

Candidate number:
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King's College London

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B.Sc. EXAMINATION

6CCP3212 Statistical Mechanics

Examiner: Dr Eugene Lim

**Examination Period 2
(Summer 2020)**

Time allowed: THREE hours

Candidates may answer as many parts as they wish from SECTION A, but the total mark for this section will be capped at 40.

Candidates should also answer TWO questions from SECTION B. No credit will be given for answering a further question from this section. The approximate mark for each part of a question is indicated in square brackets.

Calculators may be used. The following models are permitted: Casio fx83 and Casio fx85.

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Physical Constants

Permittivity of free space	$\epsilon_0 = 8.854 \times 10^{-12} \text{ F m}^{-1}$
Permeability of free space	$\mu_0 = 4\pi \times 10^{-7} \text{ H m}^{-1}$
Speed of light in free space	$c = 2.998 \times 10^8 \text{ m s}^{-1}$
Gravitational constant	$G = 6.673 \times 10^{-11} \text{ N m}^2 \text{ kg}^{-2}$
Elementary charge	$e = 1.602 \times 10^{-19} \text{ C}$
Electron rest mass	$m_e = 9.109 \times 10^{-31} \text{ kg}$
Unified atomic mass unit	$m_u = 1.661 \times 10^{-27} \text{ kg} = 931.494 \text{ MeV } c^{-2}$
Proton rest mass	$m_p = 1.673 \times 10^{-27} \text{ kg}$
Neutron rest mass	$m_n = 1.675 \times 10^{-27} \text{ kg}$
Planck constant	$h = 6.626 \times 10^{-34} \text{ J s}$
Boltzmann constant	$k_B = 1.381 \times 10^{-23} \text{ J K}^{-1} = 8.617 \times 10^{-11} \text{ MeV K}^{-1}$
Stefan-Boltzmann constant	$\sigma = 5.670 \times 10^{-8} \text{ W m}^{-2} \text{ K}^{-4}$
Gas constant	$R = 8.314 \text{ J mol}^{-1} \text{ K}^{-1}$
Avogadro constant	$N_A = 6.022 \times 10^{23} \text{ mol}^{-1}$
Molar volume of ideal gas at STP	$= 2.241 \times 10^{-2} \text{ m}^3$
One standard atmosphere	$P_0 = 1.013 \times 10^5 \text{ N m}^{-2}$

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Useful Information

Maxwell Relations

$$\left(\frac{\partial P}{\partial T}\right)_V = \left(\frac{\partial S}{\partial V}\right)_T, \quad \left(\frac{\partial T}{\partial V}\right)_S = -\left(\frac{\partial P}{\partial S}\right)_V,$$

$$\left(\frac{\partial S}{\partial P}\right)_T = -\left(\frac{\partial V}{\partial T}\right)_P, \quad \left(\frac{\partial V}{\partial S}\right)_P = \left(\frac{\partial T}{\partial P}\right)_S.$$

Fundamental Equation of Thermodynamics

$$dE = TdS - PdV + \mu dN$$

Thermodynamic Potentials

$$F = E - TS, \quad \Phi = E - TS + PV, \quad H = E + PV.$$

with differentials

$$dF = -SdT - PdV + \mu dN, \quad d\Phi = -SdT + VdP + \mu dN, \quad dH = TdS + VdP + \mu dN.$$

Heat Capacities

$$C_V = T \left(\frac{\partial S}{\partial T}\right)_V = \left(\frac{\partial E}{\partial T}\right)_V, \quad C_P = T \left(\frac{\partial S}{\partial T}\right)_P = \left(\frac{\partial H}{\partial T}\right)_P.$$

Microcanonical Ensemble Entropy

$$S = k_b \ln \Omega$$

Canonical Partition Function and formulas

$$Z = \sum_r e^{-\beta E_r}, \quad P_r = \frac{1}{Z} e^{-\beta E_r}, \quad \langle X \rangle = \sum_r P_r X_r,$$

$$F = -k_b T \ln Z, \quad S = k_b \frac{\partial}{\partial T} (T \ln Z), \quad \text{Mean Energy } \langle E \rangle = - \left(\frac{\partial \ln Z}{\partial \beta} \right)$$

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Grand Canonical Ensemble Partition Function

$$\mathcal{Z} = \sum_r e^{-\beta(E_r - \mu N_r)} ,$$

Mean Energy $\langle E \rangle + \mu \langle N \rangle = - \left(\frac{\partial \ln \mathcal{Z}}{\partial \beta} \right)$, Mean Particle Number $\langle N \rangle = \frac{1}{\beta} \left(\frac{\partial \ln \mathcal{Z}}{\partial \mu} \right)$.

Fermi-Dirac Distribution

$$\langle N_{\mathbf{n}} \rangle = \frac{1}{e^{\beta(E_{\mathbf{n}} - \mu)} + 1} .$$

Bose-Einstein Distribution

$$\langle N_{\mathbf{n}} \rangle = \frac{1}{e^{\beta(E_{\mathbf{n}} - \mu)} - 1} .$$

Thermal de Broglie wavelength

$$\lambda = \sqrt{\frac{2\pi\hbar^2}{mk_bT}} .$$

Stirling's Formula

$$\ln N! \approx N \ln N - N , \quad N \gg 1$$

Polylog integrals

$$\int_0^\infty \frac{x^{n-1}}{e^x + 1} dx = (1 - 2^{1-n}) \Gamma(n) \zeta(n) , \quad (n > 0),$$

and

$$\int_0^\infty \frac{x^{n-1}}{e^x - 1} dx = \Gamma(n) \zeta(n) , \quad (n > 1),$$

with Riemann Zeta function

$$\zeta(p) \equiv \sum_{n=1}^{\infty} \frac{1}{n^p} ,$$

and the Gamma function

$$\Gamma(n) \equiv \int_0^\infty x^{n-1} e^{-x} dx .$$

The Gamma function for $n > 0$ integers is

$$\Gamma(n) = (n - 1)! , \quad n \in \mathcal{N} - \{0\} .$$

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Common values for half-integer Gamma functions

$$\Gamma(1/2) = \sqrt{\pi}, \quad \Gamma(3/2) = \frac{\sqrt{\pi}}{2}, \quad \Gamma(5/2) = \frac{3\sqrt{\pi}}{4}, \quad \Gamma(7/2) = \frac{15\sqrt{\pi}}{8}.$$

and Zeta functions

$$\zeta(3/2) = 2.612, \quad \zeta(2) = \frac{\pi^2}{6}, \quad \zeta(5/2) = 1.341, \quad \zeta(3) = 1.202, \quad \zeta(7/2) = 1.127.$$

Gaussian Integral

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

Geometric Sum

$$\sum_{n=0}^{n=\infty} x^n = \frac{1}{1-x}, \quad |x| < 1.$$

A derivative identity between x , y and z with a single constraint $x(y, z)$

$$\left(\frac{\partial x}{\partial y}\right)_z \left(\frac{\partial y}{\partial z}\right)_x \left(\frac{\partial z}{\partial x}\right)_y = -1$$

Differential transform from $f(x, y) \rightarrow f(x, z)$ for a function $f(x, y)$ with a constraint $x = x(y, z)$

$$\left(\frac{\partial f}{\partial x}\right)_z = \left(\frac{\partial f}{\partial x}\right)_y + \left(\frac{\partial f}{\partial y}\right)_x \left(\frac{\partial y}{\partial x}\right)_z.$$

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SECTION A

Answer SECTION A in an answer book.

Answer as many parts of this section as you wish. Your total mark for this section will be capped at 40.

1.1 State the zeroth, 1st and 2nd Laws of Classical Thermodynamics.

[3 marks]B

1.2 State what is meant by the *Thermodynamic limit* of statistical mechanics.

[3 marks]B

1.3 State which of the following are exact differentials. Integrate the equation if it is exact.

(i) $dG(x, y) = (2xe^{yx} + yx^2e^{yx})dx + x^3e^{yx}dy.$

(ii) $dG(x, y, z) = y^2z^{-1}dx + 2yxz^{-1}dy - xy^2z^{-2}dz.$

(iii) $dG(x, y) = -2ydx + 2xdy.$

[9 marks]P

1.4 A thermodynamic system is described by the Dieterici equation of state given by

$$P = \frac{k_b T N}{V - b} e^{-\frac{aN}{k_b T V}}.$$

For fixed N , $a > 0$, $b > 0$ and by arguing that the system has to be stable under *isothermal* compression, show that

$$k_b T > \frac{aN(V - b)}{V^2}.$$

[6 marks]U

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1.5 Recall that the entropy of a system can be written in the Shannon form as

$$S = -k_b \sum_i P_i \ln P_i$$

where P_i is the probability of the i -th microstate occurring. Calculate the entropy of a fair 6-sided die.

Suppose the die is *loaded* (i.e. not a fair die) such that the chances of getting a 6 at every throw is 50%, and with the other 50% of the time evenly distributed among the other numbers. Show that the entropy is

$$S = k_b \ln(2\sqrt{5}) .$$

[8 marks] P

1.6 Starting from the fundamental equation of thermodynamics, and by using T and V as our state variables, show that

$$\left(\frac{\partial E}{\partial V}\right)_T = -P + T \left(\frac{\partial P}{\partial T}\right)_V .$$

Suppose for a particular gas, the energy only depends on T and not V , show that its equation of state is given by

$$P = f(V)T .$$

where $f(V)$ is any function of constants and V .

[8 marks]U

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1.7 The Maxwell-Boltzmann distribution of a gas at temperature T is given by

$$f(v)e^{-mv^2/2k_bT} = \sqrt{\frac{2}{\pi}} \left(\frac{m}{k_bT} \right)^{3/2} v^2 e^{-mv^2/2k_bT} ,$$

where the absolute velocity is

$$v = \sqrt{v_x^2 + v_y^2 + v_z^2} .$$

Calculate (i) $\langle v_x \rangle$ (ii) $\langle v_y^2 \rangle$ (iii) $\langle v_x^2 v_y^2 v_z^2 \rangle$.

You may use any theorems without proof.

[8 marks]B

1.8 The density of states for a bosonic quantum mechanical system with vanishing chemical potential $\mu = 0$ is given by

$$g(E) = \alpha E^{5/2} .$$

where $\alpha > 0$ is a dimensionful constant. Calculate the mean energy $\langle E \rangle$ of this system for a canonical ensemble with fixed β . You may leave the final answer in terms of the Γ and ζ functions.

[8 marks]B

1.9 Consider the following Landau Functional

$$F(T) = F_0(T) + \alpha(T - T_c)m^2 + bm^4 ,$$

where T_c is the critical temperature, and $\alpha > 0$, $b > 0$ are constants. Find the equilibrium points of this functional. Plot $F(T)$ for the two cases where $T < T_c$ and $T > T_c$. What is the order of the phase transition that this functional models? Justify your assertion.

[7 marks]B

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Solutions

1.1 Bookwork

1.2 $N \rightarrow \infty$ and $V \rightarrow \infty$ with $N/V \rightarrow \text{const.}$

1.3 (i) Exact. $G(x, y) = x^3 e^{yx}$ (ii) Exact. $G(x, y, z) = xy^2 z^{-1}$. (iii) Inexact.

1.4 Stability of (from bookwork) implies that $\left(\frac{\partial P}{\partial V}\right)_T < 0$, or

$$\left(\frac{\partial P}{\partial V}\right)_T = \frac{k_b T N}{V - b} \left(-\frac{1}{V - b} + \frac{aN}{k_b T V^2}\right) e^{-\frac{aN}{k_b T V}}. \quad (1)$$

which gives the required condition.

1.5 The probability of each microstate in a n -th sided die is $P_i = 1/n$, so $S = -k_b \sum_i P_i \ln P_i = k_b n \times (1/n) \ln n = k_b \ln n$. For 6 sided die this is $S = k_b \ln 6$. For the loaded die $P_6 = 1/2$ and $P_i = 1/10$ for $i = 1, 2, 3, 4, 5$, then $S = -k_b(0.5 \ln(1/2) + (5/10) \ln(1/10)) = k_b \ln 2\sqrt{5}$.

1.6 First part is bookwork. Using the identity in the Rubric, with $f \rightarrow E$, $x \rightarrow V$, $y \rightarrow S$ and $z \rightarrow T$, we get

$$\left(\frac{\partial E}{\partial V}\right)_T = \left(\frac{\partial E}{\partial V}\right)_S + \left(\frac{\partial E}{\partial S}\right)_V \left(\frac{\partial S}{\partial V}\right)_T \quad (2)$$

But now from the fundamental equation $dE = TdS - PdV$, i.e.

$$\left(\frac{\partial E}{\partial S}\right)_V = T, \quad \left(\frac{\partial E}{\partial V}\right)_S = -P \quad (3)$$

gets us

$$\left(\frac{\partial E}{\partial V}\right)_T = -P + T \left(\frac{\partial S}{\partial V}\right)_T, \quad (4)$$

and then using the Maxwell relation $\left(\frac{\partial S}{\partial V}\right)_T = \left(\frac{\partial P}{\partial T}\right)_V$

$$\left(\frac{\partial E}{\partial V}\right)_T = -P + T \left(\frac{\partial P}{\partial T}\right)_V. \quad (5)$$

If $\left(\frac{\partial E}{\partial V}\right)_T = 0$, then $P = T \left(\frac{\partial P}{\partial T}\right)_V$, and the solution for this equation is $P = f(V)T$.

1.7 (i) 0 by symmetry (ii) $k_b T/m$ by equipartition theorem $\langle mv^2/2 \rangle = (1/2)k_b T$ (iii) $(k_b T/m)^3$.

1.8 The integral is

$$\langle E \rangle = \int \frac{g(E)E}{e^{\beta E} - 1} dE = \beta^{-9/2} \alpha \int \frac{x^{7/2}}{e^x - 1} dx = \beta^{-9/2} \alpha \Gamma(9/2) \zeta(9/2) . \quad (6)$$

1.9 Finding the minima by $\partial F / \partial m = 0$, gets us the equilibrium solutions $m = 0$, $m = \pm \sqrt{-a/2b}$ where $a = \alpha(T - T_c)$. For the system to model a 2nd order phase transition, $\partial^2 F / \partial T^2$ must be discontinuous at $T = T_c$, and this is true since

$$\lim_{T \rightarrow T_c^-} \frac{\partial^2 F}{\partial T^2} - \lim_{T \rightarrow T_c^+} \frac{\partial^2 F}{\partial T^2} = \frac{\alpha^2}{2b} , \quad (7)$$

and the system is discontinuous at 2nd order.

SECTION B - Answer TWO questions
Answer SECTION B in an answer book

- 2) A simple magnetic system can be described by two independent state variables. These state variables include the magnetic field H , the temperature T , the internal energy E , the entropy S and the *magnetization* M defined by

$$M \equiv \frac{\bar{\mu}_N}{V} ,$$

where $\bar{\mu}_N$ is the total mean magnetic moment of the magnet and V is the volume of the system. (Note that V is not a state variable of magnetic systems.)

The 1st Law of Thermodynamics for the system is given by

$$dE = \delta Q + HdM .$$

- (a) For the state variables mentioned above (H , S , T , E and M), which are extensive and which are intensive?

[4 marks] U

- (b) The heat capacities at constant M and H for a magnetic system can be defined as

$$C_M \equiv \left(\frac{\delta Q}{dT} \right)_M , \quad C_H \equiv \left(\frac{\delta Q}{dT} \right)_H ,$$

respectively. By using T and M as the pair of independent state variables, show that

$$C_M = \left(\frac{\partial E}{\partial T} \right)_M \quad \text{and} ,$$

$$C_H = C_M + \left(\left(\frac{\partial E}{\partial M} \right)_T - H \right) \left(\frac{\partial M}{\partial T} \right)_H .$$

Hence prove the following differential relationship

$$dE = C_M dT + \left[\frac{C_H - C_M}{\left(\frac{\partial M}{\partial T} \right)_H} + H \right] dM .$$

[10 marks] U

QUESTION CONTINUES ON NEXT PAGE
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(c) A *Curie magnet* is a magnetic system described by the equation of state

$$M = a \frac{H}{T} ,$$

and the relationships

$$\left(\frac{\partial E}{\partial M} \right)_T = 0 , \quad C_M = bT ,$$

where $a > 0$ and $b > 0$ are positive definite constants.

Assuming that $E(T = 0, M = 0) = 0$, find $C_H(T, M)$ and $E(T, M)$ for a Curie magnet.

[10 marks] U

(d) Using your results in (c) and (d), show that for an adiabatic change (i.e. $dQ = 0$), the temperature changes with respect to the magnetization as

$$\frac{dT}{dM} = \frac{M}{ab} .$$

[6 marks] U

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Solution 2

(a) M and T are intensive, S , H and E are extensive.

(b) From $E(T, M)$

$$dE = \left(\frac{\partial E}{\partial T} \right)_M dT + \left(\frac{\partial E}{\partial M} \right)_T dM, \quad (8)$$

and combining with the first law in (b) we get

$$dQ = dE - HdM = \left(\frac{\partial E}{\partial T} \right)_M dT + \left(\left(\frac{\partial E}{\partial M} \right)_T - H \right) dM. \quad (9)$$

Then the heat capacities follows from the above

$$C_M = \left(\frac{dQ}{dT} \right)_M = \left(\frac{\partial U}{\partial T} \right)_M, \quad (10)$$

and

$$C_H = \left(\frac{dQ}{dT} \right)_H = C_M + \left(\left(\frac{\partial E}{\partial M} \right)_T - H \right) \left(\frac{\partial M}{\partial T} \right)_H. \quad (11)$$

Hence

$$C_H - C_M = \left(\left(\frac{\partial E}{\partial M} \right)_T - H \right) \left(\frac{\partial M}{\partial T} \right)_H \quad (12)$$

which rearranging gets us

$$\left(\frac{\partial E}{\partial M} \right)_T = \frac{C_H - C_M}{\left(\frac{\partial M}{\partial T} \right)_H} + H. \quad (13)$$

Plugging this back into the dU relationship we get the required relationship.

(c) For $E(T, M)$, from

$$dE = \underbrace{\left(\frac{\partial E}{\partial T} \right)_M}_{C_M=bT} dT + \underbrace{\left(\frac{\partial E}{\partial M} \right)_T}_0 dM \quad (14)$$

Integrating

$$E(T, M) = \int_0^T bT' dT' = \frac{1}{2}bT^2 + f(M). \quad (15)$$

But from $\left(\frac{\partial E}{\partial M} \right)_T = f'(M) = 0$ (given), $f(M) = \alpha$ where α is some constant. Hence $E(T, M) = \frac{1}{2}bT^2 + \alpha$. But now imposing $E(T = 0, M = 0) = 0$, we see that $\alpha = 0$. Thus the final answer is $E(T) = \frac{1}{2}bT^2$.

For C_H , we calculate

$$\left(\frac{\partial M}{\partial T}\right)_H = -\frac{aH}{T^2} \quad (16)$$

using the equation of state $M = aH/T$. Then using the $E(T) = \frac{1}{2}bT^2$ above, $\left(\frac{\partial E}{\partial M}\right)_T = 0$ and hence using the result in (c),

$$C_H = C_M + (0 - H)\left(-\frac{aH}{T^2}\right) = bT + \frac{M^2}{a} . \quad (17)$$

(d) Using the first law with $dQ = 0$, we get from (c)

$$\frac{dT}{dM} = -\frac{\left(\frac{\partial E}{\partial M}\right)_T - H}{C_M} \quad (18)$$

and plugging in our results from (d) for the Curie magnet we immediately get $dT/dM = M/ab$.

- 3) A gas of N indistinguishable and non-interacting atoms is held in a spherically symmetric *neutral atom trap* with potential $V(r) = ar$ where $r = \sqrt{x^2 + y^2 + z^2}$, such that the energy per particle is given by the Hamiltonian

$$H = \frac{\mathbf{p}^2}{2m} + V(r) ,$$

where m is the mass of each particle. The constant $a > 0$ denotes the strength of the potential. The gas is in thermal equilibrium with temperature T .

- (a) Is the potential attractive or repulsive? Explain your answer.

[4 marks] P

- (b) Show that the single particle partition function has the following form

$$Z_1 = AT^\alpha a^\beta ,$$

where A , α and β are constants. Find α and β .

(Hint: Recall that $\int_{-\infty}^{\infty} f(r) dx dy dz = 4\pi \int_0^{\infty} r^2 f(r) dr$.)

[8 marks] P

- (c) Using your result in (b), write down the partition function for the system of N particles, and derive the entropy S of the system as a function of N , Z_1 and T . (Hint: You may find Stirling's formula useful.)

[6 marks] P

- (d) Calculate the mean energy per particle of the system $\langle E \rangle$. Verify that this result is consistent with the Equipartition theorem.

[6 marks] U

- (e) The gas can be cooled if the potential is lowered reversibly by decreasing the strength of the potential a while no heat is allowed to be exchanged with the surroundings, $\dot{d}Q = 0$. Under these conditions, show that $T(a)$ is a power law of the form

$$T = T_0 \left(\frac{a}{a_0} \right)^\gamma ,$$

with initial values T_0 and a_0 . Find γ . (Hint: You may find your result in (c) useful.)

[6 marks] U

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Solution 3

(a) Since the energy E of the particle increases as a function of r for $a > 0$, the probability of the particle $P \propto e^{-\beta E}$ decreases, hence the particle is most likely to be found in at the origin $r = 0$. Thus it is an *attractive* potential.

(b) The single particle partition function is

$$Z_1 = \frac{1}{(2\pi\hbar)^3} \underbrace{\int dp_x dp_y dp_z e^{-\beta(p_x^2 + p_y^2 + p_z^2)}}_{(2\pi m/\beta)^{3/2}} \underbrace{\int dx dy dz e^{-\beta ar}}_{\int_0^\infty 4\pi r^2 e^{-\beta ar} dr} \quad (19)$$

$$= \frac{1}{(2\pi\hbar)^3} \left(\frac{2\pi m}{\beta}\right)^{3/2} \times 4\pi \left(\frac{1}{a\beta}\right)^3 \underbrace{\int_0^\infty x^2 e^{-x} dx}_2 \quad (20)$$

$$= \frac{8\pi(2\pi m)^{3/2} k_b^3}{(2\pi\hbar)^3} T^{9/2} a^{-3} . \quad (21)$$

Thus $\alpha = 9/2$ and $\beta = -3$.

(c) The partition function for the system of N particles is

$$Z = \frac{1}{N!} Z_1^N . \quad (22)$$

The free energy is $F = -k_b T \ln Z = -N k_b T (\ln Z_1/N + 1)$ using Stirling's formula, and hence the entropy is then

$$S = - \left(\frac{\partial F}{\partial T} \right) = N k_b \left(\ln \frac{Z_1}{N} + \frac{11}{2} \right) . \quad (23)$$

(d) The mean energy of the system is given by

$$\langle E \rangle = - \left(\frac{\partial \ln Z}{\partial \beta} \right) = \frac{9}{2} N k_b T . \quad (24)$$

The equipartition theorem is $\langle x \partial H / \partial x \rangle = k_b T$ for $x = (p_x, p_y, p_z, x, y, z)$. The momenta has the usual result $\langle p_x^2 / m \rangle = k_b T / 2$ per particle. The potential term is a bit more tricky

$$\langle x_i \frac{\partial H}{\partial x_i} \rangle = \frac{a x_i^2}{\sqrt{x^2 + y^2 + z^2}} \quad (25)$$

where $x_i = (x, y, z)$. Then

$$\langle V \rangle = \langle a\sqrt{x^2 + y^2 + z^2} \rangle = \left\langle x \frac{\partial H}{\partial x} + y \frac{\partial H}{\partial y} + z \frac{\partial H}{\partial z} \right\rangle = 3k_b T . \quad (26)$$

Thus the mean energy per partile is

$$\langle E \rangle = 3k_b T + \frac{3}{2}k_b T = \frac{9}{2}k_b T \quad (27)$$

so the total mean energy of the system is $(9/2)Nk_b T$ which is the same as above.

- (e) In a reversible process S is constant, so from the result of (c), Z_1 is constant. And hence from the result of (b), $T^{9/2}a^{-3} = \text{constant}$, or $T^{9/2} \propto a^3$ and hence

$$T = T_0 \left(\frac{a}{a_0} \right)^{2/3} \quad (28)$$

i.e. $\gamma = 2/3$.

4) A quantum mechanical system has n possible energy levels, each with energies $E_k = (k^2 - 1)\Delta$ for $k = 1, 2, 3, \dots, n$ where $\Delta = \hbar\omega$ has units of energy as usual. Each energy level exhibits a *degeneracy* of k^2 (i.e. each energy level has k^2 quantum states with different quantum numbers). The system is in thermal equilibrium with a heat bath of temperature $T = 1/k_b\beta$.

(a) A single *fermion* of spin $s = 1/2$ is placed in this system (you may call the two possible quantum states spin- \uparrow and spin- \downarrow). Show that the partition function for this system is given by

$$Z_f = 2e^{\beta\Delta} \sum_{k=1}^{k=n} k^2 e^{-k^2\beta\Delta} .$$

[8 marks] U,P

(b) *Two* non-interacting and indistinguishable fermions of spin $s = 1/2$ are placed in this system. Derive a formula for the total number of microstates as a function of n , $\Omega(n)$. Using your formula, show that for $n = 3$, $\Omega(n = 3) = 378$.

(*Hint* : You may find the formula

$${}^N C_M = \frac{N!}{M!(N - M)!} ,$$

useful.)

[8 marks] U

(c) For the system described in (b), what is the most likely microstate the system will be in at very low temperatures $\beta\Delta \gg 1$? Justify your answer.

[4 marks] U

(d) N non-interacting and indistinguishable spin $s = 0$ *bosons* are placed in this system. Derive the partition function for this system. Show that in the limit of very high temperatures $\beta\Delta \ll 1$, the partition function is

$$\lim_{\beta\Delta \ll 1} Z \rightarrow \frac{1}{N!} \left(\sum_{k=1}^{k=n} k^2 \right)^N .$$

In this limit, which microstate, if any, is the most likely microstate for this system? Argue that this corresponds to the *classical limit*.

[10 marks] P

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Solution 4

- (a) The partition function for a single $s = 1/2$ fermion is

$$\begin{aligned}
 Z &= \sum_{k=1}^{k=n} (2s+1)k^2 e^{-\beta E_k} \\
 &= \sum_{k=1}^{k=n} 2k^2 e^{-\beta(k^2-1)\Delta} \\
 &= 2e^{\beta\Delta} \sum_{k=1}^{k=n} k^2 e^{-k^2\beta\Delta}
 \end{aligned} \tag{29}$$

- (b) Let N be the total number of possible energy “slots” each fermion can occupy. Since each energy level k has a degeneracy of k^2 , N is given by

$$N = \sum_{k=1}^{k=n} k^2 . \tag{30}$$

For $s = 1/2$, each fermion has two possible states, let's call them \uparrow and \downarrow . Now the two fermions can either occupy a single slot or two separate slots. If they occupy a single slot, the occupation is must be $\uparrow\downarrow$ by Pauli exclusion principle, and hence there is a total of N such microstates. If they occupy two separate slots, there are ${}^N C_2$ ways of choosing two such slots, and for each choice, there are four possibilities $\uparrow\uparrow, \uparrow\downarrow, \downarrow\downarrow, \downarrow\uparrow$, for a total of $4 \times {}^N C_2$. Thus the total number of microstates is

$$\Omega(n) = N + 4 \cdot {}^N C_2.$$

For $n = 3$, we get $N = 1 + 4 + 9 = 14$, and $\Omega(3) = 14 + 4 \cdot 14!/2!(12!) = 378$.

- (c) The probability for a fermion to be in the k -th energy level is $P = (1/Z)e^{-\beta(k^2-1)\Delta}$, so for $\beta\Delta \ll 1$, the $e^{-k^2\beta\Delta} \rightarrow 1$ faster for larger k , so the most likely state is the $k = 1$ state. For a 2 fermion system, the most likely microstate is then $\uparrow\downarrow$ at the $k = 1$ state.
- (d) For non-interacting indistinguishable bosons, we can calculate the partition function for a single boson first which is

$$Z_1 = e^{\beta\Delta} \sum_{k=1}^{k=n} k^2 e^{-\beta k^2 \Delta} . \tag{31}$$

The total partition function is then the N -th product over Z_1 , divided by $N!$ (for indistinguishable particles), we have

$$Z = \frac{1}{N!} \prod_N Z_1 = \frac{1}{N!} e^{N\beta\Delta} \left(\sum_{k=1}^{k=n} k^2 e^{-\beta k^2 \Delta} \right)^N \tag{32}$$

In the limit of high temperatures $e^{\pm\beta\Delta} \rightarrow 1$, so we get

$$\lim_{\beta\Delta \ll 1} Z \rightarrow \frac{1}{N!} \left(\sum_{k=1}^{k=n} k^2 \right)^N . \quad (33)$$

as required.

In this limit, all the configurations are equally probable, and hence this corresponds to the classical limit. (Another way of explaining is to note that \hbar has vanished from the final result.)