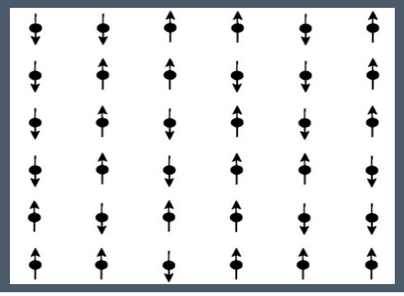

Exploring Magnetism in Solid Lattices with Efficient Monte Carlo Simulations

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ABSTRACT

A Monte Carlo simulation was implemented for a square Ising lattice of interacting atomic spins to collect independent measurements of the crystal's magnetization at varying times. Due to the stochastic updating algorithm for the spin sites, one system state was strongly correlated with the next state. To retain the validity of the magnetization average and variance calculations and minimize their bias, the simulation needed to only collect data when the states were nearly uncorrelated. Evidently, the time steps required for the 30x30 (dimensions in site numbers) lattice's spin autocorrelation to drop below 10% ranged from ~20 steps when far from the critical temperature (ferromagnetic to paramagnetic phase change) to ~200 steps when very close to the critical temperature. The next step to improve the Monte Carlo simulation efficiency is to train a neural network to more quickly calculate the probabilities of flipping spins on the lattice.

ISING LATTICE MODEL

- Square grid of regularly spaced stationary atoms
- Each atom has an up arrow (+1) or down arrow (-1) representing its spin S_i
- Each pair of nearest neighboring atoms are coupled with strength J > 0 indicating a ferromagnet
- **Known lowest energy state: ordered spins**
- **Question: At what temperature will the ordering of the spins disappear?**

$$E = -J \sum_{<ij>,\, i \neq j}^{N} S_i * S_j$$

METROPOLIS TIME STEPS

- Recreate the time-dependent behavior of a material's magnetism
- **Monte Carlo:** Stochastic update scheme for the lattice in time steps (configuration s to s')
- Each instant: propose individual spins flips
- Classical Maxwell-Boltzmann distribution: **Likelihood of a state change** depends on energy change Delta E and temperature T (Boltzmann constant k_B = 1)
- Number of updates may be less than the number of proposals

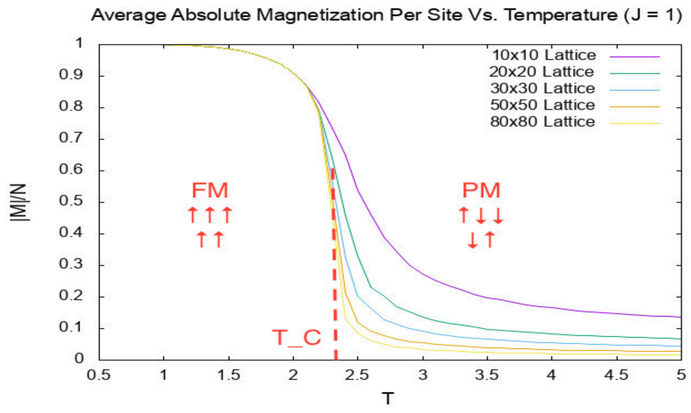
$$P(S_i \longrightarrow -S_i) = P(s')/P(s) = e^{-\Delta E/k_B T}$$

1. Tell the computer how to calculate the lattice's energy
2. Have it **tend** toward states of lower energy **more often**
3. See what happens

- **Compare** with the trends observed experimentally
- Record the system magnetization at each instant—sum of all the spin values

$$M = \sum_{i=1}^{N} S_i$$

DATA/CRITICAL SLOWING

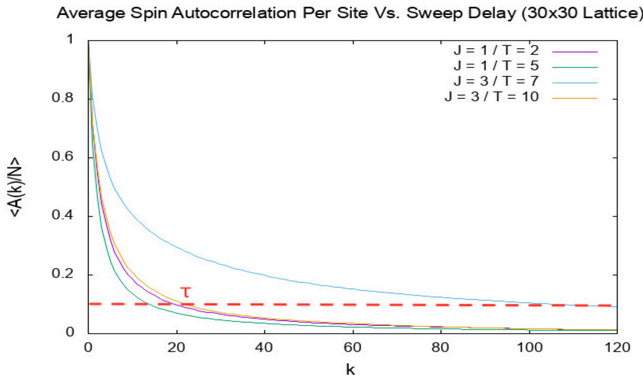


Lattice's average magnetization at different temperatures. Ferromagnetic (ordered spin sites) at low temperatures and paramagnetic (disordered spin directions) above a critical temperature (better defined for larger systems).

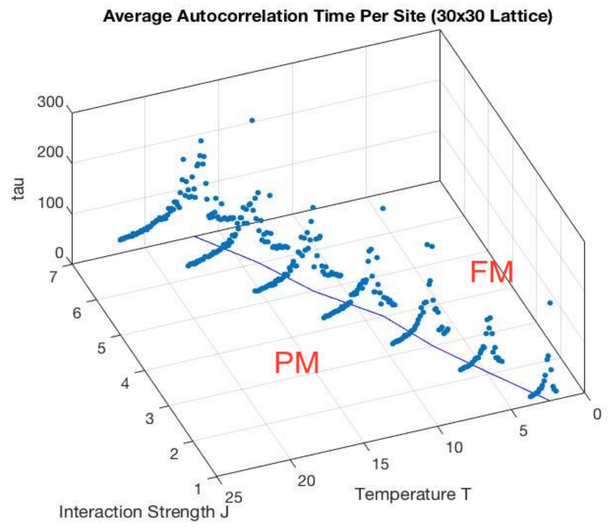
CORRELATED STATES

- **Why would highly correlated magnetization data problematic?**
- Autocorrelation A: quantifies expected relatedness of any two collected measurements separated by a time lag k
- N = number of values taken for a single site's spin
- S_bar = time average for a single site's spin
- Sigma squared = time variance for a single site's spin
- Threshold autocorrelation time tau: lag k required for the measurements to lose correlation (A below 10%)

$$A(k) = \frac{\sum_{i=1}^{N-k}(S_{i+k} - \bar{S})(S_i - \bar{S})}{\sigma^2(N - k)}$$



Spin autocorrelation seems to decay with increasing wait times until intersecting the 10% threshold



Required autocorrelation time tau (blue dots) grows very large near the lattice's phase transition (solid blue line). This is the Monte Carlo **critical slowing problem**, and it makes the simulation very inefficient around these conditions

CITATIONS

Lattice diagram:
http://sadrnezhaad.ir/mahdi/index.php/physics/26-ising-model-and-simulation

Jacques K. March 2008. Introduction to Monte Carlo methods for an Ising Model of a Ferromagnet [thesis]. [Mansfield (CT)]: University of Connecticut.