UNIVERSITY OF DUBLIN

X-MA3443-1

TRINITY COLLEGE

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FACULTY OF ENGINEERING, MATHEMATICS AND SCIENCE

SCHOOL OF MATHEMATICS

JS Theoretical Physics & JS/SS Mathematics
JS & SS Two Subject Moderatorship

Trinity Term 2013

MA3443/MA3444 - STATISTICAL PHYSICS I/II

Monday, May 13 LUCE UPPER 14.00 — 17.00

Drs. C. Thomas and S. Sint

Credit will be given for the best 3 questions answered in each section.

All questions have equal weight of 20 points.

'Formulae & tables' are available from the invigilators, if required.

Non-programmable calculators are permitted for this examination—please indicate the make and model of your calculator on each answer book used.

The time allowed for this paper is 3 hours for students registered for both MA3443 and MA3444. For students registered for just one of the modules the time allowed is 2 hours

$dU = TdS - PdV$ $dU = dQ - PdV$ $dQ = dU + PdV$

$\left(\frac{\partial U}{\partial T}\right)_P dU + \left(\frac{\partial U}{\partial V}\right) dV$

 $C_V = \left(\frac{\partial U}{\partial T}\right)_V$

C_V

Section MA3443 — Statistical Physics I

Credit will be given for the best 3 questions answered in this section.

1. (a) What are extensive and intensive quantities? Provide three examples of each. (4 marks)

   (b) Give Kelvin's and Clausius' statements of the second law and show that they are equivalent. (6 marks)

   (c) Consider a solid body with heat capacity C at constant volume. Assuming the volume remains constant, show that the entropy change of the body in a transformation from temperature T_i to temperature T_f is

$T_f = T_i e^{\Delta S/C}$

$$\Delta S = S_f - S_i = C \ln(T_f/T_i) \ .$$

   Hence derive an expression for the final temperature when two such solid bodies with initial temperatures T_1 and T_2 (both with heat capacity C) are brought into equilibrium in a reversible transformation. (5 marks)

   (d) Considering the same two bodies, show that the final temperature is $T_f = \frac{1}{2}(T_1 + T_2)$ if they are instead brought directly into thermal contact (irreversibly). Show that the entropy change is positive in this case. (5 marks)

$\Delta Q = C_V(\Delta U)$

$dQ = C_V$

$C_V =$

T_i

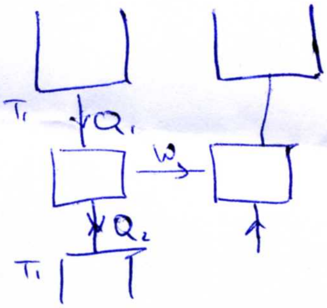
$dS = \frac{dQ}{T}$ $dS = \int \frac{dQ}{T}$

$T_f = T_1 e^{\Delta S/C} = T_2 e^{\Delta S_2/C}$

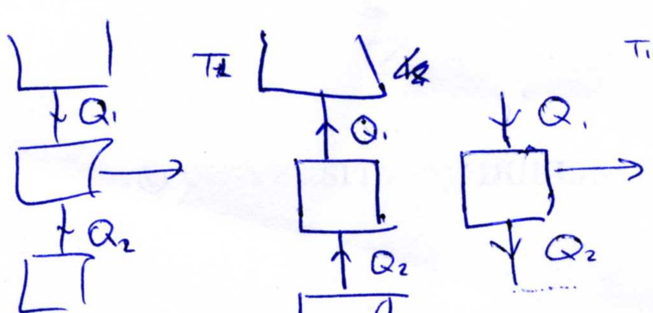
$\Delta S_1 = C \ln(T_f/T_1)$

$\Delta S_2 = C \ln(T_f/T_2)$

cold → hot



Clausius:



$\Delta S_1 + \Delta S_2 = C \ln$

$\ln(a) + \ln(b) = \ln ab$

U F TS $u(S,V,N)$ $F = U - TS$

PV H G $G = U - TS + PV$

2. (a) Explain what is meant by a first order phase transition? What distinguishes it from a second order phase transition? (5 marks)

   (b) What is the relevant thermodynamic potential to consider at constant temperature and pressure? Using this thermodynamic potential, prove that the chemical potentials, μ, of two phases at a phase coexistence curve are equal. (5 marks)

   (c) Derive the Clausius-Clapeyron equation for the phase coexistence curve,

$$\frac{dp}{dT} = \frac{l}{T(v_1 - v_2)},$$

$dU = TdS - PdV + \mu dN$ $\qquad \frac{T(s_1 - s_2)}{T(v_1 - v_2)} \qquad \frac{S_I - S_{II}}{V_I - V_{II}}$

$dF = dU - TdS - SdT$

   where $l = T(s_1 - s_2)$ is the latent heat, $s_i = S_i/N_i$ (specific entropy) and $v_i = V_i/N_i$ (specific volume). (5 marks)

$= \mu N$

   (d) Consider a system at constant pressure where phase I is stable for $T > T_0$, phase II is stable for $T < T_0$ and there is a first order phase transition at T_0. Prove that $l > 0$ in a transition from phase II to phase I. (5 marks)

   [Hint: consider $S = -\left(\frac{\partial G}{\partial T}\right)_{P,N}$ for each phase.] T

C TN
GC Tμ
MC EN

3. (a) What systems are described by canonical, grand canonical and microcanonical ensembles? Under what conditions is the choice of ensemble irrelevant? (5 marks)

   (b) Consider a classical ideal gas of ultrarelativistic particles with energies $\epsilon = |\vec{p}|c$. Compute the grand canonical partition function, Z_Ω, and hence show that the grand potential is,

$$\Omega = -\frac{4\pi z V}{c\beta^2 h^3},$$

   where $z = e^{\beta\mu}$, $\beta = \frac{1}{kT}$, V is the volume and μ is the chemical potential. (5 marks)

   (c) Using the result for Ω, derive expressions for the pressure and the average number of particles, $\bar{N}$, in such a gas. Hence derive the equation of state in terms of P, V, T and $\bar{N}$, and derive an expression for the chemical potential. (6 marks) T, μ

   (d) Without evaluating any additional integrals, obtain an expression for the equation of state for an ideal gas of relativistic particles with energies $\epsilon = \sqrt{|\vec{p}|^2c^2 + m^2c^4}$. (4 marks) ε

$dU = TdS - PdV + \mu dN$

$-TS$

$\boxed{\begin{matrix} U & F \\ H & G \end{matrix}}$ $\quad F = U - TS \quad dF = dU - TdS - SdT = -SdT - PdV + \mu dN$

$G = U - TS + PV \quad dG = dU - TdS + PdV + VdP = -SdT + VdP + \mu dN$

4. Recall the cluster expansion, $Q_N = \sum_{m_1,m_2,\ldots,m_N} S(m_1, m_2, \ldots, m_N)$ with $S(m_1, m_2, \ldots, m_N) = c_1^{m_1} c_2^{m_2} \ldots c_N^{m_N} \mathcal{S}$, of the canonical partition function, $Z_N = \frac{1}{N!\lambda^{3N}} Q_N$, where $Q_N \equiv \int d^{3N}x \prod_{i<j}(1 + f_{ij})$, $f_{ij} \equiv e^{-\beta V(\vec{x}_i - \vec{x}_j)} - 1$, and where c_l is a cluster integral.

   (a) Describe why the cluster expansion is useful and give the requirements on the potential, $V(\vec{x}_i - \vec{x}_j)$, for the expansion to be appropriate. (5 marks)

   (b) Explain the significance of $S(m_1, m_2, \ldots, m_N)$ and $\mathcal{S}$, and give the general constraint on $\{m_1, m_2, \ldots, m_N\}$. (5 marks)

   (c) Derive a general expression for $\mathcal{S}$. (5 marks)

   (d) Enumerate all possible $(m_1, m_2, \ldots, m_N)$ that contribute to Q_5 and give a diagrammatic representation for $S(3, 1, 0, 0, 0)$ and $S(1, 2, 0, 0, 0)$. Explicitly expand the $S(3, 1, 0, 0, 0)$ contribution in terms of f_{ij} and hence verify the general expression for $\mathcal{S}$ in this case. (5 marks)

Section MA3444 — Statistical Physics II

Credit will be given for the best 3 questions answered in this section.

5. Consider a relativistic gas of massless bosons in two space dimensions. The energy-momentum relation is thus given by $\varepsilon(p) = c|\mathbf{p}| \equiv cp$, where the 2-dimensional momentum $\mathbf{p}$ has only 2 components, (p_1, p_2). Particle number conservation is assumed.

   (a) Obtain the grand canonical partition function and the average particle density in a finite 2-dimensional volume, $V_2 \equiv L^2$, as a sum over momenta (assume periodic boundary conditions). (5 marks)

   (b) Consider the regime of large volume ($V_2 \longrightarrow \infty$) and obtain the grand canonical partition function and the average particle density as integrals over momenta. Then change variables to give the results in terms of the functions $g_l(z)$ of Eq. (1). (You may ignore potential problems with the zero-momentum terms in the sums). (5 marks)

   (c) For a given temperature, is there a critical density beyond which the system forms a Bose-Einstein condensate? If so determine the critical density. You may assume the following result ($0 \leq z < 1$):

$$g_l(z) = \frac{1}{\Gamma(l)} \int_0^\infty \mathrm{d}x \frac{x^{l-1}}{z^{-1}\mathrm{e}^x - 1} = \sum_{n=1}^{\infty} \frac{z^n}{n^l}, \tag{1}$$

   (5 marks)

   (d) Explain for which choices of parameters you expect the equation of state to approach the corresponding classical result. In this regime, verify that this is the case and compute the first quantum correction to the classical equation of state. (5 marks)

6. Consider the Einstein model of a solid, where each atom is held in place by a harmonic oscillator potential with the same frequency ω for all atoms. The quantum mechanical canonical partition function for such a system of uncoupled harmonic oscillators is given by

$$Z_N = \left[2\sinh\left(\frac{1}{2}\beta\hbar\omega\right)\right]^{-3N}$$

(a) Compute the internal energy U and its behaviour for low and high temperature. (5 marks)

(b) Calculate the specific heat C_V and discuss its low temperature and high temperature limits. (5 marks)

(c) Obtain the entropy. Does it behave according to the third law of thermodynamics? (5 marks)

(d) The canonical partition function of the corresponding classical system is given by

$$Z = \frac{1}{N!}\left(\beta\hbar\omega\right)^{-3N}$$

Compute the internal energy and specific heat C_V and compare with the results obtained above. (5 marks)

$2^2\ 2^{3+4}$

$(N)\ e^{-\beta E}$

$$\frac{\rho(\varepsilon_1)}{\rho(\varepsilon_2)} = \frac{\rho(\varepsilon_1+\varepsilon)}{\rho(\varepsilon_2+\varepsilon)} \qquad Q = \sum z_n Z_N$$

$Q = \sum (N) e^{-\beta E}$

$$\rho(\varepsilon_1)\rho(\varepsilon_2+\varepsilon) = \rho(\varepsilon_1+\varepsilon)\rho(\varepsilon_2)$$

T

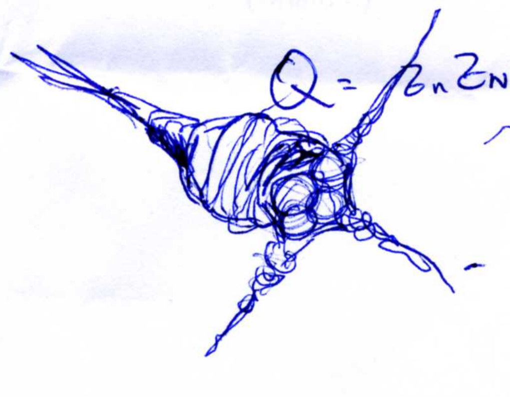
$Z =$

$\cancel{\rho e}\ \rho(\varepsilon_1) = e^{\varepsilon_1}$

L=

$$e^{\varepsilon_1} e^{\varepsilon_2+\varepsilon} = e^{\varepsilon_1+\varepsilon} e^{\varepsilon_2}$$

$Q = \sum z_n Z_N$



7. The density matrix ρ is a quantum mechanical operator with the properties

$$(i) \quad \rho^\dagger = \rho, \qquad (ii) \quad \mathrm{tr}(\rho) = 1, \qquad (iii) \quad \langle\varphi|\rho|\varphi\rangle \geq 0.$$

where the last equation holds for any element $|\varphi\rangle$ of the Hilbert space.

Consider the complex 2-by-2 matrix

$$A = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix},$$

with complex numbers $\alpha, \beta, \gamma, \delta$.

(a) Determine the conditions to be satisfied by $\alpha, \beta, \gamma, \delta$ so that A has the properties (i) and (ii). Parameterise the resulting matrix in terms of α and β. (5 marks)

(b) Work out the condition on α and β which follows from imposing (iii).
Hint: reformulate property (iii) in terms of the eigenvalues of ρ. (5 marks)

(c) The resulting matrix has all the properties of a density matrix for a 2-state system and can thus be written in the form

$A\lambda = \lambda I$

$$A = p|1\rangle\langle 1| + (1-p)|2\rangle\langle 2|,$$

with orthonormal states $|1\rangle, |2\rangle$, and $0 \leq p \leq 1$. How is p related to α, β? Compute the associated entropy,

$$S = -k\,\mathrm{tr}(A \ln A),$$

$e^x =$

and determine the value of p which maximises the entropy. (5 marks)

(d) Under which condition for α and β does A become a projector, i.e. $A^2 = A$? (5 marks)

$f(x) = f(a) + f'(a)x$ $\quad 1 - \frac{1}{x}$ $\quad \frac{1}{0.}$

$\ln 20$ $\quad 1 - x$ $\quad e^{1.12}$

$f(x+h) = f(x) + f'(x)h + f''(x)h^2$

$1 + x + \frac{x^2}{2}$ $\quad \log(1.12)$

$-\log x + \frac{1}{x}h +$

$e^x = 1 + x = y$ $\quad \log(0) =)$ $\quad \log(0.1$

8. Consider the 1-dimensional Ising model with N spins and Hamiltonian

$$\hat{H} = -\sum_{i=1}^{N-1} J_i s_i s_{i+1}. \qquad (s_i = \pm 1, i = 1, \ldots, N)$$

(a) Give the definition of the canonical partition function Z_N and determine the number of spin configurations. (5 marks)

(b) Enlarge the chain by a further spin s_{N+1} and show that the partition function satisfies the recursion relation

$$Z_{N+1} = 2Z_N \cosh(\beta J_N).$$

Q

$Z_N = C(N)e^{-\beta E}$ T, N

$C(N)e^{-\beta E}$

(5 marks)

(c) For a single spin there is no interaction and the partition function is given by

$$Z_1 = \sum_{s=\pm 1} \exp(0) = 2.$$

$e^{-\beta E}$

Using this initial value compute Z_N with the help of the above recursion relation. (5 marks)

(d) Using the result for Z_N compute the expectation value $\langle s_i s_{i+j} \rangle$.

Hint: first justify that this expectation value can be re-written as $\langle s_i s_{i+j} \rangle = \langle (s_i s_{i+1})(s_{i+1} s_{i+2}) \cdots (s_{i+j-1} s_{i+j}) \rangle$ and then consider derivatives of the canonical partition function with respect to the couplings J_i. (5 marks)

Q

$Z_N = \sum^{C} e^{-\beta E}$

$Z_N =$