

**PHYSICS 115/242**  
**Monte Carlo Simulation Project**

**Due on Monday, June 2.**

This is a long time off, but you should start it soon. 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

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} S_i S_j, \quad (1)$$

where there are  $N$  spins  $S_i$  which take values  $\pm 1$ , 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. The appendix describes one convenient way of implementing periodic boundary conditions.

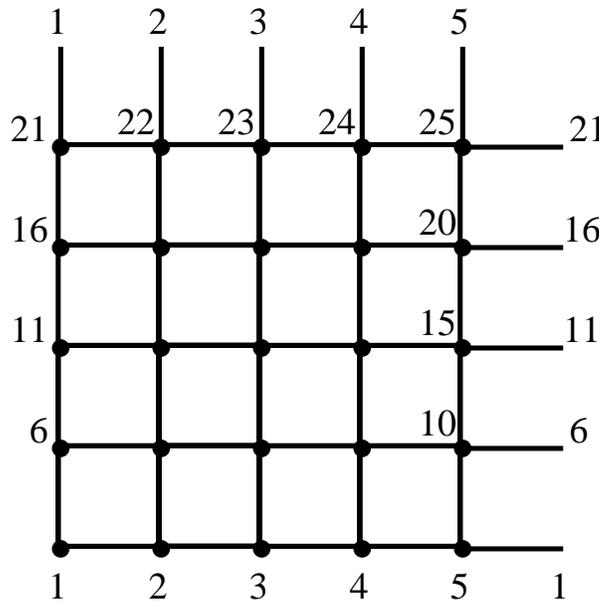


Figure 1: A  $5 \times 5$  lattice with periodic boundary conditions.

This model has a phase transition at temperature

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

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

$$m = \frac{1}{N} \sum_{i=1}^N S_i. \quad (3)$$

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 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  $T_c$  it 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 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 to this theory, the size dependence in the data is a function of the ratio of the system size  $L$  to the correlation length  $\xi$  (of an infinite system). As discussed in class, the range of the correlations grows as we approach the transition, and, in fact,  $\xi$  diverges according to

$$\xi \propto |T - T_c|^{-\nu}, \quad (4)$$

where  $\nu$  is a “critical exponent”. For the two-dimensional Ising model, the exact solution yields

$$\boxed{\nu = 1}. \quad (5)$$

The claim in finite-size scaling is, therefore, that the ratio

$$\frac{L}{\xi} \propto L|T - T_c|^\nu \quad (6)$$

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

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

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

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

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 zero above  $T_c$  and varies below  $T_c$  as  $\propto (T_c - T)^\beta$ , where  $\beta$  is another critical exponent. For the two-dimensional Ising model the exact solution gives

$$\boxed{\beta = 1/8.} \quad (9)$$

Hence,

$$\langle m^2 \rangle \rightarrow 0, \quad \text{for } L^{1/\nu}(T - T_c) \gg 1, \quad (T > T_c) \quad (10a)$$

$$\langle m^2 \rangle \rightarrow (T_c - T)^{2\beta}, \quad \text{for } L^{1/\nu}(T_c - T) \gg 1, \quad (T < T_c), \quad (10b)$$

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  $x \rightarrow -\infty$ . In addition, the  $T$  dependence must be  $(T_c - T)^{2\beta}$ . These two conditions require that

$$f(x) \propto (-x)^{2\beta}, \quad (x \rightarrow -\infty), \quad (11)$$

and

$$y = -\frac{2\beta}{\nu}. \quad (12)$$

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

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

where  $T_c, \nu$  and  $\beta$  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  $T_c, \nu$  and  $\beta$ , 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

$$\boxed{P(m) = L^\lambda \tilde{P} ( L^\lambda m, L^{1/\nu} (T - T_c) ) ,} \quad (14)$$

where  $\tilde{P}(x, y)$  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,  $(\lambda)$ , must equal the power of  $L$  in the prefactor, and normalization then follows provided  $\int \tilde{P}(x, y) dx = 1$ .

In fact we must have

$$\boxed{\lambda = \beta/\nu} \quad (15)$$

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  $T < T_c, L \rightarrow \infty$ . To show this, note that we are considering the limit  $y \rightarrow -\infty$ . In this limit, if the scaling function has the form  $\tilde{P}(x, y) \propto (-y)^{2\beta} \bar{P}(x)$ , where  $\bar{P}(x)$  is a function of  $x$ , then Eq. (10b) is obtained provided  $\lambda = \beta/\nu$ . In fact,  $\bar{P}(x)$  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 which are *dimensionless*, i.e. 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

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

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

The finite-size scaling form for  $g_L$  is then

$$\boxed{g_L = \tilde{g}((T - T_c) L^{1/\nu})}, \quad (17)$$

where  $\tilde{g}(x)$  is a scaling function which has the properties  $g(x) \rightarrow 0$  for  $x \rightarrow \infty$  and  $g(x) \rightarrow 1$  for  $x \rightarrow -\infty$ . 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://young.physics.ucsc.edu/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,  $T_c, \mu$  and  $2\beta/\nu$ .

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

## A Implementing periodic boundary conditions

This appendix discusses one convenient way of implementing boundary conditions. For compactness we will just consider one-dimension. In the project, which considers two dimensions, you will have two nested loops, one over  $x$  and the other over  $y$ , and you apply the same scheme for both of them.

The sites are labeled by an index  $i$  which runs from 0 to  $L - 1$ . We need two more indices to label the neighbors of site  $i$ , namely  $ip$  which is the site to the right of  $i$ , and  $im$  which is the site to the left. Normally  $ip = i + 1$  and  $im = i - 1$ . However, a correction is needed either if  $i = L - 1$  because then  $ip = 0$  rather than  $L$ , or if  $i = 0$  because then  $im = L - 1$  rather than  $-1$ . Instead of putting a lot of `if` statements in the code, which are messy to read and slow down execution, the following scheme works simply and elegantly:

```
im = L-2;
i = L-1;
for (ip = 0; ip < L; i++)
{
    .....
    im = i;
    i = ip;
}
```

where  $\dots$  indicates the rest of the code. Note that we sum over  $ip$ , not  $i$ , and the last two assignments cause  $i$  and  $im$  to “chase their tails” round the periodic boundary conditions. Check this by verifying that the successive values of  $im, i$  and  $ip$  are as follows:

$im$	$i$	$ip$
$L - 2$	$L - 1$	0
$L - 1$	0	1
0	1	2
1	2	3
$\vdots$	$\vdots$	$\vdots$
$L - 3$	$L - 2$	$L - 1$