Faculty of Science and Engineering
School of Physical Sciences
Department of Mathematical Sciences

Exam Contact: —
Contact No/Email: ---

UNIVERSITY OF LIVERPOOL

SPECIMEN 1

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 random walk that starts at $x = 0$ and consists of N steps. At each step, the walker moves forward by an unknown distance $\ell > 0$ with probability $p = 0.4$, moves backward by the same distance with probability $q = 0.3$, or doesn't move at all.

(a) What is the probability that the walker doesn't move for one step?

[2 marks]

(b) What are the mean μ and variance σ^2 of the single-step process?

[5 marks]

(c) For $N \gg 1$, what is the expectation value for the final position of the walk as a function of N?

[3 marks]

(d) For $N = 100$ steps, use the central limit theorem to estimate the probability that the walk ends at the expectation value from part (c). Recall that the probability distribution can be approximated as a constant within a small interval. In case you don't have a calculator, feel free to leave your answer in terms of $\sqrt{2\pi}$ and similar factors.

[8 marks]

2. Consider a micro-canonical system of N indistinguishable particles in thermodynamic equilibrium in volume V. The number of micro-states for internal energy E is

$$M = \frac{1}{N!} \frac{1}{\left(\frac{3}{2}N\right)!} \left(\frac{V}{\lambda_m^3}\right)^N E^{3N/2},$$

where $\lambda_m \equiv \sqrt{2\pi\hbar^2/m}$ and m is the mass of each particle.

(a) What is the entropy of this system?

[4 marks]

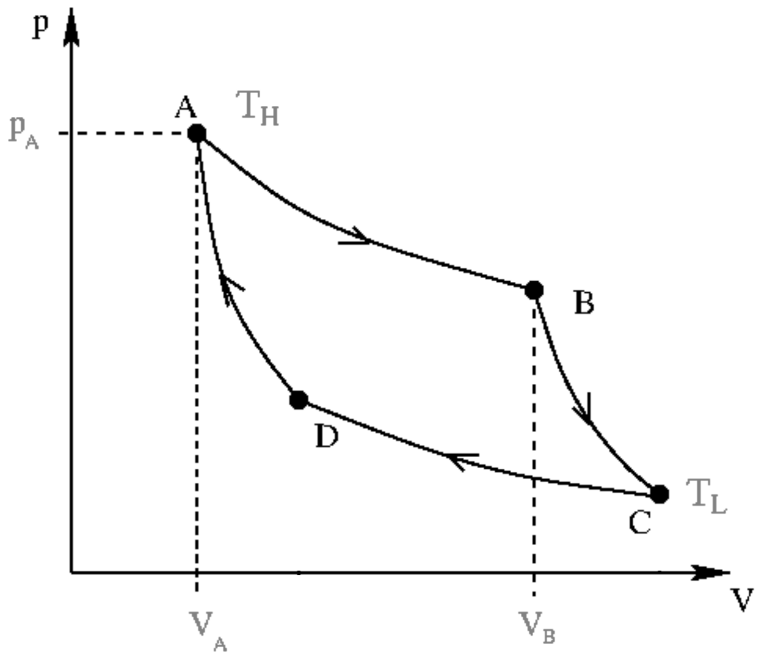
(b) Derive a relation between this system's temperature T and its energy E.

[5 marks]

(c) Applying Stirling's formula for $N \gg 1$, express the chemical potential μ of this system as a function of particle number, volume and temperature.

[8 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 $A \to B$ and $C \to D$ are both isothermal while the processes $B \to C$ and $D \to A$ are both adiabatic. Five quantities are given as inputs: The pressure P_A at point A; The volume V_A at point A; The volume $V_B > V_A$ at point B; The temperature T_H at point A; The temperature T_L at point C.



(a) Calculate the temperatures $\{T_B, T_D\}$, the pressures $\{P_B, P_C, P_D\}$ and the volumes $\{V_C, V_D\}$ in terms of the input quantities.

[8 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 (some or all 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) Calculate the efficiency of the cycle, $\eta = \frac{W_{\text{done}}}{Q_{\text{in}}}$, in terms of (some or all of) the input quantities.

[5 marks]

4. Consider a gas of photons in a volume V with inverse temperature $\beta = 1/T$ and chemical potential $\mu = 0$. The grand-canonical potential is

$$\Phi(\beta, \mu) = \frac{VT}{c^3 \pi^2} \int_0^\infty \omega^2 \log\left[1 - e^{-\beta(\hbar\omega - \mu)}\right] d\omega \,.$$

(a) Show that $\langle E \rangle = \alpha V T^4$ and calculate the constant α. You might find it useful to check the formula sheet for definite integrals.

[6 marks]

(b) Calculate $\langle N \rangle$ and show that the entropy of the gas is constant if $\langle N \rangle$ is constant.

[8 marks]

(c) Calculate the pressure

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

to show $PV = \gamma \langle E \rangle$ and find the constant γ.

[6 marks]

(d) Show that the equation of state has the form $PV = \kappa \langle N \rangle T$ and calculate the constant κ.

[5 marks]

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

$$Z(\beta, N) = \sum_{\{s_i\}} \exp\left[-\beta E\left(s_i\right)\right] = \sum_{\{s_i\}} \exp\left[\beta \sum_{(ij)} s_i s_j\right] .$$

(a) For a one-dimensional Ising model with $N = 10$ spins and periodic boundary conditions, how many configurations of spins appear in the sum $\sum_{\{s_i\}}$ defining the partition function above?

How many interaction terms $s_i s_j$ appear in the sum $\sum_{(ij)}$ defining the internal energy $E\left(s_i\right)$ for each spin configuration?

Using a computer that can compute one billion $s_i s_j$ terms per second, how long would it take to fully evaluate the partition function?

[8 marks]

(b) For a two-dimensional Ising model with $N = 100$ spins on a 10×10 square lattice with periodic boundary conditions, how many configurations of spins appear in the sum $\sum_{\{s_i\}}$ defining the partition function above?

How many interaction terms $s_i s_j$ appear in the sum $\sum_{(ij)}$ defining the internal energy $E\left(s_i\right)$ for each spin configuration?

Using a computer that can compute one billion $s_i s_j$ terms per second, how long would it take to fully evaluate the partition function?

[8 marks]

FORMULA SHEET

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

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

(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

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

(d) The **entropy** for a statistical ensemble with micro-states ω_i, $i = 1, \cdots, M$ 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:

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

(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 ith micro-state:

- Partition function Z:

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

- Helmholtz free energy:

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

- Entropy S and internal energy $\langle E\rangle$:

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

- 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 ith micro-state:

- Partition function Z_g:

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

- Grand-canonical potential:

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

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

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

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

- Thermal de Broglie wavelength:

$$\lambda_{\mathrm{th}}(T) = \sqrt{\frac{2\pi\hbar^2}{mT}}$$

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

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

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

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

- 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:**

$$\int_{-\infty}^{\infty} e^{-a(x+b)^2}\,dx = \sqrt{\frac{\pi}{a}},\ a > 0, \qquad \int_0^{\infty} x^2 \log\left[1 - e^{-x}\right] dx = -\frac{\pi^4}{45},$$

$$\int_0^{\infty} \frac{x^3}{e^x - 1}\,dx = \frac{\pi^4}{15}, \qquad \int_0^{\infty} \frac{x^2}{e^x - 1}\,dx = 2\zeta(3),$$

where $\zeta(s)$ is the Riemann zeta function.