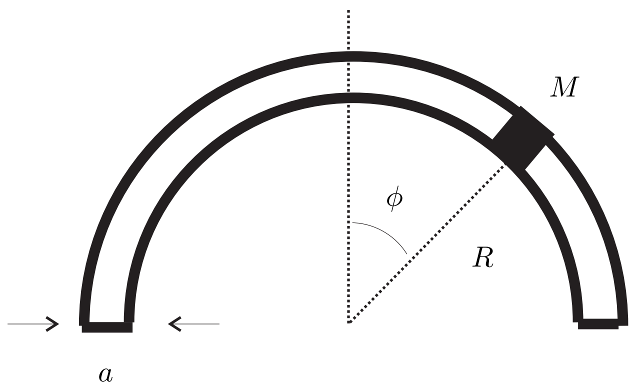
P653 HW3

Due Sept. 15, 2005

Problem 1. Alben model (Plischke and Bergersen 3.14)

The symmetry breaking aspect of second order phase transitions can be nicely illustrated in a simple mechanical model [R. Alben, American Journal of Physics **40**, 3 (1972)]. An airtight piston of mass M is inside a tube of cross sectional area a. The tube is bent into a semicircular shape of radius R.



The system is kept at temperature T. On each side of the piston there is an ideal gas consisting of N atoms. The volume to the right of the piston is $aR(\pi/2+\phi)$, while the volume to the left is $aR(\pi/2-\phi)$. Using the free energy of an ideal gas, $F = -Nk_B[1-\ln(N\lambda^3/V)]$, one finds

$$F = MgR\cos(\phi) - Nk_BT\left[2+\ln\left(\frac{aR(\pi/2+\phi)}{N\lambda^3}\right)+\ln\left(\frac{aR(\pi/2-\phi)}{N\lambda^3}\right)\right],$$

where $\lambda^2 = \hbar^2/(2\pi m k_B T)$.

1.1. Show by minimizing the free energy that the system undergoes a symmetry breaking phase transition ($\phi \neq 0$) at a temperature

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

Solution 1.1. Making F stationary, we find

$$\frac{\partial F}{\partial \phi} = -MgR\sin(\phi) + \frac{2Nk_BT\phi}{(\pi/2)^2 - \phi^2} = 0.$$

It suffices to consider $\phi \geq 0$ in which case,

$$\begin{aligned} MgR\sin\phi &\leq MgR\phi \\ \frac{2Nk_BT\phi}{(\pi/2)^2 - \phi^2} &\geq \frac{2Nk_BT\phi}{(\pi/2)^2}. \end{aligned}$$

Thus if $MgR < 8Nk_BT/\pi^2$ the only possible solution is $\phi = 0$.
Looking at the curvature

$$\left.\frac{\partial^2 F}{\partial \phi^2}\right|_{\phi=0} = -MgR + \frac{8Nk_BT}{\pi^2},$$

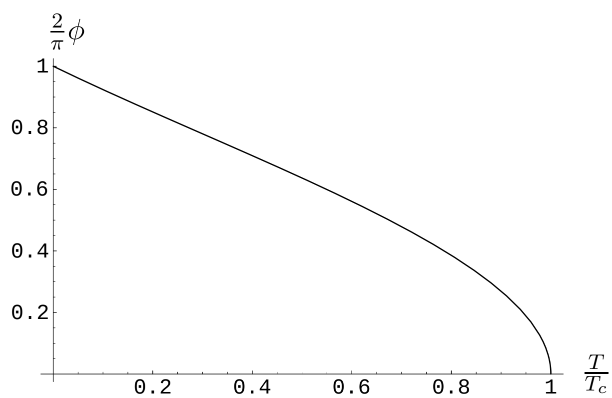
we see that the $\phi = 0$ solution is a local maximum if $MgR > 8Nk_BT/\pi^2$, Therefore, in this low temperature regime, the minimum must occur at nonzero ϕ.

1.2. Plot the "order parameter" ϕ vs T/T_c for $T < T_c$.

Solution 1.2. The angle ϕ obeys

$$\frac{T}{T_c} = \frac{1 - (2/\pi)^2\phi^2}{\phi}\sin(\phi),$$

which gives



1.3. Describe what happens to the phase transition if the number of atoms on the left and right side of the piston is $N(1-\delta)$ and $N(1+\delta)$ respectively.

Solution 1.3. In the $T - \delta$ plane, there is a critical point at $T = T_c$ and $\delta = 0$. A first order phase transition line extends from T_c to $T = 0$.

1.4. At a certain temperature the right chamber (containing $N(1+\delta)$ molecules) is found to contain a puddle of liquid coexisting with its vapor. Which of the following statements may be true at equilibrium:

1. The left chamber will contain a liquid in coexistence with its vapor.
2. The left chamber contains only vapor.
3. The left chamber contains only liquid.

Solution 1.4. In the coexistence region, the free energy per particle of the liquid and gaseous phases must be the same. Thats why they coexist! Therefore the free energy of the fluid on the right hand side has no ϕ dependence, and can be ignored.
We now consider each of the possibilities:
1. The left chamber contains a liquid in coexistence with its vapor. By the above argument, the only ϕ dependence of F is $F = MgR\cos(\phi)$. The piston therefore moves to one side until one side becomes all gas or all liquid. Therefore, this is not a possibility.
2. The left chamber contains only vapor. This may be locally stable if $\phi > 0$ so the pressure on the left is smaller than the pressure on the right. If $\delta > 0$ then this will be only locally stable (metastable), but if $\delta < 0$ this will be the global minimum of the free energy.
3. The left chamber contains only liquid. This may be stable if $\phi < 0$ so the pressure on the left is greater than the pressure on the right. If $\delta < 0$ then this will be only locally stable (metastable), but if $\delta > 0$ this will be the global minimum of the free energy.

Problem 2. Bethe Approximation (Plischke and Bergersen sec. 3.4)

Here we work through a more general mean field theory for the Ising model, where we include some short range correlations. As before, we select out one site, with spin σ_0, but we also select out all q of its neighboring sites. We assume that none of the neighbors are neighbors to each-other. The Hamiltonian of these $q+1$ sites will be approximated by

$$H_c = -J\sigma_0 \sum_{j=1}^{q} \sigma_j - h\sigma_0 - h' \sum_{j=1}^{q} \sigma_j.$$

The h' is the effective field that each of the q neighbors feels, which includes the effect of all the spins (except σ_0) which are their neighbors.

2.1. Calculate the partition function for this cluster

$$Z_c = \sum_{\sigma_j=\pm 1} e^{-\beta H_c}.$$

Solution 2.1.

$$
\begin{aligned}
Z_c &= \sum_{\{\sigma_k\}} e^{-\beta H_c} \\
&= \sum_{\sigma_0} e^{\beta h \sigma_0} \left[\sum_{\sigma_1} e^{\beta(J\sigma_0 + h')\sigma_1} \right] \cdots \left[\sum_{\sigma_q} e^{\beta(J\sigma_0 + h')\sigma_q} \right] \\
&= \sum_{\sigma_0} e^{\beta h \sigma_0} \left[2\cosh[\beta(J\sigma_0 + h')] \right]^q \\
&= e^{\beta h} \left[2\cosh[\beta(J + h')] \right]^q + e^{-\beta h} \left[2\cosh[\beta(J - h')] \right]^q .
\end{aligned}
$$

2.2. Write an expression for $\langle \sigma_0 \rangle$ when $h = 0$.

Solution 2.2.

$$
\begin{aligned}
\langle \sigma_0 \rangle &= \frac{1}{\beta} \frac{\partial \log Z_c}{\partial h} \bigg|_{h=0} \\
&= \frac{1}{Z_c} \left\{ \left[2\cosh[\beta(J + h')] \right]^q - \left[2\cosh[\beta(J - h')] \right]^q \right\} .
\end{aligned}
$$

2.3. Write an expression for $\langle \sigma_j \rangle$ when $h = 0$.

Solution 2.3. If $j \neq 0$ we have

$$
\begin{aligned}
\langle \sigma_j \rangle &= \frac{1}{\beta q} \frac{\partial \log Z_c}{\partial h'} \bigg|_{h=0} \\
&= \frac{1}{Z_c} \left\{ 2\sinh[\beta(J + h')] \left[2\cosh[\beta(J + h')] \right]^{q-1} - 2\sinh[\beta(J - h')] \left[2\cosh[\beta(J - h')] \right]^{q-1} \right\} .
\end{aligned}
$$

2.4. Since the ferromagnet is translationally invarient, we require $\langle \sigma_j \rangle = \sigma_0$. Show that this requirement leads to the formula

$$
\frac{\cosh^{q-1}[\beta(J + h')]}{\cosh^{q-1}[\beta(J - h')]} = e^{2\beta h'} . \tag{1}
$$

Solution 2.4. Equating the two expressions, gives

$$
\begin{aligned}
& \left[\cosh[\beta(J + h')] - \sinh[\beta(J + h')] \right] \left[2\cosh[\beta(J + h')] \right]^{q-1} \\
= \; & \left[\cosh[\beta(J - h')] - \sinh[\beta(J - h')] \right] \left[2\cosh[\beta(J - h')] \right]^{q-1} .
\end{aligned}
$$

Noting that $\cosh(A) - \sinh(A) = e^{-A}$, we arrive at the desired expression.

Equation (1) always has the solution $h' = 0$. When $h' \to \infty$, the left hand side approaches a constant while the right hand side diverges. Therefore a sufficient condition to have a solution with $h' \neq 0$ is to have the slopes $\partial_{h'}\mathbf{L.H.S} > \partial_{h'}\mathbf{R.H.S.}$ at $h' = 0$.

2.5. Find the slopes at $h' = 0$, and thereby find the critical temperature, at which the solutions for $h' \neq 0$ exist.

Solution 2.5. Equating these slopes gives

$$k_B T_c = \frac{J}{\operatorname{arctanh}[1/(q-1)]}.$$

2.6. For the $1-D$ Ising model, $q = 2$. What is the critical temperature predicted by this approximation? Is this better than our previous mean field approximation?

Solution 2.6. Setting $q = 1$ we get $T_c = 0$, which agrees with the exact result.

2.7. For the $2-D$ Ising model on a square lattice, $q = 4$. What is the critical temperature?

Solution 2.7. Setting $q = 4$ gives $k_B T_c = 2.89J$.

2.8. What is the critical temperature in the limit of large q? How does this compare with our previous mean field approximation?

Solution 2.8. At large q we recover our previous mean field result, $q\beta J = 1$.

2.9. Near the transition temperature show that the magnetization obeys $m(h = 0) \propto |T - T_c|^\beta$. Find β.

Solution 2.9. For T near T_c, m and h' are linearly related. Therefore $h' \propto |T - T_c|^\beta$, and it suffices to find how h' varies with T.
One needs to expand equation (1) in powers of h' and in powers of $T - T_c$. The algebra is simplified if we first symmetrize the expression, writing (1) as

$$e^{-\beta h'/(q-1)} \frac{\cosh(\beta(J + h'))}{\cosh(\beta J)} - e^{\beta h'/(q-1)} \frac{\cosh(\beta(J - h'))}{\cosh(\beta J)} = 0.$$

Expanding to cubic order in h', we find

$$a(T)(\beta h) + b(T)(\beta h)^3 + \cdots = 0,$$

where $a(T) = 2\tanh(\beta J) - 2/(1-q) = a_1(T - T_c) + \cdots$ and $3b(T) = \tanh(\beta J)[3/(q-1)^2 + 1] - [3/(q-1) + 1/(q-1)^3] = b_0 + b_1(T - T_c) + \cdots$, where a_1, b_0, and b_1 are all non-zero.
To lowest order in $T_c - T$, one finds

$$h^2 = a_1/b_0(T - T_c),$$

and $\beta = 1/2$.

Problem 3. Latent Heat (Plischke and Bergersen 3.11)

Consider the Landau free energy

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

and assume that $b > 0$, $c < 0$, and $d > 0$ so that a first-order transition takes place. Derive an expression for the latent heat of transition. [Hint: read section 3.7]

Solution 3.1. This free energy has three local minima: $m = 0, \pm m_0$, where the latter are the solutions to the quadratic equation $dm_0^4 + cm_0^2 + b = 0$. The phase transition occurs when the free energy of the symmetry broken phase $m = \pm m_0$ is equal to that of the symmetric phase. As shown in section 3.7 this occurs when $b = (3/16)c^2/d$, corresponding to $m_0^2 = -(3/4)c/d$.
The latent heat is given by the product $L = T\delta S$, where δS is the entropy difference between the two phases. The entropy is simply $S = \partial G/\partial T$, where the derivative is taken while holding fixed $\partial G/\partial m = 0$. This gives

$$L = -\frac{b'T}{2}m_0^2 + \frac{c'T}{4}m_0^4 + \frac{d'T}{6}m_0^6,$$

where primes denote derivatives with respect to T.