The following problems
from the 1995, 1996 and 1997
Written Ph.D. Qualifying Exams
are provided without solutions.

They can be used
as a study aid
to create practice exams, etc.

1997

STATISTICAL MECHANICS

1. A toy model for DNA consists of a zipper-like structure with N pairs of 'teeth' (each pair of teeth corresponding to a base-pair). The bond between the partners in each base-pair can either be closed or open. If a bond is open, the energy associated with it is ϵ, while if a bond is closed the energy associated with it is zero. The zipper can be opened from both ends simultaneously, but it cannot be opened from the center. Thus if the bond i is broken, either all the bonds $1 \ldots i-1$ or all the bonds $i+1 \ldots N$ (or both) must be open. The system is in equilibrium at temperature T. Calculate the Helmholtz free energy and the expectation value for the number of open bonds for $N\epsilon >> k_BT$.

1997

STATISTICAL MECHANICS

2. Consider the spin-1/2 Ising model in a transverse field, whose Hamiltonian is given by

$$\mathcal{H} = -\sum_{\langle i,j\rangle} J_{ij}\sigma_i^z\sigma_j^z - h\sum_i \sigma_i^x ,$$

where the σ_i^α are Pauli spin matrices, and h is the transverse field. Assume that the interactions, J_{ij} act between nearest neighbors and are of strength J. Let the number of nearest neighbors of a given site be z. For sufficiently high temperature or transverse field the system will be in a paramagnetic state and otherwise it will be in a ferromagnetic state.

a.) Find a self-consistent expression for the magnetization $m \equiv \langle\sigma_i^z\rangle$ in the ferromagnetic region, in the mean field approximation. Note: The mean field is a vector.

b.) Find an implicit expression for the critical line separating the paramagnetic and ferromagnetic phases. (Assume that the transition is continuous so this is the line where $m \to 0$). What is the value of the critical temperature when $h = 0$, (i.e. the regular Ising model), and what is the critical value of h at $T = 0$?

c.) Give a rough sketch of the phase diagram, the $h-T$ plane, showing the paramagnetic region, where $m = 0$, and the ferromagnetic region, where $m \neq 0$.

d.) Show that $\langle\sigma_i^x\rangle$ is independent of T below T_c, within this approximation.

1997

STATISTICAL MECHANICS

3. A classical gas of N particles is in thermal equilibrium at temperature T. The particles interact with each other via a potential $U(r)$. Each particle has a mass m.

(a) What is the probability distribution for the x component of the velocity of a particle, $P(v_x)$?

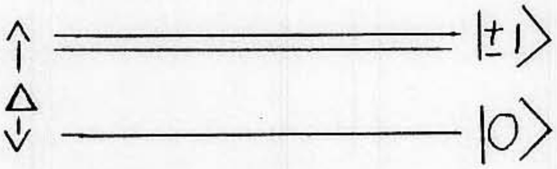
(b) At any given time, one particle has the largest value of $|v_x|$. Call this value $v_{x,max}$. Write down the expression for the probability distribution of $v_{x,max}$. Your answer can involve integrals.

(c) In the limit of very large N, calculate the average value of $v_{x,max}$, to leading order in $\log N$.

1996

STATISTICAL MECHANICS

1. A spin-1 ion in a crystal has its energy levels split by its environment such that the $|S_z = 0>$ state is an energy Δ below the $|S_z = \pm 1>$ states (see sketch).



A magnetic field h in the x direction is added which gives a term in the Hamiltonian

$$-hS_x$$

a) This gives rise to a non-zero expectation value $< S_x >$. Find the susceptibility, χ, as a function of T, where χ is defined by

$$< S_x >= h\chi \quad (h \to 0)$$

I suggest you proceed as follows:
(i) Show that $\chi = \frac{\partial^2 f}{-\partial h^2}|_{h=0}$ where f is the free energy of the ion.
(ii) Calculate the change in the energy of the levels to 2nd order in h.
(iii) Hence, calculate the free energy up to 2nd order in h and so determine χ.

b) Show that for $k_B T \gg \Delta$, $\chi \propto \frac{1}{T}$ (Curie law), and that $\chi \to$ const. as $T \to 0$.

n.b. The non-zero matrix elements of S_x are:

$$\langle 0|S_x| \pm 1\rangle = \langle \pm 1|S_x|0\rangle = \frac{1}{\sqrt{2}}$$

in units where Planck's constant, $\hbar$, is unity.

1996

STATISTICAL MECHANICS

2. One place where it gets very hot is the early universe. Phase transitions probably occurred at various times. We study one.

a. Write down the free energy for a free, non-relativistic spin one particle (Bose-Einstein statistics) as an integral over momenta. Don't evaluate the integral.

b. Write down the free energy for a free, *relativistic* spin one particle by making the replacement

$$\frac{p^2}{2m} \to \sqrt{p^2 + m^2}$$

(use units with $c = 1$). How does this result compare to that for a free photon gas?

c. Assuming that $T \gg m$, expand the integrand in the expression and write out the term which is first order in m^2. In order to get rid of parts which are independent of temperature, subtract from the integrand its value at $T = 0$, and then do the resulting integral.

d. At zero temperature, the ground state energy in the standard model has the form

$$-am^2 + bm^4.$$

Add the temperature dependent contribution you found in part *d*. In the standard model, the mass is dynamical, which means that it will always sit at the minimum value of the free energy. Does this system undergo a phase transition? What is the order?

(Hint:) You need to remember that the free energy for a system of bosons is

$$F = -T \sum_n \ln(1 - e^{-\beta E_n}).$$

You will need the integral

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

1996

STATISTICAL MECHANICS

3. Statistical Mechanics of a Lock. Consider a combination lock with N digits. Each digit takes on the values $0 \ldots 9$. If the correct combination is found, the lock opens and the energy is $-N\epsilon < 0$. Otherwise the energy of the lock is 0. The lock is kept at a temperature T.

(a) Calculate the partition function $Z(T)$, and the free energy.

(b) Calculate the energy, entropy and free energy per digit in the limit of large N. Calculate the specific heat.

(c) The digits are simultaneously flipped randomly with a frequency of ω. Estimate the average time it takes to find the correct combination.

1995

STATISTICAL MECHANICS

1. Consider a (fictional!) one-dimensional non-interacting gas of N particles in a container of length L with the Hamiltonian

$$\mathcal{H} = \sum_j \epsilon(p_j)$$

where the single particle energy $\epsilon(p)$ behaves as $\epsilon(p) \approx p^2$ for small p and $\epsilon(p) \approx \alpha \ln|p| + \gamma \ln\ln|p|$ for large $|p|$.

a) Show that the canonical partition function cannot be defined for $T > T_c$, and find T_c.

b) How does the mean energy per particle diverge as $T \to T_c$ for (i) $\gamma = 0$ and (ii) $\gamma = 3\alpha$.

c) For $\gamma = 3\alpha$, what happens if u, the energy per particle, is large, and the gas is isolated from its surroundings?

1995

STATISTICAL MECHANICS

2. Colloidal spherical particles of radius a and mass M dispersed in a solvent are seen to undergo Brownian motion. The cause is a *fluctuating force*, $F(t)$ that arises from collisions with the solvent molecules. The solvent has a viscosity η, and the system is at a temperature T. The equation of motion of a particle is

$$M\frac{d^2x}{dt^2} + 6\pi\eta a\frac{dx}{dt} = F(t).$$

The average over time of $F(t)$ is zero, and the force at different times is uncorrelated: $\langle F(t)F(t')\rangle \propto \delta(t-t')$, where $\langle\ \rangle$ denote an average over different realizations of $F(t)$.

a) Show that a measurement of the mean square displacement, $\langle \Delta x^2 \rangle$, as a function of time can be used to determine Boltzmann's constant k_B.

b) The system (the solvent and the colloidal particles) is confined between two parallel horizontal plates, with vertical coordinates $z = \pm L$. Due to boundary effects from the plates, the viscosity η felt by a colloidal particle now depends on its height. If $\eta(z) = \eta_0/(1 - z^2/L^2)$, obtain an expression for the mean square horizontal displacement as a function of time, for long times, assuming $a << L$. (Do not forget gravity.) *Hint: For long times, the particle distribution in the z direction comes to thermal equilibrium, calcluate this distribution first. From part (a) we know the diffusion coefficient for the particle in a particular plane. Put these facts together.*

1995

STATISTICAL MECHANICS

3. Consider an Ising antiferromagnet on a square lattice where $S_i, S_j = \pm 1$ and S_i and S_j are the spins on the two sublattices. The exchange interaction is between nearest neighbors only. A uniform field H is applied along the spin ordering direction of one sublattice.

a) Write the Hamiltonian for this system.

b) Write an approximate Hamiltonian in the mean field approximation, where each spin sees only the average behavior of its neighbors. Use this approximation for the remaining calculations.

c) Calculate $< S_i >$. Your answer may be expressed in terms of $< S_j >$.

d) Calculate $< S_j >$ in a similar way.

e) For $H = 0$, calculate the transition temperature T_c.

f) Calculate the susceptibility near T_c.

g) Show that the staggered magnetization $M_s =< S_i > - < S_j >$ goes to zero at T_c to first order in H.

h) For $H = 0$, show that the staggered magnetism near T_c has the behaviour $M_s \sim (\frac{T-T_c}{T_c})^\beta$, and calculate β.

1998

Statistical Mechanics
(do 2 out of 3 problems)

Please do **EACH** problem you attempt on a **SEPARATE** paper.
Put your name on each paper.

STATISTICAL MECHANICS

1. Consider a classical pendulum, weakly coupled to a heat bath, near the surface of the earth, consisting of a mass m on a massless, rigid rod of length L. The mass swings freely in one plane with the angle θ defined as shown in the figure. Although you should check that the solutions that you obtain for calculations below agree with your expectations, you must show your calculations for credit.

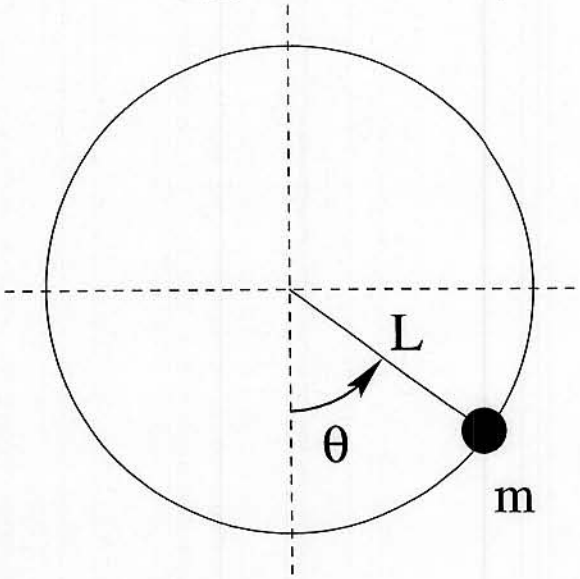
a. Write an expression for the average height of the mass as a function of the temperature T. Although your answer should be expressed in a simple form, you do not need to solve the integral.

b. Calculate from this expression the limiting value of the average height as $T \to \infty$ (you must show your work).

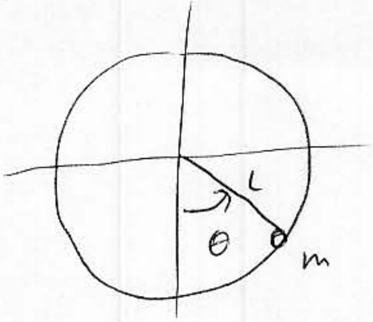
c. Calculate the average height as $T \to 0$. Your answer must include the leading T dependence.

d. Repeat parts a, b and c for the average energy.

e. Sketch the heat capacity for this system.



Stat Mech #1 1998 1/2



$$h = -L\cos\theta$$

$$E = \tfrac{1}{2} m L^2 \dot\theta^2 - mgL\cos\theta$$

a) $$\langle h\rangle = -L\frac{\int_0^\pi \cos\theta \, e^{-(\frac{1}{2} m L^2 \dot\theta^2 - Lmg\cos\theta)\beta} \, d\dot\theta \, d\theta}{\int_0^\pi e^{-(\frac{1}{2} m L^2 \dot\theta^2 - Lmg\cos\theta)\beta} \, d\dot\theta \, d\theta}$$

$$\langle h\rangle = -\frac{L\int_0^\pi \cos\theta \, e^{mgL\beta\cos\theta} \, d\theta}{\int_0^\pi e^{mgL\beta\cos\theta} \, d\theta}$$

b) for $\beta \to 0$, $T \to \infty$

$$\langle h\rangle \approx \frac{-L\int_0^\pi \cos\theta \, d\theta}{\int_0^\pi d\theta} = 0$$

c) for $\beta \to \infty$, $T \to 0$

$$E \simeq \tfrac{1}{2} m L^2 \dot\theta^2 - mgL + \tfrac{1}{2} mgL\theta^2$$

$$h \simeq -L + \tfrac{1}{2} L\theta^2$$

$$\langle\theta^2\rangle = \frac{\int_0^\infty \theta^2 e^{-\frac{1}{2} mgL\beta\theta^2} \, d\theta}{\int_0^\infty e^{-\frac{1}{2} mgL\beta\theta^2} \, d\theta} = \frac{kT}{\cancel{2}mgL}$$

$$\langle h\rangle \simeq -L + \frac{1}{2}\frac{kT}{mg}$$

Stat Mech #H1998 4L

d) $$\langle \dot\theta^2 \rangle = \frac{\int_0^\infty \dot\theta \, e^{-\frac{1}{2} m L^2 \dot\theta^2 \beta} \, d\dot\theta}{\int_0^\infty e^{-\frac{1}{2} m L^2 \dot\theta^2 \beta} \, d\dot\theta} = \frac{kT}{mL^2}$$

$$E = \tfrac{1}{2} m L^2 \dot\theta^2 + mgh$$

$$\langle E \rangle = \tfrac{1}{2} kT - mgL \frac{\int_0^\pi \cos e^{mgL\beta\cos\theta} \, d\theta}{\int_0^\pi e^{mgL\beta\cos\theta} \, d\theta}$$

for $\beta \to 0$, $T \to \infty$

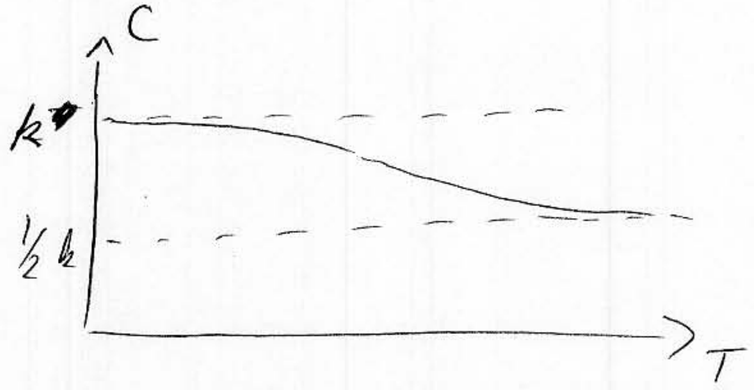
$$\langle E \rangle \simeq \tfrac{1}{2} kT$$

for $\beta \to \infty$, $T \to 0$

$$\langle E \rangle = \tfrac{1}{2} kT - mgL + \tfrac{1}{2} kT$$

$$\langle E \rangle = kT - mgL$$

e)



STATISTICAL MECHANICS

2. A one dimensional system consists of a point mass m attached to a linear spring with spring coefficient k. The other end of the spring is tethered to a wall which is completely impenetrable. Thus the equilibrium position of the spring is at the wall.

a. First consider the system to be classical and calculate the average energy as a function of temperature.

b. Now consider the system to be quantum mechanical and calculate the average energy as a function of temperature.

c. Show that your answer in part (b) goes to your answer in part (a) in the limit of high temperature. Evaluate your answer in part (b) at zero temperature.

SOLUTION Stat Mech #2 1998

(a) The potential energy is $V(x) = V_0(x) + W(x)$, where $V_0 = \frac{1}{2}kx^2$ is the potential of a linear spring, and $W(x)$ represents the potential of the wall which is infinite for $X < 0$ and zero otherwise. The average energy is the sum of the kinetic and potential energy. By the equipartition theorem, the kinetic energy is $K_BT/2$. The average of the potential energy is

$$\frac{\int_0^\infty e^{-\beta V_0(x)} V_0(x) dx}{\int_0^\infty e^{-\beta V_0(x)} dx}$$

By symmetry we can change the limits so as to go from $-\infty$ to ∞. This is identical to the average potential energy of a spring without a wall, which by the equipartition theorem is $k_BT/2$. Thus the sum of the kinetic and potential energies yields k_BT.

(b) The quantum problem with a wall is like the problem without a wall except that the boundary condition at zero is different. We require that the wave function at the wall is zero. Without the wall, the energy is $E_n = \hbar\omega_0(n + \frac{1}{2})$. $\omega_0 = \sqrt{k/m}$ is the oscillation frequency. With the wall, the even n solutions are not allowed since they violate the boundary condition at zero. However the odd n solutions are allowed. Therefore

$$E_n = \hbar\omega_0(\frac{1}{2} + 1 + 2n).$$

for $n = 0, 1, 2, \ldots$. This can be rewritten as

$$E_n = \hbar\omega_2 n + E_0.$$

where $\omega_2 = 2\omega_0 = 2\sqrt{k/m}$, and $E_0 = \frac{3}{2}\omega_0$. The average energy

$$\langle E \rangle = E_0 + \hbar\omega_2 \langle n \rangle$$

The term $\langle n \rangle$ is identical to the average occupation of bosons at energy $\hbar\omega_2$ (with zero chemical potential). This is the Bose-Einstein distribution

$$\langle n \rangle = \frac{1}{e^{\beta\hbar\omega_2} - 1}$$

Therefore

$$\langle E \rangle = E_0 + \frac{\hbar\omega_2}{e^{\beta\hbar\omega_2} - 1}$$

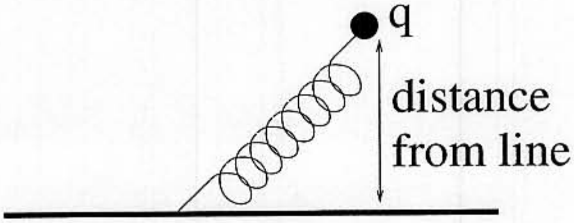
(c) At high temperatures, $\beta \to 0$ so that

$$e^{\beta\hbar\omega_2} - 1 \approx \beta\hbar\omega_2$$

Substituting this into the answer for (b) and ignoring the zero point energy term, which is negligible, we obtain $\langle E \rangle \to k_BT$ as $k_BT \to \infty$. When $T = 0$ we have the zero point energy $E_0 = \frac{3}{2}\omega_0$.

STATISTICAL MECHANICS

3. Consider an infinite line charge with charge per unit length λ, which can either be positive or negative. One end of a massless linear spring is attached to it, and the other side has a charge q and mass m. Call the spring constant k, and treat this system classically at finite temperature T.



a. Write down the partition function for this system.
b. Calculate the average distance between the charge and the line as a function of T and λ.
c. Find the region in the λ-T plane where this average value is zero.

SOLUTION Stat Mech #3 1998

(a) The potential energy of the spring is $U_{sp}(\mathbf{r}) = \frac{1}{2}kr^2$. The potential energy of the line charge can be calculated from the electric field which in turn can be obtained from Gauss's law: $2\pi rE \;=\; \lambda/\epsilon_0$ (SI units). Therefore $E = \lambda/2\pi\epsilon_0 r$. Since $\mathbf{E} = -\nabla V$ The electric potential energy is

$$U_{el} = qV = -\frac{q\lambda}{2\pi\epsilon_0}\ln r.$$

Adding these two energies together

$$Z = \int_0^\infty e^{-(\frac{1}{2}k(r^2+z^2)-\frac{q\lambda}{2\pi\epsilon_0}\ln r)/T}2\pi r dr dz \int e^{-(\frac{1}{2}m(v_x^2+v_y^2+v_z^2)/T}dv_x dv_y dv_z$$

(b) The average value of r is

$$\langle r\rangle \;=\; \frac{\int e^{-H/T}r2\pi r dr dz dv_x dv_y dv_z}{\int e^{-H/T}2\pi r dr dz dv_x dv_y dv_z}$$

The velocities and z integrals cancel leaving

$$\langle r\rangle \;=\; \frac{\int_0^\infty e^{-(\frac{1}{2}k(r^2+z^2)-\frac{q\lambda}{2\pi\epsilon_0}\ln r)/T}r^2 dr}{\int_0^\infty e^{-(\frac{1}{2}k(r^2+z^2)-\frac{q\lambda}{2\pi\epsilon_0}\ln r)/T}r dr}$$

Let $u \equiv \frac{1}{2T}kr^2$ and define $K \equiv \frac{q\lambda}{2\pi\epsilon_0 T}$. Then $rdr = \frac{1}{2}d(r^2) = \frac{T}{k}du$. Simplifying,

$$\langle r\rangle \;=\; \sqrt{\frac{2T}{k}}\frac{\int_0^\infty e^{-(u-K\ln r)}\sqrt{u}du}{\int_0^\infty e^{-(u-K\ln r)}du}$$

which can be expressed as

$$\frac{\sqrt{\frac{2T}{k}}\int_0^\infty e^{-(u-\frac{K}{2}\ln u)}\sqrt{u}du}{\int_0^\infty e^{-(u-\frac{K}{2}\ln u)}du} \;=\; \sqrt{\frac{2T}{k}}\frac{\int_0^\infty e^{-u}u^{\frac{(K+1)}{2}}}{\int_0^\infty e^{-u}u^{\frac{K}{2}}}$$

This can be written in terms of Gamma functions

$$\sqrt{\frac{2T}{k}}\frac{\Gamma(\frac{K}{2}+\frac{3}{2})}{\Gamma(\frac{K}{2}+1)}$$

(c) For sufficiently strong attractive forces, the denominator diverges. The divergence occurs when $u^{K/2}$ diverges faster than u^{-1}, or when $K < -2$. Therefore the region in parameter-space where the the average is zero is

$$\frac{q\lambda}{2\pi\epsilon_0 T} < -2$$

1999

Statistical Mechanics
(do 2 out of 3 problems)

Please do **EACH** problem you attempt on a **SEPARATE** paper.
Put your name on each paper.

STATISTICAL MECHANICS - 1

1. Consider an infinite one-dimensional chain of ferromagnetic Ising spins. Each spin has the value $S = \pm 1$ and interacts only with its immediate neighbors with interaction strength $J > 0$ and the Hamiltonian $H = -J \sum_{<ij>} S_i S_j$.

a. Find the exact partition function of this system.

b. Find the energy of this system as a function of temperature and sketch the result.

c. Find the specific heat of this system as a function of temperature and sketch the result.

d. Does this system have long range order at finite temperature? How do you know this from your solution?

SM#1(1)

Qual Problem #1

$$S_i = \pm 1 \qquad \mathcal{H} = -J \underset{\langle ij \rangle}{\sum} S_i S_j$$

nearest neighbors

$$Z = \underset{\substack{\text{all} \\ \text{possible} \\ \text{spin} \\ \text{config}}}{\sum} e^{J\beta \sum_{\langle ij \rangle} S_i S_j}$$

enumerate possibilities

$\cdots + S_1 S_2 + S_2 S_3 + \cdots$ each bond acts like spin

1 1	1 1	1 1
1 -1	-1 1	-1 -1
-1 1	1 1	
-1 -1	-1 1	-1 1
-1 1	1 -1	1 -1
-1 -1	-1 -1	-1 -1
1 1	1 -1	1 1
1 -1	-1 -1	1 -1
		-1 1

each occurs twice

let $z_1 = e^{J\beta} + e^{-J\beta} = 2\cosh J\beta$

$$Z = 2\left(2\cosh J\beta\right)^N = 2\left(2\cosh J\beta\right)^N$$

for $N \to \infty$

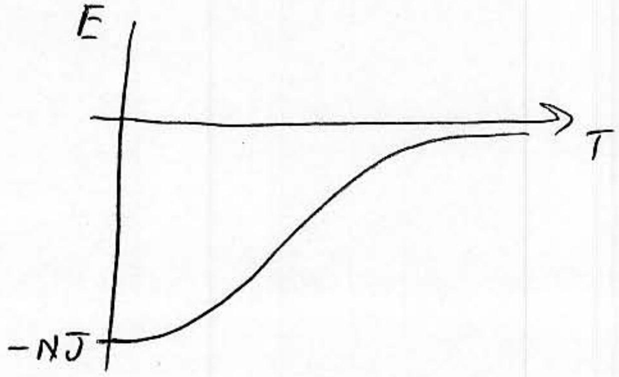
$$Z \approx \left(2\cosh J\beta\right)^N = \left(e^{J\beta} + e^{-J\beta}\right)^N$$

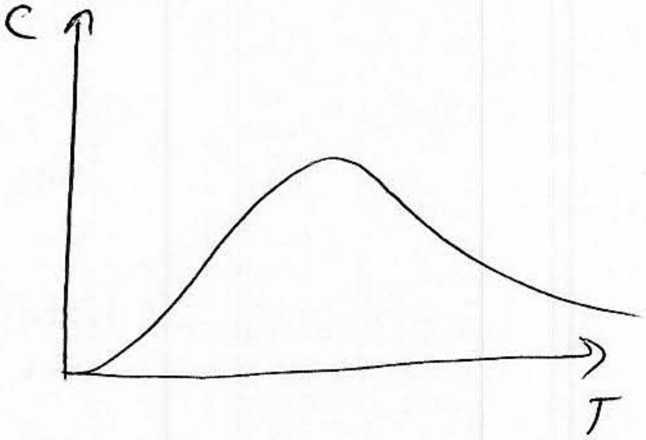
$$E = -\frac{\partial}{\partial\beta} \ln Z = \frac{-JN\left(e^{J\beta} + e^{-J\beta}\right)^{N-1}\left(e^{J\beta} - e^{-J\beta}\right)}{\left(e^{J\beta} + e^{-J\beta}\right)^N}$$

SM#1(2)

$$E = -JN \tanh(J\beta)$$

$$C = -k\beta^2 \frac{\partial E}{\partial \beta} = Nk\left(\frac{J}{kT}\right)^2 \operatorname{sech}^2\left(\frac{J}{kT}\right)$$





there is no singular behavior, so there is no long range order transition

2. Consider a crystal that is formed of two elements, A and B, and has the chemical formula AB_2 [eg, $SrCl_2$]. In this crystal there are N_A A sites and N_B B sites; $N_B = 2\,N_A$. The Gibbs free energy is given by $G = G_0 + U_A n_A + U_B n_B - ST$ for this case.

a. Consider vacancies on both the A and B sites. For this problem assume no other defects are present. The energy to form an A site vacancy is u_A and to form a B site vacancy, u_B. Let there be n_A vacancies on A sites and n_B vacancies on B sites. Write down the Gibbs free energy in terms of the configurational entropy and caculate the equilibrium value of n_A and n_B for a given value of temperature T. What is the ratio n_A/n_B?

b. Next consider only site-antisite disorder in which pairs of atoms are on the opposite site. (Neglect other defects here). Let u_{ex} be the energy to interchange an A and B atom. Let n_b be the number of B atoms on A sites and n_a be the number of A atoms on B sites. ($n_a = n_b = n$). Again use the Gibbs free energy to calculate the equilibrium number of site-antisite defects [ie calculate n] at a temperature T. Assume $n << N_A$ or N_B.

SM#2(1)

Solution.

a) $G = G_0 + u_A n_a + u_B n_b - ST$

$S = k_B \ln W \quad ; \quad W = \frac{N_A!}{(N_A-n_a)!\, n_a!} \frac{N_B!}{(N_B-n_b)!\, n_b!}$

use Stirlings approx $\ln N! = n \log N - N$.

$S = k_B \{ \ln(N_A!\, N_B!) - \ln(N_A-n_a)! - \ln n_a! - \ln(N_B-n_b)! - \ln n_b! \}$

Require $\frac{\partial G}{\partial n_a} = \frac{\partial G}{\partial n_b} = 0$.

$\frac{\partial G}{\partial n_a} = u_A - k_BT \frac{\partial}{\partial n_a} \{ -(N_A-n_a)\ln(N_A-n_a) + (N_a-n_a) - n_a \ln(n_a) + n_a \}$

$0 = u_A - k_BT \left[\ln(N_A-n_a) - \cancel{\frac{N_A-n_a}{N_A-n_a}(-1)} \cancel{-1} - \ln n_a - \cancel{n_a}/n_a + \cancel{1} \right]$

$-\frac{u_A}{k_BT} = \ln \frac{n_a}{N_A-n_a} \Rightarrow n_a = (N_A-n_a)\, e^{-u_A/kT}$

$n_a = N_A/(1+e^{+u_A/kT})$

n_b is similar

$n_b = (N_B-n_b)\, e^{-u_B/kT}$

$n_b = \frac{N_b}{1+e^{u_B/kT}}$

$\frac{n_a}{n_b} = \underset{\overset{\shortparallel}{1/2.}}{\frac{N_A}{N_B}} \frac{1+e^{u_B/kT}}{1+e^{u_A/kT}}$

If $u/kT \gg 1$, $\frac{n_a}{n_b} \simeq 1/2\, e^{(u_B-u_A)/kT}$

SM#2(2)

Solutions cont'd.

b) Site - antisite.

$$W = \frac{N_A!}{(N_A - n_B)!\, n_B!} \quad \frac{N_B!}{(N_B - n_A)!\, n_A!}$$

with $n_B = n_A \underset{2}{=} n$,

$$W = \frac{N_A!\, N_B!}{(N_A - n)!\, n!\, (N_B - n)!\, n!}$$

$$G = G_0 + U_{ex}\, n - k_BT \ln W.$$

$$\frac{\partial G}{\partial n} = U_{ex} - k_BT \frac{\partial}{\partial n}\left\{ -\ln (N_A - n)!\ 2\ln n! - \ln (N_B - n)! \right\}$$

$$0 = U_{ex} + k_BT \frac{\partial}{\partial n}\left\{ (N_A - n)\ln(N_A - n) - (N_A - n) + 2(n \ln n - n) + (N_B - n)\ln(N_B - n) - (N_B - n) \right\}$$

$$0 = U_{ex} + k_BT\Big[-\ln(N_A - n) - \cancel{\frac{N_A - n}{N_A - n}} \cancel{+1} + 2\ln n + \cancel{2} - \cancel{2}$$

$$- \ln(N_B - n) \cancel{-1} + \cancel{1} \Big]$$

$$-\frac{U_{ex}}{k_BT} = \ln \frac{n^2}{(N_A - n)(N_B - n)}$$

For n small ($n << N_A, N_B$)

$$n^2 \simeq N_A N_B\, e^{-U_{ex}/k_BT}$$

$$n = \sqrt{N_A N_B}\ e^{-\frac{U_{ex}}{2k_BT}} = \sqrt{2}\, N_A\, e^{-\frac{U_{ex}}{2k_BT}} \quad (N_B = 2N_A).$$

3. If the energy stored in the rotational and vibrational modes is not too large, we may approximate the Hamiltonian of a diatomic molecule by

$$\mathcal{H} = \mathcal{H}_{transl} + \mathcal{H}_{rot} + \mathcal{H}_{vib}$$

neglecting any effect of the rotation on the vibrational modes and the effect of the vibrational distortions on the moment of inertia, I. In a dilute gas, the density of will be low enough so that the translational motion can be treated classically. The energy of rotation is:

$$E_j = \frac{\hbar^2 j(j+1)}{2I}$$

where $j = 0, 1, 2 \ldots$ is the rotational quantum number. The state with quantum number j has degeneracy $2j+1$ (we have, for simplicity, assumed that the two atoms in the diatomic molecule are different). The vibrational degree of freedom may be taken to be that of a simple harmonic oscillator with frequency ω_v.

a. Find a general expression for the energy at temperature T.

b. Determine the energy and specific heat for the following cases:

(i) $T \ll \theta_r \ll \theta_v$

(ii) $\theta_r \ll T \ll \theta_v$

(iii) $\theta_r \ll \theta_v \ll T$.

where

$$\theta_r \equiv \frac{\hbar^2}{2Ik_B}, \qquad \theta_v \equiv \frac{\hbar\omega_v}{k_B}\ .$$

Hint: The Euler summation formula,

$$\sum_{n=0}^{\infty} f(n) = \int_0^{\infty} f(x)dx + \frac{1}{2}f(0) - \frac{1}{12}f'(0) + \ldots$$

may be useful.

c. Show that the specific heat per molecule is approximately $\frac{3}{2}k_B$, $\frac{5}{2}k_B$, and $\frac{7}{2}k_B$ respectively in the three ranges.

Statistical Mechanics Questions

Solutions

1/(a) The free energy (and hence the energy and specific heat is a sum of three terms

$$f = f_{trans} + f_{vib} + f_{rot}$$

where f is the free energy per molecule. Hence

$$\underset{\substack{\uparrow \\ \text{energy/mol}}}{u} = -\frac{\partial}{\partial\beta}(\beta f), \qquad \underset{\substack{\uparrow \\ \text{specific heat/mol.}}}{C} = \frac{\partial u}{\partial T} \qquad (u = u_{trans} + u_{vib} + u_{rot}, \text{ etc.}$$

By equipartition the translational part of the energy is $u_{trans} = \frac{3}{2}k_B T$, so $C_{trans} = \frac{3}{2}k_B$ in all 3 regions.

For the vibrational part

$$Z_{vib} = e^{-\frac{1}{2}\beta\hbar\omega_v}\sum_{n=0}^{\infty} e^{-n\beta\hbar\omega_v} = \frac{e^{-\frac{1}{2}\theta_v/T}}{1-e^{-\theta_v/T}} = \frac{1}{2\sinh(\theta_v/2T)}$$

$$u_{vib} = -\frac{\partial}{\partial\beta}\ln Z_{vib} \ast \quad \text{so} \quad \frac{u_{vib}}{k_B} = \frac{\theta_v}{2}\coth\left(\frac{\theta_v}{2T}\right)$$

For the rotational part

$$Z_{rot} = \sum_{j=0}^{\infty}(2j+1)e^{-\hbar^2 j(j+1)/(2k_B T I)} = \sum_{j=0}^{\infty}(2j+1)e^{-j(j+1)\theta_r/T}$$

$$u_{rot} = -\frac{\partial}{\partial\beta}\ln Z_{rot}.$$

(b) (i) $T \ll \theta_{rot} \ll \theta_{vib}$

$$\frac{u_{vib}}{k_B} = \frac{\theta_v}{2}\left(1 + 2e^{-\theta_v/T}\cdots\right),$$ ∴ C_{vib} is exponentially small

$$Z_{rot} = 1 + 3e^{-2\theta_r/T}, \quad u_{rot} = 6k_B\theta_r e^{-2\theta_r/T}$$

∴ u_{rot} and C_{rot} are exponentially small.

∴ $C = \frac{3}{2}k_B$ (+ exponentially small corrections) per molecule

1 (b)(ii). U_{trans} and U_{vib} are same as in (i).

For the rotational motion, use the Euler formula

$$Z_{rot} = \int_0^{\infty} dj\,(2j+1)\,e^{-j(j+1)\theta_r/T} + \frac{1}{2} - \frac{2}{6} + O\left(\frac{\theta_r}{T}\right)$$

$$= \frac{T}{\theta_r} + \overset{\text{const}}{[illegible]} + O(\theta_r/T)$$

$$U_{rot} = k_B\left(T - \overset{\text{const.}}{\theta_r} + O\left(\frac{1}{T}\right)\right) \qquad \underline{C_{rot}} = k_B\left[1 + O\left(\frac{\theta_r}{T}\right)^2\right]$$

Hence $\underline{C = \frac{5}{2}k_B.}$

b(iii) U_{trans} and U_{rot} are the same as in (ii)

$$U_{vib} = \frac{\theta_v k_B}{2}\left[\frac{2T}{\theta_v} + \frac{1}{3}\frac{1}{2}\left(\frac{\theta_v}{2T}\right) + \dots\right] = k_B\left[T + O\left(\frac{\theta_v}{T}\right)^2\right]$$

$$\therefore \underline{C_{vib} = k_B}\left[1 + O\left(\theta_v/T\right)^2\right]$$

Hence $\underline{C = \frac{7}{2}k_B.}$

2000

Statistical Mechanics
(do 2 out of 3 problems)

Please do **EACH** problem you attempt on a **SEPARATE** paper.
Put your name on each paper.

Put your name, section name and problem # on each sheet you turn in.
Do only two problems. Do not do all three problems.

STATISTICAL MECHANICS - 1

1. Consider an intrinsic semiconductor with a filled valence band and an empty conduction band at $T = 0$. As T increases, some of the electrons will be thermally excited across the gap, $E_G = \epsilon_c - \epsilon_v$, where ϵ_c is the bottom of the conduction band and ϵ_v is the top of the valence band. Treat the valence band as a hole-band. Assume parabolic energy bands such that the density of states for electrons is

$$g_e(\epsilon) = C_e(\epsilon - \epsilon_c)^{1/2} \quad C_e = \frac{1}{2\pi^2}(\frac{2m_e}{\hbar^2})^{3/2}$$

$$g_h(\epsilon) = C_h(\epsilon_v - \epsilon)^{1/2} \quad C_h = \frac{1}{2\pi^2}(\frac{2m_h}{\hbar^2})^{3/2}$$

where m_e and m_h are the electron and hole effective masses.

a. Using Fermi-Dirac statistics, give equations for the number of electrons in the conduction band, n_o, and the number of holes, p_o, in the valence band. Leave as integrals, but write the integrals in terms of a dimensionless variable (Hint: remove the T-dependence).

b. Set $n_o = p_o$ to determine an equation for the chemical potential (Fermi energy ϵ_f) as a function of T.

c. In the non-degenerate case (ϵ_f is in the gap between bands),

$$f(\epsilon) \approx e^{\epsilon_f/kT}e^{-\epsilon/kT}.$$

Using this expression, show

$$n_o \approx N_c e^{\frac{\epsilon_f - \epsilon_c}{kT}}; p_o = N_v e^{-\frac{\epsilon_v - \epsilon_f}{kT}},$$

where

$$N_c = 2(\frac{m_e kT}{2\hbar^2\pi})^{3/2}; N_v = 2(\frac{m_h kT}{2\hbar^2\pi})^{3/2}.$$

(Note $\int_0^\infty y^{1/2}e^{-y}dy = \frac{1}{\sqrt{\pi}}$.)

d. Use equations in part (c) above to show

$$\epsilon_f = \frac{1}{2}(\epsilon_v + \epsilon_c) + \frac{3}{2}kT\ell n(m_h/m_e).$$

Statistical

SM#1

Detailed Balance in intrinsic semiconductors.
Consider an intrinsic semiconductor with a filled valence band and an empty conduction band at $T=0$. As T increases, some of the electrons will be thermally excited across the gap $\mathcal{E}_G = \mathcal{E}_c - \mathcal{E}_v$ where $\mathcal{E}_c$ is the bottom of the conduction band & $\mathcal{E}_v$ is the top of the valence band. Treat the valence band as a hole-band. Assume parabolic energy bands such that the density of states for electrons is

$$g_e(\mathcal{E}) = C_e\,(\mathcal{E}-\mathcal{E}_c)^{1/2} \qquad C_e = \frac{1}{2\pi^2}\left(\frac{2m_e}{\hbar^2}\right)^{3/2}$$

$$g_h(\mathcal{E}) = C_h\,(\mathcal{E}_v-\mathcal{E})^{1/2}. \qquad C_h = \frac{1}{2\pi^2}\left(\frac{2m_h}{\hbar}\right)^{3/2}$$

where m_e & m_h are the electron & hole effective masses.

a) Using Fermi Dirac statistics, ~~write~~ give equations for the number of electrons in the conduction band n_0 & the number of holes p_0 in the valence band. Leave as integrals, but write integral in terms of a dimensionless ~~parameter~~ variable (Hint remove T dep.)

b) Set $n_0 = p_0$ to determine an equation for the chemical potential (Fermi energy $\mathcal{E}_f$) as a function of T.

c) In non-degenerate case ($\mathcal{E}_f$ is in gap between bands) $f(\mathcal{E}) \simeq e^{+\mathcal{E}_f/kT}\, e^{-\mathcal{E}/kT}$. Using this expression show

$$n_0 \cong N_c\, e^{\frac{(\mathcal{E}_f-\mathcal{E}_c)}{kT}} \;,\; p_0 = N_v\, e^{-\frac{(\mathcal{E}_v-\mathcal{E}_f)}{kT}}$$

where $N_c = 2\left(m_e kT/2\hbar^2\pi\right)^{3/2}$; $N_v = 2\left(m_h kT/2\hbar^2\pi\right)^{3/2}$

[Note $\int_0^\infty y^{1/2} e^{-y}\, dy = 2/\sqrt{\pi}$] [but don't need it]

d) Solve equations in c) above to show

$$\varepsilon_F = 1/2\,(\varepsilon_v + \varepsilon_c) + 3/2 \ln\left(m_h/m_e\right)$$

SM#1

Solution

a) Number of carriers $= \int g(\mathcal{E}) f(\mathcal{E})\, d\mathcal{E}$ in general

Conduction band

$$n_0 = \int_{\mathcal{E}_c}^{\infty} g_c\, f(\mathcal{E})\, d\mathcal{E} = C_c \int (\mathcal{E}-\mathcal{E}_c)^{1/2} f(\mathcal{E})\, d\mathcal{E}$$

$$= C_c (kT)^{3/2} \int_{\mathcal{E}_c/kT} \left(\frac{\mathcal{E}-\mathcal{E}_c}{kT}\right)^{1/2} \frac{1}{1+e^{(\mathcal{E}-\mathcal{E}_F)/kT}} \frac{d\mathcal{E}}{kT}$$

$$= C_c (kT)^{3/2} \int_0^{\infty} y^{1/2} \frac{1}{1+e^{y-\eta_0}}\, dy \qquad \eta_0 = \frac{\mathcal{E}_c-\mathcal{E}}{kT}$$

For valence band

$$p = \#\text{ of empty states} = \int_{-\infty}^{\mathcal{E}_v} \underset{\uparrow \text{ holes}}{g_v(\mathcal{E})} \underset{\uparrow \text{ electrons}}{\overset{\text{holes}}{\overbrace{[1-f(\mathcal{E})]}}}\, d\mathcal{E}$$

If we rewrite in terms of holes, with $\mathcal{E}$ measured from top of valence band, and note

$$1-f(\mathcal{E}) = \frac{e^{+(\mathcal{E}-\mathcal{E}_F)/kT}}{1+e^{+(\mathcal{E}-\mathcal{E}_F)/kT}} = \frac{1}{1+e^{-(\mathcal{E}-\mathcal{E}_F)/kT}}$$

$$= \frac{1}{1+e^{+(\mathcal{E}_F-\mathcal{E})/kT}}$$

$$p_0 = C_h (kT)^{3/2} \int_0^{\infty} y^{1/2} \frac{1}{1+e^{y-\eta_0'}}\, dy \qquad \eta_0' = \frac{\mathcal{E}_v-\mathcal{E}_F}{kT}$$

b) $n_0 = p_0 \Rightarrow$

$$C_c (kT)^{3/2} \int_0^{\infty} y^{1/2} \frac{1}{1+e^{y-\eta_0}}\, dy = C_h (kT)^{3/2} \int y^{1/2} \frac{1}{1+e^{y-\eta_0'}}\, d$$

Need to solve integrals in terms of η_0 + η_0' to get $\mathcal{E}_F$

SH#1

c) The non-degenerate case

$$\frac{1}{1+e^{y-y_0'}} \approx e^{-y} e^{y_0'}$$

Then equation [illegible] becomes

$$C_e (kT)^{3/2} e^{+y_0} \int_0^\infty y^{1/2} e^{-y} \, dy = C_h (kT)^{3/2} e^{+y_0'} \int_0^\infty y^{1/2} e^{-y} \, dy$$

$$\Rightarrow \frac{C_e}{C_h} = \left(\frac{m_e}{m_h}\right)^{3/2} = e^{-\frac{(\mathcal{E}_F-\mathcal{E}_c)}{kT}} e^{\frac{(\mathcal{E}_v-\mathcal{E}_c)}{kT}}$$

$$\cong e^{-\frac{2\mathcal{E}_F}{kT}} e^{\frac{\mathcal{E}_c+\mathcal{E}_v}{kT}}$$

Take logs

$$\frac{2\mathcal{E}_F}{kT} = \frac{\mathcal{E}_c+\mathcal{E}_v}{kT} + \frac{3}{2}\ln\left(\frac{m_h}{m_e}\right)$$

$$\mathcal{E}_F = \frac{\mathcal{E}_c+\mathcal{E}_v}{2} + \frac{3}{2} kT \ln\left(m_h/m_e\right)$$

STATISTICAL MECHANICS - 2

2. Two particles slide on a ring of radius R. The potential energy between them is

$$U = U_0 \log(\theta)$$

where U_0 is a constant and θ is the angle subtended by the first particle, the center of the ring and the second particle. The masses of the two particles are m_1 and m_2 respectively. Treat this system classically. The system is in contact with a heat bath of temperature T.

a. Write down the partition function for the system.

b. Calculate the free energy, F, as a function of temperature.

c. Calculate the energy, as a function of temperature.

d. At what temperature is there a singularity in F?

SM #2
Solution

STATISTICAL MECHANICS - 2

2. 1. Two particles slide on a ring of radius R. The potential energy between them is

$$U = U_0 \log(\theta)$$

where U_0 is a constant and θ is the angle subtended by the first particle, the center of the ring and the second particle. The masses of the two particles are m_1 and m_2 respectively.

Treat this system classically. The system is in contact with a heat bath of temperature T.

description

[(a)] Write down the partition function for the system.

Angular momentum L, and θ are canonically conjugate.

$$Z = \int_{-\infty}^{\infty} dL_1 \int_{-\infty}^{\infty} dL_2 \int_{-\pi}^{\pi} d\theta_1 \int_{-\pi}^{\pi} d\theta_2 e^{-H/k_B T}$$

where

$$H = \frac{1}{2}(\frac{L_1^2}{m_1 R^2} + \frac{L_2^2}{m_2 R^2}) + U_0 \log(\ min(|2\pi - |\theta_1 - \theta_2||, |\theta_1 - \theta_2|)$$

[(b)] Calculate the free energy, F, as a function of temperature.

Separate the kinetic and potential terms $Z \equiv Z_K Z_U$, we have

$$Z_K = \sqrt{2\pi T m_1 R^2}\sqrt{2\pi T m_2 R^2} = 2\pi T R^2 \sqrt{m_1 m_2}$$

Since the system has rotational invariance, we can fix particle 1 to $\theta_1 = 0$ and let θ_2 range from $-\pi$ to π. Then the integration over θ_1 gives just a factor of 2π.

$$Z_U = 2\pi \int_{-\pi}^{\pi} e^{-U_0 \log(|\theta|)/k_B T} = 4\pi \int_0^{\pi} \theta^{-U_0/k_B T} d\theta$$

integration is only defined for $U_0/k_B T \ < \ 1$

$$\frac{4\pi}{1 - U_0/k_B T} \pi^{1 - U_0/k_B T}$$

The free energy $F = -k_B T \log Z$

[(c)] Calculate the energy, as a function of temperature.

The energy E is related to the partition function through

$$E = -\frac{\partial \log Z}{\partial \beta}$$

SM#2

with $\beta = 1/k_BT$.

From above, the energy is the sum of a kinetic and a potential part. The kinetic part by the equipartition theorem gives a contribution to the energy of $E_K \;=\; 2k_BT/2 = k_BT$. The potential part is

$$E_U \;=\; -\frac{\partial}{\partial\beta}(-\log(1-U_0\beta)(1-U_0\beta)\log\pi \;=\; U_0(\frac{1}{U_0\beta-1} \;+\; \log\pi)$$

[(d)] At what temperature is there a singularity in F?

From (c) this happens when $U_0/k_BT = 1$ or

$$T = U_0/k_B.$$

STATISTICAL MECHANICS - 3

3. Consider the following Landau expansion for the free energy of a material undergoing a phase transition with order parameter m:

$$F(m) = a(T) + \frac{b(T)}{2}m^2 + \frac{c}{4}m^4 + \frac{d}{6}m^6 + ...,$$

where c and d are assumed independent of the temperature, $c < 0$, $d > 0$, and

$$b(T) = \alpha(T - T^\star).$$

a. Explan why the transition is first order (i.e. m vanishes discontinuously). Also explain why the transition is not at $T^\star$. Sketch the free energy versus m for different temperatures, one of which (clearly marked) should be at the transition temperature T_c and another should be at $T^\star$.

b. Determine the value of m as T approaches T_c from below.

c. Determine the latent heat of transition. Note: You are given that the energy U is related to the free energy by $U = \partial(\beta F)/\partial\beta$, where $\beta = 1/(k_B T)$.

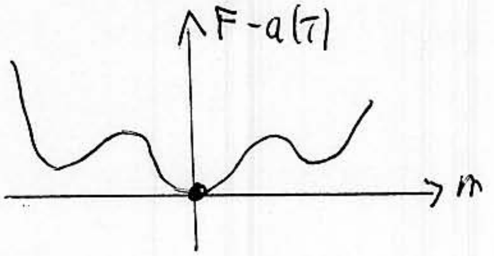
Statistical Mechanics (Solutions)

①

SM#3

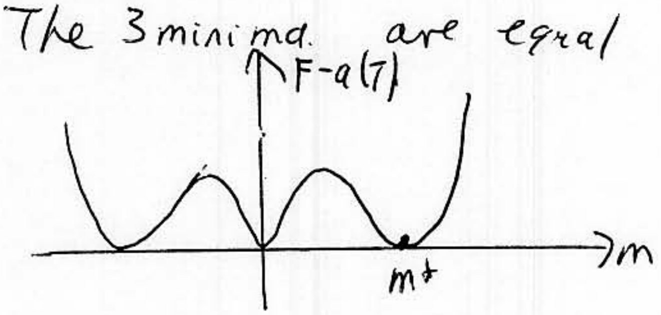
1) $F = a(T) + \frac{b(T)}{2} m^2 + \frac{c}{4} m^4 + \frac{d}{6} m^6$

(a) $T > T_c$

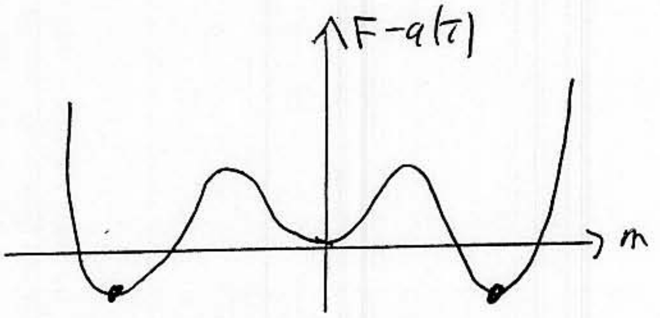


Need to find minimum of F $\Rightarrow$ $m = 0$

$T = T_c$ The 3 minima are equal

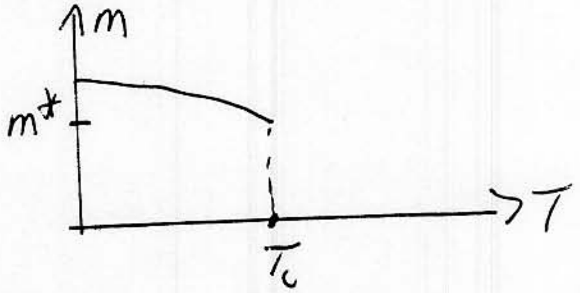


$T < T_c$



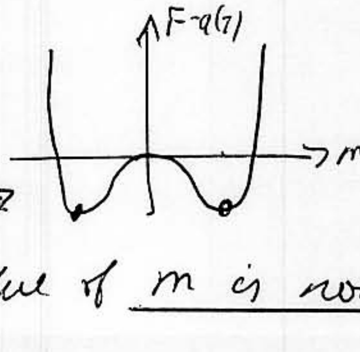
The sol^n with $m \neq 0$ are the equilibrium solution.

Hence



i.e Transition is discontinuous, (1st order)

Note at $T = T^*$ ~~we have~~ the coefficient of m^2 is zero so we have →



and the equilibrium value of m is non-zero

i.e. $T_c > T^*$

(b) ~~A~~ The equilibrium magnetization is given by $\frac{\partial E}{\partial m}=0$, i.e. <u>either</u> $m=0$

<u>or</u> $b + cm^2 + dm^4 = 0$ ①

In addition, at T_c, $\left.F-a(T)\right|_{h}^{=0}$ at the ~~non zero~~ solutions with non-zero m, i.e

$$\frac{b}{2}m^2 + \frac{c}{4}m^4 + \frac{d}{6}m^6 = 0$$

which, for $m \neq 0$, can be written

$$b + \frac{c}{2}m^2 + \frac{d}{3}m^3 = 0 \qquad ②$$

m^* is the simultaneous solution of ① and ②, i.e subtracting

$$\frac{c}{2}m^{*2} + \frac{2d}{3}m^{*4} = 0$$

Remembering that $c<0$ this gives

$$\underline{\underline{m^* = \sqrt{\frac{-3c}{4d}}}}$$

(c) The latent heat is the change in energy, ΔU, at the transition.

$$\text{Since } U = \frac{\partial}{\partial \beta}(\beta F) = F - \beta\frac{\partial F}{\partial \beta} = F + T\frac{\partial F}{\partial T}$$

$$\Delta U = \underbrace{\Delta F}_{=0} + T\frac{\partial}{\partial T}\Delta F = \underline{T_c \left.\frac{\partial}{\partial T}\Delta F\right|_{T_c}}$$

Now $\Delta F = \frac{b(T)}{2}m^2 + \frac{c}{4}m^4 + \frac{d}{6}m^6$ (at $T=T_c$)

so $$\frac{\partial}{\partial T}\Delta F = \frac{\alpha}{2}m^{*2} + \left.\frac{\partial m}{\partial T}\right|_{T_c}\Big(\underbrace{bm^* + cm^{*3} + dm^{*5}}_{=0 \text{ from } ①}\Big)$$

Hence $$\underline{\Delta U = \alpha T_c\left(\frac{-3c}{8d}\right)}$$

Legendre Polynomials

1. Generating function:

$$g(t,x) = (1 - 2xt + t^2)^{-1/2} = \sum_{n=0}^{\infty} P_n(x) t^n$$

2. Recursion relations

$$(2n+1)xP_n(x) = (n+1)P_{n+1}(x) + nP_{n-1}(x)$$

$$(1-x)^2 P_n''(x) - 2xP_n'(x) + n(n+1)P_n(x) = 0$$

3. Normalization

$$\int dx [P_n(x)]^2 = \frac{2}{2n+1}$$

Spherical Harmonics

1. $\ell = 0$:

$$Y_{00} = \frac{1}{\sqrt{4\pi}}$$

2. $\ell = 1$:

$$Y_{1,\pm 1} = \mp\sqrt{\frac{3}{8\pi}} \sin(\theta) e^{\pm i\phi} \qquad Y_{10} = \sqrt{\frac{3}{4\pi}} \cos(\theta)$$

2. Green's function:

$$\frac{1}{|\vec{x} - \vec{x}'|} = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{m=l} \frac{1}{2l+1} \frac{r_<^l}{r_>^{l+1}} Y^*_{lm}(\theta', \phi') Y_{lm}(\theta, \phi)$$

Bessel's Equation:

$$\frac{d^2R}{dx^2} + \frac{1}{x}\frac{dR}{dx} + (1 - \frac{\nu^2}{x^2})R = 0$$

Spherical Bessel Functions

$$j_\ell(kr) \to \frac{\sin(kr - \ell\pi/2)}{kr}$$

$$n_\ell(kr) \to -\frac{\cos(kr - \ell\pi/2)}{kr}$$

$$j_o(\rho) = \frac{\sin(\rho)}{\rho} \qquad n_o(\rho) = -\frac{\cos(\rho)}{\rho}$$

$$j_1(\rho) = \frac{\sin\rho}{\rho^2} - \frac{\cos(\rho)}{\rho}$$

Gamma Function

1. Integral Representation:

$$\Gamma(z) = \int_0^{\infty} dt e^{-t} t^{z-1}$$

2. Functional relation:

$$\Gamma(z+1) = z\Gamma(z)$$

3. Special values:

$$\Gamma(1) = 1 \qquad \Gamma(1/2) = \sqrt{\pi}$$

Zeta Function

1. Integral representations:

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

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

2. Special values:

$$\zeta(0) = -\frac{1}{2} \qquad \zeta(3/2) = 2.612 \qquad \zeta(2) = \frac{\pi^2}{6}$$

$$\zeta(5/2) = 1.341 \qquad \zeta(4) = \frac{\pi^4}{90}$$

Classical Mechanics

1. Euler-Lagrange equations:

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} = \frac{\partial L}{\partial q_i}$$

2. Force in a rotating frame:

$$\vec{F}_{eff} = \vec{F} - m\vec{a}_f - m\dot{\vec{\omega}} \times \vec{r} - m\vec{\omega} \times (\vec{\omega} \times \vec{r}) - 2m\vec{\omega} \times \vec{v}_r$$

where v_r is the velocity with respect to the rotating axes, a_f is the acceleration of the moving frame with respect to the fixed axes.

Quantum Mechanics

1. Harmonic Oscillator:

$$H = \hbar\omega(\frac{1}{2} + a^\dagger a)$$

$$a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle \qquad a|n\rangle = \sqrt{n}|n-1\rangle$$

2. Angular momentum:

$$J_\pm = J_1 \pm iJ_2 \qquad J_\pm|j\ m\rangle = \sqrt{j(j+1) - m(m\pm 1)}|j\ m-1\rangle$$

3. Spherically symmetric potentials:

$$\Psi_{Elm}(r,\theta,\phi) = R_{El}(r)Y_{lm}(\theta,\phi) = \frac{\rho_{El}(r)}{r}Y_{lm}$$

$$[-\frac{d^2}{dr^2} + \frac{2m}{\hbar^2}(V(r) + \frac{l(l+1)\hbar^2}{2mr^2} - E)]\rho_{El}(r) = 0$$

3. Partial Wave Expansion:

$$f(\theta) = \frac{1}{k}\sum_{\ell=0}^{\infty}(2\ell+1)e^{i\delta_\ell}\sin(\delta_\ell)P_\ell(\cos(\theta))$$

$$\sigma = \frac{4\pi}{k^2}\sum_{\ell=0}^{\infty}(2\ell+1)\sin^2\delta_\ell$$

For resonance,

$$\cot(\delta_n) = -(E - E_r)\frac{2}{\Gamma}$$

4. Born Approximation

$$f(\Omega) = -\frac{m}{e2\pi\hbar^2}\int d^3\vec{r}\,' e^{-i\vec{q}\cdot\vec{r}\,'}V(\vec{r}\,')$$

Useful Integrals

1.

$$\int \frac{x^2 dx}{(x^2+b^2)^{1/2}} = \frac{x}{2}\sqrt{x^2+b^2} - \frac{b^2}{2}\ln(x + \sqrt{x^2+b^2})$$

Electromagnetism

1. Energy density:

$$u = \frac{1}{8\pi}(\vec{E}^2 + \vec{B}^2)$$

2. Poynting vector

$$\vec{S} = \frac{c}{4\pi}(\vec{E} \times \vec{B})$$

3. Maxwell stress tensor:

$$T_{ij} = \frac{1}{4\pi}(E_iE_j + B_iB_j - \frac{1}{2}(\vec{E}^2 + \vec{B}^2)\delta_{ij})$$

4. Dipole moment

$$\vec{p} = \int d^3x\vec{x}\rho(\vec{x})$$

5. Quadrupole moment:

$$Q_{ij} = \int d^3x(3x_ix_j - r^2\delta_{ij})\rho(\vec{x})$$

Vector Analysis

1. Cross product

$$(\vec{A} \times \vec{B})_i = \epsilon_{ijk}A_jB_k$$

2. ϵ tensor:

$$\epsilon_{123} = 1, \epsilon_{213} = -1, \epsilon_{112} = 0, \text{etc.}$$

$$\epsilon_{ijk}\epsilon_{ilm} = \delta_{jl}\delta_{km} - \delta_{jm}\delta_{kl}$$

2001

Statistical Mechanics

(Turn in 2 out of 3 problems.)

Do **each problem on SEPARATE** paper.
Write your **NAME, SECTION, PROBLEM #** on each sheet you turn in.
Turn in **ONLY two problems**. Do not turn in all three problems.

Qualifying Exam Copy Disclaimer:

Solutions are submitted at an early stage in the Written Qualifying Exam preparation process. No effort is made to update solutions. Some questions may have been changed since the solution was written. Solutions may contain errors, inaccuracies and/or omissions. Use them cautiously.

If similar or related questions appear on any exam, errors, inaccuracies and/or omissions in these materials will not be cause for any change in score or outcome.

STATISTICAL MECHANICS - 1

1. A gas of molecules at temperature T has a density of n molecules per unit volume, which is low enough to treat the molecules as almost non-interacting. Each molecule has a dipole moment of magnitude p that can point in any direction. Calculate the dipole moment per unit volume as a function of p, the electric field E, and T. Treat the system classically.

Hint: The energy of a dipole in a field is $U = -\vec{p} \cdot \vec{E}$.

SM1 1/1

Problems

1. A gas of molecules at temperature T has a density of n molecules per unit volume, which is low enough to treat the molecules as almost non-interacting. Each molecule has a dipole moment of magnitude p that can point in any direction. Calculate the dipole moment per unit volume as a function of p, E, and T. Treat the system classically

Hint: The energy of a dipole in a field is $U = -\mathbf{p} \cdot \mathbf{E}$.

Solution

$\mathbf{p}$ aligns with the field in the direction of the field. It's magnitude is $< U > /E$. Take E in the z direction.

$$< U >= \frac{\int d\phi \int d\cos(\theta) \exp(-\beta Ep\cos(\theta)) Ep\cos(\theta)}{\int d\phi \int d\cos(\theta) \exp(-\beta Ep\cos(\theta))}$$

Where $U = Ep\cos(\theta)$

So we calculate

$$Z \equiv \int d\cos(\theta) \exp(-\beta Ep\cos(\theta)) \;\propto\; \int_{-pE}^{pE} dU \exp(-\beta U)$$

and note that

$$< U >= \frac{\partial \ln Z}{\partial \beta}$$

Integrating we obtain

$$Z = \frac{1}{\beta}\sinh(\beta pE)$$

Therefore

$$< U >= pE\frac{\cosh(\beta pE)}{\sinh(\beta pE)} - \frac{1}{\beta} \;=\; pE\coth(\beta pE) - \frac{1}{\beta}$$

So that the dipole moment per unit volume is $n < U > /E >$ which is

$$N(p\coth(\beta pE) - \frac{1}{\beta E})$$

2. Consider a ferromagnet, which for long wavelengths has a continuous dispersion $\epsilon(\vec{k}) = \alpha k^2$, where $\vec{k}$ is the reciprocal wave vector for magnons.

a. Calculate the specific heat for a three dimensional ($d = 3$) system valid at low temperatures where the dispersion relation above holds.

b. Do the same for $d = 2$.

c. Show that for the same number of spins, the $d = 2$ system will have a larger specific heat than the $d = 3$ system as $T \to 0$, according to the answers obtained in parts a and b above.

d. Very briefly explain why does this not make sense and what is wrong with our assumptions that produce this result.

Problem #2 Solution

a) $D(k) = \frac{V}{(2\pi)^3} 4\pi k^2 dk = \frac{V}{2\pi^2} k^2 dk$

$$U_3 = \frac{V}{2\pi^2} \int_0^\infty \frac{k^2 \epsilon(k)}{e^{\beta \epsilon(k)} - 1} dk = \frac{V\alpha}{2\pi^2} \int_0^\infty \frac{k^4\, dk}{e^{\alpha\beta k^2} - 1}$$

let $z = (\alpha\beta)^{1/2} k \qquad dk = (\alpha\beta)^{-1/2} dz \qquad k^2 = (\alpha\beta)^{-1} z^2$

$$U_3 = \frac{V\alpha}{2\pi^2} (\alpha\beta)^{-5/2} \int_0^\infty \frac{z^4}{e^{z^2} - 1} dz$$

$$U_3 = \frac{V (kT)^{5/2}}{2\pi^2 \alpha^{3/2}} \int_0^\infty \frac{z^4}{e^{z^2} - 1} dz = D T^{5/2}$$

where D = const

$$C_3 = \tfrac{5}{2} D T^{3/2}$$

b) $D(k) = \frac{A}{(2\pi)^2} 2\pi k\, dk = \frac{A}{2\pi} k\, dk$

$$U_2 = \frac{A\alpha}{2\pi} \int_0^\infty \frac{k^3\, dk}{e^{\alpha\beta k^2} - 1} = \frac{A\alpha}{2\pi} (\alpha\beta)^{-2} \int_0^\infty \frac{z^3 dz}{e^{z^2} - 1}$$

$$U_2 = \frac{A (kT)^2}{2\pi \alpha} \int_0^\infty \frac{z^3 dz}{e^{z^2} - 1} = B T^2$$

where B = const

$$C_2 = 2BT$$

c) $\frac{C_2}{C_3} = \frac{4}{5} \frac{B}{D} T^{-1/2} \to \infty$ as $T \to 0$, so C_2 dominates

d) at very low T, the densities of state are not continuous and the problem must be treated with discrete states. Treating them as continuous leads to the result that the ~~state~~ system with fewer degrees of freedom has a higher specific heat, ~~and~~ which is not correct.

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

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

where $J > 0$. Use $\hbar = 1$.

a. Find the energy levels. Hint: Use $\left(\vec{S}_{tot}\right)^2 = \left(\vec{S}_1 + \vec{S}_2\right)^2$, where $\vec{S}_{tot}$ 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_{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) $T \to 0$ and (ii) $T \to \infty$? Explain how you could have obtained these values from elementary considerations without first determining the free energy.

Statistical Mechanics.

$\mathcal{H} = J \vec{S}_1 \cdot \vec{S}_2$ Spin - 1.

(a) $\vec{S}_1 \cdot \vec{S}_2 = \frac{1}{2}\left(\vec{S}_{tot}^{\,2} - \vec{S}_1^{\,2} - \vec{S}_2^{\,2} \right)$

$\vec{S}_{tot}^{\,2} = S_{tot}(S_{tot}+1)$, $S_1^2 = 1.2 = 2$

Hence Energy levels are $\frac{J}{2}\left[S_{tot}(S_{tot}+1) - 4 \right]$

$= -2J$ $S_{tot} = 0$ degeneracy 1.
$-1J$ $S_{tot} = 1$ degeneracy 3
$1J$ $S_{tot} = 2$ degeneracy 5.

(b) Partition function, let $h = \beta J$

$$Z = e^{2h} + 3e^{h} + 5e^{-h}.$$

$$\underline{F = -k_B T \ln\left[e^{2h} + 3e^{h} + 5e^{-h} \right]}$$

$$\frac{S}{k_B} = \frac{-\partial F}{k_B \partial T} = \ln\left[e^{2h} + 3e^{h} + 5e^{-h} \right] - \frac{TJ}{k_B T^2}\left[\frac{2e^{2h} + 3e^{h} - 5e^{-h}}{e^{2h} + 3e^{h} + 5e^{-h}} \right]$$

$$= -\frac{F}{T} + \frac{U}{T}.$$

$F = U - TS$
$S = \frac{U}{T} - \frac{F}{T}$

$$U = -J\left[\frac{2e^{2h} + 3e^{h} - 5e^{-h}}{e^{2h} + 3e^{h} + 5e^{-h}} \right]$$

(c) $\underline{T \to 0}$ $\frac{S}{k_B} = \ln e^{2h} - \frac{J}{k_B T} \times 2 = \underline{\underline{0}}$

$\underline{T \to \infty}$ $\underline{\frac{S}{k_B} = \ln 9}$

$\underline{T \to 0}$ g.s. is non degenerate & $S = \ln$ degeneracy $\underline{\underline{= 0}}$

$\underline{T \to \infty}$ 9 states with equal occupation $\Rightarrow \underline{S = k_B \ln 9.}$

Legendre Polynomials

1. Generating function:

$$g(t,x) = (1-2xt+t^2)^{-1/2} = \sum_{n=0}^{\infty} P_n(x)t^n$$

2. Recursion relations

$$(2n+1)xP_n(x) = (n+1)P_{n+1}(x) + nP_{n-1}(x)$$

$$(1-x)^2P_n''(x) - 2xP_n'(x) + n(n+1)P_n(x) = 0$$

3. Normalization

$$\int dx[P_n(x)]^2 = \frac{2}{2n+1}$$

Spherical Harmonics

1. $\ell = 0$:

$$Y_{00} = \frac{1}{\sqrt{4\pi}}$$

2. $\ell = 1$:

$$Y_{11} = -\sqrt{\frac{3}{8\pi}}\sin(\theta)e^{i\phi} \qquad Y_{10} = \sqrt{\frac{3}{4\pi}}\cos(\theta)$$

3. Green's function:

$$\frac{1}{|\vec{x}-\vec{x}'|} = 4\pi\sum_{l=0}^{\infty}\sum_{m=-l}^{m=l}\frac{1}{2l+1}\frac{r_<^l}{r_>^{l+1}}Y_{lm}^*(\theta',\phi')Y_{lm}(\theta,\phi)$$

Bessel's Equation:

$$\frac{d^2R}{dx^2} + \frac{1}{x}\frac{dR}{dx} + (1-\frac{\nu^2}{x^2})R = 0$$

Spherical Bessel Functions

$$j_\ell(kr) \to \frac{\sin(kr-\ell\pi/2)}{kr}$$

$$n_\ell(kr) \to -\frac{\cos(kr-\ell\pi/2)}{kr}$$

$$j_o(\rho) = \frac{\sin(\rho)}{\rho} \qquad n_o(\rho) = -\frac{\cos(\rho)}{\rho}$$

$$j_1(\rho) = \frac{\sin\rho}{\rho^2} - \frac{\cos(\rho)}{\rho}$$

Gamma Function

1. Integral Representation:

$$\Gamma(z) = \int_0^{\infty} dte^{-t}t^{z-1}$$

2. Functional relation:

$$\Gamma(z+1) = z\Gamma(z)$$

3. Special values:

$$\Gamma(1) = 1 \qquad \Gamma(1/2) = \sqrt{\pi}$$

Fourier Transform

1. Discrete Fourier transform:

$$f(x) = \sum_{m=-\infty}^{\infty} c_m e^{\frac{2\pi i m x}{L}} \qquad c_m = \frac{1}{L}\int_o^L dx\ f(x)e^{-\frac{2\pi i m x}{L}}$$

2. Continuous Fourier Transform:

$$f(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \tilde{d}k\ f(k)e^{ikx} \qquad \tilde{f}(k) = \int_{-\infty}^{\infty} dx\ e^{-ikx} f(x)$$

Zeta Function

1. Integral representations:

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

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

2. Special values:

$$\zeta(0) = -\frac{1}{2} \qquad \zeta(3/2) = 2.612 \qquad \zeta(2) = \frac{\pi^2}{6}$$

$$\zeta(5/2) = 1.341 \qquad \zeta(4) = \frac{\pi^4}{90}$$

Classical Mechanics

1. Euler-Lagrange equations:

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} = \frac{\partial L}{\partial q_i}$$

2. Force in a rotating frame:

$$\vec{F}_{eff} = \vec{F} - m\vec{a}_f - m\dot{\vec{\omega}} \times \vec{r} - m\vec{\omega} \times (\vec{\omega} \times \vec{r}) - 2m\vec{\omega} \times \vec{v}_r$$

where v_r is the velocity with respect to the rotating axes, a_f is the acceleration of the moving frame with respect to the fixed axes.

Quantum Mechanics

1. Harmonic Oscillator:

$$H = \hbar\omega(\frac{1}{2} + a^\dagger a)$$

$$a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle \qquad a|n\rangle = \sqrt{n}|n-1\rangle$$

2. Angular momentum:

$$J_\pm = J_1 \pm iJ_2 \qquad J_\pm|j\ m\rangle = \sqrt{j(j+1) - m(m\pm 1)}|j\ m\pm 1\rangle$$

3. Spherically symmetric potentials:

$$\Psi_{Elm}(r,\theta,\phi) = R_{El}(r)Y_{lm}(\theta,\phi) = \frac{\rho_{El}(r)}{r}Y_{lm}$$

$$[-\frac{d^2}{dr^2} + \frac{2m}{\hbar^2}(V(r) + \frac{l(l+1)\hbar^2}{2mr^2} - E)]\rho_{El}(r) = 0$$

4. Partial Wave Expansion:

$$f(\theta) = \frac{1}{k}\sum_{\ell=0}^{\infty}(2\ell+1)e^{i\delta_\ell}\sin(\delta_\ell)P_\ell(\cos(\theta))$$

$$\sigma = \frac{4\pi}{k^2}\sum_{\ell=0}^{\infty}(2\ell+1)\sin^2\delta_\ell$$

For resonance,

$$\cot(\delta_n) = -(E-E_r)\frac{2}{\Gamma}$$

5. Born Approximation

$$f(\Omega) = -\frac{m}{e2\pi\hbar^2}\int d^3\vec{r}' e^{-i\vec{q}\cdot\vec{r}'}V(\vec{r}')$$

Useful Integrals

1.

$$\int\frac{x^2dx}{(x^2+b^2)^{1/2}} = \frac{x}{2}\sqrt{x^2+b^2} - \frac{b^2}{2}\ln(x+\sqrt{x^2+b^2})$$

2.

$$\int_{-\infty}^{\infty}dx\frac{\sin^2(x)}{x^2} = \pi$$

Electromagnetism

1. Energy density:

$$u = \frac{1}{8\pi}(\vec{E}^2+\vec{B}^2)$$

2. Poynting vector

$$\vec{S} = \frac{c}{4\pi}(\vec{E}\times\vec{B})$$

3. Maxwell stress tensor:

$$T_{ij} = \frac{1}{4\pi}(E_iE_j + B_iB_j - \frac{1}{2}(\vec{E}^2+\vec{B}^2)\delta_{ij})$$

4. Dipole moment

$$\vec{p} = \int d^3x\vec{x}\rho(\vec{x})$$

5. Quadrupole moment:

$$Q_{ij} = \int d^3x(3x_ix_j - r^2\delta_{ij})\rho(\vec{x})$$

Vector Analysis

1. Cross product

$$(\vec{A}\times\vec{B})_i = \epsilon_{ijk}A_jB_k$$

2. ϵ tensor:

$$\epsilon_{123} = 1, \epsilon_{213} = -1, \epsilon_{112} = 0, \text{etc.}$$

$$\epsilon_{ijk}\epsilon_{ilm} = \delta_{jl}\delta_{km} - \delta_{jm}\delta_{kl}$$

Complex Analysis

1. Principal Part or Principal Value, an example:

$$\text{PP}\frac{1}{x-x_o} = \frac{1}{2\pi i}(\frac{1}{x-x_o-i\epsilon} - \frac{1}{x-x_o+i\epsilon})$$

Equivalently, one can do integrals over a small circle in the complex plane about x_o, weighted with $\frac{1}{2\pi i}$.

PHYSICAL CONSTANTS

Revised 1989 by B.N. Taylor. Based mainly on the "1986 Adjustment of the Fundamental Physical Constants" by E.R. Cohen and B.N. Taylor, Rev. Mod. Phys. 59, 1121 (1987). The figures in parentheses after the values give the 1-standard-deviation uncertainties in the last digits; the uncertainties in parts per million (ppm) are given in the last column. The uncertainties of the values from a least-squares adjustment are in general correlated, and the laws of error propagation must be used in calculating additional quantities; the full variance matrix is given in the cited paper. The set of constants resulting from the 1986 adjustment has been recommended for international use by CODATA (Committee on Data for Science and Technology), and is the most up-to-date, generally accepted set available.

Quantity	Symbol, equation	Value	Uncert. (ppm)
speed of light	c	299 792 458 m s^{-1}	(exact)*
Planck constant	h	6.626 075 5(40)$\times 10^{-34}$ J s	0.60
Planck constant, reduced	$\hbar \equiv h/2\pi$	1.054 572 66(63)$\times 10^{-34}$ J s	0.60
		= 6.582 122 0(20)$\times 10^{-22}$ MeV s	0.30
electron charge magnitude	e	1.602 177 33(49)$\times 10^{-19}$ C = 4.803 206 8(15)$\times 10^{-10}$ esu	0.30, 0.03
conversion constant	$\hbar c$	197.327 053(59) MeV fm	0.30
conversion constant	$(\hbar c)^2$	0.389 379 66(23) GeV^2 mbarn	0.59
electron mass	m_e	0.510 999 06(15) MeV/c^2 = 9.109 389 7(54)$\times 10^{-31}$ kg	0.30, 0.59
proton mass	m_p	938.272 31(28) MeV/c^2 = 1.672 623 1(10)$\times 10^{-27}$ kg	0.30, 0.59
		= 1.007 276 470(12) u = 1836.152 701(37) m_e	0.012, 0.020
deuteron mass	m_d	1875.613 39(57) MeV/c^2	0.30
unified atomic mass unit (u)	(mass C^{12} atom)/12 = (1 g)/N_A	931.494 32(28) MeV/c^2 = 1.660 540 2(10)$\times 10^{-27}$ kg	0.30, 0.59
permittivity of free space	$\left.\begin{array}{l}\epsilon_0\\ \mu_0\end{array}\right\}\ \epsilon_0\mu_0 = 1/c^2$	8.854 187 817 ... $\times 10^{-12}$ F m^{-1}	(exact)
permeability of free space		$4\pi \times 10^{-7}$ N A^{-2} = 12.566 370 614 ... $\times 10^{-7}$ N A^{-2}	(exact)
fine structure constant	$\alpha = e^2/4\pi\epsilon_0\hbar c$	1/137.035 989 5(61)[†]	0.045
classical electron radius	$r_e = e^2/4\pi\epsilon_0 m_e c^2$	2.817 940 92(38)$\times 10^{-15}$ m	0.13
electron Compton wavelength	$\bar{\lambda}_e = \hbar/m_e c = r_e\alpha^{-1}$	3.861 593 23(35)$\times 10^{-13}$ m	0.089
Bohr radius ($m_{\text{nucleus}} = \infty$)	$a_\infty = 4\pi\epsilon_0\hbar^2/m_e e^2 = r_e\alpha^{-2}$	0.529 177 249(24)$\times 10^{-10}$ m	0.045
wavelength of 1 eV/c particle	hc/e	1.239 842 44(37)$\times 10^{-6}$ m	0.30
Rydberg energy	$hcR_\infty = m_e e^4/2(4\pi\epsilon_0)^2\hbar^2 = m_e c^2\alpha^2/2$	13.605 698 1(40) eV[§]	0.30
Thomson cross section	$\sigma_T = 8\pi r_e^2/3$	0.665 246 16(18) barn	0.27
Bohr magneton	$\mu_B = e\hbar/2m_e$	5.788 382 63(52)$\times 10^{-11}$ MeV T^{-1}	0.089
nuclear magneton	$\mu_N = e\hbar/2m_p$	3.152 451 66(28)$\times 10^{-14}$ MeV T^{-1}	0.089
electron cyclotron freq./field	$\omega^e_{\text{cycl}}/B = e/m_e$	1.758 819 62(53)$\times 10^{11}$ rad s^{-1} T^{-1}	0.30
proton cyclotron freq./field	$\omega^p_{\text{cycl}}/B = e/m_p$	9.578 830 9(29)$\times 10^{7}$ rad s^{-1} T^{-1}	0.30
gravitational constant	G_N	6.672 59(85)$\times 10^{-11}$ m^3 kg^{-1} s^{-2}	128
		= 6.707 11(86)$\times 10^{-39}$ $\hbar c$ (GeV/c^2)$^{-2}$	128
standard grav. accel., sea level	g	9.806 65 m s^{-2}	(exact)
Avogadro number	N_A	6.022 136 7(36)$\times 10^{23}$ mol^{-1}	0.59
Boltzmann constant	k	1.380 658(12)$\times 10^{-23}$ J K^{-1}[§]	8.5
		= 8.617 385(73)$\times 10^{-5}$ eV K^{-1}[§]	8.4
Wien displacement law constant	$b = \lambda_{\max}T$	2.897 756(24)$\times 10^{-3}$ m K[§]	8.4
molar volume, ideal gas at STP	$N_A k$(273.15 K)/(1 atmosphere)	22.414 10(19)$\times 10^{-3}$ m^3 mol^{-1}[§]	8.4
Stefan-Boltzmann constant	$\sigma = \pi^2 k^4/60\hbar^3 c^2$	5.670 51(19)$\times 10^{-8}$ W m^{-2} K^{-4}[§]	34
Fermi coupling constant	$G_F/(\hbar c)^3$	1.166 37(2)$\times 10^{-5}$ GeV^{-2}	17
weak mixing angle	$\sin^2\theta_W$	0.2259±0.0046	
$W^\pm$ boson mass	m_W	80.6±0.4 GeV/c^2	
Z^0 boson mass	m_Z	91.161±0.031 GeV/c^2	

[redacted]

2002

STATISTICAL MECHANICS

(Do only 2 out of 3 problems)

Please do **EACH** problem you attempt on a **SEPARATE** paper.
Put your name on each paper.

1. Consider a large system of N non-interacting particles in a magnetic field $\vec{B}$, each fixed in position and carrying a magnetic moment $\vec{\mu}$ that can point either in the same direction as $\vec{B}$ or in the opposite direction.

a. Find the entropy for the system in terms of the number, n, of spins pointing against the field.

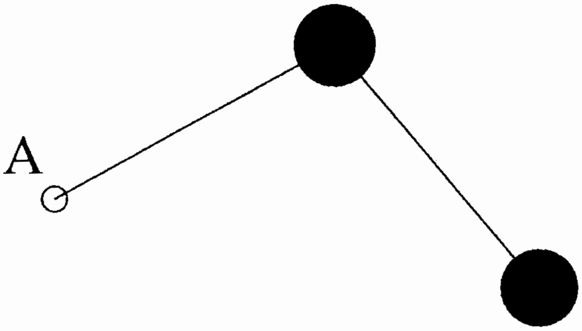
b. Find the maximum of the entropy in terms of n.

c. Find the conditions under which the temperature of the system is negative.

d. How can the system be prepared such that it has a negative temperature?

e. If the system has a negative temperature and is put into contact with a system with a positive temperature, which way will heat flow?

2. Consider a classical double pendulum in the absence of gravity as shown below.

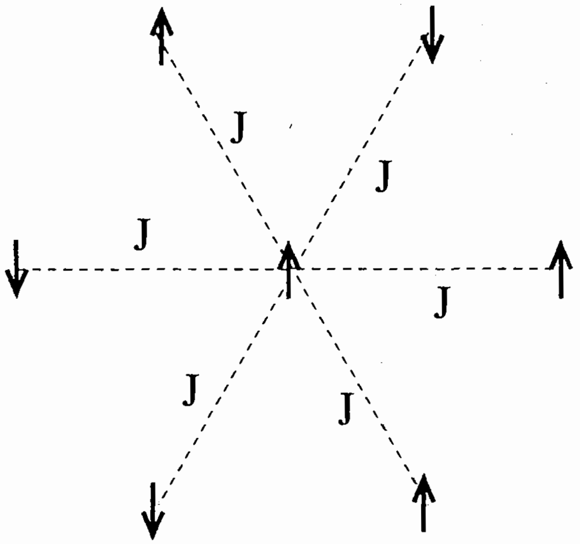


It consists of two rigid rods tethered at point A, with all joints freely hinged. The system is in contact with a heat bath at temperature T. The masses of the two rods and their moments of inertia are the same. The masses of the two black spheres are the same. For simplicity, consider the problem in two dimensions.

a. Calculate the probability distribution for the end to end vector between the point A and the end sphere.

b. Calculate the energy as a function of temperature.

3. N Ising spins $S_i = \pm 1$, where $i = 1, 2, 3, ...N$ are all connected to a central spin s_0, but not each other, through a ferromagnetic coupling J as shown below.



They are all in a uniform magnetic field. The Hamiltonian for the system is

$$H = -J \sum_{i=0}^{N} S_0 S_i - h \sum_{i=0}^{N} S_i \quad .$$

a. Calculate the partition function for arbitrary N.
b. For very large N, calculate $< S_1 >$ as a function of β and h.
c. In the large N limit, state if there is a discontinuity in $< S_1 >$ as a function of h and for what temperature(s) it appears. Calculate the size of the discontinuity.

Qualifier #1 [redacted]

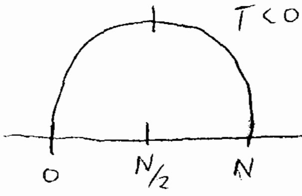
STAT MEC
2002

9) $\Omega = \dfrac{N!}{n!(N-n)!}$

$S = k_B \ln \Omega \simeq k_B\{N \ln N - n \ln n - (N-n)\ln(N-n)\}$

$\dfrac{\partial S}{\partial n} = 0$ for maximum entropy

$\dfrac{\partial S}{\partial n} = -k_B\{\ln n - \ln(N-n)\} = 0$



$n = N - n \qquad n = \dfrac{N}{2}$

$\dfrac{1}{T} = \left(\dfrac{\partial S}{\partial U}\right)_V \qquad S_{max} = k_B[N \ln N - \cancel{2}N \ln \tfrac{1}{2}N]$

$= k_B N \ln 2$

$U = n\mu B + (N-n)(-\mu B) = 2n\mu B - N\mu B$

$dU = 2\mu B\, dn$

$T = \dfrac{2\mu B}{(\partial S/\partial n)}$ for $\dfrac{\partial S}{\partial n} < 0$ we have $T < 0$

this can be achieved by a field reversal done quickly

$$\frac{dS}{dt} = \frac{dU_A}{dt}\left(\frac{\partial S_A}{\partial U_A}\right)_V + \frac{dU_B}{dt}\left(\frac{\partial S_B}{\partial U_B}\right)_V$$

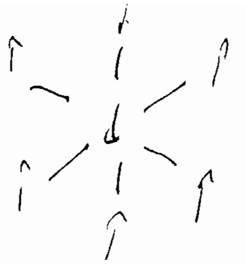
$$= \frac{dU_A}{dt}\left[\left(\frac{\partial S_A}{\partial U_A}\right)_V - \left(\frac{\partial S_B}{\partial U_B}\right)_V\right]$$

$$= \frac{dU_A}{dt}\left[\frac{1}{T_A} - \frac{1}{T_B}\right] > 0 \qquad \text{2nd Law}$$

if $T_A < 0$ & $T_B > 0$, then

$\dfrac{dU_A}{dt} < 0$, so heat flows from A to B

STAT MECH III



$$H = -(h + J S_0) \sum_{i=1}^{N} s_i$$

$$Z = Z(s_0 = -1) + Z(s_0 = +1)$$

$$= \left(e^{-\beta(h-J)} + e^{\beta(h-J)}\right)^N$$

$$+ \left(e^{-\beta(h+J)} + e^{\beta(h+J)}\right)^N$$

$$= 2^N\left[\cosh^N(\beta(h-J)) + \cosh^N(\beta(h+J))\right]$$

$$\langle s_1 \rangle = \frac{1}{N}\left\langle \sum_{i=1}^{N} s_i \right\rangle = +\frac{T}{N}\frac{\partial \ln Z}{\partial h}$$

for $h > 0$ $\lim_{N \to \infty}$ $\ln Z = N \ln 2 + N \ln \cosh(\beta(h+J))$

$h < 0$ " " $=$ " $+ N \ln \cosh(\beta(h-J))$

$$\therefore \langle s_1 \rangle = +\frac{T}{N} N \tanh(\beta(h+J)) \cdot \beta = + \tanh(\beta(h+J)) \quad h >$$

$$= \tanh(\beta(h-J)) \quad h <$$

discontinuity @ $h = 0$ of $2 \tanh(\beta J)$

Statistical Mechanics

2003

[redacted]

1. *Specific heat due to interaction with the walls.*
The partition function for a classical system of particles is given by

$$Z = \frac{1}{N!\,(2\pi\hbar)^{3N}} \int \prod_{i=1}^{N} \left(d^3p_i d^3r_i\right) \exp\left(-\mathcal{H}[\vec{p},\vec{r}]/k_BT\right)$$

where $\mathcal{H}[\vec{p},\vec{r}]$ is the Hamiltonian, which depends on the coordinates $\{\vec{r}_i\}$ and momenta $\{\vec{p}_i\}$ of the N particles.

   (a) A classical non-interacting gas is repelled by the walls of its container. The force can be represented by a step in the potential energy which is W a short distance ℓ from the wall and zero further away.

   Find an expression for the additional energy produced by this effect in terms of k_B, T, W, ℓ, N, the volume of the gas V, and the wall area A.

   (b) Assuming that $V \gg A\ell$, show that the corresponding extra specific heat, ΔC, tends to zero when k_BT is very large or very small compared with W, but that

$$\Delta C \sim Nk_B\frac{\ell A}{V}$$

   when k_BT is of order W.

2003

Statmech Solutions [redacted]

1. $$Z = \frac{1}{N!\,(2\pi\hbar)^{3N}} \int \prod (d^3p_i\, d^3q_i)\, e^{-\beta \mathcal{H}}$$

where $\mathcal{H} = \sum_i \frac{\vec{p}_i^{\,2}}{2m} + \sum_i U(\cancel{q}\vec{r}_i)$ where

$$U(\vec{r}_i) = \begin{cases} W & \text{if } \vec{r}_i \text{ is within a distance } l \text{ of the walls} \\ 0 & \text{otherwise.} \end{cases}$$

(a) $Z = Z_{KE}\, Z_{PE}$ where

$$Z_{KE} = (1) \int \prod_i d^3p_i \; e^{-\sum_i \beta p_i^2/2m}$$

$$Z_{PE} = \int \prod d^3r_i \; e^{-\sum \beta U(\vec{r}_i)}$$

$$= \mathfrak{z}_{PE}^{\,N} \quad \text{where } \mathfrak{z}_{PE} = \int d^3r\, e^{-\beta U(\vec{r})} \underline{= V - Al + Al e^{-\beta W}}$$

Hence $F = F_{KE} + F_{PE}$ and $U = U_{KE} + U_{PE}$

We are interested in U_{PE} where

$$U_{PE} = N\frac{\partial}{\partial\beta}\left(-\cancel{\beta}\ln \mathfrak{z}_{PE}\right) = \frac{NAlWe^{-\beta W}}{V + Al(e^{-\beta W} - 1)} \simeq \underline{\underline{\frac{Al}{V} W e^{-\beta W}}}$$

(b) Specific Heat

$$C_{PE} = \frac{\partial U_{PE}}{\partial T}$$

$$\Rightarrow \underline{\frac{C_{PE}}{Nk_B} = \left(\frac{W}{k_B T}\right)^2 e^{-\beta W} \frac{Al}{V}}$$

$T \to \infty \quad \Rightarrow \quad \left(\frac{W}{T}\right)^2 \to 0$

$T \to 0 \quad \Rightarrow \quad e^{-W/T} \to 0$

For $k_B T = W$, $\quad \underline{C_{PE} \sim Nk_B \frac{Al}{V}}$

2. *Elasticity due to entropy*
Consider a simple model of a polymer constrained to lie in one-dimension. The polymer consists of N segments ($N \gg 1$), of unit length, which can either point to the right or to the left along a line.

   (a) Calculate the free energy, F, of the system at a temperature T as a function of the end to end distance, x.
   Note: There is no energy in this problem, only entropy, so you need to think about the *number* of configurations with a given value of x.

   (b) Show that
   $$F(x) = F(0) + \frac{1}{2}Kx^2$$
   (*i.e.* one has Hooke's law: Force $= -Kx$) as long as x is small compared with the fully stretched length of the polymer.

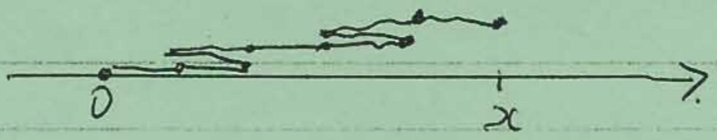
   (c) Show that the elastic constant, K, is proportional to temperature.

Note: This is believed to be the why rubber, which consists of cross-linked polymers, has an elastic constant which *increases* with T, whereas most substances get softer as they heat up so their elastic constant *decreases.*

Stat Mech Solutions, [redacted]

(2003)

2)



(a) Let there be N_r segments which go to right
N_L - - - - - - - - left

Clearly $N_r + N_L = N$ so $N_r = \frac{1}{2}(N+x)$
$N_r - N_L = x$. $N_l = \frac{1}{2}(N-x)$

How many ways are there of choosing N_r segment to right

Ans. Binomial coefficient $g(N,x) = \frac{N!}{N_L!\,N_r!} = \underline{\frac{N!}{\left[\frac{N}{2}(1+x)\right]!\,\left[\frac{N}{2}(1-x)\right]!}}$

Free energy

$$\underline{\underline{F = -k_B T \ln g(N,x).}}$$

(b) From Stirlings approximation

$$\ln g(N,x) = \ln N! - \ln\left[\left(\frac{N}{2}(1+x)\right)!\right] - \ln\left[\left(\frac{N}{2}(1-x)\right)!\right]$$

$$\hat{=} N\ln N - N - \left\{\frac{N}{2}(1+x)\ln\left[\frac{N}{2}(1+x)\right] - \frac{N}{2}(1+x)\right\}$$
$$- \left\{\frac{N}{2}(1-x)\ln\left[\frac{N}{2}(1-x)\right] - \frac{N}{2}(1-x)\right\}$$

$$= \cancel{N\ln N} - \frac{N}{2}(1+x)\ln[\cancel{N}(1+x)] - \frac{N}{2}(1-x)\ln[\cancel{N}(1-x)] + N\ln 2.$$

For $x \ll N$, expand to lowest non vanishing order in x

$$\ln[g(N,x)] = N\left[\ln 2 - \frac{x^2}{2}\right]$$

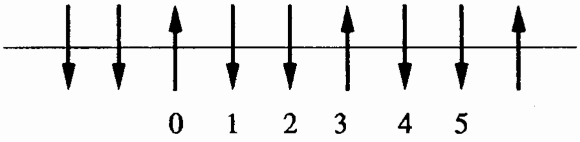
Hence $F = F_0 + k_B T\, N \frac{x^2}{2}$

(c) ~~(d)~~ Force constant k is given by $\underline{K = N k_B T}$ (i.e. $\propto T$)

[redacted]

STATISTICAL MECHANICS - 1

2. Consider a long linear chain of N Ising spins, where the spin value is $S_i = \pm 1$ and the interaction between spins is $-J$, where $J > 0$.



1) Write the Hamiltonian for this system.
2) Write the partition function for this system.
3) Rewrite the partition function for this system having summed over the odd numbered spins.
4) Rewrite the partition function again, but in the same form as the original Hamiltonian, but with the sum over the even spins only, multiplied by a function only of the temperature, and at different effective temperature, T'. This could be written in the form

$$Z(N,T) = f(T)^{N/2} Z(N/2,T') \tag{1}$$

Show the equation for T' in terms of T and the equation for $f(T)$. Is the new temperature higher or lower than the original one?
5) Explain why this exercise demonstrates that the system never has a phase transition or long-range order.

Solution

1) $\mathcal{H} = -J \sum_{i=-\infty}^{\infty} S_i S_{i+1}$

2) $Z = \sum e^{J\beta(\cdots + S_0S_1 + S_1S_2 + S_2S_3 + S_3S_4 + \cdots)}$

3) $Z = \sum \cdots e^{J\beta(S_0S_1 + S_1S_2)} e^{J\beta(S_2S_3 + S_3S_4)} \cdots$

$$Z = \sum \cdots \left[e^{J\beta(S_0+S_2)} + e^{-J\beta(S_0+S_2)}\right]\left[e^{J\beta(S_2+S_4)} + e^{-J\beta(S_2+S_4)}\right]\cdots$$

4) $$e^{J\beta(S_0+S_2)} + e^{-J\beta(S_0+S_2)} = f(T)\, e^{+J\beta' S_0 S_2}$$

for $S_0 = S_2 = 1, -1$

$$e^{2J\beta} + e^{-2J\beta} = f(T)\, e^{J\beta'}$$

for $S_0 = -S_2 = 1, -1$

$$2 = f(T)\, e^{-J\beta'}$$

divide to get $\cosh 2J\beta = e^{2J\beta'}$

$$2J\beta' = \ln(\cosh 2J\beta)$$

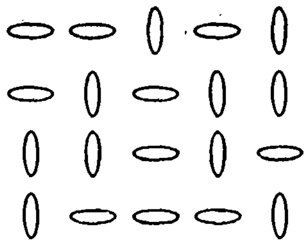
$$T' = \frac{2J}{k \ln(\cosh 2J/kT)} \qquad T' > T$$

$$f(T) = 2e^{J\beta'} = 2\cosh^{1/2}(2J\beta)$$

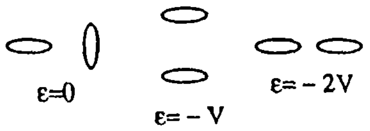
$$f(T) = 2\cosh^{1/2}\left(\frac{2J}{kT}\right)$$

5) there are no singular points where a transition takes place. Since the system is disordered at high T, it must always be disordered and no long-range order can take place

3. Cigar shaped molecules are arranged on a square lattice, as illustrated in the sketch below:



Each molecule may be oriented only along the x or y axes. The molecules interact only if they are nearest neighbors, and the energy of this interaction may be 0, -V or -2V (V > 0) depending on the relative orientation of the molecules.



This system will undergo a phase transition to an ordered state at low temperature. Within a mean field approximation use the effective field on each molecule to calculate, self consistently,the transition temperature. Then determine (again in mean field) either the value (if continuous) or the discontinuity (if discontinuous) of the system at the transition temperature. *for:*

(a) the *energy*

(b) the entropy

The self consistency condition is that the normalized weight associated with the 0 orientation should be p, i.e.

$$p = \frac{\exp[6pV\beta]}{\exp[6pV\beta] + \exp[6(1-p)V\beta]}$$

Writing $p = \frac{1}{2}(1+f)$, we obtain

$$f = \tanh[3V\beta f].$$

This always has a solution $f=0$. At low temperatures, however, the $f=0$ solution loses stability to a pair of solutions at $f = \pm f_0$. As for magnets, the critical temperature is found by expanding the RHS in powers of f, which yields

$$3V\beta_c = 1.$$

For $\beta \gtrsim \beta_c$, $f \approx 0$. For $3V\beta = 1+\epsilon$, expanding in powers of f we have

$$f = (1+\epsilon) f - \frac{[(1+\epsilon)f]^3}{3} + \dots$$

i.e., $-\epsilon f \approx -\frac{f^3}{3}$, so that $f = \pm\sqrt{3\epsilon} + O(\epsilon^{3/2})$

This is a second order transition, so that the energy and entropy are continuous, but the specific heat is not

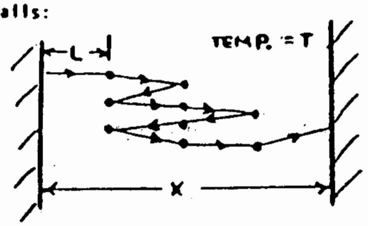
a) ~~not~~. The energy per molecule at T_c is given by $-\frac{\partial}{\partial\beta} \ln Z$

$$= p\cdot(-6pV) + (1-p)(-6(1-p)V)$$

$$= (\text{since } f_c = 0) \quad -3V$$

b) The entropy per molecule at T_c is found by using $S = -k\sum p_i \ln p_i$. Since both the 0 and the ⬭ orientation have probability $= \frac{1}{2}$ at T_c, $S = k\ln 2$.

5. There is a chain consisting of $n>>1$ links at temperature T, between two walls:



Let the length of each link be L and let the distance between the endpoints be x. The joints between the links are frictionless and turn freely. No external forces, other than the connections to the walls at the two endpoints, act on the chain. Consider this as a one-dimensional problem, i.e., each link can assume only one of the two orientations: •→• OR •←•

a) Find the entropy of this chain as a function of x.

b) Determine the relation between the temperature of the chain and the force (tension) which is necessary to maintain the distance x.

5. a) If there are n_+ links pointing forward and n_- pointing backwards,

$$n_+ - n_- = x/L$$
$$n_+ + n_- = n$$

So that

$$n_+ = \tfrac{1}{2}(n + x/L)$$
$$n_- = \tfrac{1}{2}(n - x/L)$$

The number of configurations we can construct is ${}^{n}C_{n_+}$. Therefore the entropy is

$$S = k_B \ln \Omega = k_B \left\{ n \ln n - n - n_+ \ln n_+ + n_+ - n_- \ln n_- + n_- \right\}$$

Expanding this expression in powers of x,

$$S = k_B \left\{ n \ln n - \left[\frac{n}{2} \ln n/2 + \frac{1}{2}\frac{x}{L} \cdot \frac{x}{nL}\right] \times 2 \right\}$$
$$= k_B \left\{ n \ln 2 - x^2/nL^2 + O(x^3) \right\}$$

b) $dF = -S\,dT + f\,dx$, $F = U - TS = -TS$.

$$f = \partial F/\partial x \Big|_T = 2 k_B T x / n L^2$$

Bonus: If we stretch a rubberband, $dU = dQ + f dx = 0$

We see that the energy spent in stretching the band flows out to the environment as heat. (In real rubber, although $U \neq 0$, $-TS$ dominates the free energy, so assuming $U = 0$ is not a bad approximation).

(One can also derive, from this expression, that i) stretched rubber left to itself will spontaneously contract in an irreversible process ii) when we heat rubber it will contract.)

[redacted]
Statistical/04

2004
STATISTICAL MECHANICS
(Turn in 2 0ut of 3 Problems)

INSTRUCTIONS:
DO EACH PROBLEM ON SEPARATE PAPER.

WRITE YOUR NAME, SECTION, PROBLEM# ON EACH SHEET YOU TURN IN.

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

Statistical Mechanics #1

1. Consider a one-dimensional Ising model with ferromagnetic coupling $J > 0$ on a chain with N sites, with randomly placed impurity atoms. The impurity atoms are located between lattice sites, and destroy the ferromagnetic coupling. Thus the energy of a spin configuration is given by

$$E = -J \sum_{i=1}^{N-1} n_i S_i S_{i+1}$$

where $S_i = \pm 1$ is the Ising spin on the i'th site, and $n_i = 0$ if there is an impurity atom on the i'th bond while $n_i = 1$ otherwise. Assume that N is extremely large. You should take free boundary conditions rather than periodic boundary conditions.

(a) For the pure system, i.e. all the n's are equal to 1, calculate the free energy and energy per site.

(b) Calculate the free energy per site if the impurity atoms are free to drift in and out of the chain, i.e. the impurity variables $\{n_i\}$ are in equilibrium with the spin variables.

(c) In part b, what is $1 - \langle n_i \rangle$, the average density of impurity atoms?

Statistical Mechanics #2

2. Consider non interacting fermions with spin 1/2 at finite temperature. The specific heat at finite temperature, as measured in the lab, is given by

$$C = \left(\frac{\partial U}{\partial T}\right)_N = -k_B\beta^2\left(\frac{\partial U}{\partial \beta}\right)_N$$

where U is the internal energy and $\beta = 1/(k_B T)$.

(a) Write down expressions for the energy and mean number of particles N in the grand canonical ensemble in terms of the Fermi function

$$f(\epsilon) = \frac{1}{\exp(\beta(\epsilon - \mu) + 1}$$

(where μ is the chemical potential), and the density of states $g(\epsilon)$.

(b) In order to keep the number of particles constant show that μ must vary with β as

$$\left(\frac{\partial \mu}{\partial \beta}\right)_N = -\left(\frac{\partial N}{\partial \beta}\right)_\mu / \left(\frac{\partial N}{\partial \mu}\right)_\beta .$$

(c) Hence find an expression for the specific heat involving partial derivatives of U and N, assumed to be functions of μ and β.

(d) Write the partial derivatives in part 2c in terms of integrals over $f'(\epsilon)$.

(e) By using the Sommerfield expansion

$$\int A(\epsilon) f'(\epsilon)\, d\epsilon = -\left[A(\mu) + \frac{\pi^2}{6}k_B^2 T^2 A''(\mu) + \cdots\right],$$

(which you are **not** required to prove), valid at low-T, where $A(\epsilon)$ is an arbitrary function, evaluate each of the partial derivatives in part 2e to lowest order in T, and hence determine the specific heat at low temperature to leading order. *Note:* You should find the specific heat to be linear in T.

Statistical Mechanics #3

3. Consider electromagnetic radiation inside a cubic box of volume V at temperature T.

   (a) Calculate the allowed wave-vectors for the photons. To make this simpler, you can consider periodic boundary conditions for an $L \times L \times L$ box.

   (b) Calculate the density of states of the photons, that is, the number of states in frequency range ω to $\omega + d\omega$.

   (c) State what is the average number of photons that occupy a single state at frequency ω if the temperature is T?

   (d) Calculate the energy density per unit frequency range inside the box.

   (e) Show that the answer to part d has a maximum at $\omega = \omega_c$ where

$$\hbar\omega_c = C\, k_B T$$

   where C is a numerical constant. You should explain how C is obtained but you do not need to determine its numerical value.

Qualifying Examination, 2004

Statistical Mechanics

Solutions

1. (a) If all the n_i are equal to 1 we just have the regular one-dimensional Ising model with energy

$$E = -J \sum_{i=1}^{N-1} S_i S_{i+1} \,.$$

With free boundary conditions, the simplest way to determine the partition function is to trace out an end spin, $i = N$ say, since this is independent of spin S_{N-1}. The sum gives

$$\sum_{S_N = \pm 1} e^{\beta J S_{N-1} S_N} = e^{\beta J} + e^{-\beta J} = 2\cosh \beta J \,.$$

The process can be repeated for spins $N-1, N-2, \cdots, 3, 2$. This just leaves spin S_1 which then has no coupling and summing over it gives a factor of 2. Hence the partition function is given by

$$Z = 2(2\cosh\beta J)^{N-1} \,.$$

The free energy per site is given by $f = -N^{-1} k_B T \ln Z$, i.e.

$$\boxed{f = -k_B T \ln(2\cosh\beta J)\,,}$$

in which the difference between $N-1$ and N has been neglected (valid for large N). The energy per site, u, is given by

$$u = \frac{\partial}{\partial \beta}(\beta f) = \boxed{-J\tanh\beta J\,.}$$

Note: These results can also be obtained by transfer matrices.

(b) We now repeat the procedure in the first part but including the n_i. We start by tracing out the end spin S_N and the end bond n_{N-1}:

$$\sum_{n_{N-1}=0,1} \sum_{S_N=\pm 1} e^{\beta J n_{N-1} S_{N-1} S_N} = 2 + e^{\beta J} + e^{-\beta J} = 2(1 + \cosh\beta J)\,. \qquad (1)$$

Repeating for spins $N-1, N-2, \cdots, 3, 2$ we get

$$Z = 2^N (1 + \cosh\beta J)^{N-1} \,.$$

The free energy per site is therefore

$$\boxed{f = -k_B T \ln(2 + 2\cosh\beta J)\,,}$$

Note: Again, these results can also be obtained by transfer matrices.

(c) Now $1 - \langle n_i \rangle$ is the ratio of the statistical sum with n_i fixed to be zero divided by the total statistical sum. This is given by the ratio of the terms in Eq. (1) with $n_i = 0$ to the total in Eq. (1), i.e.

$$1 - \langle n_i \rangle = \frac{2}{2(1+\cosh\beta J)} = \boxed{\frac{1}{1+\cosh\beta J}}\,.$$

2. (a) The expressions for the energy, U, and mean number of particles, N, are

$$\boxed{U = 2\int_0^\infty \epsilon f(\epsilon)g(\epsilon)\,d\epsilon\,,}$$

$$\boxed{N = 2\int_0^\infty f(\epsilon)g(\epsilon)\,d\epsilon\,,}$$

(the factor of 2 comes from the spin degeneracy).

(b) We need $dN = 0$, i.e.

$$0 = dN = \left(\frac{\partial N}{\partial \mu}\right)_\beta d\mu + \left(\frac{\partial N}{\partial \beta}\right)_\mu d\beta$$

and so

$$\boxed{\left(\frac{\partial \mu}{\partial \beta}\right)_N = -\left(\frac{\partial N}{\partial \beta}\right)_\mu \Big/ \left(\frac{\partial N}{\partial \mu}\right)_\beta .}$$

(c) The specific heat is given by

$$\begin{aligned} C &= -k_B\beta^2\left(\frac{\partial U(\beta,\mu)}{\partial \beta}\right)_N = -k_B\beta^2\left[\left(\frac{\partial U}{\partial \beta}\right)_\mu + \left(\frac{\partial U}{\partial \mu}\right)_\beta \left(\frac{\partial \mu}{\partial \beta}\right)_N\right] \\ &= \boxed{-k_B\beta^2\left[\left(\frac{\partial U}{\partial \beta}\right)_\mu - \left(\frac{\partial U}{\partial \mu}\right)_\beta \left(\frac{\partial N}{\partial \beta}\right)_\mu \Big/ \left(\frac{\partial N}{\partial \mu}\right)_\beta\right]} . \end{aligned}$$

(d) The partial derivatives in the last section can easily be obtained from the results in part. 2a:

$$\begin{aligned} \left(\frac{\partial U}{\partial \beta}\right)_\mu &= \boxed{\frac{2}{\beta}\int_0^\infty \epsilon(\epsilon-\mu)f'(\epsilon)g(\epsilon)\,d\epsilon} \\ \left(\frac{\partial U}{\partial \mu}\right)_\beta &= \boxed{-2\int_0^\infty \epsilon f'(\epsilon)g(\epsilon)\,d\epsilon\,,} \\ \left(\frac{\partial N}{\partial \beta}\right)_\mu &= \boxed{\frac{2}{\beta}\int_0^\infty (\epsilon-\mu)f'(\epsilon)g(\epsilon)\,d\epsilon\,,} \\ \left(\frac{\partial N}{\partial \mu}\right)_\beta &= \boxed{-2\int_0^\infty f'(\epsilon)g(\epsilon)\,d\epsilon\,,} \end{aligned}$$

(e) Using the Sommerfield expansion, the expressions in the last part can be written, to leading order in T,

$$\begin{aligned} \left(\frac{\partial U}{\partial \beta}\right)_\mu &= -\frac{4}{\beta}\frac{\pi^2}{6}k_B^2T^2(\mu g'(\mu)+g(\mu))\,, \\ \left(\frac{\partial U}{\partial \mu}\right)_\beta &= 2\mu g(\mu)\,, \\ \left(\frac{\partial N}{\partial \beta}\right)_\mu &= -\frac{4}{\beta}\frac{\pi^2}{6}k_B^2T^2 g'(\mu)\,, \\ \left(\frac{\partial N}{\partial \mu}\right)_\beta &= 2g(\mu) \end{aligned}$$

Combining we get

$$C = k_B \beta^2 \frac{4}{\beta} g(\mu) \frac{\pi^2}{6} k_B^2 T^2 = \boxed{\frac{2}{3}\pi^2 k_B^2 T g(\mu)},$$

which is linear in T.

3. (a) Calculate the allowed wave-vectors for the photons. To make this simpler, you can consider periodic boundary conditions for an $L \times L \times L$ box.

With plane waves, continuity implies

$$\boxed{\mathbf{k} = (2\pi/L)(n_x\hat{\imath} + n_y\hat{\jmath} + n_z\hat{k})\,,}$$

where the n's take on all integral values. There are 2 distinct polarization states at every allowed value of k.

(b) Calculate the density of states of the photons, that is, the number of states in frequency range ω to $\omega + d\omega$.

The number of k-values per unit volume of k-space is $(L/2\pi)^3$ and so

$$\tilde{g}(k)dk = 2\left(\frac{L}{2\pi}\right)^3 4\pi k^2 dk\,,$$

where $\tilde{g}(k)dk$ is the number of states for which $|\mathbf{k}|$ lies between k and $k + dk$. Now $\omega = ck$, and so, in terms of ω rather than k, we have

$$g(\omega)d\omega = \tilde{g}(k)dk = 2\left(\frac{L}{2\pi}\right)^3 4\pi k^2 dk = 2\left(\frac{L}{2\pi}\right)^3 4\pi\left(\frac{\omega}{c}\right)^2 \frac{1}{c}d\omega\,.$$

Equating the first and last expressions in the previous equation gives

$$\boxed{g(\omega) = \frac{L^3}{c^3\pi^2}\,\omega^2\,.}$$

(c) At a temperature T, what is the average number of photons that occupy a single state at frequency ω?

Photons are bosons, and have no constraint on total number. Hence they obey the Planck distribution. Since the energy of a photon is $E = \hbar\omega$ we have

$$\boxed{\langle n\rangle = \frac{1}{e^{\beta\hbar\omega} - 1}\,.}$$

(d) Calculate the energy density per unit frequency range inside the box.

The energy in the frequency range ω to $\omega + \omega$ is $\langle n\rangle\hbar\omega g(\omega)d\omega$. Dividing by L^3 to get the energy per unit volume, and denoting the result by $e(\omega)d\omega$ we have

$$\boxed{e(\omega) = \frac{\hbar\omega^3}{c^3\pi^2}\frac{1}{e^{\beta\hbar\omega} - 1}\,.}$$

(e) Show that the answer to part 3d has a maximum when $\hbar\omega = C\,k_BT$.

We need to find the maximum of

$$\omega^3\frac{1}{e^{\beta\hbar\omega} - 1}$$

with respect to ω. This is at $\omega = \omega_c$ where

$$3\omega_c^2\frac{1}{e^{\beta\hbar\omega_c} - 1} = \omega_c^3\beta\hbar\frac{e^{\beta\hbar\omega_c}}{(e^{\beta\hbar\omega_c} - 1)^2}$$

or

$$3k_BT = \hbar\omega_c \frac{1}{1 - e^{-\beta\hbar\omega}}.$$

Letting $\boxed{\hbar\omega_c = Ck_BT}$ we have

$$\boxed{C = 3(1 - e^{-C}).}$$

(You are not required to determine the value of C. The actual value is about 2.82.)

Master

Problems + Solutions

2005
STATISTICAL MECHANICS
(Turn in 2 0ut of 3 Problems)

INSTRUCTIONS:

DO EACH PROBLEM ON SEPARATE PAPER.

WRITE YOUR NAME, SECTION, PROBLEM# ON EACH SHEET YOU TURN IN.

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

Qualifying Exam 05

Statistical Mechanics 1

---

1. If the energy stored in the rotational and vibrational modes is not too large, we may approximate the Hamiltonian of the diatomic molecule by

$$\mathcal{H} = \mathcal{H}_{transl} + \mathcal{H}_{rot} + \mathcal{H}_{vib},$$

neglecting any effect of the centrifugal forces on the vibrational modes and the effect of the vibrational distortions on the moment of inertia, I. In a dilute gas, the density will be low enough so that the translational motion can be treated classically. The energy of rotation is:

$$\epsilon_j = \frac{\hbar^2 j(j+1)}{2I}$$

where $j = 0, 1, 2, \cdots$ is the rotational quantum number. The state with quantum number j has degeneracy $2j+1$ (we have, for simplicity, assumed that the two atoms in the diatomic molecule are different). The vibrational degree of freedom may be taken to be that of a simple harmonic oscillator with frequency ω_{vib}.

Determine the specific heat per molecule in the following limits:

(a)

$$T \ll \theta_{rot} \equiv \frac{\hbar^2}{2Ik_B} \ll \theta_{vib} \equiv \frac{\hbar\omega_{vib}}{k_B},$$

(b)

$$\theta_{rot} \ll T \ll \theta_{vib},$$

(c)

$$\theta_{rot} \ll \theta_{vib} \ll T.$$

Note: The Euler summation formula

$$\sum_{n=0}^{\infty} f(n) = \int_0^{\infty} f(n)\, dn + \tfrac{1}{2}f(0) + \tfrac{1}{12}f'(0) + \cdots$$

may be useful in evaluating the vibrational contribution for $T \gg \theta_{rot}$. (Which term on the right hand side dominates in this limit?)

Qualifying Exam 05

Statistical Mechanics 2

Consider a fixed number, N, of monatomic Bosons in a three-dimensional box of size $L \times L \times L$.

(a) For a large box (large enough that the spacing between the single-particle energy levels is very small, so the levels can be treated as a continuum for most purposes) find the density of states as a function of the energy $\epsilon = \hbar^2 k^2/(2m)$.

(b) For one state of wave vector $\vec{k}$, write the grand partition function, $Z_G(\vec{k})$. Your expression will include the chemical potential μ.

(c) Using the grand potential, $\Phi_G(\vec{k}) = -k_B T \ln Z_G(\vec{k})$, where k_B is the Boltzmann constant, derive the Bose-Einstein distribution, $n(\vec{k})$, for the number of bosons in state $\vec{k}$.

(d) Show that the chemical potential cannot be positive.

(e) Show that there is a critical temperature, T_c, for which the chemical potential becomes zero (in our approximation) and give its value.

(f) Explain what must happen when the temperature becomes less than T_c and why the equations derived above completely miss this important part of the physics (*i.e.* Bose-Einstein condensation).

Note: You are given that

$$\int_0^\infty \frac{z^{1/2}\,dz}{e^z - 1} = 2.315\,.$$

Qualifying Exam 05

Statistical Mechanics 3

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

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

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.

(b) Calculate the magnetization as a function of temperature close to the phase transition.

Qualifying Examination, 2005

Statistical Mechanics: Solutions

[redacted]

1. The **translational** motion can be treated classically. Classical equipartition gives $U_{trans} = \frac{3}{2} k_B T$ (per molecule) and so

$$\boxed{C_{trans} = \tfrac{3}{2} k_B \qquad (\text{all } T)\,.} \tag{1}$$

The **vibrational** motion is that of a simple harmonic oscillator for which we have

$$U = \left(\frac{1}{\exp(\beta \hbar \omega_{vib}) - 1} + \frac{1}{2} \right) \hbar \omega_{vib}\,, \tag{2}$$

where, as usual, $\beta \equiv (k_B T)^{-1}$. This can easily be derived from the partition function

$$Z = \sum_{n=0}^{\infty} \exp(-\beta(n + \tfrac{1}{2})\hbar\omega)\,.$$

Eq. (2) gives

$$\begin{aligned} U &= \left(\exp(-\beta \hbar \omega_{vib}) + \frac{1}{2} \right) \hbar \omega_{vib} \qquad (\theta_{vib} \gg T) && (3) \\ &= k_B T \qquad (\theta_{vib} \ll T), && (4) \end{aligned}$$

and so

$$\begin{aligned} C &= k_B \left(\frac{\hbar \omega_{vib}}{k_B T} \right)^2 \exp(-\beta \hbar \omega_{vib}) = \boxed{k_B \left(\frac{\theta_{vib}}{T} \right)^2 \exp\left(-\frac{\theta_{vib}}{T} \right) \qquad (\theta_{vib} \gg T)\,,} && (5) \\ &= \boxed{k_B \qquad (\theta_{vib} \ll T)}, && (6) \end{aligned}$$

The **rotational** energy is determined from the rotational partition function

$$Z_{rot} = \sum_{j=0}^{\infty} (2j+1) \exp(-j(j+1)\beta\theta_{vib})\,. \tag{7}$$

At low T only the first two terms contribution

$$Z_{rot} \simeq 1 + 3 \exp(-2\beta k_B \theta_{vib})\,. \tag{8}$$

The energy is obtained from $U_{rot} = -(\partial/\partial\beta)\ln Z_{rot}$ which gives

$$U_{rot} \simeq -\left(\frac{\partial}{\partial\beta}\right)[3\exp(-2\beta k_B\theta_{vib})] = 6k_B\theta_{vib}\exp(-2\beta k_B\theta_{vib})\,. \tag{9}$$

Hence the rotational specific specific heat is given by

$$\boxed{C_{rot} = 12k_B\left(\frac{\theta_{vib}}{T}\right)^2\exp(-2\beta k_B\theta_{vib}) \qquad (\theta_{vib} \gg T)\,.} \tag{10}$$

At high temperatures we use the summation formula given

$$\sum_{j=0}^{\infty}(2j+1)\exp(-j(j+1)\beta\theta_{vib}) = \int_{j=0}^{\infty}(2j+1)\exp(-j(j+1)\beta\theta_{vib}) + \tfrac{1}{2} + \tfrac{1}{12}f'(0) + \cdots + \ldots\,, \tag{11}$$

where $f(x) = (2x+1)\exp(-x(x+1)\beta\theta_{vib})$. The integral gives

$$\int_0^{\infty}(2j+1)\exp(-j(j+1)\beta\theta_{vib})\,dj = \frac{T}{\theta_{vib}}\,. \tag{12}$$

We are interested region where $T \gg \theta_{vib}$ where the integral is much larger than the constant $1/2$ in Eq. (11). Furthermore $f'(0)$ has a piece which is independent of β (and hence is also negligible compared with the integral) and a piece of order $\theta_{vib}\beta$ which is even smaller. Hence, at high T the sum is given, to a good approximation, by the integral. This gives

$$U_{vib} \simeq -\left(\frac{\partial}{\partial\beta}\right)\ln\left(\frac{T}{\theta_{vib}}\right) = k_BT\,. \tag{13}$$

Hence the specific heat is given by

$$\boxed{C_{vib} = k_B \qquad (\theta_{vib} \ll T)\,.} \tag{14}$$

The specific heat in the regions specified in the question can then be obtained by combining the above boxed expressions.

i) a) $k_x = \frac{\pi}{L} n_x$, $k_y = \frac{\pi}{L} n_y$, $k_z = \frac{\pi}{L} n_z$

$$D(k)dk^2 = \frac{L^3}{2\pi^2} k^2 dk \qquad k_x, k_y, k_z \geq 0$$

$$\epsilon = \frac{\hbar^2 k^2}{2m} \qquad k^2 = \frac{2m\epsilon}{\hbar^2}$$

$$d\epsilon = \frac{\hbar^2}{m} k\,dk = \frac{\hbar^2}{m}\sqrt{\frac{2m\epsilon}{\hbar^2}}\, dk$$

$$dN(\epsilon)d\epsilon = \frac{V(2m)^{3/2}}{4\pi^2\hbar^3} \epsilon^{1/2} d\epsilon \qquad V = L^3$$

$$D(\epsilon)d\epsilon = \frac{L^3(2m)^{3/2}}{4\pi^2\hbar^3} \epsilon^{1/2} d\epsilon$$

b) $Z = 1 + e^{-(\epsilon(\vec{k}) - \mu)\beta} + e^{-2(\epsilon(\vec{k}) - \mu)\beta)} + \cdots$

$$Z = \frac{1}{1 - e^{-(\epsilon(\vec{k}) - \mu)\beta}}$$

c) $\phi_\epsilon = k_B T \ln(1 - e^{-(\epsilon - \mu)\beta})$

$$n(\vec{k}) = -\left(\frac{\partial \phi}{\partial \mu}\right)_{T,V} = \frac{1}{e^{(\epsilon-\mu)\beta} - 1}$$

d) suppose $\mu > 0$

for $T \to 0$, $n(0) < 0 \Rightarrow \mu \geq 0$

e) $$N = \frac{V}{2\pi^2}\int_0^\infty \frac{k^2 dk}{e^{(\epsilon(\vec{k}) - \mu)\beta} - 1}$$

as T is lowered, $\mu \to 0$ at T_c

$$N = \frac{V}{2\pi^2}\int_0^\infty \frac{k^2 dk}{e^{\epsilon(\vec{k})\beta_c} - 1} \qquad \text{let } x^2 = \frac{\hbar^2}{2m} k^2 \beta_c$$

$$\beta_c = \frac{1}{k_B T_c}$$

$$N = \frac{V}{2\pi^2}\left(\frac{2m k_B T_c}{\hbar^2}\right)^{3/2} \int_0^\infty \frac{x^2 dx}{e^{x^2} - 1}$$

$$k_B T_c = 3.31 \frac{\hbar^2}{m}\left(\frac{N}{V}\right)^{2/3} = 3.31 \frac{\hbar^2}{m} \rho^{2/3}$$

note: will need value of integral.

$$\int_0^\infty \frac{z^{1/2}dz}{e^z-1} = 2\int_0^\infty \frac{x^2dx}{e^{x^2}-1} = 2.315$$

on cheat sheet or in probl.

1. $$H = -\frac{J}{2}\sum_{\langle ij\rangle} \vec{S}_i\cdot\vec{S}_j \qquad \vec{S}_i = \pm\hat{i}, \pm\hat{j}$$

$$\doteq - \sum_i \vec{S}_i\cdot\vec{h} \qquad \vec{h} = \langle \vec{S}_i\rangle J\nu, \quad \nu = 6$$

take $\vec{h} \parallel \hat{i}$ (symmetry is broken in any of the 4 directions)

$$\langle S_x\rangle = \frac{1\cdot e^{\beta h} + 2\cdot 0\cdot e^{0} - 1\cdot e^{-\beta h}}{Z}, \quad Z = e^{\beta h} + 2e^{0} + e^{-\beta h}$$

$$= \frac{2\sinh\beta h}{2\cosh\beta h + 2} = \frac{\sinh(\beta h)}{\cosh(\beta h) + 1}$$

(a) For small h: $$\langle S_x\rangle \doteq \frac{\beta h + \frac{1}{3!}(\beta h)^3}{2 + \frac{(\beta h)^2}{2!}}$$

$$= \frac{\beta h}{2}\,\frac{\left(1 + \frac{(\beta h)^2}{6}\right)}{1 + \frac{(\beta h)^2}{4}} = \frac{\beta h}{2}\left(1 - \frac{1}{12}(\beta h)^2\right)$$

So linearizing: $\langle S_x\rangle = \frac{\beta_c h}{2} = \frac{\beta_c J\nu}{2}\langle S_x\rangle$

$$\Rightarrow \beta_c = \frac{2}{J\nu} \Rightarrow T_c = \frac{J\nu}{2} = 3J$$

1. Cont'd

close to T_c:

$$\langle S_x \rangle = \frac{\beta \langle S_x \rangle J \nu}{2} \left(1 - \frac{1}{12} \left(\beta \langle S_x \rangle J \nu \right)^2 \right)$$

$$\Rightarrow 1 = \beta T_c \left(1 - \frac{1}{3} (\beta T_c)^2 \langle S_x \rangle^2 \right)$$

$$1 - \frac{1}{3} (\beta T_c)^2 m^2 = \frac{1}{\beta T_c} \Rightarrow m^2 \doteq \left(1 - \frac{1}{\beta T_c} \right) \cdot \frac{3}{(\beta T_c)^2}$$

$$\therefore \quad m = \pm \sqrt{3(1 - T/T_c)} \quad \text{for } T \text{ close to } T_c \quad T < T_c$$

$$0 \quad \text{for } T > T_c$$

2006
STATISTICAL MECHANICS
(Turn in 2 out of 3 Problems)

INSTRUCTIONS:

DO EACH PROBLEM ON SEPARATE PAPER.

WRITE YOUR NAME, SECTION, PROBLEM# ON EACH SHEET YOU TURN IN.

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

Qualifying Exam 06

Statistical Mechanics Problem 1

Consider the following Landau expansion for a material undergoing a phase transition with order parameter m:

$$F(m) = a(T) + \frac{1}{2}b(T)\,m^2 - \frac{1}{3}c\,m^3 + \frac{1}{4}d\,m^4 + \cdots\ , \tag{1}$$

where $c > 0, d > 0$ and

$$b(T) = \alpha\,(T - T^{\star}).$$

(a) Explain why the transition is first order *i.e.* m vanishes discontinuously.
Note: You should sketch the free energy versus m for different temperatures, one of which (clearly marked) should be the transition temperature T_c, and another of which should be at $T^{\star}$.

(b) Determine the value of m as T approaches T_c from below, assuming that this value is small so higher terms in the Landau expansion than those shown explicitly in Eq. (??) can be neglected.

(c) Show that

$$T_c - T^{*} = \frac{2c^2}{9\alpha\,d}\ .$$

Qualifying Exam 06

Statistical Mechanics Problem 2

Consider the nearest-neighbor Ising model in one dimension in a magnetic field h, which has Hamiltonian

$$\mathcal{H} = -J\sum_{i=1}^{N} S_i S_{i+1} - h\sum_{i=1}^{N} S_i,$$

where J is the nearest-neighbor interaction. Periodic boundary conditions are applied, so $S_{N+1} = S_1$.

(a) Using the method of transfer matrices, or otherwise, compute the magnetization $m \equiv \langle S_i \rangle$. (Assume $N \to \infty$.)

(b) Show that for small h,

$$m = \chi h,$$

where the susceptibility χ is given by

$$\chi = \frac{1}{k_B T} \exp\left(\frac{2J}{k_B T}\right).$$

Qualifying Exam 06

Statistical Mechanics Problem 3

A tall vertical cylinder contains a monoatomic classical ideal gas of N molecules of ma in a gravitational field near the surface of the earth.

(a) Show that the pressure in the cylinder at height z is given by

$$P(z) = P_0 \exp\left(-\frac{mgz}{k_B T}\right).$$

(b) A piston of mass M is initially clamped at a height h_0 from the bottom of the cyli The whole system is in equilibrium at temperature T_i, and the volume above the p is a vacuum. The clamp is released, and a new equilibrium is eventually establi Calculate the final height h of the piston and the amount of heat Q provided t system, if it is maintained at constant temperature T_i.

(c) Now assume that the system is thermally insulated. Derive two equations implicitly give the final height h and the final temperature T_f.
Note: You are not required to solve these equations.

1 SM#2
Solution

Solution

Calculate the partition function

$$Z = \sum_{S_1 \ldots S_N} e^{-\beta H} \tag{2}$$

by making the change of variables to the new set: $\sigma = S_i S_{i+1}$, $i = 1, 2, \ldots, N-1$ and S_1. Expressing H in terms of these variables gives:

$$H = -\sum_{i=1}^{N} J_1 \sigma_i + J_2 \sigma_i \sigma_{i+1} \tag{3}$$

which is equivalent to a nearest neighbor Ising model in an external field, where the coupling is J_2 and the external field (h) is J_1.

The calculation of $< S_i S_{i+1} >$ now becomes equivalent to calculating $< \sigma >$, that is, the average magnetization.

This is a standard problem solved in most graduate books on stat mech. The transfer matrix technique is probably the easiest way to calculate Z. Once that is obtained, $< \sigma_i >$ is obtain by differentiation:

$$< \sigma_i >= \frac{1}{N} < \sum_{i=1}^{N} \sigma_i >= T \frac{\partial \log Z}{\partial T} = \frac{\sinh(\beta J_1) + \frac{\sinh(\beta J_1)\cosh(\beta J_1)}{\sqrt{\sinh^2(\beta J_1) + \exp(-4\beta J_2)}}}{\cosh(\beta J_1) + \sqrt{\sinh^2(\beta J_1) + \exp(-4\beta J_2)}} \tag{4}$$

Qualifying Exam 06

Statistical Mechanics Problem 3: Solution

(a) *If the number of molecules per unit volume is* $n(z)$ as a function of the height z, we have

$$dP/dz = -nmg.$$

Also, the ideal gas law is

$$P(z) = n(z)k_BT.$$

Combining these last two expressions and solving gives

$$\boxed{P(z) = P_0 \exp[-mgz/(k_BT)].} \tag{1}$$

(b) If the area of the cylinder is A, we know that, to balance the forces on the piston,

$$P(h) = Mg/A.$$

Also,

$$\int_0^h P(z)dz = k_BT_i \int_0^h n(z)dz = k_BT_iN/A.$$

Integrating Eq. (??) with respect to z and eliminating P_0 gives

$$P(h)(k_BT_i/mg)\{\exp[mgh/(k_BT_i)] - 1\} = k_BT_iN/A.$$

It follows that

$$\boxed{\exp[mgh/(k_BT_i)] - 1 = Nm/M,}$$

which gives h.

Since the internal energy of the gas is unchanged, the heat supplied is just the work done to change the height of the piston.

$$\boxed{Q = Mg(h - h_i).}$$

(c) In this case, all the initial steps are the same as the previous case, except that T_i is replaced by T_f. Therefore

$$\boxed{\exp[mgh/(k_BT_f)] - 1 = Nm/M.}$$

Since no heat is supplied, the change in potential energy of the piston plus the change in the internal energy of the gas is zero, so

$$\boxed{Mg(h - h_i) + (3/2)Nk_B(T_f - T_i) = 0.}$$

These two equations implicitly give T_f and h.

Qualifying Exam 06

Statistical Mechanics Problem 1 : Solution

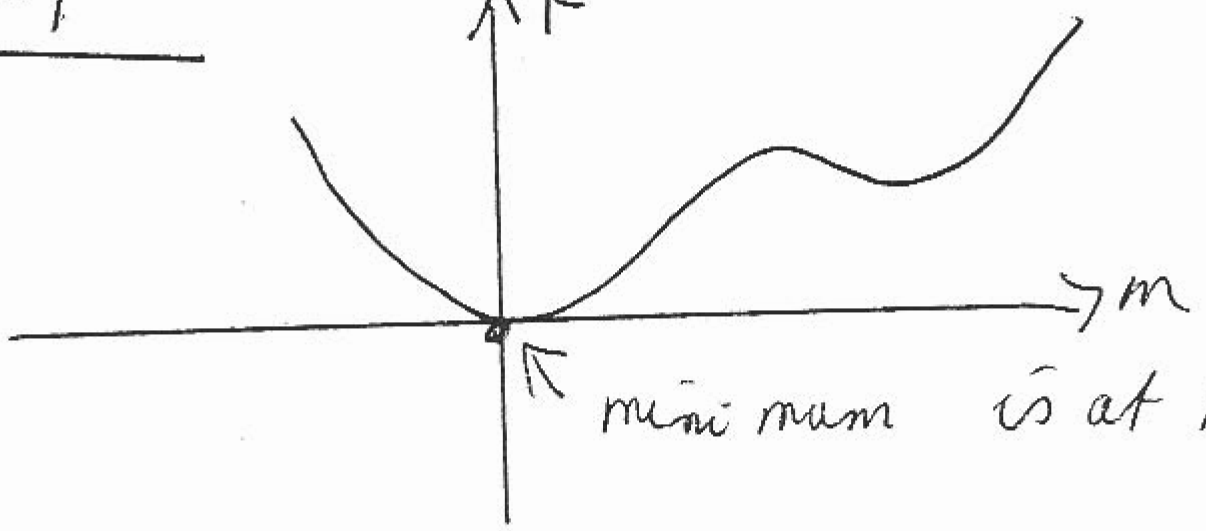
1/ $F(m) = a(T) + \frac{1}{2} b(T) m^2 - \frac{c}{3} m^3 + \frac{d}{4} m^4 + \dots$

where $b(T) = \alpha(T - T^*)$

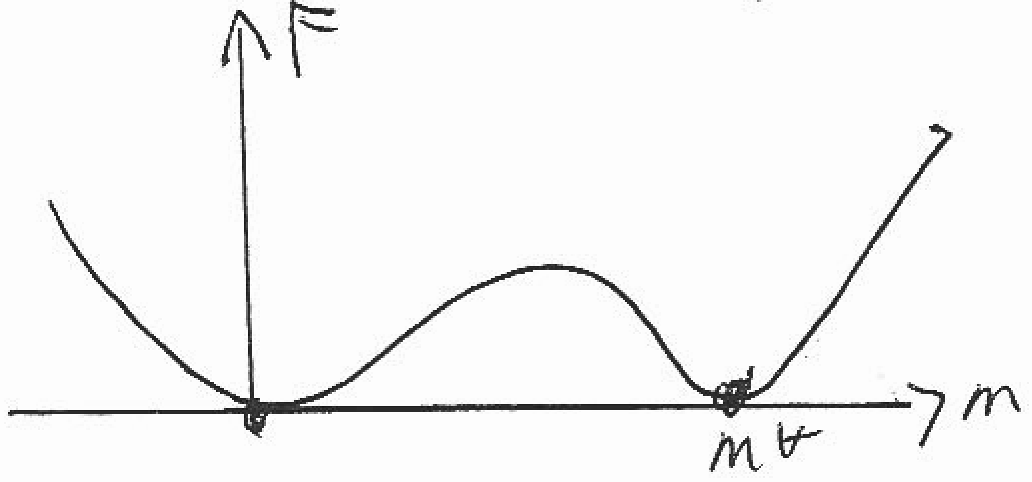
let $\hat{F}(m) = F(m) - a(T)$

(a) ↑ smooth part which does not play a role.

- At high-T



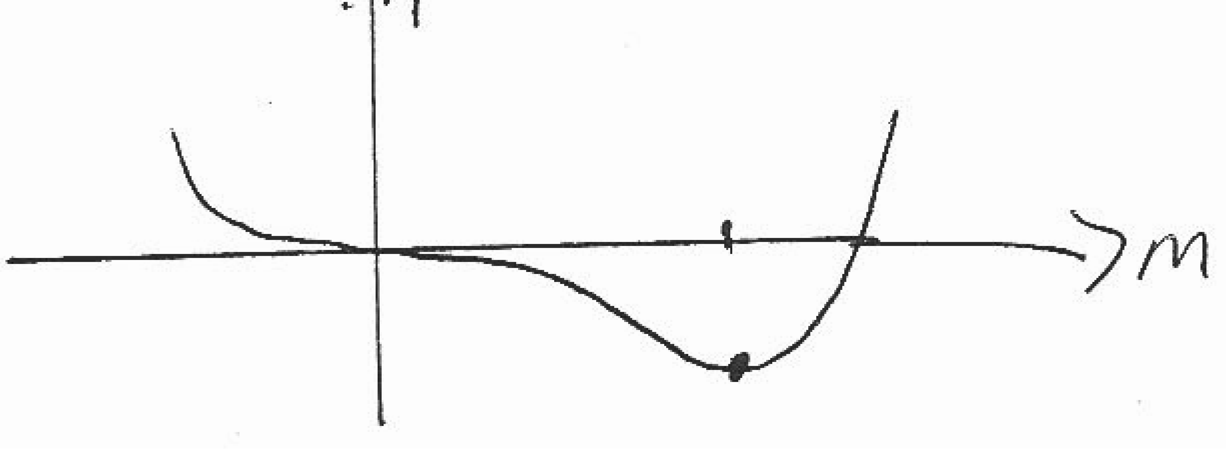
- As T is lowered the 2nd minimum will hit the axis



$T = T_c$

This is T_c because the minimum at $m = m^*$ has the same free energy that at $m = 0$

- As T is lowered further the minimum at non-zero m is the lowest. T^* is where the curvature of $m=0$ vanishes.



$T = T^*$

(b) m^* is determined by $\left.\frac{\partial \tilde{F}}{\partial m}\right|_{m^*} = \tilde{F}(m^*) = 0$, i.e.

$$\alpha (T_c - T^*) m^* - c m^{*2} + d m^{*3} = 0 \qquad ①$$

$$\frac{\alpha}{2} (T_c - T^*) m^{*2} - \frac{c}{3} m^{*3} + \frac{d}{4} m^{*4} = 0 \qquad ②$$

$$① \div m^* \Rightarrow \alpha (T_c - T^*) = c m^* - d m^{*2} \qquad ③$$

$$2 \times ② \div (m^*)^2 \Rightarrow \alpha (T_c - T^*) = \frac{2}{3} c m^* - \frac{d}{2} m^{*2} \qquad ④$$

$$③ - ④ \quad \frac{1}{3} c m^* - \frac{d}{2} m^{*2} = 0$$

$$\Rightarrow m^* = \frac{2c}{3d}$$

(c) Substitute into ③

$$\alpha (T_c - T^*) = \frac{2}{3} \frac{c^2}{d} - \frac{4}{9} \frac{c^2}{d} = \frac{2}{9} \frac{c^2}{d}$$

FALL 2007
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 (SM), PROBLEM #, AND PAGE # ON EACH SHEET YOU TURN IN.

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

YOU MAY USE A CALCULATOR, BUT THE USE OF IPODS, MP3 PLAYERS, AND CELL PHONES IS NOT PERMITTED.

Qualifying Exam 07

Statistical Mechanics Problem 1

Consider the spin-1 Ising model

$$\mathcal{H} = -\sum_{\langle i,j \rangle} J_{ij} S_i S_j,$$

in which the spins S_i take values $1, 0$ and -1. The interactions J_{ij} are equal to 1 if i and j are nearest neighbors and 0 otherwise. Assume the spins lie on a simple cubic lattice (i.e. there are 6 neighbors).

1. Find the transition temperature, T_c, in the mean field approximation.
   Note: You may assume that the transition is continuous.

2. Show that just below T_c, the magnetization per spin, $m \equiv \langle S_i \rangle$, varies as

   $$m \propto (T_c - T)^\beta ,$$

   and determine β.

Statistical Mechanics (2007): Solution #1

1. We consider the spin–1 Ising model

$$\mathcal{H} = -\sum_{\langle i,j \rangle} J_{ij} S_i S_j,$$

in which the spins S_i take values 1, 0 and -1. The interactions J_{ij} are equal to 1 if i and j are nearest neighbors and 0 otherwise. The spins have 6 neighbors.

(a) In the mean field approximation the instantaneous field acting on spin i,

$$H_i = \sum_j J_{ij} S_j,$$

is replaced by its average value $H_i \to \sum_j J_{ij} \langle S_j \rangle = \sum_j J_{ij} m = 6m$, where $m \equiv \langle S_j \rangle$ is the magnetization per site (the same for all sites by symmetry). The effective Hamiltonian for site i is then $-H_i S_i$ which gives the self-consistent expression for the magnetization

$$m = \frac{e^{6\beta m} - e^{-6\beta m}}{e^{6\beta m} + 1 + e^{-6\beta m}} = \frac{2 \sinh 6\beta m}{1 + 2\cosh 6\beta m}. \qquad (1)$$

⑥

Assuming that the transition is continuous, it occurs when $m \to 0$. Expanding the RHS gives

$$m = \frac{12\beta m}{3},$$

which gives

$$\boxed{k_B T_c = 4\,.}$$

(b) Expanding Eq. (1) in powers of m gives

$$m = \frac{12\beta m\left[1 + (6\beta m)^2/6 + \cdots\right]}{1 + 2\left[1 + (6\beta m)^2/2 + \cdots\right]} = 4\beta m\left[1 - 6(\beta m)^2 \cdots\right]\,.$$

Noting that T is close to T_c, we can write this, to leading order in $T_c - T$, as

$$m\left(\frac{T_c}{T} - 1\right) = 24(\beta_c m)^3\,.$$

④

Dividing by m we get

$$\boxed{m^2 \propto (T_c - T)\,,}$$

so

$$\boxed{\beta = 1/2\,.}$$

Qualifying Exam 07

Statistical Mechanics Problem 2

Consider an infinite parallel plate capacitor in which the plates are perpendicular to the x axis and located at $x = \pm L$. It is filled with a solution consisting of an equal number of positive and negative ions of charge $\pm q$. The average number of positive ions per unit volume is n_0. The capacitor is in equilibrium at a temperature T. The voltage difference between the plates is V_0.

Find the density of positive and negative ions $n_{\pm}(x)$ as a function of x. Assume that $qV_0 \ll k_B T$.

Note: You will need to use statistical mechanics to obtain the density of the positive and negative ions in terms of the potential $V(x)$. You will then need to use electrostatics to relate the potential to the net charge density.

Solution #2

2. Let us choose $V(\pm L) = \pm\frac{1}{2}V_0$ so, by symmetry, $V(x)$ is an odd function of x. The density of positive/negative ions is given in terms of the potential by

$$n_\pm(x) = n_0 \exp[\mp\beta q V(x)] \approx n_0[1 \mp \beta q V(x)], \tag{2}$$

where the prefactor can be seen to be n_0 because the average over x of the last expression is then equal to n_0.

Next we use Poisson's equation to relate the charge density, $n_+(x) - n_-(x)$, to the potential,

$$\frac{d^2V}{dx^2} = -\frac{q}{\epsilon_0}(n_+ - n_-) \approx \frac{2\beta q^2 n_0}{\epsilon_0}V, \tag{3}$$

where we noted that V only depends on x. The solution to this equation with the required boundary conditions is

$$V(x) = \frac{1}{2}V_0\frac{\sinh\kappa x}{\sinh\kappa L}, \tag{4}$$

with $\kappa^2 = 2\beta q^2 n_0/\epsilon_0$. Therefore

$$\boxed{n_\pm(x) \approx n_0\left[1 \mp \frac{1}{2}\beta q V_0 \frac{\sinh\kappa x}{\sinh\kappa L}\right].} \tag{5}$$

Qualifying Exam 07

Statistical Mechanics Problem 3

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

1. Calculate the exact number of allowed configurations $\Gamma(N, m)$ of the particles and thus the total entropy $S_{\text{tot}} = k_B \ln \Gamma(N, m)$.
2. Consider a subset of n lattice sites with $n^2 \ll N - m$. What is the natural log of the probability that these sites will *all* be unoccupied?

   Note: For this part you should also assume $N - m \gg 1$, and use Stirling's approximation in the form $\ln(k!) = k \ln k - k$ for $k \gg 1$. Your final answer should have a linear dependence on n.

Solution #3

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

4 tot

$$\Gamma(N,m) = \frac{N!}{(N-m)!m!} \tag{6}$$

so

$$\boxed{S_{tot} = k_B \ln(\frac{N!}{(N-m)!m!}).} \tag{7}$$

(b) The probability that a state will have all n sites unoccupied is

6 tot

$$P_n = \frac{\Gamma(N-n,m)}{\Gamma(N,m)} \tag{8}$$

← +3

so

$$\ln P_n = \ln\left(\frac{\Gamma(N-n,m)}{\Gamma(N,m)}\right) = \ln\left(\frac{N-n)!}{(N-m-n)!m!}\frac{(N-m)!m!}{N!}\right). \tag{9}$$

We can regroup this as

$$\ln P_n = \ln\frac{(N-n)!}{N!} + \ln\frac{(N-m-n)!}{(N-m)!} \tag{10}$$

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:

$$\ln P_n \approx -n\ln N + n\ln(N-m) = \boxed{n\ln\left(\frac{N-m}{N}\right).} \tag{11}$$

← +3

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 $n^2/N \ll 1$. Hence this is a legitimate expansion.

Note: The answer is easily understood by noting that the probability of a site being empty is $\frac{N-m}{N}$, and, for $n \ll N-m$, these probabilities are all statistically independent, so the probability that all n sites are empty is $(\frac{N-m}{N})^n$.

FALL 2008
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 (SM), PROBLEM #, AND PAGE # ON EACH SHEET YOU TURN IN.

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

YOU MAY USE A CALCULATOR, BUT THE USE OF IPODS, MP3 PLAYERS, AND CELL PHONES IS NOT PERMITTED.

Qualifying Exam 08

Statistical Mechanics. Problem 1

Consider a cube of width L with a piston of zero thickness dividing the inside into two isolated chambers. Both the left and the right hand side are each filled with N non-interacting fermions. The ones on the left are spin 3/2 particles, but the ones on the right are spin 1/2 particles, and both gases are at the same temperature.

1. State the condition for thermodynamic equilibrium.
2. Consider the very high temperature (classical) limit. What is the the average position of the piston l (measured from the left side of the box).
3. Now consider the limit of zero temperature. Find the Fermi momentum and the Fermi energy on both sides of the container. The side lengths are assumed large so that the energy levels form a continuum.
4. Still in the limit of zero temperature, calculate the average position of the piston l (measured from the left side of the box).

Note: Ignore relativistic effects.

Solution

1. The pressures are equal.

2. In the limit of infinite temperature, the behavior is classical, so the number of the internal states of the particles is irrelevant and the pressure of the gas as a function of density and temperature is independent of the spin. Therefore the position of the piston is $L/2$.

3. The number of internal states of a particle is $g = 2S + 1$, where S is the spin. g states will be occupied for each point in k-space. The ratio of the degeneracy of the spin 3/2 to spin 1/2 particles is $g_1/g_2 = 2$.

   Because for a free particle the kinetic energy $= p^2/2m \propto k^{-2}$, the Fermi energy $E_F \propto l^{-2}$ where l is the width of the region containing the gas.

   Also the Fermi energy should only depend on density, $E_F = f(\rho)$ but the g-fold degeneracy due to internal degrees of freedom, will lower the above density by a factor $1/g$, in other words $E_F = f(\rho/g)$. Since ρ scales as N/l^3, $E_F = \tilde{f}((N/g)/l^3)$, but from above is also $\propto 1/l^2$ implying $f(x) \propto x^{2/3}$.

   Hence
   $$E_{tot} = KN\left(\frac{N}{V}\right)^{2/3} g^{-2/3},$$
   where K is a prefactor of no interest to this calculation.

   Alternatively The density of states is equal to $CVg\epsilon^{1/2}$, where C is an unimportant constant and V is the volume. Hence the Fermi energy is given by
   $$N = C'Vg\epsilon_F^{3/2}$$
   The total energy is given by
   $$CVg\int_0^{\epsilon_F} \epsilon^{1/2}\epsilon\, d\epsilon = C''Vg\epsilon_F^{5/2} \propto N^{5/3}/(Vg)^{2/3},$$
   in agreement with above.

4. Therefore the pressure
   $$P = -\frac{\partial E_{tot}}{\partial V} = K(2/3)(N/V)^{5/3}g^{-2/3}$$

Equating the pressure on the two sides:

$$l^{-5/3}{g_1}^{-2/3} = (L - l)^{-5/3}{g_2}^{-2/3}$$

so that

$$l = \frac{L}{(g_1/g_2)^{2/5} + 1} = \frac{L}{2^{2/5} + 1}$$

Qualifying Exam 08

Statistical Mechanics. Problem 2

Consider a three-dimensional gas of ideal spinless non-relativistic bosons at a given pressure P and temperature T. The bosons can be absorbed 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 treated classically, and assumed to be in equilibrium with the (ideal) quantum two-dimensional adsorbed gas.

1. State the condition for thermodynamic equilibrium between the two gases.
2. Calculate the Grand potential Ω of the classical 3-d gas and hence obtain its chemical potential in terms of P and T.
3. Determine the surface density of the 2-d gas in terms of the temperature and its chemical potential.
4. Hence compute the surface density in the layer as a function of P and T.

Note: You may find the result

$$\int_0^\infty \frac{dx}{a\exp[x]-1} = -\ln(1-1/a)$$

to be useful.

SOLUTION:

1. Since the two gases are in equilibrium and can exchange particles and energy, they are at the same temperature and chemical potential.

2. Let the chemical potential be μ. Then, for the classical 3d gas the grand partition function is

$$\sum_N \exp[\beta\mu N]\frac{V^N}{(2\pi\hbar)^{3N}}\frac{1}{N!}\left(\int \exp[-\beta p^2/(2m)]dp_x dp_y dp_z\right)^N = \exp[e^{\beta\mu}(Vmk_BT/2\pi\hbar^2)^{3/2}]. \tag{1}$$

Since $\Omega \equiv -PV = -k_BT \ln Z_{gr}$ we have

$$\Omega \equiv -PV = -Ve^{\beta\mu}k_BT\left(\frac{mk_BT}{2\pi\hbar^2}\right)^{3/2}, \tag{2}$$

and hence

$$e^{\beta\mu} = \frac{P}{k_BT}\left(\frac{2\pi\hbar^2}{mk_BT}\right)^{3/2}. \tag{3}$$

3. Also, in terms of the chemical potential and temperature, the number of particles in the two dimensional layer is

$$N_{2d} = \frac{1}{(2\pi)^2}\frac{A}{\hbar^2}\int \frac{1}{\exp\beta(\epsilon-\epsilon_0-\mu)-1}dp_x dp_y, \tag{4}$$

where $\epsilon = (p_x^2+p_y^2)/2m$. Replacing the double integral with $2\pi p dp = 2\pi m d\epsilon$, the surface density is

$$n_{2d} \equiv \frac{N_{2d}}{A} = \frac{mk_BT}{2\pi\hbar^2}\ln\frac{1}{1-e^{\beta\epsilon_0}e^{\beta\mu}}. \tag{5}$$

4. Substituting for $e^{\beta\mu}$ from Eq. (3) this gives the surface density in terms of the temperature and pressure.

Qualifying Exam 08

Statistical Mechanics. Problem 3

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

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

The spins $\mathbf{S}_i$ are unit vectors that can point along each of the six axis directions, $\pm\hat{\imath}$. $\pm\hat{\jmath}$, and $\pm\hat{k}$. The sum is over nearest neighbors, with each distinct nearest neighbor pair being counted once.

Treat this problem using the mean field approximation, and *assume* that the transition is continuous (second order).

1. Calculate the phase transition temperature.
2. Show that the magnetization varies as

   $$m \propto (T_c - T)^{1/4}$$

   close to the phase transition.

   Note: In case you are concerned about the result, the power 1/4 is unusual and comes from a cancellation of factors for this particular model.

Qualifying Exam 08

Statistical Mechanics. Problem 3 **Solutions**

The Hamiltonian is given by

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

where the spins $\mathbf{S}_\mathrm{i}$ are unit vectors that can take the values $\pm\hat{\imath}$, $\pm\hat{\jmath}$ and $\pm\hat{k}$.

1. The part of the Hamiltonian involving $\mathbf{S}_i$ is

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

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

   $$\mathbf{H}_i = J \sum_j \mathbf{S}_j \, , \qquad (2)$$

   where the sum is over the z neighbors of i ($z = 6$ here). In the mean field approximation we replace the spins in Eq. (2) by their average values so

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

   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 six directions. Let us suppose this is $\hat{\imath}$. Hence $\langle S_x \rangle$ is given self consistently by

   $$\begin{aligned} \langle S_x \rangle &= \frac{1 \cdot e^{\beta H} + 4 \cdot 0 \cdot e^0 + (-1) \cdot e^{-\beta H}}{e^{\beta H} + 4 \cdot e^0 + e^{-\beta H}} \\ &= \frac{2 \sinh \beta H}{2 \cosh \beta H + 4} = \frac{\sinh \beta H}{\cosh \beta H + 2} \, , \end{aligned}$$

   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

   $$\langle S_x \rangle = \frac{\beta H + \frac{1}{3!}(\beta H)^3 + \cdots}{3 + \frac{1}{2!}(\beta H)^2 + \cdots} \simeq \frac{\beta H}{3} \left(1 - O(\beta H)^4\right) \, , \qquad (3)$$

where the expected leading correction on the RHS (of order $(\beta H)^3$) vanishes. At T_c the terms linear in βH on both sides are equal so

$$\langle S_x\rangle = \frac{\beta_c H}{3} = 2\beta_c J\langle S_x\rangle$$

which gives

$$\boxed{k_B T_c = 2J\,.}$$

2. Eq. (3) can be written

$$\langle S_x\rangle = \frac{\beta z J\langle S_x\rangle}{2}\left(1 - \text{const.}\,(\beta z J\langle S_x\rangle)^4\right)\,.$$

Dividing out $\langle S_x\rangle$ gives

$$1 = \left(\frac{T_c}{T}\right)\left(1 - \text{const.}'\,\langle S_x\rangle^4\right)\,.$$

This can be written

$$\langle S_x\rangle^4 = \text{const.}''\left(1 - \frac{T}{T_c}\right)\,,$$

or

$$\boxed{\langle S_x\rangle \propto (T_c - T)^{1/4}\,.}$$

Note: The power is 1/4 rather than the expected 1/2 because the expected leading correction to the RHS of Eq. (3), of order $(\beta H)^3$, happens to have zero coefficient for this model.

FALL 2009
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 (SM), PROBLEM #, AND PAGE # ON EACH SHEET YOU TURN IN.

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

YOU MAY USE A CALCULATOR, BUT THE USE OF IPODS, MP3 PLAYERS, AND CELL PHONES IS NOT PERMITTED.

Qualifying Exam 09

Statistical Mechanics. Problem 1

---

1. The pressure P and energy density ρ of a particle species in thermal equilibrium at a temperature T in the early Universe can be expressed as the following integrals in momentum space, in units where $\hbar = 1$, and where $E^2(p) = |\vec{p}|^2 + m^2$ and g indicates the number of internal degrees of freedom:

$$P = g \int \frac{\mathrm{d}^3|\vec{p}|}{(2\pi)^3} f(\vec{x},\vec{p}) \frac{|\vec{p}|^2}{3E(p)}, \qquad \rho = g \int \frac{\mathrm{d}^3|\vec{p}|}{(2\pi)^3} f(\vec{x},\vec{p}) E(p) \tag{1}$$

and where the equilibrium distributions for bosons and fermions are, respectively,

$$f_B = \frac{1}{e^{(E-\mu)/T} - 1}, \qquad f_F = \frac{1}{e^{(E-\mu)/T} + 1}, \tag{2}$$

with μ the chemical potential.

   (a) Cast the expressions for P and ρ in eq. (1) as integrals over E, with the appropriate extrema of integration.

   (b) Show that $P = \rho/3$ in the relativistic limit ($T \gg m$), independently of whether the particle species is bosonic or fermionic

   (c) In the limit where $T \gg \mu$, calculate $\mathrm{d}P/\mathrm{d}T$ and show that

$$\frac{\mathrm{d}P}{\mathrm{d}T} = \frac{\rho + P}{T}. \tag{3}$$

   [Suggestion: show that $\mathrm{d}f/\mathrm{d}T = -(E/T)\mathrm{d}f/\mathrm{d}E$ *and integrate by parts the resulting integral over* E *defining* P.*]*

   (d) Consider the following expression that defines the differential of the entropy $S(V,T)$ as

$$\mathrm{d}S(V,T) = \frac{1}{T}\Big[\mathrm{d}\left(\rho(T)V\right) + P(T)\mathrm{d}V\Big]. \tag{4}$$

   Identify the coefficient functions multiplying $\mathrm{d}T$ and $\mathrm{d}V$ with the general form of the differential

$$\mathrm{d}S(V,T) = \frac{\partial S(V,T)}{\partial V}\mathrm{d}V + \frac{\partial S(V,T)}{\partial T}\mathrm{d}T \tag{5}$$

   and show that the integrability condition (equality of the mixed derivatives)

$$\frac{\partial^2 S(V,T)}{\partial V \partial T} = \frac{\partial^2 S(V,T)}{\partial T \partial V} \tag{6}$$

   is equivalent to eq. (3).

Qualifying Exam 09

Statistical Mechanics. Problem 1. Solution

---

1. (a) Since $2E\mathrm{d}E = 2|\vec{p}|\mathrm{d}|\vec{p}|$ and the integrals do not depend on angles (hence $\mathrm{d}^3|\vec{p}| \rightarrow 4\pi|\vec{p}|^2\mathrm{d}|\vec{p}|$), we have

$$\rho = g\int_m^\infty \frac{4\pi E\sqrt{E^2-m^2}\mathrm{d}E}{(2\pi)^3} f(E)E = g\int_m^\infty \frac{\sqrt{E^2-m^2}}{2\pi^2} f(E)E^2\mathrm{d}E \tag{1}$$

$$P = g\int_m^\infty \frac{(E^2-m^2)^{3/2}}{6\pi^2} f(E)\mathrm{d}E \tag{2}$$

where the extrema of integration capture the range of integration for the integrals in momentum space, where $|\vec{p}|$ goes from 0 to infinity.

(b) In the relativistic limit we can set $m = 0$ in eq. (1) and immediately verify that $P = \rho/3$ independently of the distribution function

(c) We have

$$\frac{\mathrm{d}f_{F,B}}{\mathrm{d}E} = -\frac{e^{E/T}}{T(1 \pm e^{E/T})^2} \qquad \frac{\mathrm{d}f_{F,B}}{\mathrm{d}T} = \frac{e^{E/T}\ E}{T^2(1 \pm e^{E/T})^2} \tag{3}$$

hence $\mathrm{d}f/\mathrm{d}T = -(E/T)\mathrm{d}f/\mathrm{d}E$. Now,

$$\begin{aligned} \frac{\mathrm{d}P}{\mathrm{d}T} &= \frac{g}{6\pi^2}\int_m^\infty \mathrm{d}E\ (E^2-m^2)^{3/2}\left(\frac{\mathrm{d}}{\mathrm{d}T}f\right)\mathrm{d}E = -\frac{g}{6\pi^2}\int_m^\infty \mathrm{d}E\ (E^2-m^2)^{3/2}\frac{E}{T}\frac{\mathrm{d}f}{\mathrm{d}E} \\ &= \frac{g}{6\pi^2\,T}\int_m^\infty \mathrm{d}E\ \frac{\mathrm{d}}{\mathrm{d}E}\left((E^2-m^2)^{3/2}E\right)f(E) \\ &= \frac{g}{6\pi^2\,T}\int_m^\infty \mathrm{d}E\ \left((E^2-m^2)^{3/2} + 3E^2\sqrt{E^2-m^2}\right)f(E) = \frac{P+\rho}{T} \end{aligned}$$

(d) From the identification of the coefficient functions we have

$$\frac{\partial}{\partial T}\left(\frac{1}{T}(\rho(T)+P(T))\right) = \frac{\partial}{\partial V}\left(\frac{V}{T}\frac{\mathrm{d}\rho(T)}{\mathrm{d}T}\right) \tag{4}$$

which directly gives

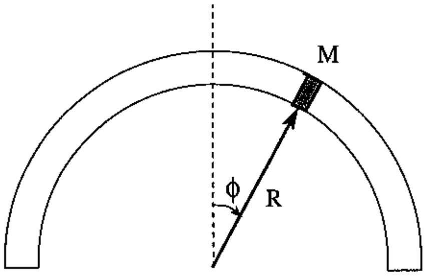
$$-\frac{\rho+P}{T^2} + \frac{1}{T}\frac{\mathrm{d}\rho}{\mathrm{d}T} + \frac{1}{T}\frac{\mathrm{d}P}{\mathrm{d}T} = \frac{1}{T}\frac{\mathrm{d}\rho}{\mathrm{d}T} \tag{5}$$

hence $\mathrm{d}P/\mathrm{d}T = (\rho+P)/T$.

Qualifying Exam 09

Statistical Mechanics. Problem 2

2. [*Alben model*]
This illustrates a second order phase transition by a mechanical model.



An airtight piston of mass m is inside a tube of cross sectional area A. The tube is bent into a semicircular shape (see Figure) of radius R. The system is kept at temperature T. On each side of the piston there is an ideal gas of N atoms. The volume of gas to the right of the piston is therefore $AR(\frac{\pi}{2}-\phi)$ and that to the left of the piston is $AR(\frac{\pi}{2}+\phi)$. You are *given* that that the free energy of an ideal gas of volume V is

$$F_{\text{ideal}} = Nk_BT\left[\ln\left(\frac{N}{V}V_Q\right)-1\right],$$

where V_Q, the "quantum volume", depends on T and the mass of the atoms, but is independent of N and V.

(a) Show that the total free energy of the system is given by

$$F = MgR\cos\phi - Nk_BT\left[\ln\left(\frac{AR(\frac{\pi}{2}+\phi)}{NV_Q}\right)+\ln\left(\frac{AR(\frac{\pi}{2}-\phi)}{NV_Q}\right)+2\right].$$

(b) By minimizing the free energy show that, at high-T, the piston is at the highest point ($\phi = 0$), but that a critical transition temperature

$$T_c = \frac{MgR\pi^2}{8Nk_B}$$

the symmetry is broken and ϕ becomes non-zero.
Note: Sketches of the free energy as a function of the angle ϕ will probably be helpful.

(c) Find the variation of ϕ with T for T slightly below T_c.

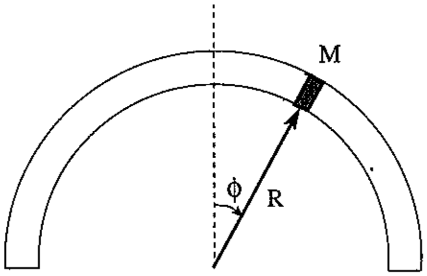
(d) Describe what happens to the phase transition if the number of atoms to the right and left side of the piston is $N(1-\delta)$ and $N(1+\delta)$ respectively.

Qualifying Exam 09

Statistical Mechanics. Problem 2. Solution

---

2. [*Alben model*]



(a) The potential energy is Mg times height $= MgR\cos\phi$. Using the expressions for the volume of the gas to the right and left of the piston, and the expression for the free energy of a gas, given in the question, the total free energy of the system is given by

$$\boxed{F = MgR\cos\phi - Nk_BT\left[\ln\left(\frac{AR(\frac{\pi}{2}+\phi)}{NV_Q}\right) + \ln\left(\frac{AR(\frac{\pi}{2}-\phi)}{NV_Q}\right) + 2\right].} \tag{1}$$

(b) Expanding the free energy in powers of ϕ assuming that ϕ is small gives

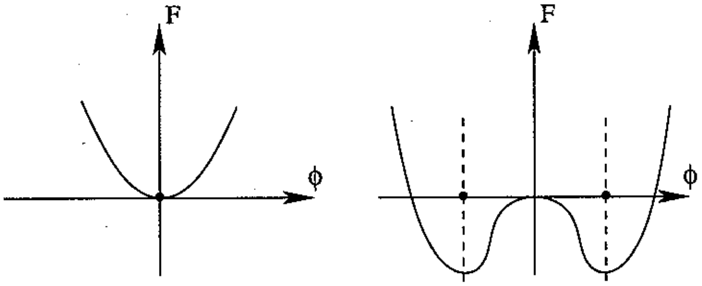
$$F = F_0 + \left(\frac{4Nk_BT}{\pi^2} - \frac{MgR}{2}\right)\phi^2 + \left(\frac{8Nk_BT}{\pi^4} + \frac{MgR}{24}\right)\phi^4 + \cdots, \tag{2}$$

where F_0 is independent of ϕ. The coefficient of the ϕ^2 term changes sign at $T = T_c$ where

$$\boxed{T_c = \frac{MgR\pi^2}{8Nk_B}.}$$

The coefficient of the ϕ^4 term is positive in the vicinity of T_c. Let's denote by C it's value at T_c, i.e.

$$C = MgR\left(\frac{1}{24} + \frac{1}{\pi^2}\right)$$



T > Tc

T < Tc

The figure shows that the minimum of the free energy is at $\phi = 0$ for $T > T_c$ and at one of two values (equal in magnitude and opposite in sign) for $T < T_c$.

(c) Neglecting the constant term F_0 we have

$$F = \frac{4Nk_B}{\pi^2}\,(T - T_c)\,\phi^2 + C\phi^4 + \cdots .$$

Minimizing for T just below T_c gives

$$\boxed{\phi^2 = \frac{2Nk_B}{\pi^2 C}\,(T_c - T)\ .}$$

(d) Equation (1) is an even function of ϕ, which is why no odd powers appear in the expansion, Eq. (2). However, if the number of atoms to the right and left side of the piston are different, $N(1-\delta)$ and $N(1+\delta)$ respectively, this symmetry is broken and odd powers will appear in the expansion, i.e.

$$F = -h\phi + A\,(T - T_c)\,\phi^2 + B\phi^3 + C\phi^4 + \cdots ,$$

where h, A, B, and C are constants. The parameters h and B are proportional to δ for small δ.

Because of the term linear in h, the equilibrium value for ϕ, obtained by minimizing the free energy, is *always* non-zero. The sharp transition is now rounded out, just as a magnetic field rounds out a transition in a magnetic system. However, if δ is small (so h is small) there will be a *rapid* increase in ϕ near T_c.

Qualifying Exam 09

Statistical Mechanics. Problem 3

---

3. Consider a triangle consisting of a single spin 1 particle interacting with two spin half particles, with the Hamiltonian

$$H = J\left[\frac{1}{2}S_1^z(\sigma_2^z + \sigma_3^z) + \sigma_2^z\sigma_3^z\right],$$

where $\sigma_j^z = \pm\frac{1}{2}$ and $S_1^z = \pm 1, 0$.

(a) Find an expression for the entropy as a function of T.

(b) Find the entropy at $T = 0$ assuming that $J > 0$.

(c) Show that the sum of the energies over all configurations vanishes. Why does it do so?

Qualifying Exam 09

Statistical Mechanics. Problem 3. Solution

---

3. (a) The twelve configurations are neatly divided into three categories: $(8, -J/4)$, $(2, J/4)$ and $(2, 3J/4)$ where (n, e) stands for the degeneracy and the energy respectively.

   Hence the free energy is given by

$$F = -k_B T \log Z = -k_B T \log\left(8e^{K/4} + 2e^{-K/4} + 2e^{-3K/4}\right),$$

   where $K = J/(k_B T)$. We get the entropy from this using $S = -\partial F/\partial T$, i.e

$$S = -\frac{J}{T}\left(\frac{2e^{K/4} - \frac{1}{2}e^{-K/4} - \frac{3}{2}e^{-3K/4}}{8e^{K/4} + 2e^{-K/4} + 2e^{-3K/4}}\right) + k_B \log\left(8e^{K/4} + 2e^{-K/4} + 2e^{-3K/4}\right). \tag{1}$$

   (b) The zero temperature entropy is $S = k_B \log(8)$ from observing that the lowest energy state has a degeneracy of 8. This result can also be obtained from Eq. (??) by taking the $T \to 0$ limit.

   (c) The sum over all energies vanishes by computation: It must do so since the trace of the Hamiltonian is zero by inspection in the basis where it is presented (i.e. summing over the spins directly).

FALL 2010
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 (SM), PROBLEM #, AND PAGE # ON EACH SHEET YOU TURN IN.

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

YOU MAY USE A CALCULATOR, BUT THE USE OF IPODS, MP3 PLAYERS, AND CELL PHONES IS NOT PERMITTED.

Qualifying Exam 2010

Statistical Mechanics. Problem 1.

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 there 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 $T^0_{ij} = 1$ for all matrix elements. The transfer matrix for $n = 1$ has $T^1_{ij} = \exp[\beta J]$ for $i = j$ and $T_{ij} = \exp[-\beta J]$ 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 $-k_BT[\ln 2 + (m/N)\ln\cosh\beta J]$. In the thermodynamic limit, this is equal to $-k_BT[\ln 2 + p\ln\cosh\beta J]$.

Qualifying Exam 2010

Statistical Mechanics. Problem 2.

---

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 condensattion at a finite temperture 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 ($N \to \infty$, $A \to \infty$, $N/A \to$ 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, $D(\varepsilon)d\varepsilon = 2\pi k dk/(2\pi/L)^2 = A k dk/(2\pi)$, 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

Statistical Mechanics. Problem 3.

---

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

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

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

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

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

$$\mathbf{H}_i = J \sum_j \mathbf{S}_j \,, \tag{3}$$

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

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

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

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

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

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

At T_c the terms linear in βH 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

$$k_B T_c = 3J \,. \tag{7}$$

(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.

$$H = 6J\langle S^x \rangle + h \,. \tag{8}$$

Using the expansion in Eq. (6) gives

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

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. Settting $T = T_c$, given by Eq. (7), we get

$$\tfrac{1}{2} h = \tfrac{1}{24} \left(2 \langle S^x \rangle \right)^3 , \tag{10}$$

and so

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

FALL 2011
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 (SM), 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, Fall 2011

Statistical Mechanics Problem 1

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

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

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 α, b and c are positive and independent of temperature T.

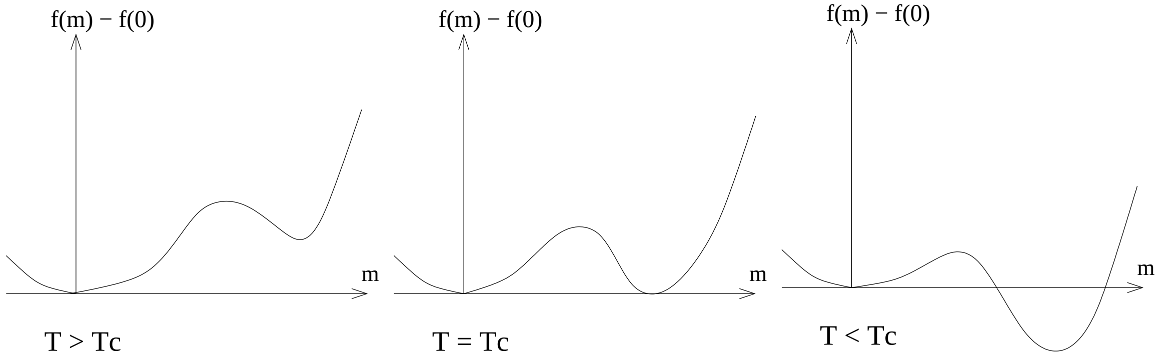
(a) Show that $m = 0$ at high T, but that there is a first order phase transtion at a temperature $T_c\,(> T_0)$ to a state with a non-zero value of m.
Note: Your answer should include sketches of f against m for (i) $T > T_c$, (ii) $T = T_c$, and (iii) $T < T_c$.

(b) Determine T_c, and the value of m for $T \to T_c^-$.

(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.

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

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

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

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

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

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 ΔS 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

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

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

Statistical Mechanics Problem 2

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 ϵ 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 $V \to \infty$?

(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 $k_BT \simeq \Delta E$ (k_B is Boltzmann's constant), since $\exp(-\Delta E/k_BT)$ 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 $k_BT \simeq \Delta E$.

Qualifying Exam Fall 2011

Statistical Mechanics. Problem 2 Solution

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 ϵ is the energy and m is the mass.

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

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

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

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

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 $V \to \infty$ $\boxed{\text{this probability tends to zero,}}$ i.e. the atom is *always un*bound.

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

$$\boxed{\frac{\Delta E}{k_BT} = \ln\left(\frac{V}{V_Q}\right).} \tag{7}$$

(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 (ΔS). 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

Statistical Mechanics Problem 3

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

Statistical Mechanics. Problem 3 Solution

(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

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

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

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

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

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

Solving,

$$h_1 = \frac{k_BT}{mg}\ln(1 + mN/M). \tag{11}$$

(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

$$U(h) = Mgh + \int_0^h \frac{\beta mgN}{A}\frac{\exp[-\beta mgz]}{1 - \exp[-\beta mgh]} mgzAdz = Mgh + Nk_BT - \frac{Nmgh}{\exp[\beta mgh] - 1}. \tag{12}$$

Using Eq.(10), we have

$$U(h_1) = Nk_BT \tag{13}$$

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

WINTER 2011
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 (SM), PROBLEM #, AND PAGE # ON EACH SHEET YOU TURN IN.

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

YOU MAY USE A CALCULATOR, BUT THE USE OF IPODS, MP3 PLAYERS, AND CELL PHONES IS NOT PERMITTED.

Winter Qualifying Exam 2010

Statistical Mechanics. Alternate Problem 1

---

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 ϵ 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 $V \to \infty$?

(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 $k_BT \simeq \Delta E$ (k_B is Boltzmann's constant), since $\exp(-\Delta E/k_BT)$ 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 $k_BT \simeq \Delta E$.

You may find the following helpful:

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

Qualifying Exam 09

Statistical Mechanics. Alternate 1. Solution

---

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 ϵ is the energy and m is the mass.

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

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

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

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

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 $V \to \infty$ $\boxed{\text{this probability tends to zero,}}$ i.e. the atom is *always un*bound.

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

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

(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 (ΔS). Hence Eq. (**??**) 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.

Winter Qualifying Exam 2010

Statistical Mechanics. Problem 2.

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 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

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

so

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

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

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

so

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

We can regroup this as

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

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:

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

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 $(\frac{N-m}{N})^n$

Winter Qualifying Exam 2010

Statistical Mechanics. Problem 3

---

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 μ, 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

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

   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

Statistical Mechanics. Problem 3. Solution

---

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 μ.

   (b) Define $\lambda = \sqrt{2\pi\hbar^2/mk_BT}$. 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
$$n_{2\mathrm{d}} = \frac{1}{\lambda^2}\int_{-\epsilon_0}^{\infty} \frac{1}{\exp[\beta(\epsilon-\mu)]-1} d(\beta\epsilon) = -\frac{1}{\lambda^2}\ln\left[1 - e^{\beta(\mu+\epsilon_0)}\right]. \tag{1}$$
   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
$$e^{\beta\mu} = \exp[\beta(U - TS + PV)/N] = \exp\left[1 - \frac{\ln Z}{N}\right] = \frac{N\lambda^3}{V} = \frac{P\lambda^3}{k_BT}, \tag{2}$$
   where we have used $U - TS = -k_BT \log Z_N$, the ideal gas law $PV = Nk_BT$, 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
$$n_{2\mathrm{d}} = -\frac{1}{\lambda^2}\ln\left[1 - \frac{P\lambda^3}{k_BT}\, e^{\beta\epsilon_0}\right].$$

Statistical Mechanics. Problem 1

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.

Statistical Mechanics. Problem 1 Solution

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

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

The heat capacity is

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

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

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

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

Statistical Mechanics. Problem 2

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.]

Statistical Mechanics. Problem 2 Solution

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.

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

Statistical Mechanics. Problem 3

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 χ, defined by

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

   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, γ, is equal 1, and C_+ is the 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 $h \to 0^+$ 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.

Statistical Mechanics. Problem 3 Solution

---

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.
$$h = a(T)m + um^3\,. \tag{4}$$
Above $T_c, m \to 0$ as $h \to 0$ so we can neglect the m^3 term. This gives
$$\chi = \frac{1}{a(T)} = \frac{1}{T_c\,\alpha}\,\frac{T_c}{(T - T_c)} = \frac{C_+}{t^\gamma} \qquad (T > T_c)\,,$$
where
$$\gamma = 1, \qquad C_+ = \frac{1}{T_c\,\alpha}\,.$$

3. Below T_c, m does not tend to zero as $h \to 0^+$. Rather, from Eq. (4), we have
$$m_{eq}^2 = -\frac{a(T)}{u}\,. \tag{5}$$
Differentiating Eq. (4) with respect to m gives
$$\chi^{-1} = a(T) + 3\,u\,m_{eq}^2 = -2a(T)\,,$$
where, to get the last equality, we used Eq. (5). Hence
$$\chi = \frac{C_-}{|t|^\gamma} \qquad (T < T_c)\,,$$
where
$$C_- = \frac{1}{2\,T_c\,\alpha}\,.$$
As a result, although C_+ and C_- individually are not universal, since they depened on the non-universal parameters T_c and α, the ratio
$$\frac{C_+}{C_-} = 2$$
is universal since it is just a number.

Statistical Mechanics. Potentially Useful Information.

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

$$\begin{aligned} dE &= TdS - PdV + \mu dN \\ F &= E - TS = -k_B T \ln Z \\ E &= \left.\frac{\partial \ln Z}{\partial(-\beta)}\right|_{V,N} \qquad\qquad \beta \equiv 1/(k_B T) \end{aligned}$$

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

Statistical Mechanics Problem 1

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 Δ 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 $\Delta \to \infty$ 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

Statistical Mechanics. Problem 1 Solution

(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 $\boxed{\text{two ground states}}$, one has $\boxed{\text{all } S_i \text{ equal to } +1}$ and the other has $\boxed{\text{all } S_i \text{ equal to } -1.}$

(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

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

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

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

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

If the transition is second order $m \to 0$ as $T \to T_c^-$, 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 $\Delta \to \infty$ the exponentials are very large and we get $\boxed{k_B T_c = zJ}$, the usual result for the Ising model.

Qualifying Exam, Winter 2012

Statistical Mechanics Problem 2

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 ϵ_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

Statistical Mechanics. Problem 2 Solution

(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 ϵ and $\epsilon+d\epsilon$ to the number of states with magnitude of wavevector between k and $k+dk$, where $\epsilon = \hbar^2k^2/2m$. i.e.

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

so

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

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 ϵ_F is found by filling the states up to ϵ_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 μB 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 μB. 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

Statistical Mechanics Problem 3

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_{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_{tot} are 0, 1, and 2 (each value once).

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

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

Qualifying Exam Winter 2012

Statistical Mechanics. Problem 3 Solution

(a) The Hamiltonian can be written as

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

Since $S_{\rm tot}$ 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

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

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

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

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

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

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

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 $T \to \infty$, 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.