PHYSICS 115/242

Monte Carlo Simulation Project

Due on Wednesday, May 25.
This is a long time off, but you you should start it right away. Come and discuss your code with me well before the deadline if you don't seem to be getting reasonable results.

Consider the Ising model discussed in class, for which the energy is given by

$$\boxed{\mathcal{H} = -J \sum_{\langle i,j \rangle} S_i S_j,} \tag{1}$$

where there are N spins S_i which take values ± 1, and the sum is over all nearest neighbor pairs on the lattice. Take $J = k_B = 1$ in the simulations.
Take a two-dimensional square lattice where each spin interacts with four neighbors. There are $N = L \times L$ sites. To avoid a surface, which gives large finite-size corrections, use periodic boundary conditions in both directions, see Fig. 1. (We will discuss in class one convenient way of implementing periodic boundary conditions.)

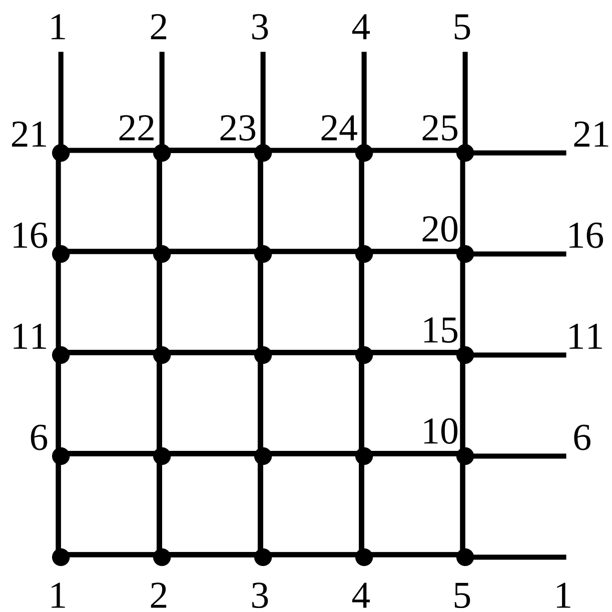

Figure 1: A 5×5 lattice with periodic boundary conditions.

This model has a phase transition at temperature

$$\boxed{T_c = \frac{2}{\ln(\sqrt{2}+1)} \simeq 2.269,} \tag{2}$$

first found by Kramers and Wannier in 1941. Some quantities like the average energy were worked out *exactly* in a major tour-de-force by Onsager in 1944. In this project you will estimate T_c from simulations.

The magnetization per spin is defined to be

$$m = \frac{1}{N} \sum_{i=1}^{N} S_i. \tag{3}$$

1. Write a C/C++/fortran program to compute $\langle m^2 \rangle$ at different temperatures and plot $\langle m^2 \rangle$ for sizes $L = 8, 16$ and 32 as a function of T *in the vicinity of* T_c. You are interested in the range of T where $\langle m^2 \rangle$ varies between a value close to 1 and and a value close to 0.

   As discussed in the handout on Monte Carlo methods you will need to do some sweeps for equilibration (when no measurements are performed) and subsequent sweeps during which measurements are made. The relaxation time is largest at the critical temperature where it varies as $\tau \propto L^z$ with z, the dynamical exponent, around 2. Below T_c is is useful to start the simulation with all spins parallel; otherwise it takes the system a long time to decide if it is going to go into the "up" spin state or the "down" spin state.

   You should indicate error bars on the points. This requires that the data you are putting into the analysis is statistically uncorrelated. The Monte Carlo handout discusses how to do this.

   You should see that $\langle m^2 \rangle$ increases as T is reduced, and that this effect is happens more suddenly at larger sizes. This is because the transition which occurs for $N = \infty$ is "rounded out" by finite-size effects, which becomes more pronounced for small sizes. You should see this rounding in your data.

2. Why did I ask you to calculate $\langle m^2 \rangle$ and not $\langle m \rangle$?

3. To get a quantitative estimate for T_c we use an assumption from "finite-size scaling", the theory used to extrapolate numerical data on finite size systems in the vicinity of a phase transition to infinite system size. According this theory, the size dependence in the data is a function of the ratio of the system size L to the correlation length ξ (of an infinite system). As discussed in class, the range of the correlations grows as we approach the transition, and, in fact, ξ diverges according to

   $$\xi \propto |T - T_c|^{-\nu}, \tag{4}$$

   where ν is a "critical exponent". For the two-dimensional Ising model, the exact solution yields

   $$\boxed{\nu = 1\,.} \tag{5}$$

   The claim, therefore, is that the ratio

   $$\frac{L}{\xi} \propto L|T - T_c|^{\nu} \tag{6}$$

   is very important in determining finite-size corrections. It is actually more useful to have $T - T_c$ appear linearly, and so we take the ratio L/ξ to the power $1/\nu$, and finite-size scaling then tells us that finite-size corrections will involve functions of

   $$L^{1/\nu}(T - T_c)\,. \tag{7}$$

As an example, the finite-size scaling form for $\langle m^2 \rangle$ is

$$\langle m^2 \rangle = L^y f\left(L^{1/\nu} (T - T_c) \right) , \tag{8}$$

where $f(x)$ is a function (called a "finite-size scaling function"). We shall see that we also need the factor of L^y multiplying the scaling function in order to get the correct behavior in the thermodynamic limit ($L \gg \xi$).

For an infinite system, $\langle m^2 \rangle$ is the square of the magnetization. The latter is is zero above T_c and varies below T_c as $\propto (T_c - T)^\beta$, where β is another critical exponent. For the two-dimensional Ising model the exact solution gives

$$\boxed{\beta = 1/8\,.} \tag{9}$$

Hence,

$$\begin{aligned}
\langle m^2 \rangle &\to 0, && \text{for } L^{1/\nu}(T - T_c) \gg 1, && (T > T_c) && \text{(10a)}\\
\langle m^2 \rangle &\to (T_c - T)^{2\beta}, && \text{for } L^{1/\nu}\,(T_c - T) \gg 1, && (T < T_c), && \text{(10b)}
\end{aligned}$$

In order to get the behavior in Eq. (10b) from Eq. (8), the L dependence must cancel between the factor of L^y and the form of the scaling function $f(x)$ for $x \to -\infty$. In addition, the T dependence must be $(T_c - T)^{2\beta}$. These two conditions require that

$$f(x) \propto (-x)^{2\beta}, \qquad (x \to -\infty)\,, \tag{11}$$

and

$$y = -\frac{2\beta}{\nu}. \tag{12}$$

Hence the data for $\langle m^2 \rangle$ should be of the following form

$$\boxed{\langle m^2 \rangle = L^{-2\beta/\nu} f\left((T - T_c)\, L^{1/\nu} \right) ,} \tag{13}$$

where T_c, ν and β are given by Eqs. (2), (5) and (9).

Verify that your data fits this form by plotting $\langle m^2 \rangle\, L^{2\beta/\nu}$ against $(T - T_c)\, L^{1/\nu}$ using the given values of T_c, ν and β, and observing that the data for different sizes "collapses" on to a common curve. Only consider data near T_c, and don't try to take large values of the parameter $x = (T - T_c)L^{1/\nu}$. The range $-5 < x < 5$ is reasonable.

Note: There are corrections to the finite-size scaling form, Eq. (13), if the sizes are too small or T is too far from T_c.

4. *(242 students only)*

   Finite-size scaling also predicts that the whole probability distribution of the magnetization per spin m, can be expressed in a finite-size scaling form

$$\boxed{P(m) = L^\lambda \widetilde{P}\left(L^\lambda\, m,\ L^{1/\nu}\, (T - T_c) \right) ,} \tag{14}$$

where $\widetilde{P}(x, y)$ is a function of two variables. The second argument is the familiar one, $y = L^{1/\nu}(T - T_c)$, and incorporates the temperature dependence. Since the distribution is normalized, i.e. $\int P(m)\, dm = 1$, the power of L multiplying m in the first argument, (λ), must equal the power of L in the prefactor, and normalization then follows provided $\int \widetilde{P}(x, y)\, dx = 1$.

In fact we must have

$$\boxed{\lambda = \beta/\nu} \tag{15}$$

in order to reproduce the expected behavior of the order parameter in Eq. (10b), $\langle m^2 \rangle \propto (T_c - T)^{2\beta}$, for $T < T_c, L \to \infty$. To show this, note that we are considering the limit $y \to -\infty$. In this limit, if the scaling function has the form $\widetilde{P}(x, y) \propto (-y)^{2\beta}\, \overline{P}(x)$, where $\overline{P}(x)$ is a function of x, then Eq. (10b) is obtained provided $\lambda = \beta/\nu$. In fact, $\overline{P}(x)$ will be two delta functions, each with weight $1/2$ at $x = \pm x_0$, where x_0 is related to the constant of proportionality in Eq. (10b).

From Eq. (14), it follows that ratios of combinations of moments such that the total power in the numerator and denominator is the same have *no* power of L multiplying the scaling function (it cancels out). A commonly studied example is the "Binder ratio", defined by

$$g_L = \frac{1}{2}\left(3 - \frac{\langle m^4 \rangle}{\langle m^2 \rangle^2}\right), \tag{16}$$

where the factors of 3 and $1/2$ are put in for convenience; they ensure that $g_L \to 1$ for $T \to 0$ and $g_L \to 0$ for $T \to \infty$ (for all L).

The finite-size scaling form for g_L is then

$$\boxed{g_L = \widetilde{g}\left((T - T_c)\, L^{1/\nu} \right)\ ,} \tag{17}$$

where $\widetilde{g}(x)$ is a scaling function which has the properties $g(x) \to 0$ for $x \to \infty$ and $g(x) \to 1$ for $x \to -\infty$. From Eq. (17) it follows that g_L should be independent of L at T_c (but dependent on L at other temperatures). The transition can therefore be found from the *intersection* of data for g_L against T for different sizes.

Compute g_L at different temperatures for sizes $L = 8, 16$ and 32. You need to determine error bars. Since g is not just a single average, but involves a ratio of different averages, it is not entirely obvious how to do this. I suggest you use the jackknife method described in `http://physics.ucsc.edu/~peter/jackboot.pdf`. Please come to my office to discuss this technique.

You should estimate T_c from the point where the data intersect. This should be very close to the exact T_c given in Eq. (2). The advantage of using a dimensionless quantity like g_L is that T_c can be determined *independently* of any other parameters. If we were to determine T_c from Eq. (13) for $\langle m^2 \rangle$ we would need to *simultaneously* fit three parameters, T_c, μ and $2\beta/\nu$.

Once you have located T_c, *determine* the exponent ν by plotting g_L against $(T - T_c)L^{1/\nu}$ and adjusting ν until the data "collapses" on to a single curve. Compare your result with the exact answer in Eq. (5).