Topic 3: Monte Carlo Simulation of Magnetic Materials (continued)

The most interesting behavior of the model occurs in the neighborhood of the phase transition from the low-temperature ferromagnetic phase to the high-temperature paramagnetic phase. Ernst Ising proved in his doctoral thesis in 1924 that the 1-D Ising model has no finite-temperature ferromagnetic phase, i.e., the Curie temperature $T_c = 0$. Kramers and Wannier showed in 1941 that the 2-D Ising model

$$\frac{k_{\rm B}T_c}{J} = \frac{2}{\ln(1+\sqrt{2})} = 2.269...$$

and in 1944, Lars Onsager found an exact analytic formula for the magnetization as a function of temperature.

Visualizing the Ising phase transition

The program cluster.c uses OpenGL graphics to display the lattice of Ising spins as it is being updated in the Monte Carlo simulation.

Dr. Michael Creutz has written a very efficient program xising.c as part of his Xtoys cellular automata programs.

These programs allow one to visualize the *critical slowing down* that occurs in the neighborhood of the phase transition. Fluctuations in the spins become strongly correlated over large distances. The *correlation length*

$$\xi(T) \sim \frac{1}{|T-T_c|^\nu} ,$$

for spin fluctuations

$$\langle s_0 s_r \rangle - \langle s \rangle^2 \sim e^{-r/\xi} ,$$

diverges at the Curie temperature. The *correlation length critical exponent* $\nu = 1$ for the 2-D Ising model. Patterns or *domains* of like spins develop near T_c, and these domains persist for long times. This implies that the successive Monte Carlo configurations are not statistically independent. This problem of *critical slowing down* has been investigated. For the 2-D Ising model simulated with the Metropolis algorithm, it can be shown that the *correlation time* τ, i.e., the minimum number of Monte Carlo steps between uncorrelated (independent) configurations in the simulation, behaves like

$$\tau \sim \xi^z , \quad \text{where} \quad z \simeq 2.125 .$$

Divergence of Heat Capacity and Susceptibility

The *heat capacity* at constant magnetic field H of the system measures the response to changes in temperature:

$$C_H = \left(\frac{\partial \langle E \rangle}{\partial T} \right)_H = \frac{1}{k_{\rm B} T^2} \left[\langle E^2 \rangle - \langle E \rangle^2 \right] .$$

Note that the heat capacity can be measured in two ways:

1. measure $\langle E \rangle$ as a function of temperature T and find the derivative numerically, or

2. measure the fluctuations of the energy at fixed temperature using the *fluctuation-dissipation formula*.

The *isothermal susceptibility* of the system measures the response to changes in magnetic field:

$$X_T = \left(\frac{\partial \langle M \rangle}{\partial H}\right)_T = \frac{1}{k_{\mathrm{B}} T}\left[\langle M^2 \rangle - \langle M \rangle^2\right] .$$

These quantities are *extensive*, i.e., proportional to the size of the system. When studying the thermodynamic limit $N \to \infty$ by simulating lattice of increasing size L, it is more appropriate to measure the heat capacity per spin

$$c_H = \frac{C_H}{N} = \frac{1}{N k_{\mathrm{B}} T^2}\left[\langle E^2 \rangle - \langle E \rangle^2\right] ,$$

and the susceptibility per spin

$$\chi_T = \frac{X_T}{N} = \frac{1}{N k_{\mathrm{B}} T}\left[\langle M^2 \rangle - \langle M \rangle^2\right] .$$

It is very interesting that these per-spin quantities actually diverge at the Curie temperature in the thermodynamic limit! The isothermal susceptibility diverges like

$$\chi_T \sim \frac{1}{|T - T_c|^{\frac{7}{4}}} ,$$

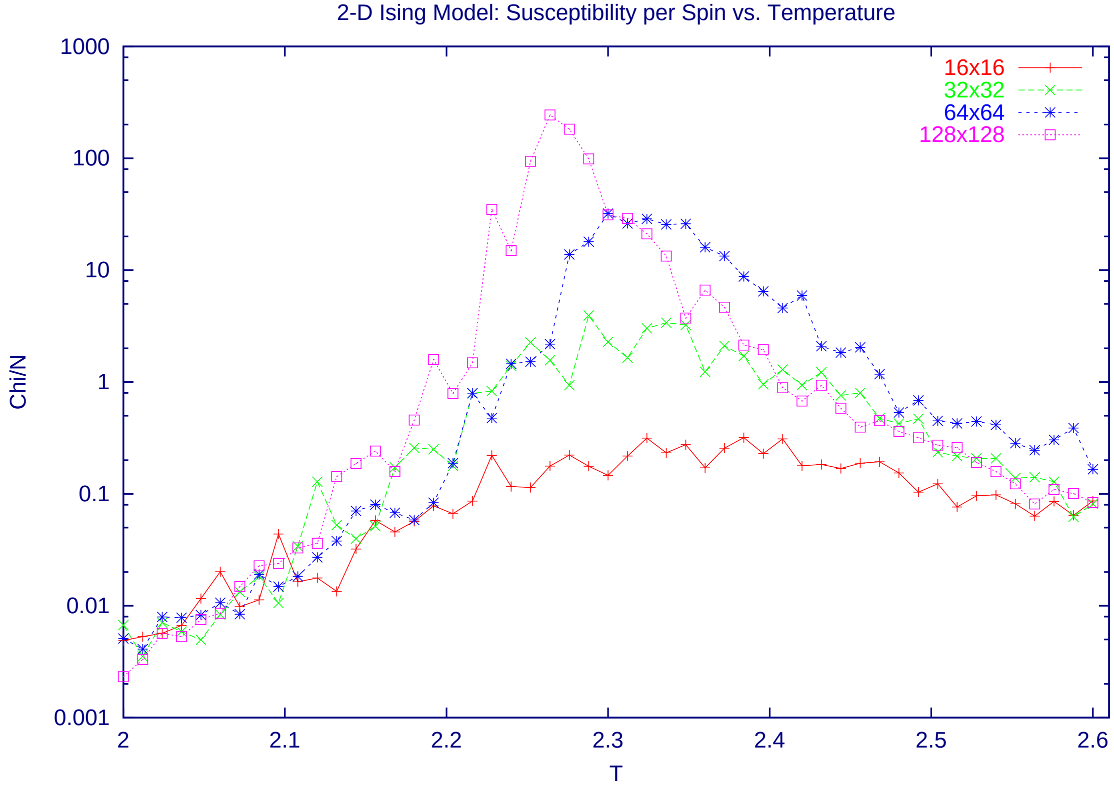
for the 2-D Ising model, while the heat capacity has a much milder logarithmic divergence

$$C_H \sim \log\left(\frac{1}{|T - T_c|}\right) .$$

How is it possible for a single spin to have a divergent heat capacity or susceptibility? The answer is that because the correlation length diverges, it is affected by an infinite number of other spins! Thus even an infinitesimal change in temperature or applied field causes a finite change in its energy or average magnetic moment.

Critical slowing down makes it difficult to simulate the Ising model close to T_c. This is illustrated by the following plot of the susceptibility per spin which was measured using the Metropolis algorithm with 10,000 thermalization steps and 20,000 production steps at each temperature value. The growth of χ with lattice size, and the uncertainties in the determination of chi are evident from the plot.

To overcome this critical slowing down one can use *cluster algorithms*, such as the Swendsen-Wang algorithm or the Wolff algorithm. These are designed to change large clusters of spins at each step rather than one spin at a time as in the Metropolis algorithm.


2-D Ising Model: Susceptibility per Spin vs. Temperature
Chi/N
T
1000
100
10
1
0.1
0.01
0.001
2
2.1
2.2
2.3
2.4
2.5
2.6
16x16
32x32
64x64
128x128