REVIEW: Derivation of the Mean Field Result

The Critical Temperature Dependence

The Mean Field Approximation assumes that there will be an average value of the spin $< s_i >$ for the $N$ electrons making up an Ising model system. The goal is to derive the temperature dependence of this average $< s >$ value. The result will be the appearance of a critical temperature $T_C$ such that the average value of the spin near $T_C$ will have a temperature dependence given by

$$< s > = \sqrt{\frac{3}{T} \left( \frac{k_B T}{zJ} \right)^3 \left( \frac{z J}{k_B} - T \right)^{1/2}} \sim (T_C - T)^\beta \quad (T < T_C)$$

$$< s > = 0 \quad (T > T_C)$$

$$T_C \equiv \frac{z J}{k_B}$$

The critical exponent $\beta = 1/2$, and the parameter $z$ is the number of nearest neighbor interactions which is 4 in this simple model. You should look at the Figure 8.4 on page 243 to appreciate the significance of this result. Essentially it indicates that above a critical temperature then no magnetic field is possible. Below the critical temperature, the magnetization grows asymptotically to its maximum value ($< s > = 1$) as the temperature approaches absolute zero.

Derivation

First introduce an external field $H$. The energy of the system with this external field is given by

$$E = -J \sum_{<ij>} s_i s_j - \mu H \sum_i s_i$$

where $\mu$ is the magnetic moment of each electron spin. Assume that there are only two spin states $\pm 1$ with energies $E_\pm = \mp \mu H$. The probabilities for being in these two states are

$$P_+ = C e^{+\mu H / k_B T} \quad P_- = C e^{-\mu H / k_B T}$$

Since the probabilities have to add up to 1 we get

$$C = \frac{1}{e^{+\mu H / k_B T} + e^{-\mu H / k_B T}}$$

This produces the average spin $< s_i >$ produced by an external field $H$ as

$$< s_i > = \sum_i s_i P_i = P_+ - P_- = \tanh \left( \frac{\mu H}{k_B T} \right)$$

The above assumed that there was no internal field, which will be the case at high enough temperatures. Now we consider that the case when internal spins produce an average internal field $H_{eff}$. We re-write the energy expression to get an equation for $H_{eff}$

$$E = - \left( J \sum_{<ij>} s_j \right) s_i - \mu H s_i \implies H_{eff} \equiv \frac{J}{\mu} \sum_i < s > = \frac{z J}{\mu} < s >$$

From the previous equation for the value of $< s >$ produced by an external field $H$ we can write a transcendental equation for the value of $< s >$ produced by $H_{eff}$, on the next page.
REVIEW: The Mean Field Result for \( < s > \)

Mean Field Transcendental Equation

Average \( < s > \) from external field \( H \): \( < s > = \tanh \left( \frac{\mu H}{k_B T} \right) \)

Expression for \( H_{\text{eff}} \) produced internally from \( < s > \): \( H_{\text{eff}} = \frac{zJ}{\mu} < s > \)

Using \( H_{\text{eff}} \) in first equation for \( < s > \): \( < s > = \tanh \left( \frac{zJ < s >}{k_B T} \right) \)

The numerical solution to the above transcendental equation obtains the average spin \( < s > \) as a function of temperature \( T \) for a given pair energy \( J \), electron magnetic moment \( \mu \), and number of nearest neighbor interactions \( z \). From the average spin \( < s > \) we get the magnetization \( M = N < s > \) for \( N \) electrons\(^1\).

It is most helpful to look at the graphical solution to this equation in two limits, as shown in Figure 8.2 on page 242. One is looking for the intersection of the hyperbolic tangent line with a straight line at 45\(^\circ\) slope. Above a certain temperature \( T_C \), as shown on the right side, there is only one trivial intersection point at \( < s > = 0 \). Below that critical temperature there are two non-trivial intersection points at \( < s > = \pm s_0 \). These values will be temperature dependent. The numerical solution of the temperature dependence is what is shown in Figure 8.4 on page 243.

Near Critical Temperature Approximation

A low values of \( x \) \( \tanh(x) \approx x - x^3/3 \). With this approximation the solution \( < s > \) is

\[
< s > \approx \frac{zJ < s >}{k_B T} - \frac{1}{3} \left( \frac{zJ < s >}{k_B T} \right)^3
\]

\[
< s > \approx \sqrt{\frac{3}{T}} \left( \frac{k_B T}{zJ} \right)^{3/2} \left( \frac{zJ}{k_B} - T \right)^{1/2} \sim (T_C - T)^\beta \quad (T < T_C)
\]

This is the result that we saw at the beginning of the derivation.

Solving a transcendental equation numerically

The simplest numerical solution for a transcendental equation is Newton’s Rule, which is also called the Newton-Raphson method, as explained in Appendix B (page 469). If one considers the general homogeneous equation \( f(x) = 0 \) and makes a guess for \( x_i \) that \( f(x_i) = 0 \), then an improved guess \( x_{i+1} \) can be obtained with an iteration

\[
x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}
\]

where \( f'(x) \) is the first derivative for \( f(x) \). As usual, the iteration is terminated when \( f(x_{i+1}) \) is deemed sufficiently close to 0. The basis of this method is that \( f(x) \) is a simply behaved function, such as \( \tanh(x) \), where convergence to the root is achieved even if the first guess is not very accurate.

\(^1\)The book’s figures such as 8.4 label the vertical axis as \( M \) instead of what is really plotted which is \( < s > \).
HOMEWORK: Solve the mean field equation as a function of $T$

Mean Field Equation for $<s>$

For temperatures $T$ below a critical temperature given by $T_C = zJ/k_B$, with $z = 4$ for the simplest nearest neighbor two dimensional approximation, then the mean field Ising model value for the average spin is the solution to the following equation

$$<s> = \tanh \left( \frac{zJ <s>}{k_B T} \right)$$

The first step is to choose a dimensionless scale for the temperature. The temperature unit is taken to be $J/k_B$, the pair energy divided by the Boltzmann constant. In this unit the critical temperature is simply $T_C = z$ or $T_C = 4$ for four nearest neighbor interactions.

Numerical solution for Mean Field Ising model

A numerical solution for the Mean Field Ising model transcendental equation for $<s>$ is contained in the program `meanField.cpp`. This program is essentially an implementation of the Newton-Raphson method following a user interface to acquire three optional input parameters: TMIN (default = 0), TMAX (8), and TSTEP (0.03).

The operation of the program is straightforward. After a dynamic allocation of arrays to contain both the numerical and the approximate analytical solutions, there is a loop over the temperatures values from TMIN to TMAX in steps of TSTEP. The transcendental equation is solved with the root finding C++ function `solveMeanValue` which take an input guess value and a particular temperature. The converged value for $<s>$ is returned by this function. The function has a hardwired fractional convergence criterion of $10^{-6}$, with a safety limit of $10^4$ for the maximum number of iterations. It is good computing practice to put in an upper limit when one is doing convergence iterations.

For this problem the Newton-Raphson equation is

$$<s>_{i+1} = <s>_i - \frac{f(<s>_i)}{f'(<s>_i)}$$

$$f(<s>) \equiv <s> - \tanh \left( \frac{zJ <s>}{k_B T} \right) \implies f'(<s>) = 1 - \frac{4.0J}{k_B T} \tanh^2(<s>)$$

The 4.0 in the derivative function represents the $z = 4$ number of nearest neighbor interactions. Defining $T$ in units of $J/k_B$ means that $J/k_B$ is set equal to unit in this program. A safety measure in the iteration loop is to check against the derivative being 0 which would cause a divide by 0 mathematical error.

The initial guess at each temperature is $<s> = 1.0$, so the positive solution is always returned. You can see from the output that the numerical solution goes to 0.0 just above the critical temperature $T_C = 4$ in units of $J/k_B$. 
HOMEWORK: Solve the mean field equation as a function of $T$

Analytic Solution near $T_C$

The program also shows the analytic solution (red curve), which is valid near and below $T_C$

$$< s > = \sqrt{\frac{3}{T}} \left( \frac{k_B T}{zJ} \right)^3 \left( \frac{zJ}{k_B} - T \right)^{1/2} \sim (T_C - T)^{\beta} \quad (T < T_C)$$

The $< s >$ displays a power law dependence near $T_C$, shows specifically the characteristics of a second order phase transition. Below $T_C$, the system is in the ferromagnetic phase with $M > 0$, while above $T_C$ the system has $M = 0$ and is said to be in the paramagnetic phase.

Deficiencies of the Mean Field solution

The Mean Field solution for the Ising model has demonstrated that there is a critical temperature $T_C = 4$ for magnetization, and that the magnetization behaves as a second order phase transition with a power law exponent $\beta = 1/2$. While these are intriguing qualitative results, the real world experiments show the quoted numbers to be wrong. Hence the Mean Field approximation itself is wrong.

The basic problem is that the Mean Field approximation ignores the long range correlations which are introduced by locally aligned pairs. Therefore, in order to solve the Ising model more exactly, we have to consider a system of $N$ electrons completely and look at all the pairs when computing the total energy. As before we will want to know the average value $< s >$ as a function of temperature. Each pair of electrons is allowed to be in an aligned or anti-aligned state according to a temperature dependent probability.
Monte Carlo Second Order Ising Model

N electron state description
A more realistic solution for the Ising Model is to consider all the N electrons in a random or Monte Carlo method. For example, if there are \( N = 9 \) electrons, we can arrange them as shown in Figure 8.5 in a 3 \( \times \) 3 square lattice. It is clear that the central electron has four nearest neighbors. However, it is not so clear what to do with all the other 8 electrons. The solution is to invoke the periodic boundary condition. This condition assumes that electrons along the nominal outer boundary of the lattice can interact with electrons on the corresponding opposite boundary, that is left side with right side and top with bottom.

You might wonder as to how the periodic boundary condition affects the quantitative outcome. The answer to that question is to go to larger square lattices, and determine whether the numerical results are stable. You can make the lattice size an input to your program. The number of electrons \( N \) will be the square of the lattice size.

Metropolis algorithm solution to the \( N \) electron Ising model
The physical problem to be solved is that the \( N \) electrons are arranged in a square lattice of size \( \sqrt{N} \) at a certain temperature \( T \). You want to know the physical parameters of that system such as the average spin value and magnetization \( \langle s \rangle, M = N \langle s \rangle \), or energy, to take two examples. This is done by using what is called the Metropolis algorithm, after its inventor nuclear physicist Nicholas Metropolis (http://en.wikipedia.org/wiki/Nicholas_Metropolis, 1915–1999). Initially, the electrons are given some arrangement of spins. Then you simulate the passage of time. For each time step each electron in turn is considered as to whether it might flip its spin orientation. If the change in spin orientation results in a reduced energy for this electron, then the spin is flipped to its opposite value. The energy changed is computed by checking the spins of the four nearest neighbors. If the change in spin orientation results in an increase of energy, symbolized as \( E_{\text{flip}} \), that change will be allowed according to a probability function.

The probability function is given by

\[
P = \exp\left(\frac{-E_{\text{flip}}}{k_BT}\right)
\]

After each time step, meaning a sweep over all the \( N \) electrons, you calculate the physical parameters of the \( N \) electron state. The first of these parameters will be for the average \( \langle s \rangle \) value, or equivalently the magnetization \( M = N \langle s \rangle \). You would look at that quantity as a function of time, at the given temperature \( T \), as shown in Figure 8.6 on page 249.

Program secondOrderIsing
The Metropolis algorithm implementation for the Ising model is named secondOrderIsing. The main difference between this program and the previous meanField program is that an explicit set of \( N \) electrons is being examined as a function of time at a given temperature. A set of physical quantities (average spin, total energy, energy variance, and spin correlation) are computed at each time step for each temperature. The mathematical center of the program is the C++ function solveSecondOrder which calls an updateSpin function to check whether a given electron’s spin should be flipped as described previously. (See the pseudo-code on page 247.)
Physical Predictions of the Second Order Ising Model

Magnetization time behavior

The first physical prediction of the more exact, second order Ising model is the temperature and time dependence of the average spin quantity \(< s(T) >\). This is shown in a series of plots such as Figure 8.6. What is plotted here is the value of \(< s >\) at each time step for a particular temperature choice \(T\) in units of \(J/k_B\). After calculating the initial values of the physical quantities, the program cycles over the temperature steps, re-initializing the spins to be all +1 before cycling over the time steps. What you see in the Figure 8.6 is the average spin after each time step. At low temperatures the average spin fluctuates close to the value \(< s > = 1\). Only if the temperature were absolute zero would the average spin be exactly 1. As the temperature is increased, these fluctuations become more pronounced. In a real system with orders of magnitude more electrons, the fluctuations would not be as dramatic or as persistent. As the temperature is raised even further, the fluctuations become larger with the system sometimes going close to a \(-1\) average for longer time intervals. Eventually, above a certain temperature, the average spin value merely fluctuates about zero.

Magnetization critical temperature behavior

It is useful to calculate the time averaged magnetization at each temperature. The secondOrderIsing program used 2000 time steps intentionally. What is done is to look at the average over the first 1000 steps, and then over the second 1000 steps, at each temperature. The equivalent textbook figure is shown on page 251. What you see in this figure is a behavior qualitatively similar to that of the Mean Field approximation. At very low temperatures the average spin value \(< s > \approx 1\), while above a certain critical temperature \(< s > \approx 0\). Near the critical temperature the average spin value drops rapidly.

Analytic studies of the second order Ising model predict a critical temperature \(T_C\)

\[
\text{Second Order Ising model: } T_C = \frac{2}{\ln(1 + \sqrt{2})} \approx 2.27
\]

You can see in Figure 8.7 that this appears to be in the middle of the steep drop of the \(< s >\) calculations. You will recall that the Mean Field approximation gave an analytic result

\[
\text{Mean Field Ising model: } T_C = 4
\]

So the Mean Field approximation is off by almost a factor of 2.

There is an even larger discrepancy for the power law exponent \(\beta\) describing the behavior of \(< s >\) just below the critical temperature

\[
< s(T) > \approx (T_C - T)^\beta
\]

\[
\text{Second Order Ising model: } \beta = \frac{1}{8}
\]

\[
\text{Mean Field Ising model: } \beta = \frac{1}{2}
\]

The physical basis for these discrepancies is that the average spin approximation does not take into account the long range correlations which are induced on the lattice. These correlations will be studied in the next lecture along with the temperature dependence of the specific heat.