

**FALL 2010  
STATISTICAL MECHANICS  
(Turn in 2 out of 3 Problems)**

**INSTRUCTIONS:**

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# Qualifying Exam 2010

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## Statistical Mechanics. Problem 1.

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A chain of  $N$  Ising spins on a ring (i.e. periodic boundary conditions) has the Hamiltonian

$$\mathcal{H} = -J \sum_{i=1}^N n_{ij} S_i S_{i+1}.$$

Here  $n_{ij}$  is independently and randomly chosen for each bond to be either 1 with probability  $p$  or 0 with probability  $1 - p$ . The bond variables are *quenched*, i.e. they are assigned specific values and are not summed over in the partition function.

- (a) Find the transfer matrix for a bond with  $n = 1$  and for a bond with  $n = 0$ .
- (b) Determine the free energy for a chain in which there are  $l$  bonds with  $n = 0$  and  $m$  bonds with  $n = 1$  (assume that  $l$  and  $m$  are large). (The sum,  $l + m$ , is the number of sites  $N$ .)
- (c) Hence determine the average free energy per site in the thermodynamic limit.

**Solution:**

The transfer matrix for a bond with  $n = 0$  has  $T_{ij}^0 = 1$  for all matrix elements. The transfer matrix for  $n = 1$  has  $T_{ij}^1 = \exp[\beta J]$  for  $i = j$  and  $T_{ij}^1 = \exp[-\beta J]$  for  $i \neq j$ . Making a unitary transformation to the eigenbasis of  $T^1$ , the transfer matrix  $\tilde{T}^1$  has entries  $2 \cosh \beta J$  and  $2 \sinh \beta J$  on the diagonal, while  $\tilde{T}^0 = 2\delta_{i1}\delta_{j1}$ . Therefore the partition function is equal to  $2^l (2 \cosh \beta J)^m$  if there are  $l$  bonds with  $n = 0$  and  $m$  bonds with  $n = 1$ . The free energy per site is  $-k_B T [\ln 2 + (m/N) \ln \cosh \beta J]$ . In the thermodynamic limit, this is equal to  $-k_B T [\ln 2 + p \ln \cosh \beta J]$ .

# Qualifying Exam 2010

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## Statistical Mechanics. Problem 2.

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1. Consider *two* two dimensional ideal gas models: (1) bosons with the dispersion relation  $\varepsilon_{\vec{k}} = \hbar^2 k^2 / 2m$ , and (2) “relativistic” bosons with the dispersion relation  $\varepsilon_{\vec{k}} = \hbar v k$ , where  $v$  is a positive constant (not necessarily equal to the speed of light). An elementary criterion for the existence of the Bose-Einstein condensation at a critical temperature  $T_B$  is  $N_T \equiv \sum_{\varepsilon_{\vec{k}} \neq 0} n(\varepsilon_{\vec{k}}, \mu = 0, T = T_B) = N$ , where  $n$  is the usual Bose-Einstein function.
  - (a) Show that this criterion leads to the conclusion that the system does not undergo a Bose-Einstein condensation at any finite temperature in the case of (1), while it does undergo a Bose-Einstein condensation at a finite temperature in the case of (2).
  - (b) In the latter case, determine  $T_B$  in terms of other quantities ( $N/A$ ,  $v$ , ...). The spin of the boson can be set to 0, and the thermodynamic limit ( $N \rightarrow \infty$ ,  $A \rightarrow \infty$ ,  $N/A \rightarrow \text{constant}$ ;  $A$  is the area) should be considered. Useful integral:  $\int_0^\infty dx x / (e^x - 1) \approx 1.645$ .

## Stat-Mech solution

1. The total number of bosons =  $N_0 + N_T$ , where  $N_0$  is the number of bosons in the lowest energy level. Within this elementary model, the condition for the Bose-Einstein condensation can be defined as

$$N_T \equiv \sum_{\varepsilon_{\vec{k}} \neq 0} n(\varepsilon_{\vec{k}}, \mu = 0, T = T_B) = N$$

The Bose-Einstein function is:

$$n(\varepsilon_{\vec{k}}, \mu, T) = \frac{1}{\exp\left(\frac{\varepsilon_{\vec{k}} - \mu}{k_B T}\right) - 1}$$

To do the sum, introduce the density of states,  $D(\varepsilon)d\varepsilon = 2\pi k dk / (2\pi/L)^2 = Ak dk / (2\pi)$ , where the sample size is assumed to be given by  $A = L \times L$ , and the periodic boundary condition is used ( $k_x = 2\pi n_x / L$ ,  $k_y = 2\pi n_y / L$ ). In the case of (1),  $D(\varepsilon)d\varepsilon = \frac{A}{4\pi} d(k^2) = \frac{mA}{2\pi\hbar^2} d\varepsilon$ , and so  $D(\varepsilon) = mA / (2\pi\hbar^2)$ . In the case of (2),  $D(\varepsilon)d\varepsilon = \frac{A}{2\pi(\hbar v)^2} \varepsilon d\varepsilon$ , and so  $D(\varepsilon) = A\varepsilon / (2\pi(\hbar v)^2)$ . The above condition  $N_T = N$  means

$$\int_0^\infty d\varepsilon D(\varepsilon) \frac{1}{\exp(\varepsilon / (k_B T_B)) - 1} = N$$

For case (1), using  $D(\varepsilon) = mA / (2\pi\hbar^2)$ , this translates to

$$\frac{m}{2\pi\hbar^2} k_B T_B \int_0^\infty dx \frac{1}{\exp(x) - 1} = \frac{N}{A}$$

Since the integral diverges (logarithmically, since the integrand  $\approx 1/x$  at small  $x$ ), the only solution to this condition is  $T_B = 0$ . Therefore, no BEC at any finite temperature.

For case (2), using  $D(\varepsilon) = A\varepsilon / (2\pi(\hbar v)^2)$ , we get

$$\frac{1}{2\pi(\hbar v)^2} (k_B T_B)^2 \int_0^\infty dx \frac{x}{\exp(x) - 1} = \frac{N}{A}$$

Using  $\int_0^\infty dx \frac{x}{\exp(x) - 1} \approx 1.645$ , we get

$$T_B = C \frac{\hbar v}{k_B} \sqrt{\frac{N}{A}}$$

where  $C \approx \sqrt{2\pi / 1.645} = 1.954$ .

# Qualifying Exam 2010

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## Statistical Mechanics. Problem 3.

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1. Consider the following Hamiltonian for spins on a three dimensional simple cubic lattice

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j. \quad (1)$$

The spins  $\mathbf{S}_i$  are unit vectors that can take four values,  $\pm\hat{x}$  and  $\pm\hat{y}$ . The sum is over nearest neighbors, with each distinct nearest neighbor pair being counted once. Treat this problem using the mean field approximation.

- (a) Calculate the phase transition temperature  $T_c$ , assuming that it is second order (continuous).  
(b) Now add a magnetic field  $\mathbf{h}$  so there is an extra term in the Hamiltonian

$$-\mathbf{h} \cdot \sum_i \mathbf{S}_i.$$

Assuming that the field is in the  $x$ -direction, calculate  $\langle S_i^x \rangle$  for small  $h$  at  $T = T_c$ .

### Solution: Statistical Mechanics Problem 3

1. The Hamiltonian is given by

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \quad (2)$$

where the spins  $\mathbf{S}_i$  are unit vectors that can take the values  $\pm\hat{x}$  and  $\pm\hat{y}$ .

(a) The part of the Hamiltonian involving  $\mathbf{S}_i$  is

$$-\mathbf{S}_i \cdot \mathbf{H}_i,$$

where  $\mathbf{H}_i$  is the local field on spin  $i$  due to its neighbors. This is given by

$$\mathbf{H}_i = J \sum_j \mathbf{S}_j, \quad (3)$$

where the sum is over the  $z$  neighbors of  $i$  ( $z = 6$  here). In the mean field approximation we replace the spins in Eq. (3) by their average values so

$$\mathbf{H}_i = J \sum_j \langle \mathbf{S}_j \rangle = zJ \langle \mathbf{S}_j \rangle \quad (\text{MF approx.}), \quad (4)$$

where in the last expression we used that  $\langle \mathbf{S}_j \rangle$  is independent of  $j$ .

The symmetry will be broken with the spins in preferentially aligned along one of the four directions. Let us suppose this is  $\hat{x}$ . Hence  $\langle S^x \rangle$  is given self consistently by

$$\begin{aligned} \langle S^x \rangle &= \frac{1 \cdot e^{\beta H} + 2 \cdot 0 \cdot e^0 + (-1) \cdot e^{-\beta H}}{e^{\beta H} + 2 \cdot e^0 + e^{-\beta H}} \\ &= \frac{2 \sinh \beta H}{2 \cosh \beta H + 2} = \frac{\sinh \beta H}{\cosh \beta H + 1}, \end{aligned} \quad (5)$$

where, remember,  $H = 6J \langle S^x \rangle$ .

Assuming the transition is second order, then, close to  $T_c$ ,  $\langle S^x \rangle$ , and hence  $H$ , is small. Expanding we get

$$\langle S^x \rangle = \frac{\beta H + \frac{1}{3!}(\beta H)^3 \dots +}{2 + \frac{1}{2!}(\beta H)^2 \dots +} \simeq \frac{1}{2} \beta H - \frac{1}{24} (\beta H)^3. \quad (6)$$

At  $T_c$  the terms linear in  $\beta H$  on both sides are equal so

$$\langle S^x \rangle = \frac{\beta_c H}{2} = 3\beta_c J \langle S^x \rangle$$

which gives

$$k_B T_c = 3J. \quad (7)$$

(b) Adding a magnetic field  $h$  in the  $x$ -direction, Eq. (5) remains unchanged but the expression for the molecular field  $H$  has the external field  $h$  added to it, i.e.

$$H = 6J \langle S^x \rangle + h. \quad (8)$$

Using the expansion in Eq. (6) gives

$$\langle S^x \rangle = \frac{1}{2} (6\beta J \langle S^x \rangle + h) - \frac{1}{24} (6\beta J \langle S^x \rangle)^3 \quad (9)$$

where we used the fact, to be confirmed at the end, that  $\langle S^x \rangle \gg h$  for small  $h$  at  $T = T_c$ , and so we omitted  $h$  compared with  $6\beta J \langle S^x \rangle$  in the cubic term. Setting  $T = T_c$ , given by Eq. (7), we get

$$\frac{1}{2}h = \frac{1}{24} (2\langle S^x \rangle)^3, \quad (10)$$

and so

$$\langle S^x \rangle = \left(\frac{3}{2}h\right)^{1/3}. \quad (11)$$

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# Qualifying Exam, Fall 2011

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## Statistical Mechanics Problem 1

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Consider the following Landau free energy for a model of a liquid crystal (Maier-Saupe model),

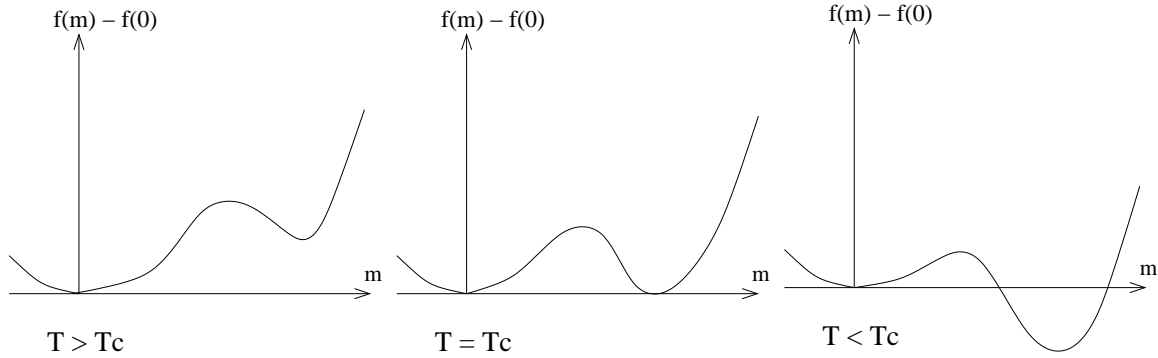
$$f = f_0(T) + \frac{1}{2}\alpha(T - T_0)m^2 - \frac{b}{3}m^3 + \frac{c}{4}m^4, \quad (1)$$

where  $m$  is the order parameter,  $f_0(T)$  is the part of the free energy that is independent of  $m$ ,  $T_0$  is a characteristic temperature, and the parameters  $\alpha, b$  and  $c$  are positive and independent of temperature  $T$ .

- (a) Show that  $m = 0$  at high  $T$ , but that there is a first order phase transition at a temperature  $T_c (> T_0)$  to a state with a non-zero value of  $m$ .  
*Note:* Your answer should include sketches of  $f$  against  $m$  for (i)  $T > T_c$ , (ii)  $T = T_c$ , and (iii)  $T < T_c$ .
- (b) Determine  $T_c$ , and the value of  $m$  for  $T \rightarrow T_c^-$ .
- (c) Determine the latent heat at the transition.

# Qualifying Exam Fall 2011

## Statistical Mechanics. Problem 1 Solution



- (a) The equilibrium value of the free energy is the minimum of  $f$ . From the sketches one sees that at high- $T$  the minimum at  $m = 0$  is the lowest, so this is the equilibrium value. However, as  $T$  is lowered, and the coefficient of the quadratic term decreases, the second minimum is lowered, and, at  $T = T_c$ , has a free energy equal to  $f(0)$ . At lower  $T$ , the minimum at positive  $m$  has the lower free energy and so this value of  $m$  is the equilibrium one.
- (b) The transition occurs where the two equations  $\partial f / \partial m = 0$  and  $f(m) = f(0)$  are simultaneously satisfied with a non-zero value for  $m$ , i.e.

$$\alpha(T_c - T_0) m - b m^2 + c m^3 = 0, \quad (2)$$

$$\frac{1}{2} \alpha(T_c - T_0) m^2 - \frac{1}{3} b m^3 + \frac{1}{4} c m^4 = 0. \quad (3)$$

We can divide these equations by powers of  $m$  since we are looking for a solution with  $m \neq 0$ , so

$$\alpha(T_c - T_0) - b m + c m^2 = 0, \quad (4)$$

$$\frac{1}{2} \alpha(T_c - T_0) - \frac{1}{3} b m + \frac{1}{4} c m^2 = 0. \quad (5)$$

Taking (4) - 2 × (5) gives

$$-\frac{1}{3} b m + \frac{1}{2} c m^2 = 0,$$

so

$$\boxed{m = \frac{2b}{3c}}.$$

Substituting this into Eq. (4) gives

$$\boxed{T_c - T_0 = \frac{2b^2}{9\alpha c}}.$$

(c) The latent heat is given by

$$L = T \Delta S,$$

where  $S$ , the entropy, is given by  $S = -\partial f / \partial T$ , and  $\Delta S$  is the change in entropy at  $T_c$ . Above  $T_c$  the entropy is given by

$$S_0 = -\frac{\partial f_0}{\partial T}.$$

Below  $T_c$  the entropy is less by an amount

$$\Delta S = \frac{1}{2} \alpha m^2 + [\alpha(T - T_0)m - b m^2 + c m^3] \frac{\partial m}{\partial T}.$$

According to Eq. (2), the expression in rectangular brackets is zero at  $T_c$  and so

$$L = T_c \Delta S = \frac{1}{2} T_c \alpha m^2 = \boxed{\frac{2}{9} \frac{\alpha b^2 T_c}{c^2}}.$$

# Qualifying Exam, Fall 2011

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## Statistical Mechanics Problem 2

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Consider *one* atom in a box of volume  $V$ . You are given that the density of states for this particle is

$$\rho(\epsilon) = \frac{V}{4\pi^2} \left( \frac{2m}{\hbar^2} \right)^{3/2} \epsilon^{1/2},$$

where  $\epsilon$  is the energy and  $m$  is the mass.

There is also *one* binding site (imagine it is somewhere on the surface of the box, but this is unimportant) of energy  $-\Delta E$  where  $\Delta E > 0$ . Hence the particle can *either* be unbound in the volume of the box *or* bound at the binding site. The temperature is  $T$ .

- (a) Find the probability that atom is bound.
- (b) What is the limit of this probability for  $V \rightarrow \infty$ ?
- (c) At what temperature is the probability of the atom being bound equal to 1/2?
- (d) You might have naively expected that the answer to the previous part would be when  $k_B T \simeq \Delta E$  ( $k_B$  is Boltzmann's constant), since  $\exp(-\Delta E/k_B T)$  is the ratio of the Boltzmann factor for the lowest energy state in the box to that for the bound state. However (unless  $V$  is really tiny) the temperature is actually much lower than this, Explain what important piece of physics is missing in the argument which gives  $k_B T \simeq \Delta E$ .

# Qualifying Exam Fall 2011

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## Statistical Mechanics. Problem 2 Solution

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We are given that the density of states for the atom in the box is

$$\rho(\epsilon) = \frac{V}{4\pi^2} \left( \frac{2m}{\hbar^2} \right)^{3/2} \epsilon^{1/2},$$

where  $\epsilon$  is the energy and  $m$  is the mass.

(a) Hence the contribution to the partition function from the “unbound” states in the box is

$$Z_{\text{unbound}} = \frac{V}{4\pi^2} \left( \frac{2m}{\hbar^2} \right)^{3/2} \int_0^\infty \epsilon^{1/2} e^{-\beta\epsilon} d\epsilon = \frac{V}{4\pi^2} \left( \frac{2mk_B T}{\hbar^2} \right)^{3/2} \int_0^\infty x^{1/2} e^{-x} dx.$$

The integral is just a number,  $\Gamma(3/2) = \frac{1}{2}\sqrt{\pi}$ , and so

$$Z_{\text{unbound}} = \frac{V}{V_Q}$$

where the “quantum volume”  $V_Q$  is given by

$$\boxed{V_Q = \left( \frac{2\pi\hbar^2}{mk_B T} \right)^{3/2}}. \quad (6)$$

In addition there is the contribution to the partition function from the single bound state,  $e^{\beta\Delta E}$ .

Hence the total partition function is

$$Z = e^{\beta\Delta E} + \frac{V}{V_Q}.$$

The probability that the atom is bound is  $e^{\beta\Delta E}$  divided by the partition function, i.e.

$$\boxed{P_{\text{bound}} = \frac{e^{\beta\Delta E}}{e^{\beta\Delta E} + V/V_Q}}.$$

(b) As  $V \rightarrow \infty$  this probability tends to zero, i.e. the atom is *always unbound*.

(c) The probability of the atom being unbound is equal to 1/2 when

$$\boxed{\frac{\Delta E}{k_B T} = \ln \left( \frac{V}{V_Q} \right)}. \quad (7)$$

- (d) Naively one might have expected that there would be “1” on the RHS of Eq. (7). However, this misses the *entropy*. In fact  $\ln(V/V_Q)$  is just  $(1/k_B)$  times) the entropy of the unbound particle in the box ( $\Delta S$ ). Hence Eq. (7) can be expressed as

$$\Delta E = T\Delta S$$

or equivalently

$$\boxed{\Delta F = 0},$$

where  $\boxed{\Delta F \equiv \Delta E - T\Delta S}$  is the *free energy* change when the particle unbinds.

# Qualifying Exam, Fall 2011

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## Statistical Mechanics Problem 3

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A tall vertical cylinder contains a monoatomic classical gas of  $N$  molecules of mass  $m$  in a gravitational field near the surface of the earth. A piston of mass  $M$  is initially clamped at a height  $h_0$  from the bottom of the cylinder. The whole system is in equilibrium at temperature  $T$  and the volume above the piston is vacuum.

- (a) Find the number density inside the cylinder as a function of height from the bottom. Hence show that the pressure exerted on the piston by the gas is given by

$$p(h_0) = \frac{mgN}{A} \frac{1}{\exp[\beta mgh_0] - 1}.$$

- (b) The piston is released, and allowed to find a new equilibrium. If the process is carried on at constant temperature, what is the new equilibrium height  $h_1$  of the piston?
- (c) How much heat is provided to the system by the environment in part (b)?

# Qualifying Exam Fall 2011

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## Statistical Mechanics. Problem 3 Solution

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- (a) From the canonical ensemble, the number density at a height  $z$  is  $n(z) = c \exp[-\beta mgz]$ , where  $c$  is some constant. Therefore the total number of molecules in the container is  $(c/\beta mg)\{1 - \exp[-\beta mgh_0]\}A$ , where  $A$  is the area of the cylinder. Since the total number of molecules is  $N$ , we have

$$n(z) = \frac{\beta mg N}{A} \frac{\exp[-\beta mgz]}{1 - \exp[-\beta mgh_0]}. \quad (8)$$

The pressure is equal to  $p = n(h_0)/\beta$ , which is equal to

$$p(h_0) = \frac{mgN}{A} \frac{1}{\exp[\beta mgh_0] - 1}. \quad (9)$$

- (b) When the system reaches equilibrium, the pressure at the top of the gas is  $p(h_1) = Mg/A$ . Using Eq.(9),

$$\frac{M}{mN} = \frac{1}{\exp[\beta mgh_1] - 1}. \quad (10)$$

Solving,

$$h_1 = \frac{k_B T}{mg} \ln(1 + mN/M). \quad (11)$$

- (c) The kinetic energy of the gas molecules is the same as it was before, since for an ideal gas the kinetic energy only depends on temperature. If the container is allowed to reach equilibrium at a height  $h$ , the potential energy of the gas and piston together is

$$U(h) = Mgh + \int_0^h \frac{\beta mg N}{A} \frac{\exp[-\beta mgz]}{1 - \exp[-\beta mgh]} mgz A dz = Mgh + Nk_B T - \frac{Nmgh}{\exp[\beta mgh] - 1}. \quad (12)$$

Using Eq.(10), we have

$$U(h_1) = Nk_B T \quad (13)$$

so that the heat supplied is  $U(h_1) - U(h_0) = Nmgh_0/(\exp[\beta mgh_0] - 1) - Mgh_0$ .

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# Winter Qualifying Exam 2010

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## Statistical Mechanics. Alternate Problem 1

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1. Consider *one* atom in a box of volume  $V$ . You are given that the density of states for this particle is

$$\rho(\epsilon) = \frac{V}{4\pi^2} \left( \frac{2m}{\hbar^2} \right)^{3/2} \epsilon^{1/2},$$

where  $\epsilon$  is the energy and  $m$  is the mass.

There is also *one* binding site (imagine it is somewhere on the surface of the box, but this is unimportant) of energy  $-\Delta E$  where  $\Delta E > 0$ . Hence the particle can *either* be unbound in the volume of the box *or* bound at the binding site. The temperature is  $T$ .

- (a) Find the probability that atom is bound.
- (b) What is the limit of this probability for  $V \rightarrow \infty$ ?
- (c) At what temperature is the probability of the atom being bound equal to 1/2?
- (d) You might have naively expected that the answer to the previous part would be when  $k_B T \simeq \Delta E$  ( $k_B$  is Boltzmann's constant), since  $\exp(-\Delta E/k_B T)$  is the ratio of the Boltzmann factor for the lowest energy state in the box to that for the the bound state. However (unless  $V$  is really tiny) the temperature is actually much lower than this, Explain what important piece of physics is missing in the argument which gives  $k_B T \simeq \Delta E$ .

You may find the following helpful:

$$\int_0^\infty x^{1/2} e^{-x} dx = \Gamma(3/2) = \frac{1}{2}\sqrt{\pi}$$

# Qualifying Exam 09

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## Statistical Mechanics. Alternate 1. Solution

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1. We are given that the density of states for the atom in the box is

$$\rho(\epsilon) = \frac{V}{4\pi^2} \left( \frac{2m}{\hbar^2} \right)^{3/2} \epsilon^{1/2},$$

where  $\epsilon$  is the energy and  $m$  is the mass.

(a) Hence the contribution to the partition function from the “unbound” states in the box is

$$Z_{\text{unbound}} = \frac{V}{4\pi^2} \left( \frac{2m}{\hbar^2} \right)^{3/2} \int_0^\infty \epsilon^{1/2} e^{-\beta\epsilon} d\epsilon = \frac{V}{4\pi^2} \left( \frac{2mk_B T}{\hbar^2} \right)^{3/2} \int_0^\infty x^{1/2} e^{-x} dx.$$

The integral is just a number,  $\Gamma(3/2) = \frac{1}{2}\sqrt{\pi}$ , and so

$$Z_{\text{unbound}} = \frac{V}{V_Q}$$

where the “quantum volume”  $V_Q$  is given by

$$\boxed{V_Q = \left( \frac{2\pi\hbar^2}{mk_B T} \right)^{3/2}}. \quad (1)$$

In addition there is the contribution to the partition function from the single bound state,  $e^{\beta\Delta E}$ .

Hence the total partition function is

$$Z = e^{\beta\Delta E} + \frac{V}{V_Q}.$$

The probability that the atom is bound is  $e^{\beta\Delta E}$  divided by the partition function, i.e.

$$\boxed{P_{\text{bound}} = \frac{e^{\beta\Delta E}}{e^{\beta\Delta E} + V/V_Q}}.$$

(b) As  $V \rightarrow \infty$  this probability tends to zero, i.e. the atom is *always unbound*.

(c) The probability of the atom being unbound is equal to 1/2 when

$$\boxed{\frac{\Delta E}{k_B T} = \ln \left( \frac{V}{V_Q} \right)}. \quad (2)$$

(d) Naively one might have expected that there would be “1” on the RHS of Eq. (??). However, this misses the *entropy*. In fact  $\ln(V/V_Q)$  is just  $(1/k_B)$  times) the entropy of the unbound particle in the box ( $\Delta S$ ). Hence Eq. (??) can be expressed as

$$\Delta E = T \Delta S$$

or equivalently

$$\boxed{\Delta F = 0},$$

where  $\Delta F \equiv \Delta E - T \Delta S$  is the *free energy* change when the particle unbinds.

# Winter Qualifying Exam 2010

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## Statistical Mechanics. Problem 2.

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A three dimensional cubic lattice has  $N$  sites. On it are  $m$  particles with  $m < N$ . There can be no more than one particle on a given site. Aside from that constraint, there are no interactions between the particles.

(a) Calculate the exact number of allowed configurations  $\Gamma(N, m)$  of the particles and thus the total entropy  $S_{tot} = k_B \ln \Gamma(N, m)$ . Assume the particles are indistinguishable.

(b) Consider a cubic subset of  $n$  lattice sites. Take  $n^2 \ll N - m$ . What is the natural log of the probability that these sites will all be unoccupied? In this case also take  $N - m \gg 1$ . Employ the approximation  $\ln(k!) = k \ln k - k$  for  $k \gg 1$ . Your final form should have a linear dependence on  $n$ .

## Solution

(a) A distinct state is delineated by a list of  $m$  distinct lattice sites, that can be given in any order. This is

$$\Gamma(N, m) = \frac{N!}{(N - m)!m!} \quad (1)$$

so

$$S_{tot} = k_B \ln\left(\frac{N!}{(N - m)!m!}\right) \quad (2)$$

(b) The probability that a state will be such that all  $n$  sites are unoccupied is

$$P_n = \frac{\Gamma(N - n, m)}{\Gamma(N, m)} \quad (3)$$

so

$$\ln P_n = \ln\left(\frac{\Gamma(N - n, m)}{\Gamma(N, m)}\right) = \ln\left(\frac{(N - n)!}{(N - m - n)!m!} \frac{(N - m)!}{N!}\right) \quad (4)$$

We can regroup this as

$$\ln P_n = \ln \frac{(N - n)!}{N!} + \ln \frac{(N - m - n)!}{(N - m)!} \quad (5)$$

With the approximation  $f(k) \equiv \ln(k!) = k \ln k - k$  for  $k \gg 1$ , we can Taylor expand the two logarithms:  $f(k_0 + \delta) \approx f(k_0) + f'(k_0)\delta$ , with an error which is the maximum value of the absolute value of the next term in the series, evaluated over the interval  $[k_0, k_0 + \delta]$ . Note  $f'(k) = \ln k$ , so expanding:

$$\ln P_n \approx -n \ln N + n \ln(N - m) = n \ln\left(\frac{N - m}{N}\right) \quad (6)$$

Note the errors in this for the first and second expansions are of order  $n^2/(N - m)$  and  $n^2/N$  respectively, but  $n^2/(N - m) \ll 1$  and therefore  $n^2/N \ll 1$ . So this is a legitimate expansion to make in this limit.

This is easily understood by saying that the probability of a site being empty is  $\frac{N - m}{N}$ , and for  $n \ll N - m$  these are all statistically independent, so the probability that all  $n$  sites are empty is  $\left(\frac{N - m}{N}\right)^n$

# Winter Qualifying Exam 2010

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## Statistical Mechanics. Problem 3

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3. A three dimensional gas of spinless non-relativistic bosons at pressure  $P$  and temperature  $T$  can be adsorbed onto a two dimensional surface layer where they are bound with energy  $-\epsilon_0 < 0$  but retain their translational degrees of freedom in two dimensions. The ideal three dimensional gas is in equilibrium with the ideal two dimensional adsorbed gas.

In this question treat the surface gas quantum mechanically and the three dimensional gas classically.

- (a) For the absorbed and non-absorbed gases to be in equilibrium with each other, what quantities must be the same for both of them?
- (b) Determine the density of absorbed bosons per unit area in terms of the chemical potential  $\mu$ , the temperature  $T$ , the mass of the particles  $m$ , and fundamental constants.

*Note:* You are given that the density of states per unit area of free, spinless particles in two-dimensions is

$$\rho_{2d}(\epsilon) = \begin{cases} \frac{m}{2\pi\hbar^2}, & (\epsilon > 0), \\ 0, & (\epsilon < 0), \end{cases}$$

i.e. it is independent of energy.

- (c) By considering the unbound (three-dimensional) bosons. and noting the answer to part 3a, compute the surface density in the layer as a function of the pressure  $P$  of the unbound gas, and  $T$ .

*Note:* It *may* be helpful to note that the classical partition function of  $N$  particles  $Z_N$  is given by

$$Z_N = \left(\frac{1}{2\pi\hbar^3}\right)^N \frac{1}{N!} \int \prod_{i=1}^N (d^3p_i d^3x_i) \exp[-\beta\mathcal{H}(\{\vec{p}, \vec{x}\})],$$

where  $\vec{p}_i$  is the momentum of the  $i$ -th particle and  $\vec{x}_i$  is its position.

# Winter Qualifying Exam 2010

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## Statistical Mechanics. Problem 3. Solution

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3. (a) For two systems to be in equilibrium if they can exchange energy with each other the temperatures must be equal. If, in addition, they can exchange particles with each other the chemical potentials must be equal. Hence here we require same the  $T$  and same  $\mu$ .
- (b) Define  $\lambda = \sqrt{2\pi\hbar^2/mk_B T}$ . From the expression for the density of states in two dimensions given in the question, and using the Bose-Einstein distribution function, the number of particles per unit area in the quantum, ideal, absorbed gas is

$$n_{2d} = \frac{1}{\lambda^2} \int_{-\epsilon_0}^{\infty} \frac{1}{\exp[\beta(\epsilon - \mu)] - 1} d(\beta\epsilon) = -\frac{1}{\lambda^2} \ln [1 - e^{\beta(\mu + \epsilon_0)}]. \quad (1)$$

This is in terms of the temperature and the chemical potential.

- (c) For the classical 3d gas with  $N$  particles the partition function can be easily computed from the expression in the question as

$$Z_N = \left( \frac{V}{(2\pi\hbar)^3} \right)^N \frac{1}{N!} \left[ \int_{-\infty}^{\infty} \exp[-\beta p^2/(2m)] dp \right]^{3N} = \frac{1}{N!} \left( \frac{V}{\lambda^3} \right)^N,$$

from which

$$e^{\beta\mu} = \exp[\beta(U - TS + PV)/N] = \exp \left[ 1 - \frac{\ln Z}{N} \right] = \frac{N\lambda^3}{V} = \frac{P\lambda^3}{k_B T}, \quad (2)$$

where we have used  $U - TS = -k_B T \log Z_N$ , the ideal gas law  $PV = Nk_B T$ , and Stirling's approximation  $\log N! \simeq N \log N - N$ . Substituting for  $e^{\beta\mu}$  from Eq. (1) into Eq. (2) we get the final result

$$n_{2d} = -\frac{1}{\lambda^2} \ln \left[ 1 - \frac{P\lambda^3}{k_B T} e^{\beta\epsilon_0} \right].$$

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Statistical Mechanics. Problem 1

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A particle of mass  $m$  is in an infinitely deep square well of width  $L$ , in one dimension. In the canonical ensemble, find approximate expressions for the specific heat (at constant  $L$ ) and the equation of state ( $P = P(L, T)$ ) in the i) low and ii) high temperature limits.

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 Statistical Mechanics. Problem 1 Solution
 

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The partition function is  $Z = \sum_n \exp[-n^2\beta\theta]$  where  $\theta = h^2/(8mL^2)$ .

i) At low temperatures, this is approximately equal to  $x(1 + x^3)$  where  $x = \exp[-\beta\theta]$ . The expectation value of the internal energy is then

$$-\frac{\partial \ln Z}{\partial \beta} = \theta \frac{x}{Z} \frac{\partial Z}{\partial x} = \theta \frac{1 + 4x^3}{1 + x^3} \approx \theta(1 + 3x^3). \quad (1)$$

The heat capacity is

$$\frac{\partial U}{\partial T} = 9x^2\theta \frac{\partial x}{\partial T} = \frac{9x^3\theta^2}{k_B T^2} = \frac{9\theta^2}{k_B T^2} \exp[-3\theta\beta]. \quad (2)$$

The one-dimensional pressure is equal to  $-\partial F/\partial L$ , where  $F$  is the Helmholtz free energy. This is equal to  $k_B T \partial \ln Z/\partial L$ . This yields

$$pL = k_B T L \frac{\partial x}{\partial L} \frac{1 + 4x^3 + \dots}{x + x^4 + \dots} = 2\theta(1 + 3x^3 + \dots). \quad (3)$$

The right hand side is a function of temperature (and various constants), and so this is the equation of state.

ii) At high temperatures,  $\beta$  is small and the sum in  $Z$  may be replaced by an integral:  $Z = \int_0^\infty \exp[-n^2\beta\theta] dn = \sqrt{\pi k_B T/4\theta} = \sqrt{2\pi m k_B T} L/h$ . The average energy is then  $-\partial \ln Z/\partial \beta = k_B T/2$ , and the specific heat is  $k_B/2$ . The equation of state is obtained from  $p = k_B T \partial \ln Z/\partial L = k_B T/L$ . Both of these are the same as the corresponding expressions for a classical one dimensional gas.

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Statistical Mechanics. Problem 2

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Two ideal Fermi gas systems occupy two compartments of a cylinder, with volumes  $V_1$  and  $V_2$ , respectively. The two compartments are separated by a freely sliding piston, and so  $V_1$  and  $V_2$  are variable, while the total volume  $V_1 + V_2$  is fixed. The number of fermions in  $V_1$  is equal to the number of fermions in  $V_2$ . The fermion in  $V_1$  has spin  $S_1$  (e.g.,  $1/2$ ) and obeys the dispersion relation

$$\varepsilon_1(\vec{k}) = \hbar v_1 k$$

while the fermion in  $V_2$  has spin  $S_2$  (e.g.,  $3/2$ ) and obeys the dispersion relation

$$\varepsilon_2(\vec{k}) = \hbar v_2 k$$

where  $v_1, v_2 > 0$  are *constant* velocity scales and  $k = |\vec{k}|$ .

The two systems are in equilibrium with each other at zero temperature. Find the ratio  $V_1/V_2$  as a function of  $v_1, v_2, S_1, S_2$ .

[A potentially helpful remark: to do this problem, you may need to consider the following important elements: (i) the density of states, (ii) the dependence of the Fermi momentum on spin and particle density, and (iii) the physical quantity, other than the temperature, equalized for these two systems in equilibrium.]

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 Statistical Mechanics. Problem 2 Solution
 

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First, since the dispersion is linear in  $k$ , the density of states  $D(\varepsilon) \propto \varepsilon^2$ . We can put  $D(\varepsilon) = A\varepsilon^2$ . At  $T = 0$ , assuming that there are  $N$  fermions, we get, by requiring that  $\int_0^{E_F} D(\varepsilon)d\varepsilon = N$  (where  $E_F$  is the Fermi energy),  $A = 3N/E_F^3$ . And, so  $D(\varepsilon) = 3N\varepsilon^2/E_F^3$ . The total energy at  $T = 0$  is  $E = \int_0^{E_F} D(\varepsilon)\varepsilon d\varepsilon = \frac{3}{4}NE_F$ .

Second, as the two systems form mutual equilibrium by equalizing the pressure, we need the expression for the pressure. Since  $T = 0$ , we note that  $F = E - TS = E$ , and  $P = -(\partial E/\partial V)_N$ . The volume dependence of  $E$  arises from  $E_F = \hbar v k_F$ . As  $k \propto 1/L$ , where  $L$  is the linear dimension of the system,  $E_F \propto V^{-1/3}$ , i.e.  $E \propto V^{-1/3}$ . So,  $P = -\partial E/\partial V = \frac{E}{3V}$ .

Combining these two results, we get  $P = \frac{NE_F}{4V} = \frac{Nvk_F}{4V}$ , where  $k_F$  is the Fermi momentum.

Now, for spin  $S$  and the number of particles  $N$ , we get  $(2S + 1)\frac{4\pi k_F^3/3}{8\pi^3/V} = N$ , and so  $k_F \propto \left(\frac{N}{(2S+1)V}\right)^{1/3}$ , up to a constant factor. Thus, we have

$$P \propto \frac{N^{4/3}v}{(2S + 1)^{1/3}V^{4/3}}$$

As  $P_1 = P_2$  and  $N_1 = N_2$  by assumption, we get the answer as follows.

$$\frac{V_1}{V_2} = \left(\frac{v_1}{v_2}\right)^{3/4} \left(\frac{2S_2 + 1}{2S_1 + 1}\right)^{1/4}$$

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 Statistical Mechanics. Problem 3
 

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Consider the Landau theory of phase transition, and for simplicity consider a scalar (Ising) order parameter  $m$ . Write the free energy as

$$F(m, h) = -hm + \frac{a(T)}{2}m^2 + \frac{u}{4}m^4 + \frac{v}{6}m^6,$$

where  $h$  is a magnetic field,  $u$  and  $v$  are assumed independent of  $T$ , and

$$a(T) = \alpha(T - T_c).$$

1. For the case of  $h = 0$  show graphically that the transition is first order (i.e. discontinuous) if  $u < 0$  and second order (i.e. continuous) if  $u > 0$ .
2. From now on assume  $u > 0$  and neglect  $v$ . Above the transition temperature  $T_c$  show that Landau theory predicts that the magnetic susceptibility  $\chi$ , defined by

$$\chi = \left. \frac{\partial m}{\partial h} \right|_{h \rightarrow 0^+},$$

diverges as

$$\chi = \frac{C_+}{t^\gamma} \quad (T > T_c),$$

where  $t \equiv (T - T_c)/T_c$  is the reduced temperature, the (universal) critical exponent,  $\gamma$ , is equal 1, and  $C_+$  is called a critical amplitude. Note that  $C_+$  is *not* universal since it depends on the parameters in the Landau free energy.

3. However, we can define the corresponding amplitude below  $T_c$  in an analogous manner, i.e.

$$\chi = \frac{C_-}{|t|^\gamma} \quad (T < T_c).$$

(You should note that, in contrast to the situation above  $T_c$ ,  $m$  itself is *not* zero in the  $h \rightarrow 0^+$  limit.) Show that the ratio  $C_+/C_-$  is universal according to Landau theory and find its universal value.

*Note:* Such critical amplitude ratios, like exponents, are believed to be universal also in an exact theory, though the universal values of amplitude ratios and exponents will, in general, be different from those predicted by Landau theory.

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 Statistical Mechanics. Problem 3 Solution
 

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1. The sketches should show that for  $u > 0$  there is a single minimum above  $T_c$  and two minima emerge continuously from this as  $T$  goes below  $T_c$ . However, if  $u < 0$ , two additional minima appear above  $T_c$  and their free energy becomes equal to that of the minimum at  $m = 0$  while  $T$  is still above  $T_c$ . When this happens, lets say at  $T = T_0$ , the transition occurs. Below  $T_0$  the magnetization jumps discontinuously to that of one of the minima with non-zero  $m$ .
2. The equilibrium magnetization is obtained minimizing the free energy with respect to  $m$ , i.e.

$$h = a(T)m + um^3. \quad (4)$$

Above  $T_c$ ,  $m \rightarrow 0$  as  $h \rightarrow 0$  so we can neglect the  $m^3$  term. This gives

$$\chi = \frac{1}{a(T)} = \frac{1}{T_c \alpha} \frac{T_c}{(T - T_c)} = \frac{C_+}{t^\gamma} \quad (T > T_c),$$

where

$$\gamma = 1, \quad C_+ = \frac{1}{T_c \alpha}.$$

3. Below  $T_c$ ,  $m$  does not tend to zero as  $h \rightarrow 0^+$ . Rather, from Eq. (4), we have

$$m_{eq}^2 = -\frac{a(T)}{u}. \quad (5)$$

Differentiating Eq. (4) with respect to  $m$  gives

$$\chi^{-1} = a(T) + 3um_{eq}^2 = -2a(T),$$

where, to get the last equality, we used Eq. (5). Hence

$$\chi = \frac{C_-}{|t|^\gamma} \quad (T < T_c),$$

where

$$C_- = \frac{1}{2T_c \alpha}.$$

As a result, although  $C_+$  and  $C_-$  individually are not universal, since they depended on the non-universal parameters  $T_c$  and  $\alpha$ , the ratio

$$\frac{C_+}{C_-} = 2$$

is universal since it is just a number.

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Statistical Mechanics. Potentially Useful Information.

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$$\int_{-\infty}^{\infty} \exp(-x^2) dx = \sqrt{\pi}$$

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

$$F = E - TS = -k_B T \ln Z$$

$$E = \left. \frac{\partial \ln Z}{\partial (-\beta)} \right|_{V,N}$$

$$\beta \equiv 1/(k_B T)$$

**WINTER 2012  
STATISTICAL MECHANICS  
(Turn in 2 out of 3 Problems)**

**INSTRUCTIONS:**

**DO EACH PROBLEM ON SEPARATE PAPER. WRITE ONLY ON THE FRONT SIDE OF EACH PAGE.**

**WRITE YOUR NAME, EXAM (CM), PROBLEM #, AND PAGE # ON EACH SHEET YOU TURN IN.**

**TURN IN ONLY TWO PROBLEMS. A THIRD PROBLEM WILL NOT BE GRADED.**

**BASIC CALCULATORS ARE ALLOWED, BUT NOT NECESSARY. THEY MUST BE NON-PROGRAMMABLE AND NON-GRAPHING CALCULATORS. THE USE OF IPODS, MP3 PLAYERS, CELL PHONES AND GRAPHING CALCULATORS WILL NOT BE PERMITTED.**

# Qualifying Exam, Winter 2012

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## Statistical Mechanics Problem 1

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Consider the following model, known as the Blume-Capel model,

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} S_i S_j - \Delta \sum_i S_i^2,$$

where  $S_i$  takes three possible states, 0, +1 and  $-1$ . Each spin interacts with  $z$  nearest neighbors, and the sum is over all nearest neighbor pairs, counted once. Take  $J > 0$  and also take the parameter  $\Delta$  to be positive.

- (a) What are the ground states of this Hamiltonian?
- (b) Derive an expression for the transition temperature,  $T_c$ , in the mean field approximation, assuming that the transition is continuous (second order).  
*Note:* Your result will be a self-consistent equation for  $T_c$ . You are not required to solve it *explicitly*.
- (c) Show that for  $\Delta \rightarrow \infty$  the result is that expected in the standard Ising model (where  $S_i = \pm 1$ ), i.e.

$$k_B T_c = z J.$$

# Qualifying Exam Fall 2012

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## Statistical Mechanics. Problem 1 Solution

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- (a) Because  $J > 0$  neighboring spins prefer to be parallel. Since  $\Delta > 0$  the states with  $S_i = \pm 1$  have lower energy than the state with  $S_i = 0$ . Hence there are two ground states, one has all  $S_i$  equal to +1 and the other has all  $S_i$  equal to -1.
- (b) All the terms involving site  $i$  can be written as

$$- \left( J \sum_j S_j \right) S_i - \Delta S_i^2.$$

In the mean field approximation we replace the spin on the neighbor by its expectation value. Writing  $m = \langle S_j \rangle$ , which is the same for all sites, the MF Hamiltonian for site  $i$  is

$$H_i^{\text{MF}} = -zJmS_i - \Delta S_i^2.$$

The expectation value of  $\langle S_i \rangle$  ( $= m$ ) obtained from  $H_i^{\text{MF}}$  is

$$m = \frac{2e^{\beta\Delta} \sinh(\beta Jzm)}{1 + 2e^{\beta\Delta} \cosh(\beta Jzm)}, \quad (1)$$

where  $\beta = 1/(k_B T)$ . This is a self-consistent equation for  $m$ .

If the transition is second order  $m \rightarrow 0$  as  $T \rightarrow T_c^-$ , so we expand the RHS of the above equation to first order in  $m$  to get

$$m = \frac{2\beta Jz e^{\beta\Delta}}{1 + 2e^{\beta\Delta}} m + O(m^3).$$

Equating the coefficients of  $m$ , we find that the transition temperature is given by the self-consistent solution of

$$\boxed{k_B T_c = \frac{2Jz e^{\beta_c \Delta}}{1 + 2e^{\beta_c \Delta}}.}$$

- (c) For  $\Delta \rightarrow \infty$  the exponentials are very large and we get  $k_B T_c = zJ$ , the usual result for the Ising model.

# Qualifying Exam, Winter 2012

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## Statistical Mechanics Problem 2

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Consider a two dimensional, non-interacting, non-relativistic electron gas of  $N$  electrons on a square surface of side  $L$  at  $T = 0$ .

- (a) Find the density of states of the system for up spins and for down spins.
- (b) Find the Fermi energy  $\epsilon_F$ .
- (c) For a small applied field  $B$ , the energy of each electron changes by  $\pm\mu B$ , depending on the sign of the spin. Find the magnetization per electron  $m$ , which is related to the difference in the number of electron spins parallel and antiparallel to the field by

$$m = \frac{N_{\uparrow} - N_{\downarrow}}{N},$$

(where, of course,  $N = N_{\uparrow} + N_{\downarrow}$ ).

# Qualifying Exam Winter 2012

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## Statistical Mechanics. Problem 2 Solution

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- (a) With periodic boundary conditions the allowed values of  $\mathbf{k}$  are

$$\mathbf{k} = \frac{2\pi}{L} (n_x, n_y),$$

where  $n_x$  and  $n_y$  are integers. Hence the density of points in  $\mathbf{k}$ -space is  $(L/2\pi)^2$ . Hence, for up spins, say, the density of states as a function of energy  $\rho_{\uparrow}(\epsilon)$  is determined from equating the number of states with energy between  $\epsilon$  and  $\epsilon + d\epsilon$  to the number of states with magnitude of wavevector between  $k$  and  $k + dk$ , where  $\epsilon = \hbar^2 k^2 / 2m$ . i.e.

$$\rho_{\uparrow}(\epsilon) d\epsilon = \frac{L^2}{(2\pi)^2} 2\pi k dk$$

so

$$\rho_{\uparrow}(\epsilon) = \frac{L^2 m}{2\pi \hbar^2} \boxed{= L^2 \frac{m}{2\pi \hbar^2}},$$

where we used that  $k dk = (m/\hbar^2) d\epsilon$ . The density of states for the down spin electrons,  $\rho_{\downarrow}(\epsilon)$  is the same. Note that, in the present case (2 dimensions) the density of states is independent of energy.

- (b) The Fermi energy  $\epsilon_F$  is found by filling the states up to  $\epsilon_F$ . Hence, if there are  $N$  electrons, we have

$$N = \epsilon_F (\rho_{\uparrow} + \rho_{\downarrow}) = \epsilon_F L^2 \frac{m}{\pi \hbar^2},$$

so

$$\boxed{\epsilon_F = \frac{\pi \hbar^2}{m} \frac{N}{L^2}}.$$

- (c) When a magnetic field is applied the energy of the up-spin states decreases by  $\mu B$  and that of the down-spin states increases by the same amount. Because the densities of states of the up spins and down spins are equal, and independent of energy, the Fermi energy stays the same. However, the lowest energy for an up spin is now  $-\mu B$  and that for a down spin is  $\mu B$ . Hence there are more up spins than down spins by an amount  $2\mu B \rho_{\uparrow}$ . In other words, the magnetization per electron is given by

$$m = \frac{N_{\uparrow} - N_{\downarrow}}{N} = \frac{L^2}{N} \frac{m}{\pi \hbar^2} \mu B = \boxed{\frac{\mu B}{\epsilon_F}}.$$

# Qualifying Exam, Winter 2012

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## Statistical Mechanics Problem 3

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Consider two spin-1 objects,  $\mathbf{S}_1$  and  $\mathbf{S}_2$ , with Hamiltonian

$$\mathcal{H} = J\mathbf{S}_1 \cdot \mathbf{S}_2,$$

where  $J > 0$ .

- (a) Find the energy levels.

*Hint:* Use  $(\mathbf{S}_{\text{tot}})^2 = (\mathbf{S}_1 + \mathbf{S}_2)^2$ , where  $S_{\text{tot}}$  is the total spin, and note that the vector rule for the addition of angular momenta states that the allowed values of the total spin quantum number  $S_{\text{tot}}$  are 0, 1, and 2 (each value once).

- (b) Find the free energy, entropy and average energy as a function of temperature,  $T$ .

- (c) What are the limits of the entropy as (i)  $T \rightarrow 0$ , and (ii)  $T \rightarrow \infty$ ? Explain how you could have obtained these values from elementary considerations without first determining the free energy.

# Qualifying Exam Winter 2012

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## Statistical Mechanics. Problem 3 Solution

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(a) The Hamiltonian can be written as

$$\mathcal{H} = \frac{J}{2} [(\mathbf{S}_1 + \mathbf{S}_2)^2 - (\mathbf{S}_1)^2 - (\mathbf{S}_2)^2] = \frac{J}{2} [S_{\text{tot}}(S_{\text{tot}} + 1) - 1 \cdot 2 - 1 \cdot 2] = \frac{J}{2} S_{\text{tot}}(S_{\text{tot}} + 1) - 2J.$$

Since  $S_{\text{tot}}$  takes values 0, 1 and 2, the energy levels are

$$\boxed{E = -2J, \quad (\text{degeneracy } 1), \quad E = -J, \quad (\text{degeneracy } 3), \quad E = J, \quad (\text{degeneracy } 5).}$$

(b) The partition function is given by

$$Z = e^{2\beta J} + 3e^{\beta J} + 5e^{-\beta J},$$

and the free energy is therefore given by

$$F = -k_B T \ln Z \quad \boxed{= -k_B T \ln (e^{2\beta J} + 3e^{\beta J} + 5e^{-\beta J})}.$$

The energy is given by  $U = \sum_l E_l P_l$  where  $P_l$  is the Boltzmann probability for state  $l$ , which gives

$$\frac{U}{J} = \frac{(-2)e^{2\beta J} + (-1)3e^{\beta J} + (+1)5e^{-\beta J}}{e^{2\beta J} + 3e^{\beta J} + 5e^{-\beta J}} \quad \boxed{= \frac{-2e^{2\beta J} - 3e^{\beta J} + 5e^{-\beta J}}{e^{2\beta J} + 3e^{\beta J} + 5e^{-\beta J}}}.$$

The entropy is given by  $S = -\partial F / \partial T$ , which, for our purposes, can be more conveniently be written as  $S = (U - F) / T$ . This gives

$$\boxed{\frac{S}{k_B} = \ln (e^{2\beta J} + 3e^{\beta J} + 5e^{-\beta J}) + (\beta J) \frac{-2e^{2\beta J} - 3e^{\beta J} + 5e^{-\beta J}}{e^{2\beta J} + 3e^{\beta J} + 5e^{-\beta J}}}.$$

(c) (a) For  $T \rightarrow 0$  we have, setting  $\beta \rightarrow \infty$  and just including the largest exponential,  $S = 2\beta J - 2\beta J \quad \boxed{= 0}.$

At  $T = 0$ , the system is definitely in the ground state, and the entropy is  $k_B$  times the log of the ground state degeneracy. Since the ground state is non-degenerate, this gives zero entropy.

(b) For  $T \rightarrow \infty$ , we set  $\beta = 0$  and so get  $S = k_B \ln 9$ . This result comes from the fact that, in this limit, 9 states are equally probable and the entropy is  $k_B$  times the log of the number of states.