UNIVERSITY OF CAMBRIDGE

NATURAL SCIENCES TRIPOS Part II

Thursday 26 May, 2022 09:00am to 11:00am

PHYSICS (1)
PHYSICAL SCIENCES: HALF SUBJECT PHYSICS (1)

Thermal and Statistical Physics

Candidates offering this paper should attempt a total of ***five*** *questions: all* ***three*** *questions from Section A and* ***two*** *questions from Section B.*

The approximate number of marks allocated to each question or part of a question is indicated in the right margin. This paper contains ***six*** *sides, including this coversheet, and is accompanied by a handbook giving values of constants and containing mathematical formulae which you may quote without proof.*

STATIONERY REQUIREMENTS	SPECIAL REQUIREMENTS
2×20 Page Answer Book	Mathematical Formulae handbook
Rough workpad	Approved calculator allowed
Yellow master coversheet	

You may not start to read the questions printed on the subsequent pages of this question paper until instructed that you may do so by the Invigilator.

SECTION A

*Attempt **all** questions in this Section. Answers should be concise and relevant formulae may be assumed without proof.*

1 Derive the equation of state for a system whose partition function has the form $Z = e^{-\alpha T^2 N^2/V}$. Here the symbols have the usual meaning encountered in lectures. [4]

$$F = k_B T^3 \alpha N^2/V \; ; \qquad P = k_B T^3 \alpha N^2/V^2$$

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2 A one-dimensional system of non-interacting bosons, whose particle number is not conserved, has an energy dispersion relation $\varepsilon \propto |k|$, where $|k|$ is the modulus of the wave vector. How does the heat capacity of the system vary with temperature? [4]

$$U = \int \frac{dxdk}{2\pi} \frac{\alpha|k|}{e^{\beta\alpha|k|} - 1} \;\propto\; (k_B T)^2 \int \frac{dxdw}{2\pi} \frac{w}{e^w - 1}$$

So heat capacity is a linear function of T.

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3 A pollen particle suspended in water is moving at random at room temperature. It is found to travel typically 4 μm in 100 seconds. If the particle diameter is 1 μm, estimate its root mean square velocity and velocity relaxation time. [4]

The question implies that the motion is in 3D. So r.m.s. distance is $\sqrt{6Dt}$ where $D = k_B T/\gamma$ is apparently equal to $2.67 \cdot 10^{-14}$ in SI units. So the friction constant $\gamma = 1.5 \cdot 10^{-7}$ in the same units (at room T). The particle mass is obtained assuming the density same as water (1000 kg/m3), i.e. $m = 5.2 \cdot 10^{-16}$kg, and the velocity relaxation time $\tau = m/\gamma = 3.5 \cdot 10^{-9}$s. The r.m.s velocity is simply $\sqrt{k_B T/m} = 0.0027$m/s.

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SECTION B

Attempt two questions from this section

4 The Ising model of ferromagnetism has the energy (Hamiltonian) written as

$$H = -m_0 B \sum_i^N \sigma_i - J \sum_{ij(nn)} \sigma_i \sigma_j \, ,$$

where we take N spins σ_i, which can either point up ($\sigma = 1$) or down ($\sigma = -1$), to sit on a simple cubic 3D crystalline lattice of spacing a. The summation in the interaction energy term is over nearest neighbours. The standard parameters used are: B the external magnetic field, m_0 the magnetic moment of the spin, and $J > 0$ the interaction energy. In this formulation, the average magnetisation M is related to the mean magnetic moment $m = m_0 \langle \sigma \rangle$ via $M = Nm/V$ with V the volume of the lattice.

(a) Explain the mean field approximation in the context of the Ising model described, and write down the effective mean-field Hamiltonian. [3]

(b) For zero external magnetic field, show that the self-consistent equation to constrain the average spin takes the form

$$\langle \sigma \rangle = \tanh \left(\frac{6J \langle \sigma \rangle}{k_B T} \right) ,$$

and define the Curie temperature T_c of the ferromagnetic phase transition. [5]

(c) By expanding the effective mean-field Hamiltonian in powers of the mean magnetic moment m around $m = 0$, obtain the free energy per spin for the Landau theory in the form

$$F = \text{const} - mB + \alpha (T - T_c) m^2 + \beta m^4 .$$ [5]

(d) Study the equilibrium conditions of this free energy graphically, by sketching the cubic function $2\alpha(T - T_c)m + 4\beta m^3$ against m and match it with the changing values of B. As a result, sketch the dependence of the mean magnetic moment m on B for the two cases: $T > T_c$ and $T < T_c$. [3]

(e) Using the sketch above, identify the thermodynamic equilibrium curve $m(B)$ and find the width of the hysteresis of this transition in an external magnetic field. [3]

(a) In the Hamiltonian given, in the pair-interaction term, we replace the spin variables by its mean: $\sigma_j = \langle \sigma \rangle + \delta\sigma_j$. Opening the brackets, dropping the (small) term proportional to the square of fluctuation, and recovering the spin variable via $\delta\sigma_j = \langle \sigma \rangle - \sigma_j$, we obtain:

$$H_{\text{eff}} = \frac{1}{2} z J N \langle \sigma \rangle^2 - (m_0 B + zJ\langle \sigma \rangle) \sum_i^N \sigma_i \qquad \text{for } z = 6 \text{ here}$$

where z is the (coordination) number of interactions this spin has, which arises from the remaining dummy sum $\sum_j$ with the 1/2 added to account for double counting.

(b) The mean-field Hamiltonian is analogious to the simple paramagnetic $H_0 = -\text{const}\sum_i^N \sigma_i$, which they have solved many times. For example, find the partition function of one spin $Z_1 = 2\cosh(\text{const}/kT)$, $Z_N = Z_1^N$, and

$$F = -Nk_BT\ln[2\cosh\left(\frac{m_0B + zJ\langle\sigma\rangle}{k_BT}\right)] + \frac{1}{2}zJN\langle\sigma\rangle^2,$$

pedantically keeping the constant term, as we will need it in the Landau expansion later... With B still there, we write the thermodynamic $M = -dF/dB$, and only now take $B = 0$. The result is

$$M \equiv Nm_0\langle\sigma\rangle = Nm_0\tanh\left(\frac{zJ\langle\sigma\rangle}{k_BT}\right)$$

as required.

(c) We need to Taylor-expand the free energy in powers of $M = Nm_0\langle\sigma\rangle$. Conveniently, one can expand the free energy given in (b) above in powers of $\langle\sigma\rangle$ and then substitute for M. Also, it's easier to do with $B = 0$ and then add $-M.B$ to the final expansion.

$$\cosh\left(\frac{zJ\langle\sigma\rangle}{k_BT}\right) \approx 1 + \frac{1}{2}\left(\frac{zJ\langle\sigma\rangle}{k_BT}\right)^2 + \frac{1}{24}\left(\frac{zJ\langle\sigma\rangle}{k_BT}\right)^4$$

$$\ln(2\cosh...) \approx \ln 2 + \frac{1}{2}\left(\frac{zJ\langle\sigma\rangle}{k_BT}\right)^2 + \frac{1}{24}\left(\frac{zJ\langle\sigma\rangle}{k_BT}\right)^4 - \frac{1}{2}\left[\frac{1}{2}\left(\frac{zJ\langle\sigma\rangle}{k_BT}\right)^2 + ...\right]^2 + ...$$

which gives

$$F \approx -M.B + \frac{1}{2}zJN\langle\sigma\rangle^2 - \frac{1}{2}Nk_BT\left(\frac{zJ\langle\sigma\rangle}{k_BT}\right)^2 + Nk_BT\frac{1}{12}\left(\frac{zJ\langle\sigma\rangle}{k_BT}\right)^4$$

"Per spin" is the same, but dividing everything by N (which could have been done from the start, using Z_1 only. Either will be accepted. The coefficients appear to be:

$$\alpha = \frac{zJ}{2k_BTm_0^2}(k_BT - zJ); \qquad \beta = k_BT\frac{z^4J^4}{12(k_BT)^3m_0^4}$$

Any mistake with the numerical prefactor in these will not be penalised.

(d) It's too hard to study the cubic equation for equilibrium $dF/dM = 0$, which is: $B = 2\alpha(T - T_c)m + 4\beta m^3$. Instead they are advised to plot both sides of this equation, as in the sketches below

The solution of the equilibrium condition is the crossing of the horizontal line for B and the cubic line. The sketches below each are illustrating how this equilibrium $M = Nm$ changes with B.

(e) Equilibrium transition occurs with the discontinuous jump at $B = 0$, but for the hysteresis boundaries marked in the $m(B)$ sketch above, we need to take an extra derivative: $2\alpha(T - T_c) + 12\beta m^2 = 0$ to find the turning points in the graph, which gives the value at which the unphysical negative slope of $m(B)$ starts: $m^* = \pm\sqrt{\alpha(T_c - T)/6\beta}$. We

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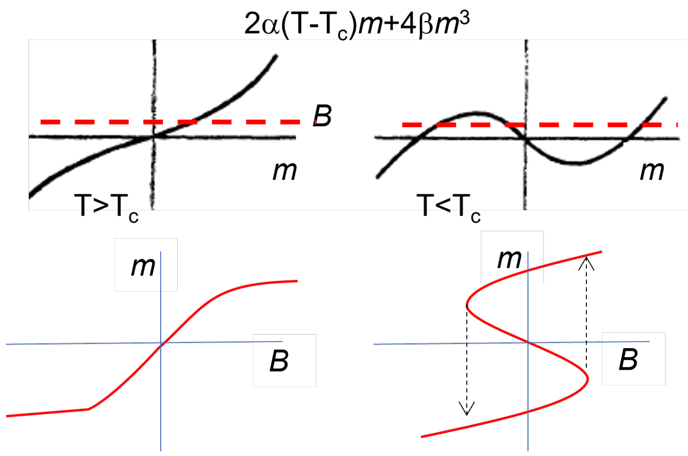

need the width of hysteresis in $\varDelta B$, which is the difference between two turning points: $\varDelta B = 2 * (2\alpha(T - T_c)m^* + 4\beta m^{*3})$, which gives

$$\varDelta B = \frac{8}{3\sqrt{6}} \frac{\alpha^{3/2}}{\beta^{1/2}} |T - T_c|^{3/2}.$$

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5 Consider an ideal gas of indistinguishable bosons with chemical potential μ.

(a) Show that the chemical potential of an ideal Bose gas cannot be positive, and sketch the dependence $\mu(T)$. [4]

(b) Explain why macroscopic occupation (that is, proportional to the number of particles, N) of the energy level with $\varepsilon = 0$ occurs when $\mu \propto -k_B T/N$. [2]

(c) Consider a large two-dimensional ideal Bose gas with N particles of mass m confined to an area A. Show that N and μ are related by

$$N = \frac{mA}{2\pi\hbar^2} \int_0^\infty \frac{1}{e^{(\varepsilon-\mu)/k_B T} - 1} \mathrm{d}\varepsilon.$$ [5]

(d) Therefore, by making the standard substitution $w = 1 - e^{-\beta[\varepsilon-\mu]}$ in the integral above, show that $\mu = k_B T \ln\left(1 - e^{-(2\pi\hbar^2/mk_B T)N/A}\right)$. Find the high-temperature limit of this chemical potential, and check that it is consistent with the classical result. [5]

(e) Using the expression for the chemical potential obtained above, or otherwise, explain why Bose-Einstein condensation does not occur in this system in the limit $N \to \infty$ with N/A constant. [3]

(a) If $\mu \geq 0$, then $\langle n(\varepsilon)\rangle = 1/(e^{\beta[\varepsilon-\mu]} - 1)$ will become infinite when $\varepsilon = \mu$ occurs, and this is not allowed. Several other perfectly valid arguments exist, e.g. the one about $\langle n(\varepsilon)\rangle$ need to be positive.

(b) The occupation of this ground state is $\langle n(0)\rangle = 1/(e^{-\beta\mu} - 1)$. When $\mu = -k_B T/N$, we have by Taylor expansion: $\langle n(0)\rangle = 1/(e^{-1/N} - 1) \approx N$. Several other valid arguments are possible.

(c)

$$N = \int \frac{d^2x\, d^2k}{(2\pi)^2} \frac{1}{e^{(\varepsilon-\mu)/k_B T} - 1} \qquad \text{for } d\varepsilon = \frac{\hbar^2}{m} k dk.$$

(d) Make standard substitution $w = 1 - e^{-\beta[\varepsilon-\mu]}$. After simple algebra:

$$N = \frac{mA}{2\pi\hbar^2} \int_{1-\exp[\beta\mu]}^{1} \frac{dw}{\beta w} = -\frac{mAk_B T}{2\pi\hbar^2} \ln\left(1 - e^{\beta\mu}\right).$$

Inverting this relation gives the required answer.

(e) The 2D problem is the cause of the logarithm that we obtained after integration $\int dw/w$. If $\mu \to 0$, then the occupation of the ground state would become $N \propto -\ln\left(1 - e^{\beta\mu}\right) \to \infty$, using the result in (d). There are many ways to answer this, for instance: we just showed in (b) that for B-E condensate we need $\mu = -k_B T/N$ but the expression $\mu = k_B T \ln\left(1 - e^{-(2\pi\hbar^2/mk_B T)N/A}\right)$ cannot give this limit.

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6 Consider the canonical ensemble of N particles of mass m interacting through a pair potential $\phi(r)$.

(a) Show that the canonical partition function can be written as

$$Z = \frac{1}{N!} \left(\frac{mk_B T}{2\pi\hbar^2}\right)^{3N/2} Z_\phi \,,$$

and write down the expression for Z_ϕ. [5]

(b) Find the difference between the internal energy of the classical gas described above, in the dilute limit, and the internal energy of an ideal gas at the same pressure and temperature. [3]

(c) For a pair potential of the form

$$\phi(r) = \begin{cases} \infty & \text{for } r < a \\ \psi(r) & \text{for } r > a \end{cases} ,$$

where $\psi(r)$ converges rapidly to zero for $r \to \infty$, show that at high temperature the internal energy difference obtained in part (b) is equal to the pair potential averaged over the relative positions of all pairs of particles: $\Delta U \approx \int_a^\infty \frac{N^2}{2V} \psi(r) d^3r$. [5]

(d) A system is described by a pair potential of the form above, with the attractive part $\psi(r) = -J/r^6$. Calculate the second virial coefficient $B_2(T)$ for this system, and obtain the Boyle temperature T^*. [6]

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[*You may use the integral* $\int_b^{\infty}[1-\exp(1/x^6)]\,x^2\mathrm{d}x \approx -1/2b^3$ *for* $b>1$.]

(a) The question implies the 3D system, with the momentum part of the partition function is $1/N!\;(1/\lambda^3)^N$, with the thermal De Broigle wavelength $\lambda = \sqrt{2\pi\hbar^2/mk_BT}$, so the remaining coordinate part is

$$Z_\phi = \int e^{-\sum_{j>i}\beta\phi(r_{ij})} d^3r_1 d^3r_2 ... d^3r_N$$

(b) $U = -\frac{\partial}{\partial\beta}\ln Z$ and for the ideal gas with $Z_0 = (V/\lambda^3)^N/N!$ it gives $U_0 = 3Nk_BT/2$. Here we have in addition the potential-energy term, so

$$U = U_0 - \frac{\partial}{\partial\beta}\ln Z_\phi = U_0 + \int\left(\sum_{j>i}\phi(r_{ij})\right)\frac{1}{Z_\phi}e^{-\sum_{j>i}\beta\phi(r_{ij})}d^3r_1d^3r_2...d^3r_N$$

(c) At high-T, we could try neglecting the Boltzmann exponentials altogether, and re-order the integration metric $...dr_idr_j$ into $d(r_{ij})dr_j$ (which has the unit Jacobian. Then every term in the sum of potentials is the same, together making: $\mathit{\Delta}U \approx \int \frac{N^2}{2V}\psi(r)d^3r$. Don't lose the $1/V$ factor that comes from the Z_ϕ in demoninator, which without the exponentials reduces to V^N.

(d) The expression studied in the lectures is $B(T) = \frac{1}{2}\int\left(1-e^{-\beta\phi(r)}\right)d^3r$. Here we have:

$$B = \frac{2}{3}\pi a^3 + 2\pi\int_a^{\infty}\left(1-e^{-\beta\psi(r)}\right)r^2dr = \frac{2}{3}\pi a^3 + 2\pi\int_a^{\infty}\left(1-e^{\beta J/r^6}\right)r^2dr$$

$$= \frac{2}{3}\pi a^3 + 2\pi\sqrt{\beta J}\int_b^{\infty}\left(1-e^{1/x^6}\right)x^2dx \quad \text{with } \; b = a/(\beta J)^{1/6}$$

Using the hinted integral, the answer is $B = \frac{2}{3}\pi a^3 - \frac{2}{3}\pi\beta J/a^3$, which gives the Boyle temperature $k_BT^* = J/a^6$, and also correctly goes to the steric limit at $T\to\infty$ and becomes negative at low T.

END OF PAPER