School of Physics & Astronomy

THE UNIVERSITY of EDINBURGH

Statistical Physics

PHYS11024 (SCQF Level 11)

Monday 18th May, 2020 14:30 - 16:30
(May Diet)

Please read full instructions before commencing writing.

Examination Paper Information

Answer **TWO** questions

Special Instructions

- Electronic Calculators must **not** be used during this examination.
- Attach supplied anonymous bar codes to *each* script book used.

Special Items

- School supplied barcodes

Chairman of Examiners: Prof J Dunlop
External Examiner: Prof E Copeland

Anonymity of the candidate will be maintained during the marking of this examination.

1. The Gibbs entropy for an assembly with available microstates labelled by j is

$$S = -k_B \sum_j p_j \ln p_j$$

where k_B is Boltzmann's constant.

a) By maximising the Gibbs entropy subject to certain constraints, which you should specify, show how one obtains the grand canonical ensemble given by

$$p_{i,N} \quad = \quad \frac{1}{\mathcal{Z}_{gc}} \exp(-\lambda_E E_{i,N}/k_B - \lambda_N N/k_B)$$

where λ_E, λ_N are Lagrange multipliers, and $\mathcal{Z}_{gc}$ is the grand canonical partition function, which you should define. **[7]**

b) Show how the Lagrange multipliers may be identified in terms of the temperature T and chemical potential μ as

$$\lambda_E = \frac{1}{T}\,, \qquad \lambda_N = -\frac{\mu}{T}\,.$$ **[4]**

c) Using the formula for the Gibbs entropy, show that the entropy in the grand canonical ensemble S_{gc} is given by

$$S_{gc} \quad = \quad k_B \ln \mathcal{Z}_{gc} + \frac{\overline{E}}{T} - \frac{\mu \overline{N}}{T}$$

where the overline denotes an average within the ensemble. **[2]**

Show how this relation is equivalent to the bridge equation relating $\mathcal{Z}_{gc}$ to the grand potential Φ, which you should define. **[2]**

Using the 1st/2nd law of thermodynamics, explain what are the natural variables for Φ. **[2]**

The density matrix for the grand canonical ensemble is written

$$\rho = \sum_{i,N} p_{i,N} |\psi_{i,N}\rangle\langle\psi_{i,N}|$$

where $|\psi_{i,N}\rangle$ is an eigenstate of the Hamiltonian operator $\hat{H}$ and number operator $\hat{N}$ with eigenvalues E_i and N, respectively.

d) Explain what are meant by pure and mixed states in quantum mechanics. **[2]**

e) Show that

$$\text{Trace}[\rho] = 1\,.$$ **[3]**

f) Show that

$$\mathcal{Z}_{gc} = \text{Trace}[\mathrm{e}^{-\beta(\hat{H}-\mu\hat{N})}]\,.$$ **[3]**

2. **a)** Explain what is meant by a radial distribution function $g(r)$ and give qualitative sketches of its form in an ideal gas, a dense liquid and a solid. **[6]**

b) A plasma with permittivity ϵ contains two freely moving ionic species with opposite charges $q_1 = -q_2$ but with the same overall number densities denoted by $n_1(\infty)$ and $n_2(\infty)$.

Derive the Poisson-Boltzmann equation for the electrostatic potential ϕ around an arbitrary charge q_0 at the origin

$$\nabla^2\phi(r) = -\sum_{i=1}^{2} \frac{q_i n_i(\infty)}{\epsilon} \mathrm{e}^{-q_i\phi(r)/kT} - \frac{q_0}{\epsilon}\delta(r) ,$$

where r is the radial distance from the origin. You should explain the terms in this equation, make clear any assumptions required and explain why the theory is mean-field in nature and why it is self-consistent. **[7]**

c) State the conditions under which one may write the Debye-Hückel equation

$$\nabla^2\phi(r) = \frac{\phi(r)}{\lambda_D^2} - \frac{q_0}{\epsilon}\delta(r)$$

and give an expression for λ_D. **[5]**

d) The solution of the Debye-Hückel equation is given by

$$\phi(r) = \frac{q_0}{4\pi\epsilon r}\mathrm{e}^{-r/\lambda_D} .$$

(You are **not** required to show this.)

Carefully explain the physical significance of λ_D. **[2]**

Define the radial distribution functions, g_{12} and g_{11}, for the two species case and sketch the forms predicted by the Debye-Hückel theory. **[5]**

3. **a)** Explain the meaning of the terms in the master equation for a random walker moving on a one-dimensional lattice with sites labelled by i:

$$\frac{\partial p_i(t)}{\partial t} = \nu(p_{i-1}(t) + p_{i+1}(t)) - 2\nu p_i(t)\ .$$ **[4]**

b) In the case of a finite system $i = 0, \ldots, L$, the reflecting boundary conditions corresponding to zero current at the boundaries are

$$\frac{\partial p_1(t)}{\partial t} = \nu(p_2(t) - p_1(t))$$
$$\frac{\partial p_L(t)}{\partial t} = \nu(p_{L-1}(t) - p_L(t))\ .$$

Write down the stationary state condition and show that the stationary state for the finite system is an equilibrium state obeying detailed balance. **[4]**

c) Now consider an infinite system $i = -\infty, \ldots, +\infty$. Show how in a continuum limit, which you should specify, one obtains the diffusion equation for the probability density of a particle

$$\frac{\partial p(x,t)}{\partial t} = D\frac{\partial^2 p(x,t)}{\partial x^2}\ .$$

You should also define the diffusion constant D in terms of the lattice spacing you use to obtain the continuum limit. **[4]**

d) Confirm that a solution of the diffusion equation, with initial condition that the particle starts at the origin, is the normalised Gaussian

$$p_G(x,t) = \frac{1}{\sqrt{4\pi Dt}} \exp\left(-\frac{x^2}{4Dt}\right)\ .$$ **[4]**

e) A particle diffuses in a fluid. At a certain time t_0 the particle has probability density $p_G(x, t_0)$. Treating the problem as one-dimensional, find and sketch the Gibbs entropy $S(t)$ as a function of time for $t > t_0$. You may use the result

$$\int_{-\infty}^{\infty} \mathrm{d}x\ p_G(x,t)x^2 = 2Dt\ ,$$

and you may ignore any time-independent contributions to S. **[5]**

f) Finally, consider the diffusive current $J = -D\frac{\partial p_G}{\partial x}$.

Sketch this current and identify any maxima and minima. **[4]**

Invigilators Information

Delivered papers 30 minutes prior to start time.

1. Course information

Course title:	Statistical Physics		
Course No:	PHYS11024		
Academic :	Martin Evans	**Contact No:**	0131 650 5294
Secretary:	Denise Couto	**Contact No:**	0131 650 7218
School:	School of Physics & Astronomy	**Contact No:**	68-8261 / 51-7525

2. Exam diet / paper information

Date of exam:	Monday 18th May, 2020	**Time of exam:**	14:30 - 16:30
Location of exam:	Patersons Land Room G1		
No of exam papers:	102		

3. Invigilators Instructions

Unissued paper returned:	Yes	**Approved Calculators :**	No
Answer on exam paper:	No	**Open Book Exam:**	No
Answer on MCQ :	No	**Script book per answer:**	See rubric
Used exam papers returned:	No	**Dictionary allowed:**	No

4. Stationery Requirement

Stationery: 16 pages x 1.

5. Items to be handed out with exam papers

Calculators (from School):	No	**Bar Codes (from School):**	Yes
Graph paper (from School:	No	**Bibles (from School)**:	No
Formula Sheets (from School):	No		

6. Additional Information

- None

Notes: