COINS
Center of Integrated Nanomechanical Systems

Computational Nanoscience

NSE C242 & Phys C203

Spring, 2008

Lecture 12:

In-Class Simulation : Ising Model

February 28, 2008

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Review

- What is a phase transition?
- How are they classified?
- What is an order parameter?
- What is an Ising model?
- For the spin 1/2 Ising model with only nearest neighbor interactions on a cubic lattice, what do we know from analytical solutions about the 1, 2, and 3 -dimensional behavior?

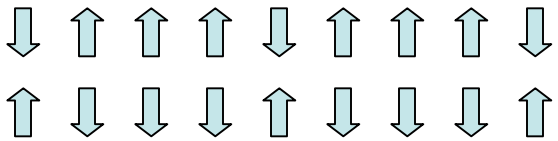
Review

- In the para-ferro magnetic transition which we will simulate today, describe using energy and entropy arguments why the phase transition occurs.
- Name (and describe) two important considerations when simulating phase transitions.
- Describe the implications of both of these for your simulation.
- Name an approach for “getting around” finite size effects?
- What is linear response, and how can we make use of it to get useful information from the fluctuations in your simulation?

Spin-Spin Correlation in the Ising Model

We are going to add one more correlation function to the series of correlation functions that we have studied so far. This correlation function is called the **spin-spin correlation function**, and it tell us how much correlation we can expect between two spins that are a given distance apart.

Consider a series of spins.



The question that this correlation function helps us understand: At a given temperature T, what is the probability that the spin at site (i+m) is aligned with the spin at site i?

If we denote spin-up with a +1 and spin-down with a -1, we can define the correlation function as

$$g(m) = \frac{\langle \sigma_i \sigma_{i+m} \rangle - \langle \sigma_i \rangle \langle \sigma_{i+m} \rangle}{1 - \langle \sigma_i \rangle \langle \sigma_{i+m} \rangle} = \langle \sigma_i \sigma_{i+m} \rangle$$

Holds for the case of zero applied field (H=0)

Spin-Spin Correlation Function

If the two sites tend to have the same spin (correlated),

$\sigma_i\sigma_{i+m}$ (-1)(-1)=1 (1)(1)=1

$$g(m) = \langle \sigma_i \sigma_{i+m} \rangle = 1$$

If the two sites have the the same spin half the time, and opposite spins half the time (completely random, uncorrelated),

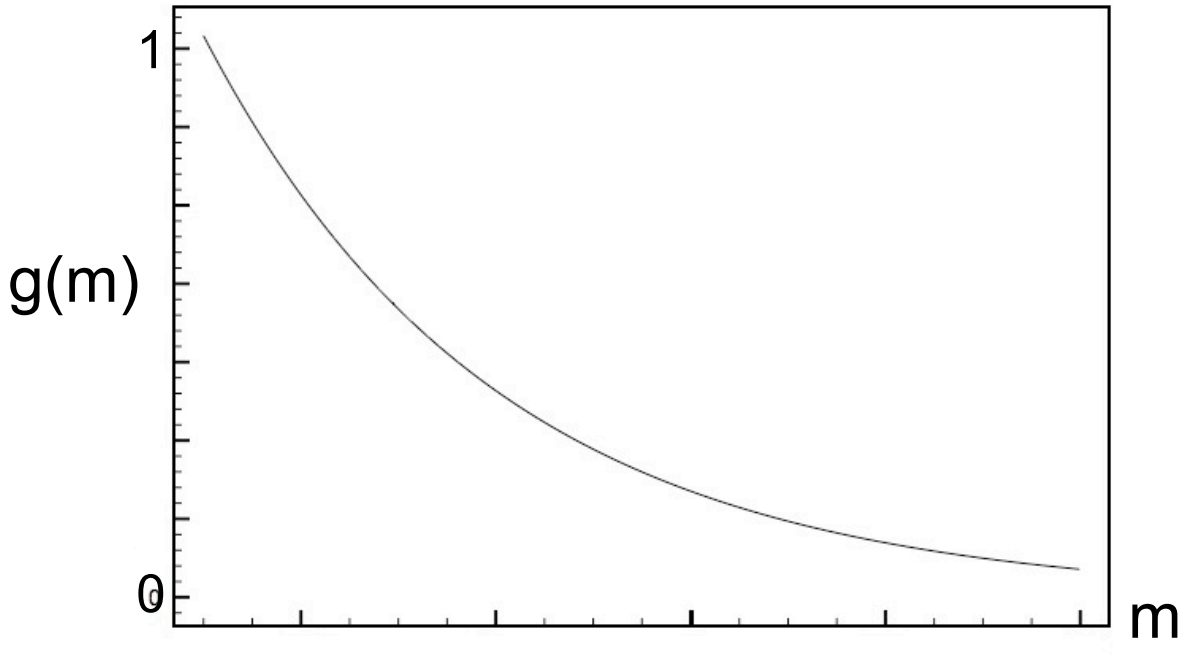
$\sigma_i\sigma_{i+m}$ (-1)(-1)=1 (1)(1)=1 (-1)(1)=-1 (-1)(1)=-1

$$g(m) = \langle \sigma_i \sigma_{i+m} \rangle = 0$$

The correlation function varies from 0 (no information) to 1 (complete correlation).

Spin-Spin Correlation Function

Qualitatively, we might expect the function g(m) to look something like this:



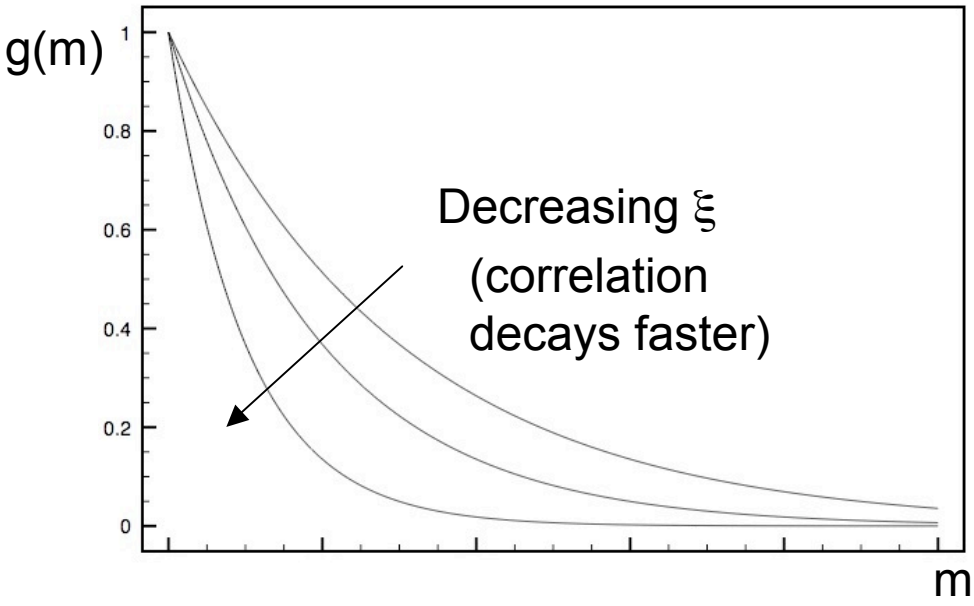
Spin-Spin Correlation Function

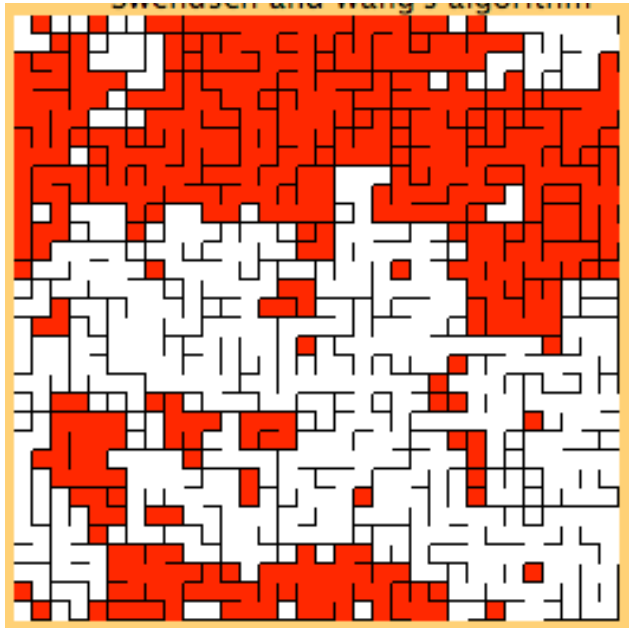
In fact, we can rigorously show that the correlation function exhibits the scaling form:

$$g(m) \sim \frac{1}{m^{v}} \exp\left[-m/\xi\right]$$

The parameter ξ is known as the **correlation length** and it varies with temperature.

ξ can be thought of as a measure of the distance over which spins will respond to what each other are doing.





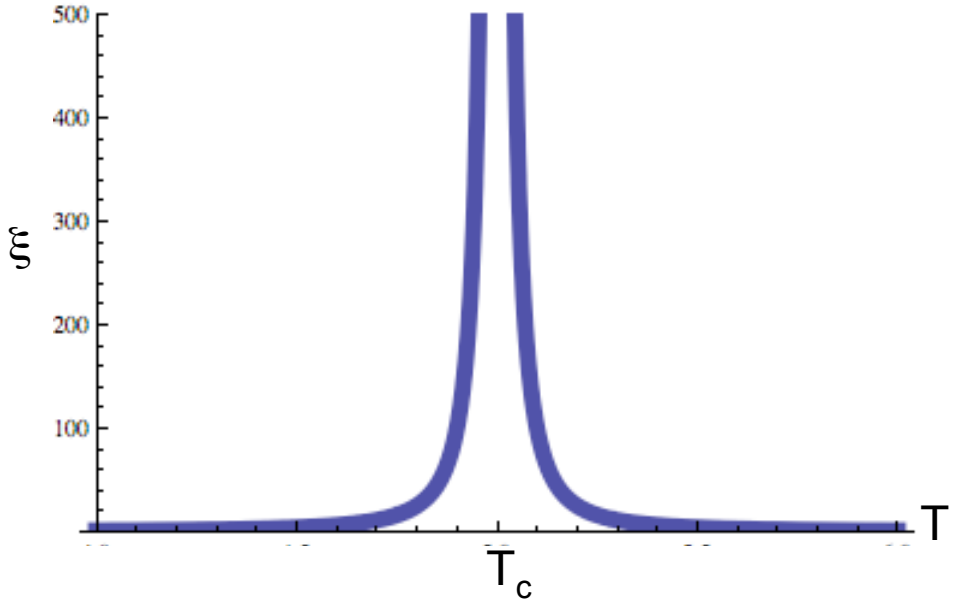
Domain structure from http://www-fcs.acs.i.kyoto-u.ac.jp/%7Eharada/monte-en.html

Correlation Length

At high T, the correlation length is low. The spins fluctuate rapidly, but they do so independently of each other.

Perhaps surprisingly, at low T, the correlation length is also low (even though the spins tend to be aligned). The point is that flipping σ_0 will hardly affect σ_n unless they are neighbors.

Near the critical temperature, the situation is different. The spins are constantly changing, but not independently. There are large domains of parallel spins which persist for a long time. Thus, spins far apart from each other are strongly correlated.



Diverging Correlation Length

This means that a given spin is infinitely aware of what it's neighbors, no matter how far away they are, are doing -- and that it is capable of responding because the thermal energy is high enough.

And, this divergence in the correlation length is responsible for the critical slowing down that we discussed last time as well as the large fluctuations in the system.

Near a phase transition, it takes an infinite amount of time for such a system to actually equilibrate during a Monte Carlo simulation. This is because every time a spin is flipped, all of it's neighbors want to respond -- and can.

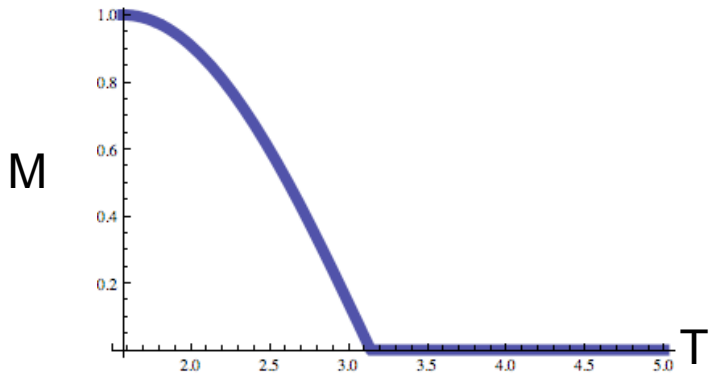
In this regime, the Metropolis approach - where one flip is switched at a time - becomes extremely inefficient for sampling phase space. We tend to rely on other approaches such as Wolff flipping (cluster flipping, where entire domains are flipped at once).

In-Class Simulation

Today, we will begin simulating the 2D Ising Model - and in the process start your next homework assignment.

The code that we will use comes to us from RPI*, and is a very nice java implementation of the Ising Model. (It actually can generalize to continuous spins for a variety of dimensions, functionality which we will not make use of today).

- We will be looking for signs of phase transitions using the 2D Ising model
- The order parameter should look something like this, in principle:



- We will look at systems of different sizes to explore finite size effects

*http://www.rpi.edu/~limc/applets/ising/ -- source code available for download!

In Class Simulation

- **First Task: Look for the formation of domain walls at low temperatures in the 2D ferromagnet for an 16x16 system.**
- Choose
  - "1" for number of z lattice points,
  - J = 1.0 for the interaction strength
  - No applied external field
  - Periodic BCs in X and Y, but not in Z
  - Make sure "Constrained To Z Axis" is checked
  - Make sure "Equalize after Resets" is checked
- For each size, vary the temperature starting from 0.0 and increasing in increments of 0.1 up to 0.4
- Do a few runs for each temperature. Can you see domain wall formation?
- Are these domains physical, or is the Metropolis scheme simply getting stuck? What might you do about this?

In Class Simulation

- **Second Task: Eyeball the transition behavior of the 2D anti-ferromagnet for an 8x8 system.**
- Choose
  - "1" for number of z lattice points,
  - J = -1.0 for the interaction strength
  - No applied external field
  - Periodic BCs in X and Y, but not in Z
  - Make sure "Constrained To Z Axis" is checked
  - Make sure "Equalize after Resets" is checked
- For each size, vary the temperature starting from 1.3 and increasing in increments of 0.3 up to 3.4
- Try to eyeball where the phase transition occurs.
- You can look at plots of average magnetization for each run to help you.
- At what size does the transition seem sharpest?

In Class Simulation & Homework

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- **GOAL: estimate the critical transition temperature and the susceptibility for the 2D easy-axis ferromagnet.**

- We will explore systems of size 4x4, 8x8, and 16x16.
- Vary the temperature from 1.3 to 3.4 in increments of 0.3
- HINT: You MUST use long runs. We are, afterall, going after the phase transition and we are limited to Metropolis algorithm. You need to equilibrate your system and then run for a long time (say 5,000 steps).
- Yes, 5,000. Even if it looks like nothing is going on, this is not the case. Those “blips” on the screen are very important to our statistics and tell us something about the system.

In Class Simulation & Homework

Center of Integrated Nanomechanical Systems

- **GOAL: estimate the critical transition temperature and the susceptibility for the 2D easy-axis ferromagnet.**

- We will explore systems of size 4x4, 8x8, and 16x16. Each of you should choose two of these sizes.
- Then, for each size, you should vary the temperature from 1.3 to 3.4 in increments of 0.3
- Thus, each of you should complete sixteen runs for this experiment.
- For each run, download the data on the magnetization. You need to record
  - average value of $|m|$. Note that this is the magnetization per site, and it is an absolute value.
  - The error in your calculation of the average
  - The number of steps over which you computed the average (~5000)
- You should see good evidence for a phase transition!
- **In order to get better statistics, send me (Elif) your results by Mar 6, which I will compile and make available on the course website. Next homework assignment will be posted today, and due Tuesday Mar 11.**

The Ising on the Cake

Now that we are concluding our discussion of Monte Carlo methods, you should be familiar with the following concepts and ideas.

- What is a Monte Carlo simulation? What can it be used for?
- Understand the following concepts:
  - Partition Functions, and evaluating average properties
  - Balance and Detailed Balance
  - Importance Sampling
  - Boltzmann Distribution
  - Metropolis Algorithm
  - Canonical Monte Carlo (NVT)
  - Grand Canonical Monte Carlo (μVT)
  - Transition State Theory
  - Phase Transitions and Order Parameters
  - Ising Models
  - Critical Slowing Down
  - Linear Response
  - Finite Size Effects
- Describe how each of the following work, and the differences between them: MD, MC, and KMC