Monte Carlo Investigations on Classical and Quantum Ising Models and Their Phase Transitions

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Summer Research Fellowship (SRF) 2020 for Science Students
Poster No: D7
UID: 3035551668
Major: Physics

Abstract

The Ising model was first raised by Wilhelm Lenz (1920) who gave it as a problem to his student Ernst Ising. Ising (1925) solved the 1-D Ising model and turned out no phase transition happens. The analytic solution of 2-D Ising model is more complicated and is obtained by Lars Onsager (1944). For 3-D model there is no analytic solution. Monte Carlo method is introduced to obtain a statistical average among numerous ensembles through which the model of any dimension can be solved easily. This research performs the Metropolis and Cluster algorithm in simulating the phase transition of 2-D Ising model. Also, since a N-D quantum system can be mapped to a (N+1)-D classical system, the phase transition of 2-D quantum Ising model is investigated as well. Based on the finite size scaling theorem, the critical points of phase transition are computed with satisfactory accuracy compared with literature values.

Introduction

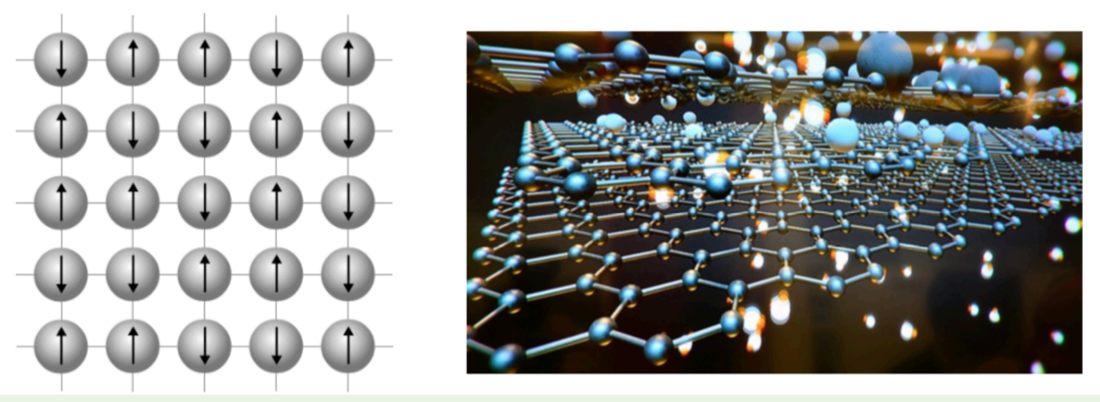
- **Ising Model:**

Ising model is a basic mathematical model that describe magnetic phase transitions, in which spins can take two values: ± 1. Consider the nearest-neighbor interaction and zero external field, the energy of the system is:

$$H = J\sum_{\langle i,j\rangle}\sigma_i^z\sigma_j^z$$

For ferromagnetism, J is negative and is taken -1 in this report. In dimension d>1, the Ising model exhibits a phase transition between a disordered (paramagnetic) state at high temperatures and an ordered (ferromagnetic) state at low temperature. The order parameter is the magnetization,

$$\boldsymbol{m} = \frac{\mathbf{1}}{N}\sum_{i=1}^{N}\sigma_i^z$$



- **Transvers Field Ising Model:**

The Hamiltonian is now with an additional term representing the transverse field in x direction.

$$H = -J\sum_{<i,j>}\sigma_i^z\sigma_j^z - h\sum_i \sigma_i^x$$

The partition function is,

$$Z = \mathrm{Tr}e^{-\beta H} = \mathrm{Tr}\left[e^{-\Delta\tau H}e^{-\Delta\tau H}e^{-\Delta\tau H}\dots e^{-\Delta\tau H}e^{-\Delta\tau H}\right]$$

In which we set $\beta = L\Delta\tau$, the product inside the trace can be viewed as a succession of imaginary time evolution operators. We introduce a complete set of σ^z eigenstates,

$$\mathbf{1} = \sum\left|\sigma_i^Z\right\rangle\left\langle\sigma_i^Z\right|$$

The partition function becomes,

$$Z = \sum\left\langle\sigma_1^Z\middle|e^{-\Delta\tau H}\middle|\sigma_L^Z\right\rangle\left\langle\sigma_L^Z\middle|e^{-\Delta\tau H}\middle|\sigma_{L-1}^Z\right\rangle\left\langle\sigma_{L-1}^Z\middle|e^{-\Delta\tau H}\middle|\sigma_{L-2}^Z\right\rangle\cdots$$

Each matrix element is found:

$$\left\langle\sigma_{l+1}^Z\middle|e^{-\Delta\tau H}\middle|\sigma_l^Z\right\rangle = \Lambda^N e^{\Delta\tau J\sum_{\langle i,j\rangle}\sigma_{i,l}^z\sigma_{j,l}^z + \gamma\sum_{\langle i,j\rangle}\sigma_{\langle i,j\rangle,l}^z\sigma_{\langle i,j\rangle,l+1}^z}$$

Then the partition function is evaluated, mapping to a (N+1)-D classical model.

$$Z = \Lambda^{NL}\sum e^{\Delta\tau J\sum_{\langle i,j\rangle}\sum_{l=1}^{L}\sigma_{i,l}^z\sigma_{j,l}^z + \gamma\sum_{\langle i,j\rangle}\sum_{l=1}^{L}\sigma_{\langle i,j\rangle,l}^z\sigma_{\langle i,j\rangle,l+1}^z}$$

$$\gamma = -\frac{1}{2}\ln\tanh(\Delta\tau h)$$

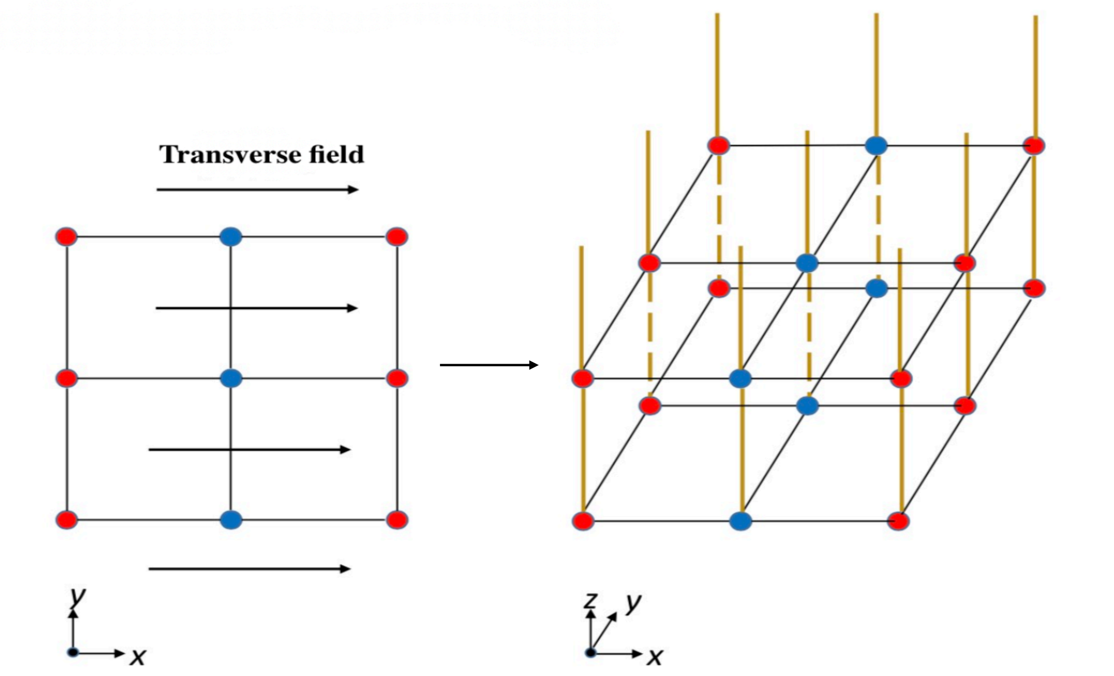


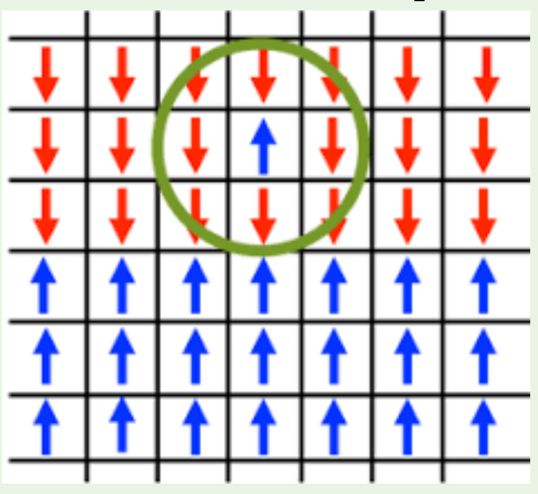
Figure 1. 2-D quantum Ising model mapping to 3-D classical Ising model. Red point represents the positive spin in z direction and blue point is negative spin.

Algorithm

- **Metropolis (local update)**

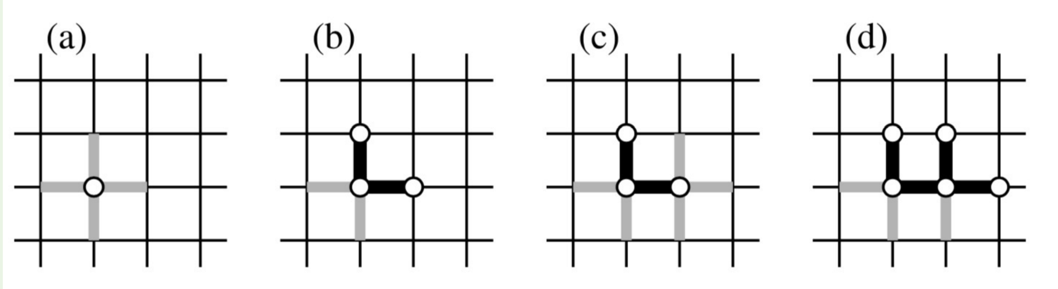
Randomly choose a spin. Consider to flip the spin σ^z to $-\sigma^z$. The probability of acceptance is,

$$P^{\text{accept}}(C_i \rightarrow C_j) = \min\left[e^{-\beta(E_j - E_i)}, 1\right]$$



- **Wolff (cluster update)**

All nearest neighbors of a random chosen spin are added to the cluster with a probability $\mathbf{P = 1 - exp(-2\beta J)}$, provided spins i and j are parallel. Once the cluster has been completed, all spins that belong to the cluster are inverted.



Compared with local update, cluster updates solve the critical slowing down phenomenon, increasing the efficiency near the critical point.

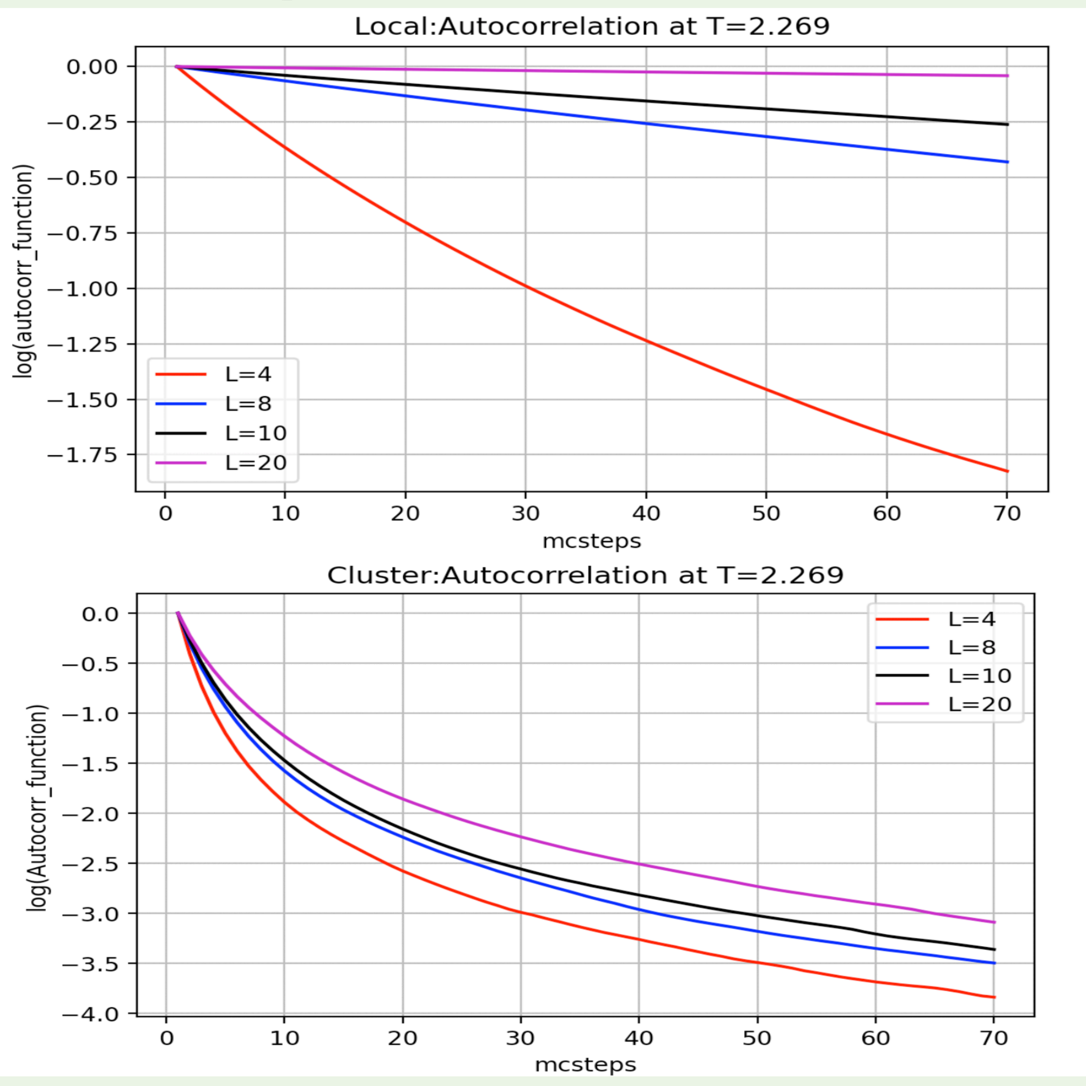


Figure 2. Comparison of autocorrelation functions of two algorithm at critical point T=2.269, smaller correlation values represent higher statistic independence. Notice that at Tc Cluster algorithm performs much better.

Results

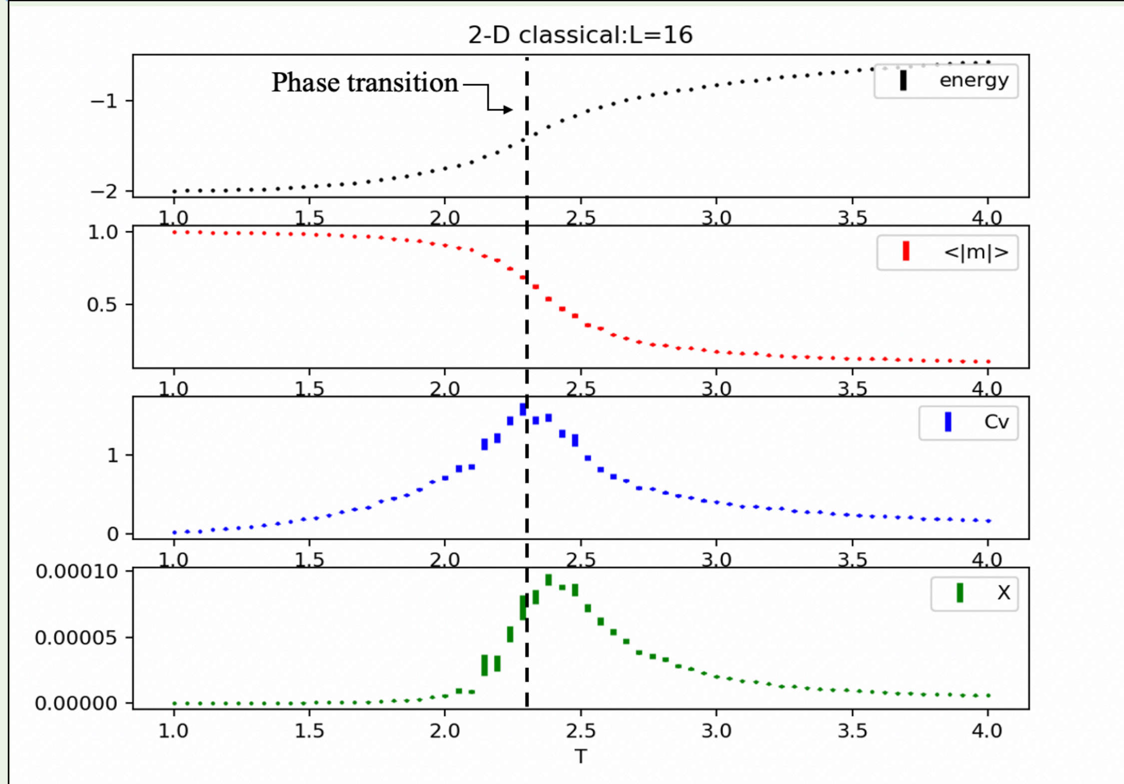


Figure 3. Physical measurables of 2-D classical Ising model against temperature. The dashed line indicates a phase transition.

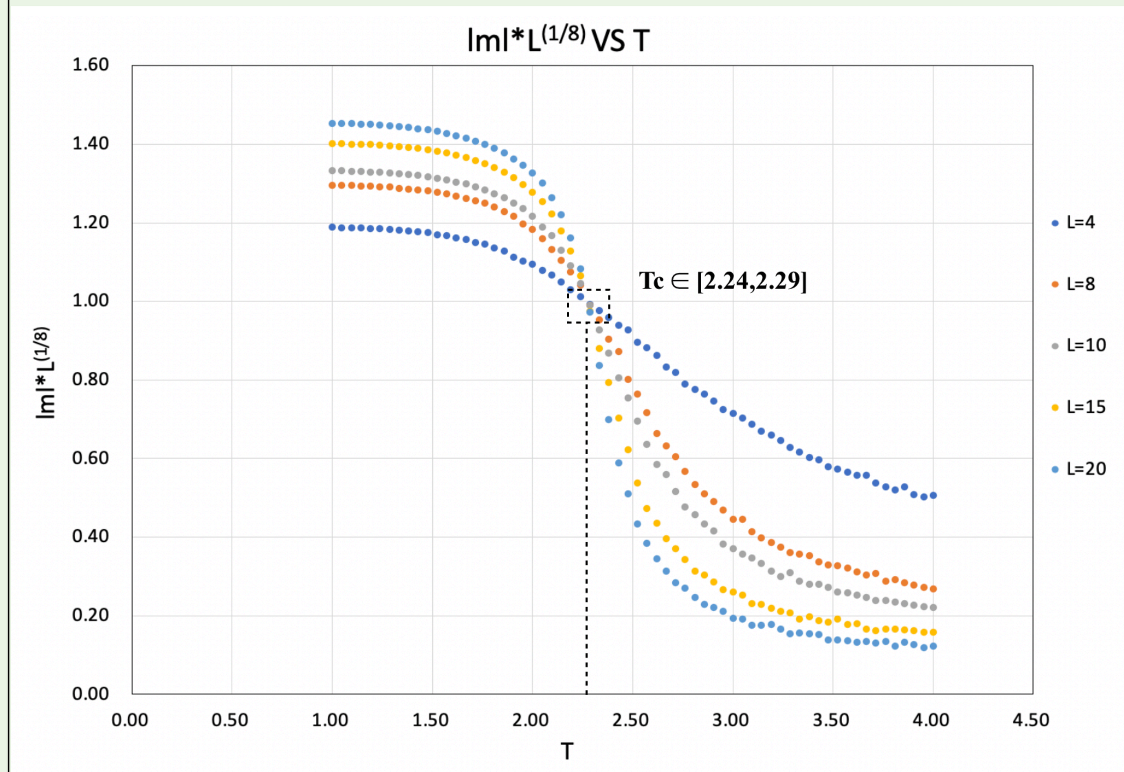


Figure 4. The result for 2-D classical Ising model. The axis is scaled such the intersection of curves for different L gives the critical point. The Tc is found in a range 2.24 to 2.29.

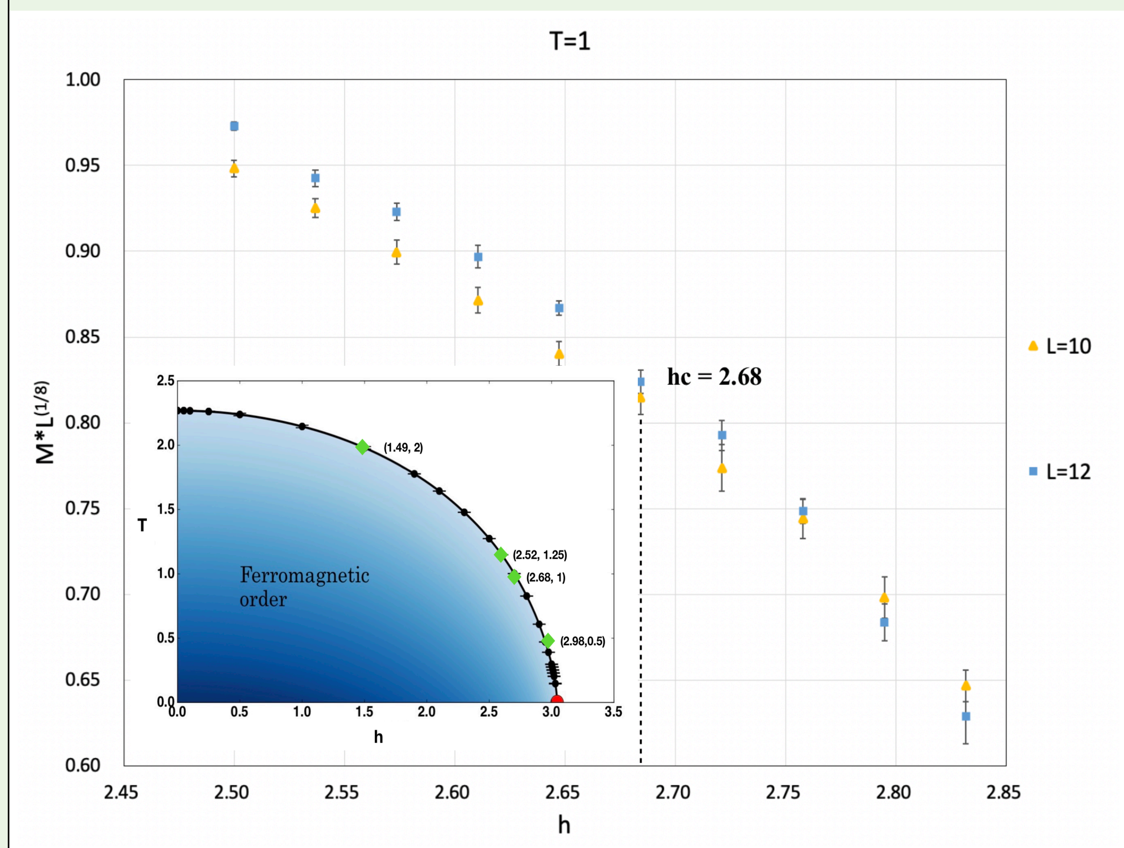


Figure 5. Critical point for 2-D quantum Ising model at T=1 as an example. The inset demonstrates the results in Ref.[3,4] of the T-h phase diagram of 2-D quantum Ising model. The green points are the data points obtained in my research, with the coordinate (h, T) in the bracket.

Conclusion

The result I get from Monte Carlo is accurate enough compared with the analytic solution, given the analytic solution of classical 2-D model is at $\mathrm{Tc} = {}^{2}/_{\ln(1+\sqrt{2})} \approx 2.269$. And in Figure 5, the results I obtained for quantum Ising model are consistent with those in Refs.[3,4]. Following the same procedure, the T-h phase boundary, separating ferromagnetic ordered state and paramagnetic state can be determined precisely. Notice that, at h=0, Tc ≈ 2.269 which is the classical case, and at T=0, hc ≈ 3.06 which is the quantum transition point at zero temperature.

Reference:

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