

# **EXAMINATION PAPER**

Examination Session: May

2019

Year:

Exam Code:

MATH4231-WE01

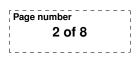
## Title:

## Statistical Mechanics IV

Time Allowed:	3 hours	
Additional Material provided:	None	
Materials Permitted:	None	
Calculators Permitted:	No	Models Permitted: Use of electronic calculators is forbidden.
Visiting Students may use dict	ionaries: No	

the the <b>AN</b> Qu	<ul> <li>Credit will be given for: the best <b>TWO</b> answers from Section A, the best <b>THREE</b> answers from Section B, <b>AND</b> the answer to the question in Section C. Questions in Section B and C carry <b>TWICE</b> as many marks those in Section A.</li> </ul>					
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**Revision:** 



## Useful formulae:

• The volume of a ball  $B^n = \{(x_1, x_2, ..., x_n) \mid x_1^2 + x_2^2 + \cdots + x_n^2 \leq R^2\}$  and the surface area of a sphere  $S^{n-1} = \{(x_1, x_2, ..., x_n) \mid x_1^2 + x_2^2 + \cdots + x_n^2 = R^2\}$  of radius R in n dimensions are:

$$\operatorname{Vol}(B^n) = \frac{\pi^{n/2}}{\Gamma(n/2+1)} R^n$$
,  $\operatorname{Area}(S^{n-1}) = \frac{2\pi^{n/2}}{\Gamma(n/2)} R^{n-1}$ .

• The one-dimensional Gaussian integral:

$$\int_{-\infty}^{\infty} dx \, e^{-ax^2} = \sqrt{\frac{\pi}{a}} \; .$$

• Stirling's formula:

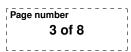
$$\log n! \approx n \, \log n - n \; .$$

• Gamma function – definition and properties:

$$\begin{split} \Gamma(x) &= \int_0^\infty e^{-t} t^{x-1} dt \qquad \operatorname{Re}(x) > 0 \ , \\ \Gamma(x+1) &= x \, \Gamma(x) \\ \Gamma\left(1/2\right) &= \sqrt{\pi} \\ \Gamma(n+1) &= n! \qquad (n \in \mathbb{N}) \ . \end{split}$$

• Dirac delta function:

$$\delta(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{i\,k\,x} \,.$$



### SECTION A

1. The energy fundamental relation expresses the internal energy E of a system in terms of the other extensive quantities like the entropy S, the volume V and the number of particles N. Consider a system whose energy fundamental relation is

$$E(S, V, N) = \alpha S^a V^{-b} N^c ,$$

for some positive constant  $\alpha$ .

- (a) Find the condition on the parameters  $\{a, b, c\}$  for which the above energy fundamental relation is acceptable.
- (b) Find the temperature T = T(S, V, N) and determine the condition on the parameters  $\{a, b, c\}$  which ensures that the 3rd Law of Thermodynamics is upheld.
- (c) Write down the enthalpy H(S, p, N) of the system.
- 2. The internal energy of a fluid is a function E(S, V, N) of its entropy S, volume V and number of particles N.
  - (a) Write down an expression for the differential dE according to the 1st Law of Thermodynamics.
  - (b) Perform a double Legendre transform with respect to the pairs of conjugate variables (S, T) and  $(N, \mu)$  to define the grand canonical potential  $\Phi(T, V, \mu)$ , and compute its differential  $d\Phi$ .
  - (c) Express the entropy S, the pressure p and the number of particles N in terms of the temperature T, the volume V and the chemical potential  $\mu$ .
  - (d) Use the extensivity of the grand canonical potential to deduce that

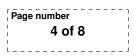
$$\Phi(T, V, \mu) = -p(T, \mu)V$$

3. The probability density for the speed of non-interacting monatomic gas particles moving in two spatial dimensions is given by the Rayleigh distribution:

$$p(v) = \frac{1}{\mathcal{N}} v \exp\left(-\frac{v^2}{2a^2}\right) , \qquad a^2 = k_B T/m . \tag{1}$$

The speed v = |v| is the modulus of the velocity vector v, and  $\mathcal{N}$  is a normalization constant.

- (a) Determine  $\mathcal{N}$  so that the probability distribution is correctly normalized.
- (b) Compute the mean  $\langle v \rangle$  and the variance  $\sigma_v^2$  of this probability distribution.
- (c) Compute the average energy of a gas particle. Is the result consistent with the equipartition theorem?
- (d) Find the probability density  $p_E(E)$  for the energy of a gas particle.



- 4. (a) Define the canonical partition function for a quantum system maintained at a fixed temperature T. How is it related to the probability distribution for the canonical ensemble?
  - (b) Consider a classical system of N identical non-interacting particles confined in a volume V in three dimensions. Compute the canonical partition function and calculate the mean energy  $\langle E \rangle$ , the free energy F and the entropy S of the system in the limit where N is large.
- 5. (a) Define the density of states g(E) of a system. Write a formula for the exact density of states g(E) of a quantum-mechanical system with energy eigenstates  $|n\rangle$  and energy eigenvalues  $E_n$ , and use it to express the canonical partition function of the system as an integral over the energies.
  - (b) A quantum-mechanical rotor with moment of inertia I has a Hamiltonian  $\hat{H}$  with eigenvalues and eigenstates given by

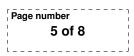
$$\hat{H}|j,m_j\rangle = \frac{\hbar^2}{2I}j(j+1)|j,m_j\rangle \equiv E_{j,m_j}|j,m_j\rangle$$

where j = 0, 1, 2, 3, ... and  $m_j = -j, -j + 1, ..., j - 1, j$ . Write an exact formula for its density of states g(E), and show that it is approximated by the density of states

$$g_{\rm c}(E) = \begin{cases} 0 , & E < 0 \\ 2I/\hbar^2 , & E > 0 \end{cases}$$

for energies such that  $|E| \gg \hbar/\sqrt{I}$ .

- 6. Consider a quantum system of N non-interacting bosons, where each boson can occupy one of the discrete one-particle states  $|r\rangle$  of energy  $E_r$ . The ground state  $|0\rangle$  has zero energy  $E_0 = 0$ .
  - (a) Write down the Bose-Einstein distribution for the average number of bosons  $\langle n_r \rangle$  that occupy state  $|r\rangle$ . For which range of the chemical potential  $\mu$  and of the fugacity  $z = e^{\beta\mu}$  is the formula sensible?
  - (b) Approximate the Bose-Einstein distribution for  $z \ll 1$ , which turns out to be a high temperature limit, to derive the classical Maxwell-Boltzmann statistics.
  - (c) Analyse the expected number  $\langle n_0 \rangle$  of bosons in the ground state in the limit where z is very close to 1. Taking into account that the system consists of a finite (though very large) number N of bosons, can z get arbitrarily close to 1? If not, estimate the maximum value of z that can be physically realised, as a function of  $N \gg 1$ .





## SECTION B

- 7. Consider a gas with a fixed number of constituents N (that is omitted in the following).
  - (a) Starting from the exact differentials of the thermodynamic potentials E(S, V), F(T, V), G(T, p) and H(S, p), derive the four Maxwell relations for the partial derivatives of S, T, V and p.
  - (b) Derive the identities

$$\frac{\partial S}{\partial T}\Big|_{p} = \frac{\partial S}{\partial T}\Big|_{V} + \frac{\partial S}{\partial V}\Big|_{T}\frac{\partial V}{\partial T}\Big|_{p}, \qquad \frac{\partial S}{\partial p}\Big|_{T} = \frac{\partial S}{\partial V}\Big|_{T}\frac{\partial V}{\partial p}\Big|_{T}.$$

(c) Show that if three variables x, y and z satisfy a constraint f(x, y, z) = 0 for all x, y and z, then

$$\frac{\partial x}{\partial y} \bigg|_z \frac{\partial y}{\partial z} \bigg|_x \frac{\partial z}{\partial x} \bigg|_y = -1 \; .$$

(d) Express the heat capacities at constant volume  $C_V$  and at constant pressure  $C_p$  in terms of derivatives of the entropy for reversible processes. Show that:

$$\begin{split} C_p - C_V &= T \frac{\partial V}{\partial T} \Big|_p \frac{\partial p}{\partial T} \Big|_V = -T \frac{\partial V}{\partial T} \Big|_p^2 \frac{\partial p}{\partial V} \Big|_T ,\\ \frac{\partial E}{\partial V} \Big|_T &= T \frac{\partial p}{\partial T} \Big|_V - p ,\\ \frac{\partial C_V}{\partial V} \Big|_T &= T \frac{\partial^2 p}{\partial T^2} \Big|_V . \end{split}$$

- 8. An isolated system consists of a fixed number N of non-interacting quantum particles, which are located at different positions in space and are therefore distinguishable. Each particle can sit in either of two states: the ground state  $|0\rangle$  or the excited state  $|1\rangle$ , which have energies  $\epsilon_0 = 0$  and  $\epsilon_1 = \epsilon$  respectively.
  - (a) Which quantities specify a macrostate of the system? Express these quantities in terms of  $\epsilon$  and of the occupation numbers  $N_0$  and  $N_1$  which count how many particles sit in the ground state and in the excited state respectively.
  - (b) Which quantities specify a microstate of the system? Relate the quantities that specify a microstate to the quantities that specify the macrostate.
  - (c) Derive a general formula for the number of microstates that realizes a given macrostate of the system, and write the discrete probability distribution for a microstate in the appropriate statistical ensemble.
  - (d) Compute the entropy S(E, N) of the system and approximate it using Stirling's formula in the thermodynamic limit of large N and E. Rewrite the result in terms of  $x_i = N_i/N$  (i = 0, 1), the "filling fractions" for the two states.
  - (e) Compute the temperature T(E, N) as a function of the energy E and the number of particles N. Invert the formula to express the energy E(T, N) in terms of the temperature T and the number of particles N.
  - (f) Analyse the low temperature and the high temperature limits of the energy: how are the two states occupied in these two limits?
- 9. Let us examine the thermodynamics of an anharmonic oscillator in one dimension.
  - (a) First consider a classical anharmonic oscillator whose Hamiltonian is

$$H(q,p) = \frac{p^2}{2m} + aq^2 + bq^4$$
,

where a and b are positive numbers. Calculate the canonical partition function and from it the heat capacity at constant volume for a system of N noninteracting indistinguishable anharmonic oscillators. You should work in the approximation where the anharmonicity is small, that is you can assume that  $b/a^2 \ll 1$  and derive your results to leading order in this small parameter.

(b) Now consider the quantum version of the above. The energy spectrum of a single oscillator is given to be

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega + x\left(n + \frac{1}{2}\right)^2\hbar\omega , \qquad n = 0, 1, 2, \dots$$

Compute the grand canonical partition function of this system, correct to leading order in the small parameter x which now measures the anharmonicity. You may use the formula

$$\frac{d^2}{dy^2} \frac{1}{2\sinh\frac{y}{2}} = \frac{3 + \cosh y}{16\sinh^3\frac{y}{2}} \ .$$



10. An ideal non-relativistic Fermi gas confined to a volume V is described by the grand canonical partition function

$$\mathcal{Z} \equiv e^{-\beta\Phi} = \prod_r (1 + z e^{-\beta E_r}) , \qquad z = e^{\beta\mu} ,$$

where r labels the one-particle states (of energies  $E_r$ ) available to a single fermion and  $\mu$  is the chemical potential.

(a) Ignoring any internal degrees of freedom, such as spin, and assuming that the energy levels are almost continuous,  $E_r \approx \hbar^2 \mathbf{k}^2/(2m)$ , so that a sum over one-particle states can be approximated by an integral

$$\sum_{r} \approx \frac{V}{(2\pi)^3} \int d^3 \boldsymbol{k} \; ,$$

show that the mean particle number  $\langle N \rangle$  of the system can be written as

$$\langle N \rangle = V \lambda^3 f_{3/2}(z)$$

where  $\lambda$  is a constant that you should determine and

$$f_{\nu}(z) = \frac{1}{\Gamma(\nu)} \int_0^\infty dx \, \frac{x^{\nu-1}}{z^{-1}e^x + 1} \, .$$

(b) Show that the mean energy is similarly given by

$$\langle E \rangle = \frac{3}{2} \frac{V \lambda^3}{\beta} f_{5/2}(z) \; .$$

(c) Using the following approximations, valid for large z,

$$f_{3/2}(z) \approx \frac{4(\ln z)^{3/2}}{3\sqrt{\pi}} \left(1 + \frac{\pi^2}{8(\ln z)^2}\right), \quad f_{5/2}(z) \approx \frac{8(\ln z)^{5/2}}{15\sqrt{\pi}} \left(1 + \frac{5\pi^2}{8(\ln z)^2}\right),$$

show that at low temperatures

$$\frac{\langle E \rangle}{\langle N \rangle} \approx \frac{3}{5} E_F (1 + O(1/\beta^2)) ,$$

where the Fermi energy  $E_F$  is to be determined in terms of the average number of particles  $\langle N \rangle$  and the volume V.





#### SECTION C

11. The Ising chain consists of a set of N spins  $s_i$ , i = 1, 2, ..., N, which can take the values  $\pm 1$  and are equally spaced on a one-dimensional periodic (*i.e.* circular) lattice. The energy for a particular configuration of spins  $\{s_i\}$  is given by

$$E[\{s_i\}] = -J \sum_{i=1}^N s_i s_{i+1} - \frac{B}{2} \sum_{i=1}^N (s_i + s_{i+1}) ,$$

where we impose the periodic boundary condition  $s_{N+1} \equiv s_1$ . Here *B* is the external magnetic field (rescaled by the dipole moment) and *J* is a coupling constant that is assumed to be positive.

- (a) Briefly describe the effect on the spins of the two contributions to the energy.
- (b) Write down the canonical partition function  $Z_N$  for the system, and prove that

$$Z_N = \operatorname{tr}(T^N) ,$$

where T is the  $2 \times 2$  transfer matrix

$$T = \begin{pmatrix} e^{\beta(J+B)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-B)} \end{pmatrix} \ .$$

Express the partition function in terms of the eigenvalues of the transfer matrix, which you should determine.

- (c) Assuming that  $N \gg 1$ , find an estimate for the partition function and the average magnetization  $m = \sum_{i=1}^{N} \langle s_i \rangle$  of the system.
- (d) Does the system exhibit spontaneous magnetization, that is a non-vanishing average magnetization at low temperatures in the absence of a magnetic field? Briefly discuss the physical interpretation of this fact.