

NATURAL SCIENCES TRIPOS Part II

Thursday 27 May 2021

11.00 am to 13.00 am

PHYSICS (1)

PHYSICAL SCIENCES: HALF SUBJECT PHYSICS (1)

THERMAL AND STATISTICAL PHYSICS

Candidates offering this paper should attempt a total of **five** questions: 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 **five** 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

 2×20 Page Answer Book Metric graph paper Rough workpad Yellow master coversheet

SPECIAL REQUIREMENTS

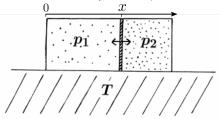
Mathematical Formulae handbook Approved calculator allowed

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.

Consider the movable barrier system below. Show that if $\partial p_j/\partial x$ (with barrier position x) is consistent with mechanical stability then the relevant thermodynamic potential is minimised (not only stationary) in equilibrium.



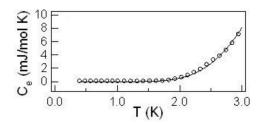
 $\begin{tabular}{ll} Movable impenetrable barrier between two gases at the same temperature T. \end{tabular}$

Consider a system of two subsystems, one labeled by J = 1, 2 the other by $m_J = -J, J$. The energy, in units of a constant ϵ , is

$$E/\epsilon = J + m_J$$
.

Can this system be viewed as two noninteracting subsystems? Explain your answer and illustrate it by the calculation of the partition function.

3 The electronic spectrum of the superconductor Mo_3Al_2C has been found to display a gap Δ ; the data below indicate that upon decreasing the temperature from 3K to 2K, the electronic contribution to the specific heat decreases approximately from 7 to 0.5 mJ mol⁻¹ K⁻¹. The critical temperature is well above 3K, thus one may take Δ to be constant in the shown temperature range. Hence, give a rough estimate for the value of Δ/k_B below 3K.



Electronic specific heat in Mo₃Al₂C at low temperatures. [A. Karki et al., Phys. Rev. B **82**, 064512, (2010).]

[4]

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SECTION B

Attempt two questions from this section

4 At high temperatures, there is significant dissociation of carbon dioxide into carbon monoxide and oxygen,

$$2CO_2 \rightleftharpoons 2CO + O_2$$
.

This question investigates the corresponding high-temperature equilibrium. Ignore internal degrees of freedom throughout.

(a) Consider a gas composed of $N_{\rm CO}$ carbon monoxide and $N_{\rm O_2}$ oxygen molecules in a volume V. Treating the molecules as classical non-interacting particles of masses $m_{\rm CO}$ and $m_{\rm O_2}$, respectively, express the partition function $Z_{\rm CO-O_2}$ and the free energy $F_{\rm CO-O_2}$ of the gas in terms of the particle numbers N_{α} , the de Broglie wavelengths λ_{α} and the volume V (here $\alpha = {\rm CO}$ or ${\rm O_2}$).

[4]

You might want to recall the ideal gas partition function $Z = (V/\lambda^3)^N/N!$ and Stirling's formula $\ln(N!) \approx N \ln(N) - N$.

(b) By combining into two CO₂ molecules, the total energy of an oxygen and two carbon monoxide molecules is lowered by ϵ . Obtain the partition function Z_{CO_2} and the free energy F_{CO_2} of a gas of N_{CO_2} carbon dioxide molecules in a volume V, again treating the molecules as classical non-interacting particles of mass $m_{\text{CO}} + m_{\text{O}_2}/2$.

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(c) Obtain the chemical potentials μ_{CO} , μ_{O_2} and μ_{CO_2} .

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(d) Express the equilibrium condition in terms of the chemical potentials. Explain your answer.

[3]

(e) Show that at high temperatures $k_{\rm B}T \gg \epsilon$, the density $n_{\rm CO_2} = N_{\rm CO_2}/V$ satisfies

$$n_{\mathrm{CO}_2} = A \, n^{3/2} \lambda_{\mathrm{CO}_2}^{3/2} \exp\left(\frac{\epsilon}{2k_{\mathrm{B}}T}\right),$$

where $n = (N_{\rm CO} + N_{\rm O_2} + N_{\rm CO_2})/V$ and A is a dimensionless coefficient of order unity.

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(a) Describe the concepts of phase transitions and order parameters. Give three examples of phase transitions and the corresponding order parameters.

[5]

Consider a three-dimensional gas of classical particles each of mass m, momentum \mathbf{p}_i and position \mathbf{r}_i in a volume V. They interact with each other via the potential $\phi(|\mathbf{r}_i - \mathbf{r}_j|) \equiv \phi(r_{ij})$. For N particles, the Hamiltonian is

$$\mathcal{H} = \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} + \frac{1}{2} \sum_{i \neq j} \phi(r_{ij}).$$

(b) Show that the grand partition function can be written as

$$\Xi = \sum_{N=0}^{\infty} \frac{1}{N!} \left(\frac{e^{\beta \mu}}{\lambda^3} \right)^N \int \prod_{i=1}^N d^3 r_i \exp \left[-\frac{\beta}{2} \sum_{i \neq j} \phi(r_{ij}) \right],$$

where
$$\mu$$
 is the chemical potential, $\lambda = \sqrt{2\pi\hbar^2\beta/m}$ and $\beta = (k_{\rm B}T)^{-1}$. [3]

The rest of the question describes the system as follows: we subdivide V into $\mathcal{N} = V/b$ cells of volume b, where b is small enough that (i) ϕ is approximately constant as \mathbf{r}_i varies within a cell and (ii) each cell is either empty or occupied by one particle. The latter feature is captured by introducing a cell occupation number $n_{\alpha} = 0, 1$ ($\alpha = 1, 2, ..., \mathcal{N}$).

(c) Show that, upon approximating integration $\int d^3r$ by summation $b\sum_{\alpha=1}^{\mathcal{N}}$,

$$\Xi \approx \sum_{n_1=0}^{1} \sum_{n_2=0}^{1} \dots \sum_{n_{\mathcal{N}}=0}^{1} \left(\frac{e^{\beta \mu} b}{\lambda^3} \right)^{\sum_{\alpha} n_{\alpha}} \exp \left[-\frac{\beta}{2} \sum_{\alpha \neq \alpha'}^{\mathcal{N}} n_{\alpha} n_{\alpha'} \phi_{\alpha \alpha'} \right], \quad (1)$$

where $\phi_{\alpha\alpha'} = \phi(|\mathbf{r}_{\alpha} - \mathbf{r}_{\alpha'}|)$ with \mathbf{r}_{α} the vector pointing to cell α .

(d) Next consider the following interaction:

$$\phi_{\alpha\alpha'} = \begin{cases} -4J & \text{if } \alpha, \alpha' \text{ are nearest neighbours (n.n.),} \\ 0 & \text{otherwise.} \end{cases}$$

Introducing σ_{α} via $n_{\alpha} = (1 + \sigma_{\alpha})/2$, show that Ξ in Eq. (1) takes the form

$$\Xi = \sum_{\sigma_1 = \pm 1} \sum_{\sigma_2 = \pm 1} \dots \sum_{\sigma_{\mathcal{N}} = \pm 1} \exp(-\beta \mathcal{H}_{eff}),$$

where, apart from a σ_{α} -independent term,

$$\mathcal{H}_{\text{eff}} = -\frac{J}{2} \sum_{\alpha \neq \alpha', \text{n.n.}}^{\mathcal{N}} \sigma_{\alpha} \sigma_{\alpha'} - h(T, \mu) \sum_{\alpha} \sigma_{\alpha}.$$

Express $h(T, \mu)$ using the parameters of the system.

(e) Using the form of \mathcal{H}_{eff} , argue that upon changing μ at constant and sufficiently low T, the system exhibits a phase transition. What is the physical meaning of the order parameter?

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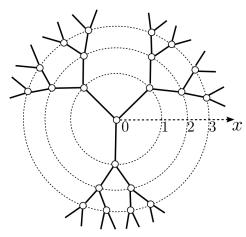
(a) Consider a one-dimensional directed random walk with probability w_{+} $(w_{-}=1-w_{+})$ for a right (left) step. Obtain the probability distribution $P_{1D}(x, N)$ for the position x relative to the starting point after N steps.

(b) Derive the Fokker Planck equation

$$\partial_t P(x,t) = D\partial_x^2 P(x,t) + C\partial_x P(x,t) \tag{2}$$

corresponding to this walk. Interpret D and C and express them in terms of the lattice constant a, the step time τ , and the bias $\epsilon = (w_- - w_+)/2$. [4]

The rest of the question considers a random walk on the lattice shown below. A step from a site to any of its z neighbours occurs with equal probability. The probability of finding the particle at distance x from the origin after N steps is denoted by P(x, N).



Lattice with z = 3. The numbers labeling the dashed circles indicate the distance x from the origin.

(c) First consider the random walk when x > 1. Show that the equation for P(x, N) is identical to that for $P_{1D}(x, N)$. Express the bias ϵ in terms of z.

(d) Focusing now near the origin, find the equations for P(1, N) and P(0, N).

(e) Consider now the Fokker-Planck equation corresponding to the evolution of P(x, N). Argue that it has the same form as Eq. (2) and specify the sign of C. What is the boundary condition at x=0?

(f) Working with the Fokker-Planck equation (2), use dimensional analysis to identify (up to a numerical factor) the characteristic time scale τ^* for the temporal decay of P(x,t) in an infinite system. Express τ^* in terms of the step time τ and z.

END OF PAPER

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