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

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

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

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

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:

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

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

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

$$\begin{aligned} \therefore\ m &= \pm\sqrt{3(1 - T/T_c)} && \text{for } T \text{ close to } T_c \quad T < T_c \\ &\ \ 0 && \text{for } T > T_c \end{aligned}$$

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

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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.

SM#1 Solution

Qualifying Exam 06

Statistical Mechanics Problem 1 : Solution

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

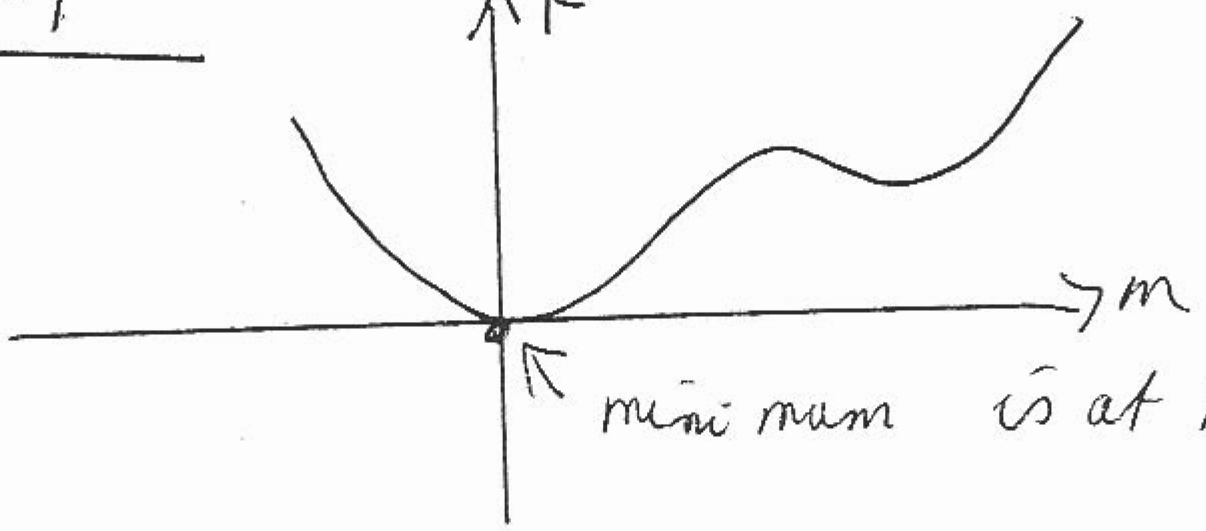
where $b(T) = \alpha(T - T^*)$

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

↑ smooth part which does not play a role.

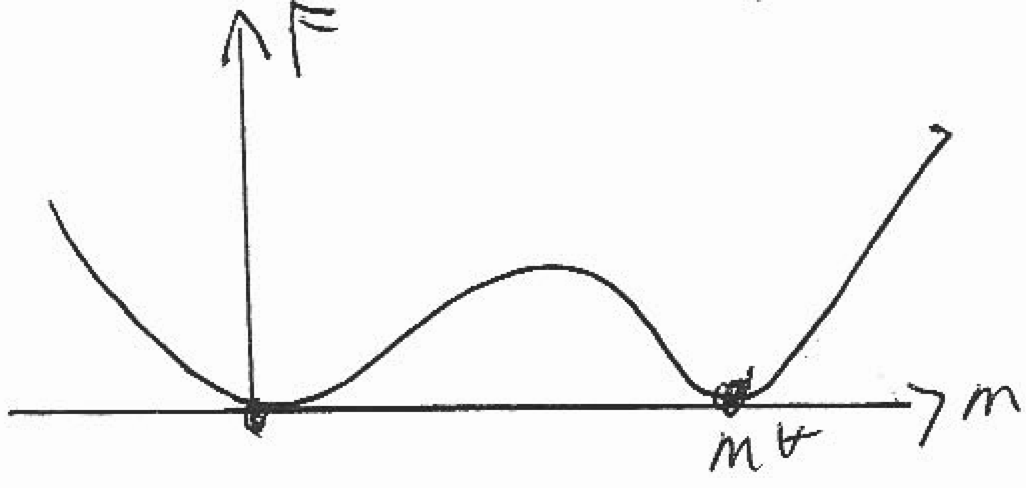
(a)

- At high-T



minimum is at $m=0$

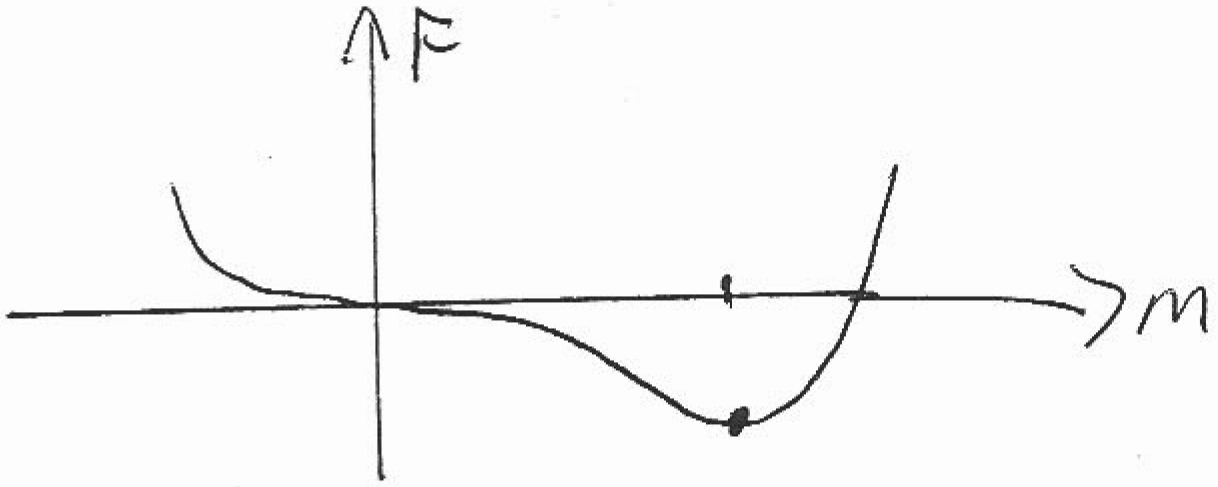
- As T is lowered the 2nd minimum will hit the axis



$T = T_c$

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.

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

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

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

$$2\times② \div (m^*)^2 \implies \alpha(T_c - T^*) = \frac{2}{3}c\,m^* - \frac{d}{2}m^{*2} \qquad ④$$

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

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

(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:

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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:

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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

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

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

   $$\mathbf{H}_i = J \sum_j \mathbf{S}_j \, , \tag{2}$$

   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

   $$\langle S_x \rangle = \frac{\beta H + \frac{1}{3!}(\beta H)^3 + \cdots}{3 + \frac{1}{2!}(\beta H)^2 + \cdots} \simeq \frac{\beta H}{3} \left(1 - O(\beta H)^4\right) \, , \tag{3}$$

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
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Qualifying Exam 09

Statistical Mechanics. Problem 1

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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

$$\rho = g\int_m^\infty \frac{4\pi E\sqrt{E^2-m^2}\mathrm{d}E}{(2\pi)^3} f(E)E = g\int_m^\infty \frac{\sqrt{E^2-m^2}}{2\pi^2} f(E)E^2\mathrm{d}E \qquad (1)$$

$$P = g\int_m^\infty \frac{(E^2-m^2)^{3/2}}{6\pi^2} f(E)\mathrm{d}E \qquad (2)$$

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

$$\frac{\mathrm{d}f_{F,B}}{\mathrm{d}E} = -\frac{e^{E/T}}{T(1\pm e^{E/T})^2} \qquad \frac{\mathrm{d}f_{F,B}}{\mathrm{d}T} = \frac{e^{E/T}\ E}{T^2(1\pm e^{E/T})^2} \qquad (3)$$

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

$$\frac{\partial}{\partial T}\left(\frac{1}{T}\left(\rho(T)+P(T)\right)\right) = \frac{\partial}{\partial V}\left(\frac{V}{T}\frac{\mathrm{d}\rho(T)}{\mathrm{d}T}\right) \qquad (4)$$

which directly gives

$$-\frac{\rho+P}{T^2} + \frac{1}{T}\frac{\mathrm{d}\rho}{\mathrm{d}T} + \frac{1}{T}\frac{\mathrm{d}P}{\mathrm{d}T} = \frac{1}{T}\frac{\mathrm{d}\rho}{\mathrm{d}T} \qquad (5)$$

hence $\mathrm{d}P/\mathrm{d}T = (\rho+P)/T$.

Qualifying Exam 09

Statistical Mechanics. Problem 2

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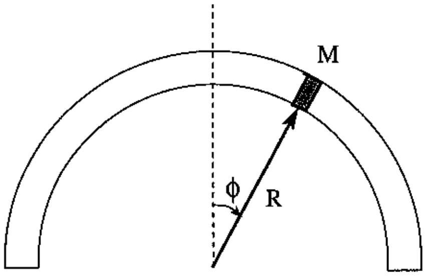
2. [*Alben model*]
This illustrates a second order phase transition by a mechanical model.



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

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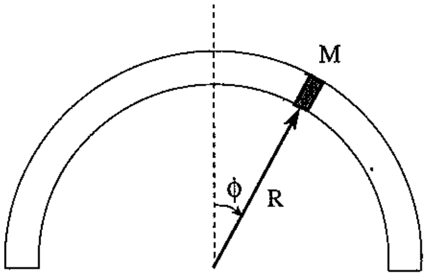
2. [*Alben model*]



(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

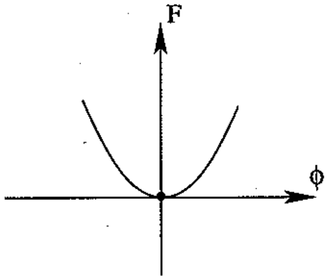
$$F = F_0 + \left(\frac{4Nk_BT}{\pi^2} - \frac{MgR}{2}\right)\phi^2 + \left(\frac{8Nk_BT}{\pi^4} + \frac{MgR}{24}\right)\phi^4 + \cdots, \tag{2}$$

where F_0 is independent of ϕ. The coefficient of the ϕ^2 term changes sign at $T = T_c$ where

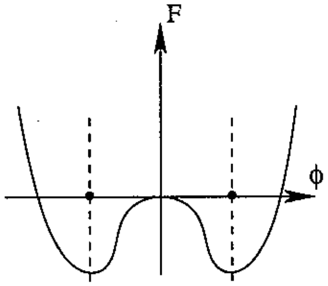
$$\boxed{T_c = \frac{MgR\pi^2}{8Nk_B}.}$$

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).