Do four of five problems!

[1.] Compute, by explicit enumeration of all the states, the partition function $Z(T)$ and average energy $\langle E \rangle(T)$ of the $N = 6$ site one dimensional Ising model with periodic boundary conditions. Verify your expression for $Z$ by checking against the exact solution $Z = (2 \cosh \beta J)^N + (2 \sinh \beta J)^N$. If you find $N = 4$ too hard to do, try $N = 4$.

[2.] Make qualitative plots of the susceptibility $\chi(T)$, and the magnetization $m(T)$ at field $B = 0$ for a system with a second order magnetic phase transition. How are the critical exponents $\beta$ and $\gamma$ defined? Make qualitative plots of the magnetization $m(B)$ for $T > T_c$, for $T = T_c$ and for $T < T_c$. How is the critical exponent $\delta$ defined? What are the Mean Field values of $\beta$, $\gamma$, and $\delta$? Discuss any relationships between the plots that occur to you. For example, does the behavior of $\chi(T)$ near $T_c$ seem plausible in terms of what happens to $m(T)$?

[3.] Write down the high and low $T$ expansions for the partition function of the Ising model on a hexagonal lattice. For high $T$ go to order ten in $\tanh \beta J$. For low $T$ go to order four in $\exp(-2\beta J)$.

[4.] Landau has a nice way of picturing any phase transition. What is it?

[5.] Suppose someone challenges you to work out Mean Field Theory (MFT) for the Ising model on the “Lieb Lattice”. See below. Unlike the square lattice we did in class, where all the sites are identical, there are two different types of sites here (one type has two neighbors and the other has four neighbors). How might you generalize MFT to such a situation? How would you formulate self-consistency? How would you go about determining $T_c$?

**Hint:** Allow $\langle S_i \rangle$ to be different depending on which type of site is being considered.

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The Lieb lattice.
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Physics 219 A
Midterm 2
Spring 2014

There are $2^6 = 64$ possible states, but they come in groups with the same energy.

\[
\begin{align*}
+ &+ + + + + \ \ \ \{ \ E = -6J \ \ \ \ g = 2.1 \\
- &- - - - - \\
\end{align*}
\]

\[
\begin{align*}
+ &+ + + + - \ \ \ \{ \ E = -2J \ \ \ \ g = 2.6 = 12 \\
- &- - - + \\
&\text{and related} \\
\end{align*}
\]

\[
\begin{align*}
+ &+ + + - - \ \ \ \{ \ E = -2J \ \ \ \ g = 2.6 = 12 \\
- &- - + + \\
&\text{and related} \\
\end{align*}
\]

\[
\begin{align*}
+ &+ + - + - \ \ \ \{ \ E = +2J \ \ \ \ g = 2 \times \frac{6.3}{2} = 18 \\
- &- + - + + \\
&\text{and related} \\
\end{align*}
\]

6 places to put first flipped spin, only 3 places for second (not allowed to be adjacent) divide by 2 because indistinguishable.
\[ \begin{align*}
\text{same: } 2 & \quad + + - - - - \quad \int \quad E = +2J \quad g = 6.2 = 12 \\
\text{note: Do} & \quad 6 \text{ places to put pair} \\
\text{not need to} & \quad \text{of flipped spins, 2 places} \\
\text{consider -----} & \quad \text{to put single flipped spin} \\
\text{background} & \quad \text{These are distinguishable} \\
\text{separately} & \quad \text{6 places to put } + + + \\
\text{6 places to put } + + + & \quad \text{notice in this case} \\
\text{do not need to consider} & \quad \text{----- background} \\
& \quad \text{separately.} \\
\text{same: } 2 & \quad + + - - - - \quad \int \quad E = -2J \quad g = 6 \\
\text{Check carefully by noting} & \quad 2 + 12 + 12 + 18 + 12 + 6 + 2 = 64 \\
\text{Another check: Expect } E \to -E \text{ symmetry} \\
\text{Indeed there are} & \quad 12 + 12 + 6 = 36 \quad E = -2J \\
& \quad 18 + 12 = 30 \quad E = +2J
\end{align*}\]
\[ Z = 2 e^{6\beta J} + 30 e^{2\beta J} + 30 e^{-2\beta J} + 2 e^{-6\beta J} \]

\[ E = -\frac{\partial}{\partial \beta} \ln Z \]
\[ = \int Z^{-1} \left[ 12 e^{6\beta J} + 60 e^{2\beta J} - 60 e^{-2\beta J} + 12 e^{-6\beta J} \right] \]

Or, if you like

\[ Z = 9 \cosh 6\beta J + 60 \cosh 2\beta J \]

\[ \langle E \rangle = 2^{-1} \int \left[ 24 \sinh 6\beta J + 120 \sinh 2\beta J \right] \]

We could check against transfer matrix / high T expansion.

\[ Z = (2 \cosh \beta J)^6 + (2 \sinh \beta J)^6 \]
\[ = (e^{\beta J} + e^{-\beta J})^6 + (e^{\beta J} - e^{-\beta J})^6 \]
\[ = e^{6\beta J} + 6 e^{4\beta J} + 15 e^{2\beta J} + 20 + 15 e^{-2\beta J} + 6 e^{-4\beta J} + e^{-6\beta J} \]
\[ + e^{6\beta J} - 6 e^{4\beta J} + 15 e^{2\beta J} - 20 + 15 e^{-2\beta J} - 6 e^{-4\beta J} + e^{-6\beta J} \]
\[ = 2 e^{6\beta J} + 30 e^{2\beta J} + 30 e^{-2\beta J} + 2 e^{-6\beta J} \]
For $T$ near $T_c$

$$m(T) \sim (T_c - T)^\beta$$

$$\chi(T) \sim \frac{1}{(T - T_c)^\gamma}$$

For $T = T_c$

$$m \sim B^{1/8}$$

Comments:

1. The plot of $M(T)$ at $B = 0$ tells us that the system spontaneously magnetizes if $T < T_c$. This suggests that its susceptibility to a magnetic field should be huge: it is about to line up even at $B = 0$ so turning on $B$ will have a large effect. Schematically:

$$M = \chi B$$

$\chi \overset{B\text{ zero}}{\rightarrow} \chi = \infty$
(2) The values of $m(B=0)$ in figure 3 are consistent with those of figure 1: If $T>T_c$, $m(B=0)$ is zero in figure 1 and also in figure 3. If $T<T_c$, $m(B=0)$ is nonzero in figure 1 and also in figure 3.

(3) The slope of $M(B)$ in figure 3 is the susceptibility $\chi$ at $T=T_c$ in figure 3, $M(B)$ crosses in $B=0$ with infinite slope (assuming $\beta > 1$). $X$ is also infinite in figure 2.

In MFT $\beta = 1/2$, $\delta = 1$, $\delta = 3$.
High $T$ expansion

$$Z = Tr e^{-\beta H} = \sum \sum \sum \frac{e^{B J}}{8^J}$$

$$= \sum \prod \left( \cosh \beta J + 1 \right)$$

$$= (\cosh \beta J)^{N_{\text{bonds}}} \sum \prod \left( 1 + \frac{N_{\text{sites}} \tanh \beta J}{} \right)$$

Small at high $T$

$\sum$ gives zero unless form closed loops from any $\sinh \beta J$ factors.

For hexagonal lattice, smallest closed loop is with six bonds.

Also if $N = \# \text{ sites}$

$$N_{\text{bonds}} = 3 \frac{N}{2}$$

You can only place hexagons on $\frac{1}{2}$ as many places as $\# \text{ sites}$

$$Z = (\cosh \beta J)^{3N/2} \left[ 1 + \frac{N}{2} t^6 + \ldots \right] 2^N$$
What about higher order? The next closed loop possible is this one: \( (\tanh \beta J)^n \)

and we need to compute number of ways it can be placed. There are \( \frac{N}{2} \) locations but 3 different orientations.

\[
Z = (\cosh \beta J)^N \left( 1 + \frac{N}{2} t^4 + \frac{3N}{2} t^{10} + \ldots \right) e^{-2N}
\]

* Given a pair of sites forming a horizontal bond, one can draw 3 \( (\tanh \beta J)^n \) diagrams.
low T expansion

Idea is to expand in flipped spins

Ground state E is Ferromagnetic \( E = -NJ^{3/2} \)

\[ Z = 2 e^{\beta N J^{3/2}} \]

\[
\begin{align*}
\text{If } N &= \text{ sites}, \\
2 \text{ FM configs: all } +1 \text{ or all } -1 & \Rightarrow \frac{3N}{2} = \text{ # bonds}
\end{align*}
\]

Next lowest E is

Energy cost is 6J

(2J for each of 3 bonds)

Can do this on any site

\[ Z = 2 e^{\beta N J^{3/2}} \left( 1 + NE^{-6\beta J} + \cdots \right) \]

or can flip 2 adjacent spins

"Breaks" 4 bonds

\[ \Rightarrow \text{ Energy cost } 8J \]

Can do this for any bond

of lattice \( \Rightarrow N = \# \text{ sites} \)

\[ \frac{3N}{2} = \text{ # bonds} \]

(again 3 bonds per site, but each bond uses 2 sites)
\[ Z = 2 e^{3\beta N} J^{1/2} \left[ 1 + Ne^{-\beta J} + \frac{3N}{2} e^{-2\beta J} + \ldots \right] \]
Landau Mean field theory pictures phase transitions in terms of the expansion of the free energy $f$ in terms of an order parameter $M$:

$$f(M) = f_0 + a(T)M^2 + b(T)M^4$$

For example, assuming $b(T) > 0$, there are 2 possible shapes for $f(M)$ depending on the sign of $a(T)$:

- $a > 0$:
  - $m = 0$ minimizes $f$.
- $a < 0$:
  - $m \neq 0$ minimizes $f$.

In Landau MFT, a phase transition occurs because $a(T)$ changes sign:

- $a(T) > 0$, $T > T_c$.
- $a(T) < 0$, $T < T_c$.

So that the order parameter $m = 0$ minimizes $f(M)$ for $T > T_c$ but $m \neq 0$ for $T < T_c$. 
Landau MFT also allows an understanding of first order transitions. If there is an $m^3$ term in $f(m)$, it is possible $f$ can evolve with $T$ so that the minimum jumps abruptly from $m = 0$ to $m = m_0$. 

$\Delta f$

$T > T_c$

$T < T_c$

Jump in $m(T)$
Let denote \( M_a = \langle S_i \rangle \) on the 4-fold coordinated sites and \( M_b = \langle S_i \rangle \) on the 2-fold coordinated sites. MFT replaces \( S_i \) by \( \langle S_i \rangle \) on the neighbors \( j \) of site \( i \). This leads to

\[
\begin{align*}
\text{\( S_a \) feels} & \quad -4Jm_b \\
\text{\( S_b \) feels} & \quad -2Jm_a \\
\end{align*}
\]

Get 2 self consistent \( \langle S_i \rangle \):

\[
\langle S_a \rangle = m_a = \tanh 4Jm_b \beta
\]

\[
\langle S_b \rangle = m_b = \tanh 2Jm_a \beta
\]

An obvious solution is \( m_a = m_b = 0 \), and this is what happens for \( T \) large (\( \beta \) small).
When will there first be a solution

to these equations with $m_a$ and $m_b$ nonzero?

One guess is to set $\tanh x = x$

$$m_a = 4J m_b \beta$$

$$m_b = 2J m_a \beta = 2J \left(4J m_b \beta \right) \beta$$

$$= 8J^2 \beta^2 m_b$$

So we need $\sqrt{8J} \beta = 1$

$$\Rightarrow k_B T_c = \sqrt{8J}$$

This is plausible in that it is in between the values

$T_c = 2J \quad \leftarrow z = 2 \text{ lattice}$

$T_c = 4J \quad \leftarrow z = 4 \text{ lattice}$