-a(x+b)^2} dx = \sqrt{\frac{\pi}{a}}, \quad \int_0^{\infty} x e^{-ax^2} dx = \frac{1}{2a}, \quad a > 0.$$