Monte carlo simulation studies of the ising model

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In this presentation

Hamiltonian of Ising model

The General ising model has two kinds of terms contributing to the Hamiltonian, they are,

Internal interaction term

- Contribution of a spin is intercting with its neighbouring spins.
- Based on model there are many terms like Nearest neighbour(NN), Next Nearest Neighbour (NNN), etc.

$$E_{int} = -\sum_{i,j} J_{ij} S_i S_j \tag{1}$$

S_i = randomly chosen spin
S_j = other interacting spin

External interaction term

- How the system reacts to external influence (external magnetic field)

$$E_{ext} = -\mu \sum_i H_i S_i \tag{2}$$

H_i = magnetic field strength
μ = magnetic permeability of system.

In both cases minus sign is used for conventional reasons.

Hamiltonian[re]

$$\mathcal{H}(S_i) = E_{int} + E_{ext} \tag{3}$$

$$\mathcal{H}(S_i) = -\sum_{i,j} J_{ij} S_i S_j - \mu \sum_i H_i S_i \tag{4}$$

where J_{ij} represents the interaction strength between spins $S_i$and S_j.

Metropolis Algorithm

To simulate the Ising model the Marcov Chain Monte Carlo (MCMC) method is used by employing the metropolis algorithm.

1. Choose an initial microstate.
2. Choose a spin at random and flip it.
3. Compute $\Delta\mathcal{H}$ for this flip. $\Delta\mathcal{H}$ is the change in the energy of the system due to the trial flip.
4. Check if, $\Delta\mathcal{H} \leq 0$ In this case the trial microstate is accepted.
5. If, $\Delta\mathcal{H} > 0$.
   - Compute the ratio of probabilities, $w = e^{-\beta\Delta\mathcal{H}}$
   - Choose a uniform random number r in the inetrval [0, 1].
   - Verify if $r \leq w$. In this case the trial microstate is accepted, otherwise rejected.
6. Repeat steps 2 through 5 until all spins of the system are tested. This sweep counts as one unit of Monte Carlo time.
7. Repeat setps 2 through 6 a sufficient number of times until thermalization, i.e. equilibrium is reached.
8. Compute the physical quantities of interest in n thermalized microstates.

Quantities computed

- **Energy per site**

$$< E >= \frac{-J}{2N} \sum_{<ij>} S_i S_j \tag{5}$$

It is divided by factor 2 to compensate for overcounting.

- **Magnetisation per site**

$$< M >= \frac{1}{N} \sum_{i} S_i \tag{6}$$

- **Specific heat capacity**

$$C = \frac{1}{T^2}(< E^2 > - < E >^2) \tag{7}$$

where $< E^2 >$ indicates average over E^2.

- **Susceptibility**

$$\chi = \frac{1}{T}(< M^2 > - < M >^2) \tag{8}$$

here N is the total lattice points or total no. of spins in system

Nearest neighbour (NN) model

The simplest Ising model is the nearest neighbour interaction model. To simplify the calculation following assumptions were made,

- The system is isotropic ($J_{ij} = J$)
- Magnetic permeability, $\mu = 1$
- External magnetic field is uniform and zero ($H_i = H = 0$)
- Natural units is adopted ($k_B = 1$)

Hamiltonian of NN model

$$\mathcal{H}(S_i) = -J \sum_{<ij>} S_i S_j \tag{9}$$

here, $< ij >$ means NN interction

1D NN model - Analytic solutions

Energy per site

$$< E >= -J \tanh\left(\frac{J}{T}\right) \tag{10}$$

Magnetisation per site

$$< M > = \tanh\left(\frac{H}{J}\right) \tag{11}$$

$$< M > = 0 \tag{12}$$

since H = 0

Specific heat capacity

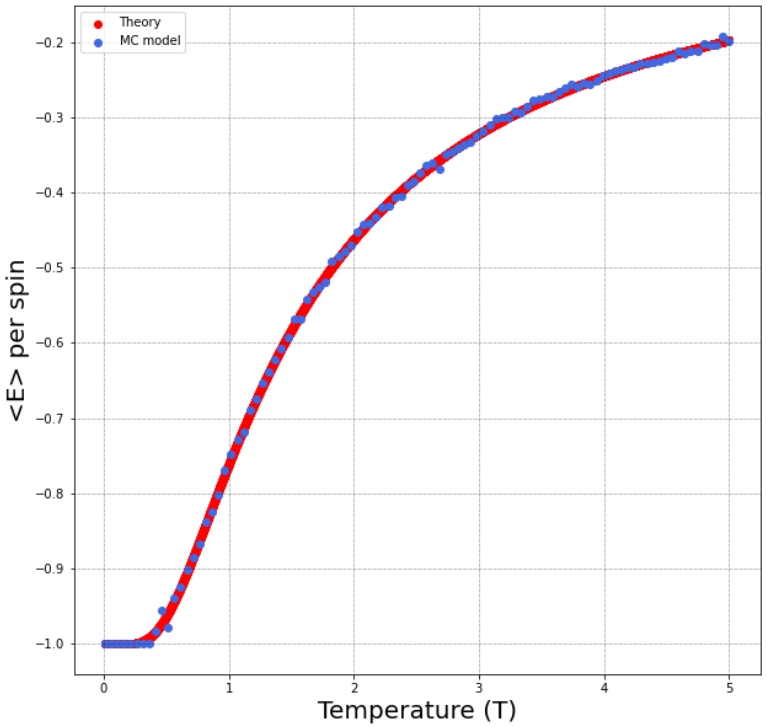
$$C = \left(\frac{J}{T}\right)^2 \frac{1}{\cosh^2(J/T)} \tag{13}$$

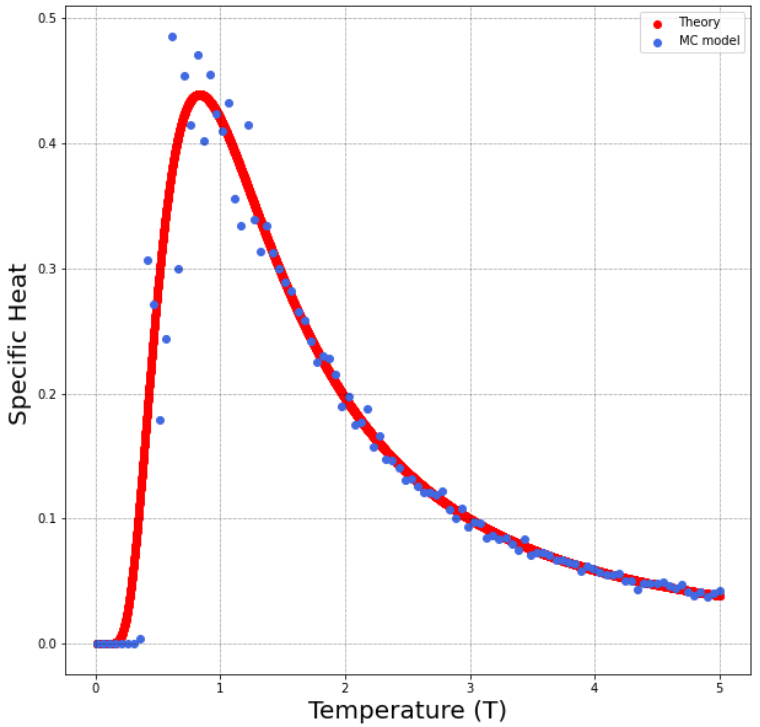
Susceptibility

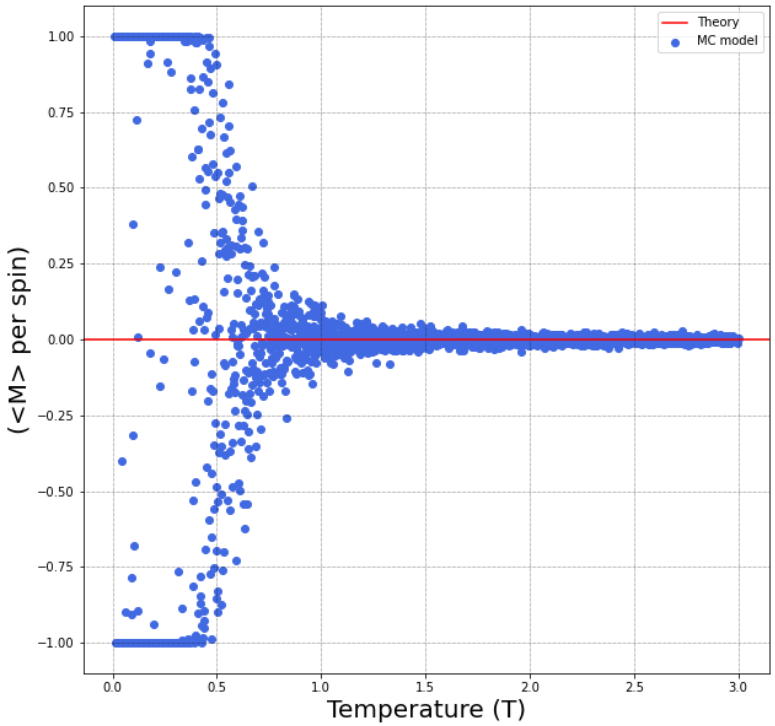
$$\chi = \left(\frac{1}{T}\right) \frac{1 + \tanh(J/T)}{1 - \tanh(J/T)} \tag{14}$$

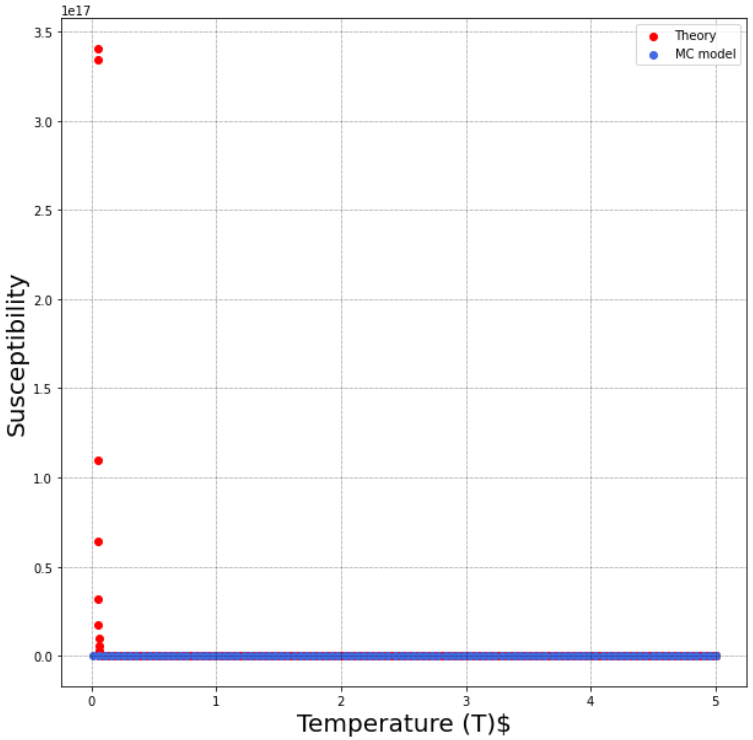
1D model - Temperature response

J is taken to be 1 here in the Hamiltonian. The system is simulated for $N = 100$ lattice points. 200 data points are obtained after 1000 thermalization MC time steps. The quantities are averaged over 1000 MC time steps after thermalization.



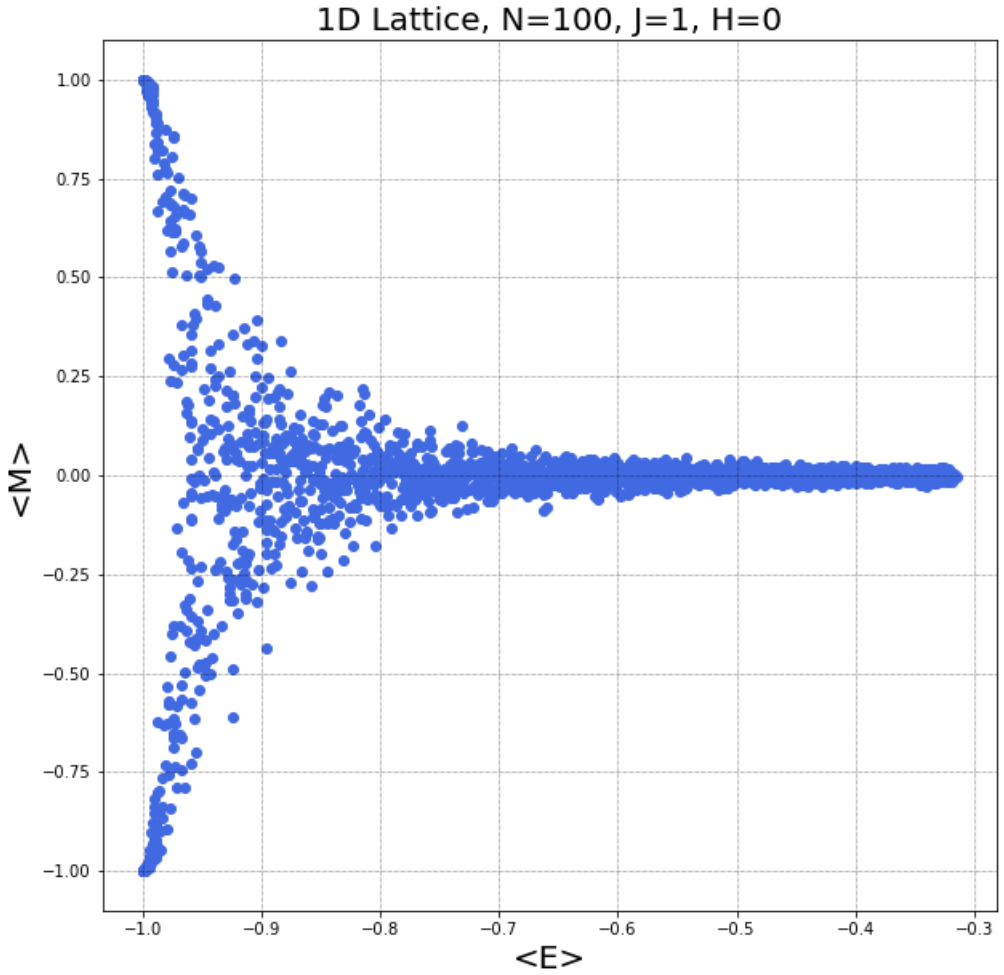






- Here, the theory is in good agreement with simulation.
- As N becomes large then the simulation and theory are more agreeing.
- There is no phase transition in the 1D Ising NN model in zero field.

The absence of phase transition is more clear from the following plot.



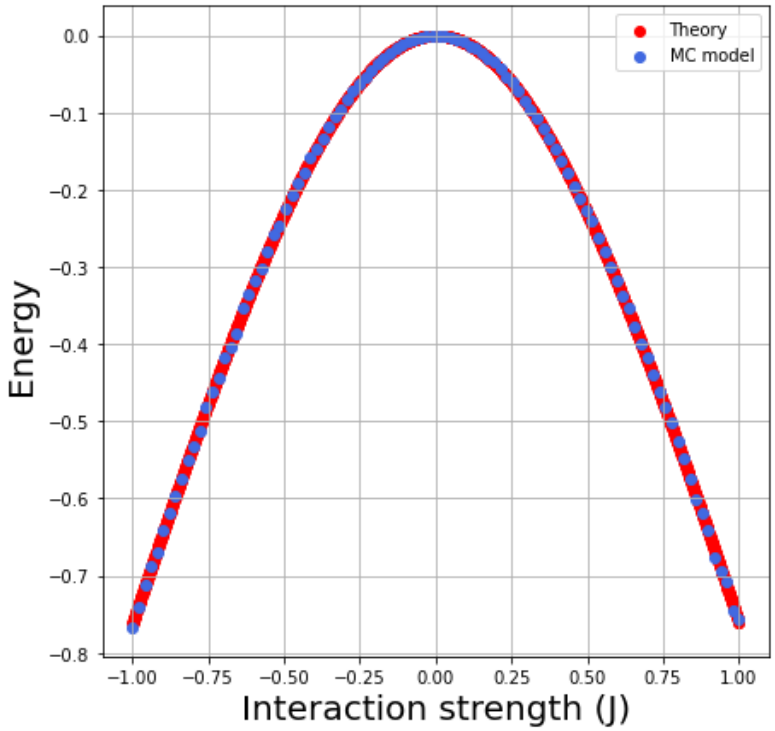
There is not any distinct ststes (phases) at low energy region. It shows that more or less the magnetization per spin fluctuates from -1 to +1 and values in between at low energy region. The system is in paramagnetic state throughout.

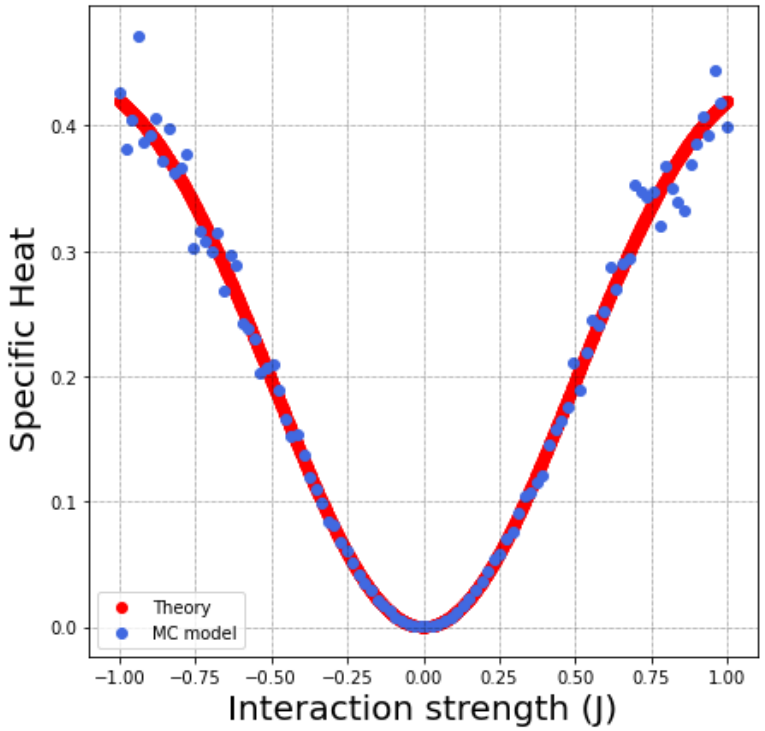
1D NN model - inteaction strength response

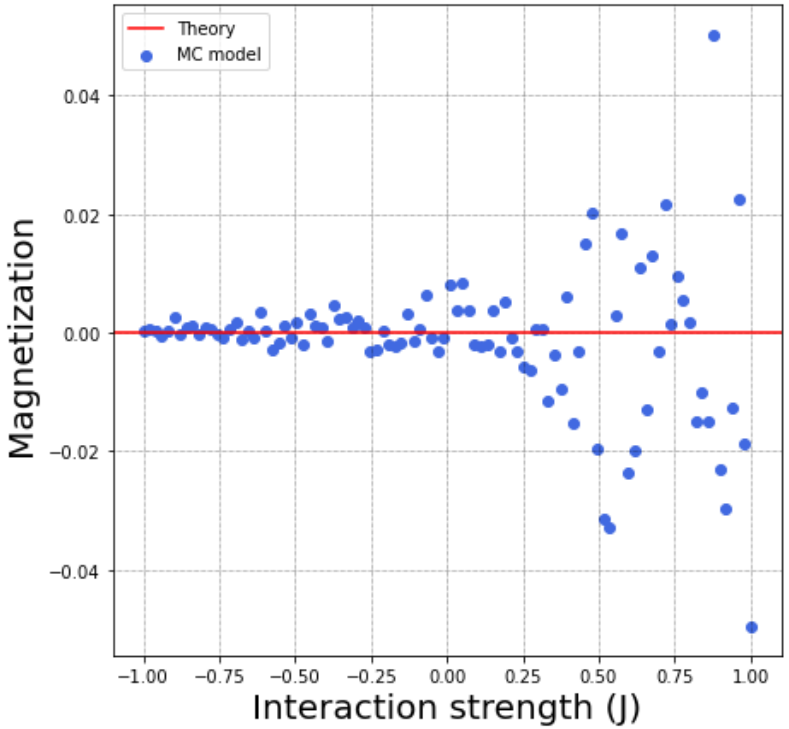
The same system is analysed for its response to different interaction strength values at fixed temperature.

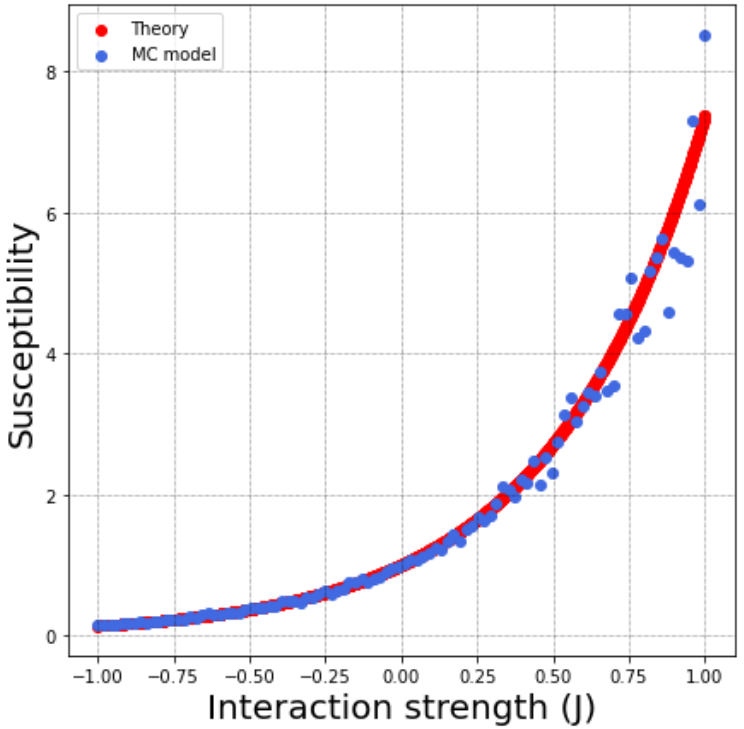
In the plots mentioned below, $N = 100$, $T = 1$, the system is allowed thermalise for 1000 MC time steps. The quantities computed are averages over 1000 MC time steps after thermalisation.

Periodic boundary condition is considered.[**reif2009fundamentals**]









- The simulation results match with theory well.
- From $J \in [-1, 0)$ the system is antiferromagnetic , this is because the susceptibility is very low here and simulated $< M >$ values are with minor fluctuations around zero indicating no net spin.
- From $J \geq 0$ the system is paramagnetic, this is because susceptibility is comparatively greater than before and simulation results show more scattered nature indicating the spins are orienting randomly.

- The interesting thing is the symmetry in Average energy per spin and specific heat capacity graph about $J = 0$ line but the phases are different.
- The above is due to the nature in which the neighbouring spins orient themselves after the interaction.
  When $J < 0$ the spin align as an alternating chain.

$$+ - + - + - + - + - + - + - + - + - + - + - +$$

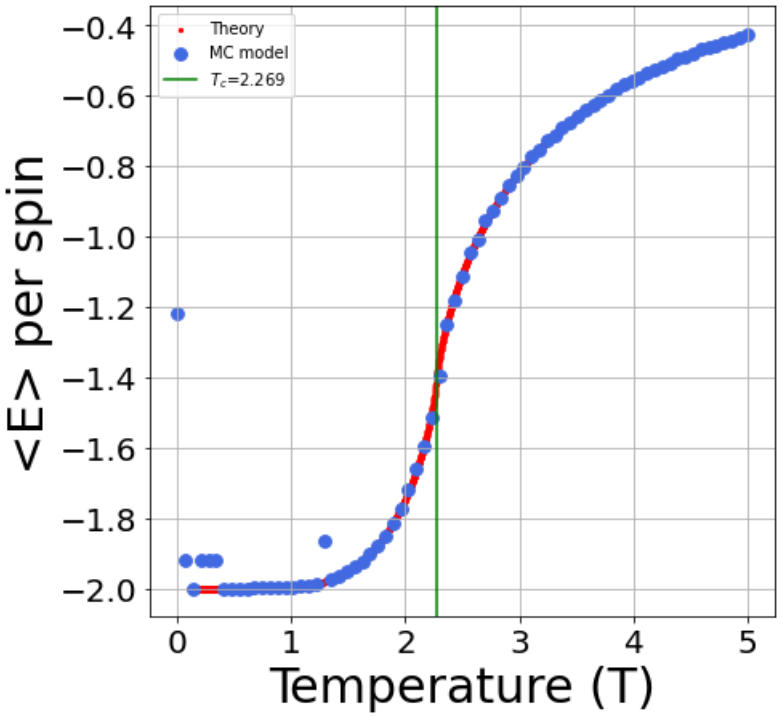
but when $J > 0$ The spins try to Orient in same direction but the thermal fluctuations don't allow them to do so and the J is not Strong enough to overcome this so it results in a random chain.

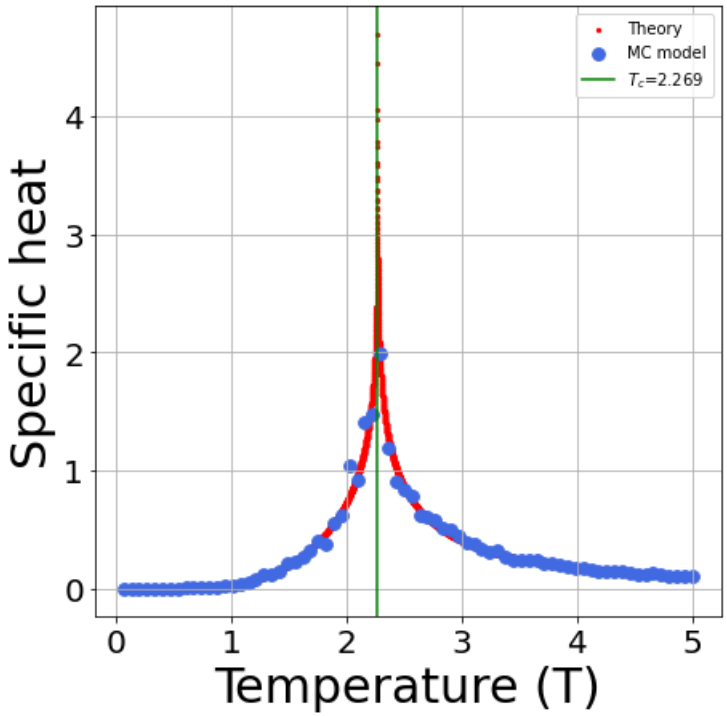
$$+ - - - + - - + + + - + - + + - - + - + -$$

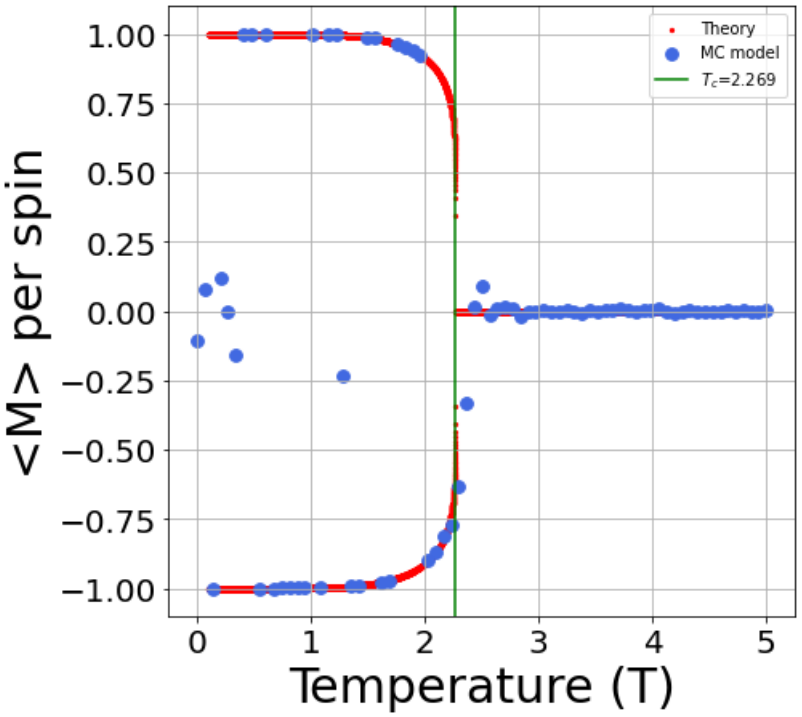
- Though configurations are different the energy value it takes is the same, this explains the symmetry.
- This is a toy model and this response study is just to compare how theory agrees with simulation. The material studied can't change its J nature abruptly from attractive to repulsive on its own in reality.

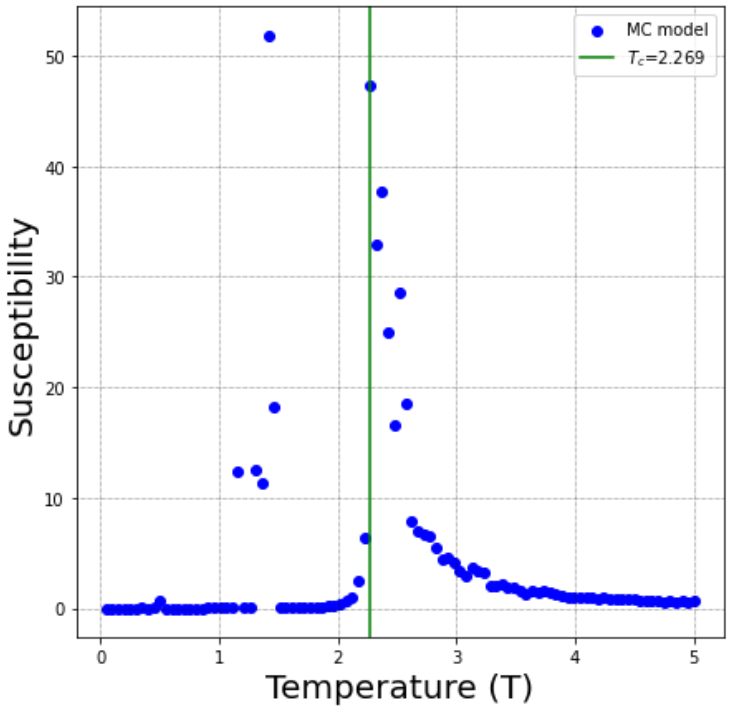
2D model - Temperature response

Any random spin of the system now has 4 nearest neighbouring spins. This plots below are the simulation of 2D lattice with, $N = 50$, $J = 1$.In this 100 data points are obtained after 1000 thermalization MC time steps. The quantities are averaged over 1000 MC time steps after thermalization. The analytical solutions are adopted from K Huang book.



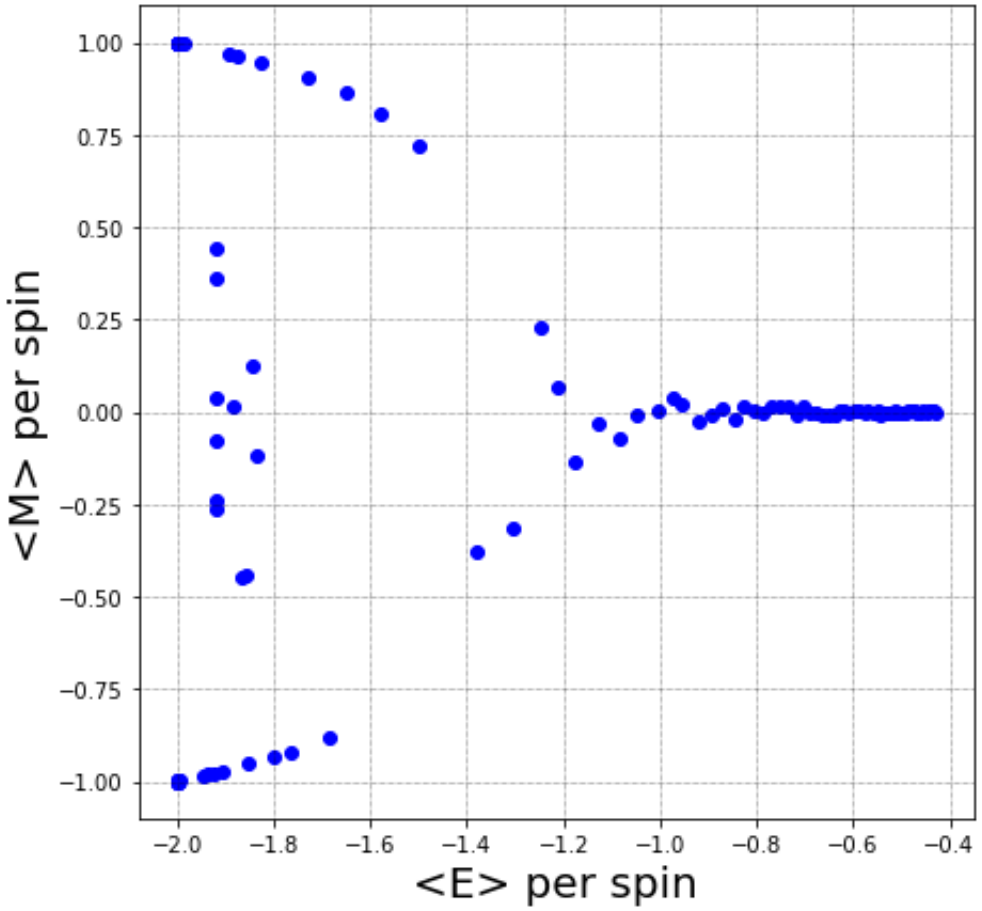






- This model also matches with the analytical solution.
- This model shows a phase transition at $T_c = 2.269$.
- $T \in [0, 2.269)$ the system is ferromagnetic. Because there exists 2 stable states for $< M >$ either $+1$ and -1 and the suceptibility is zero.
- $T > 2.269$ the system is paramagnetic. Since the magnetization and susceptibility becomes zero.

The phase transition is more clear from the graph below, where, the low energy has 2 distinct states of stable magnetization showing the ferromagnetic nature.



2D model - interaction strength response

In the plots mentioned below, $N = 10$, the system is allowed thermalise for 1000 MC time steps. The quantities computed are averages over 1000 MC time steps after thermalisation. Periodic boundary condition is considered. something interesting happens here when T values are changed.

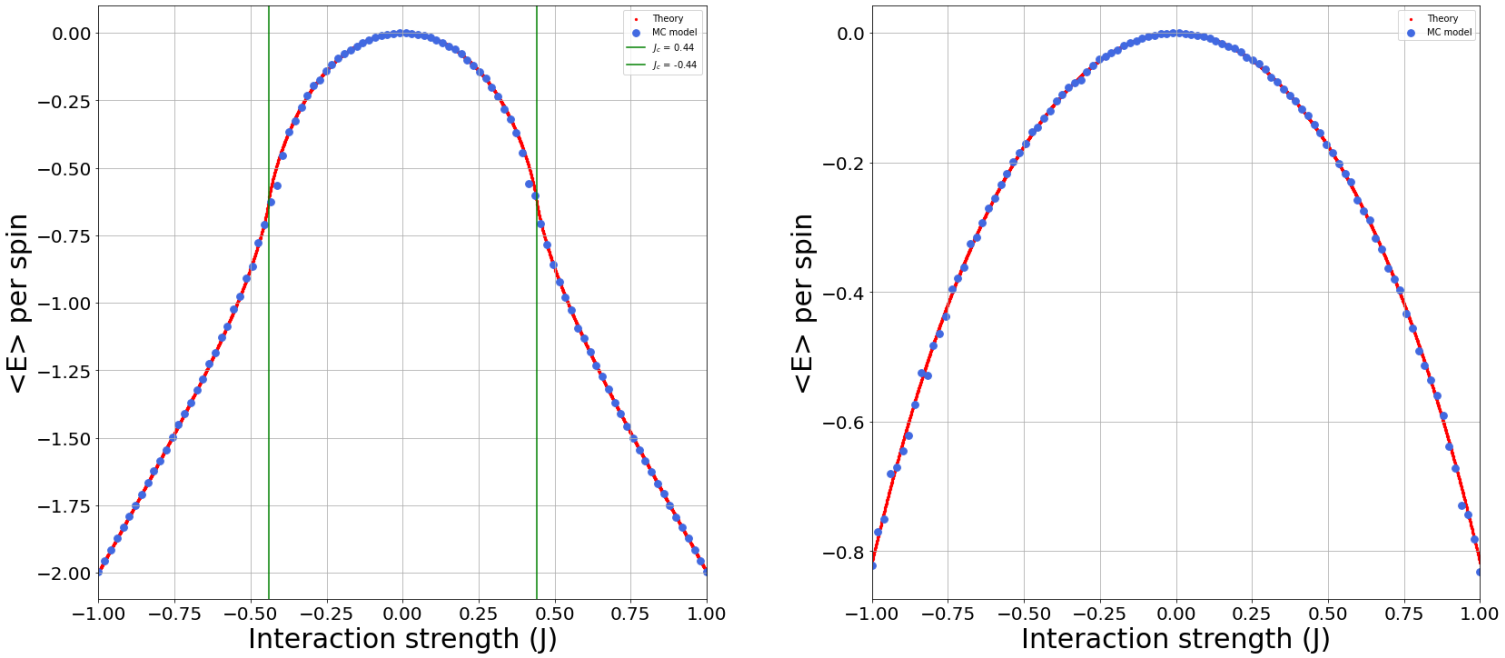


Figure: The left image ($T = 1 < T_c$) and the right image ($T = 3 > T_c$)

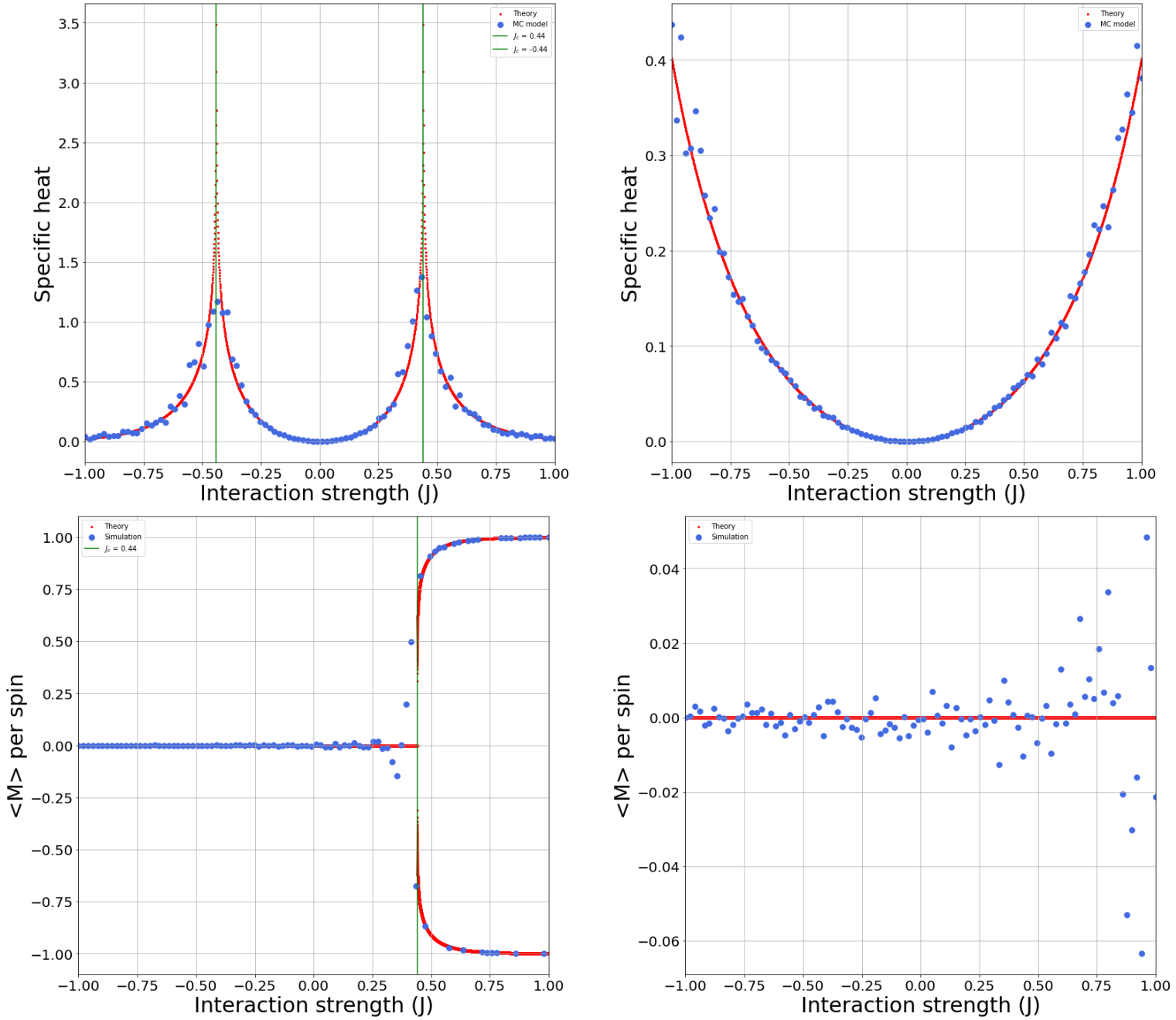


Figure: The left images ($T = 1 < T_c$) and the right images ($T = 3 > T_c$)

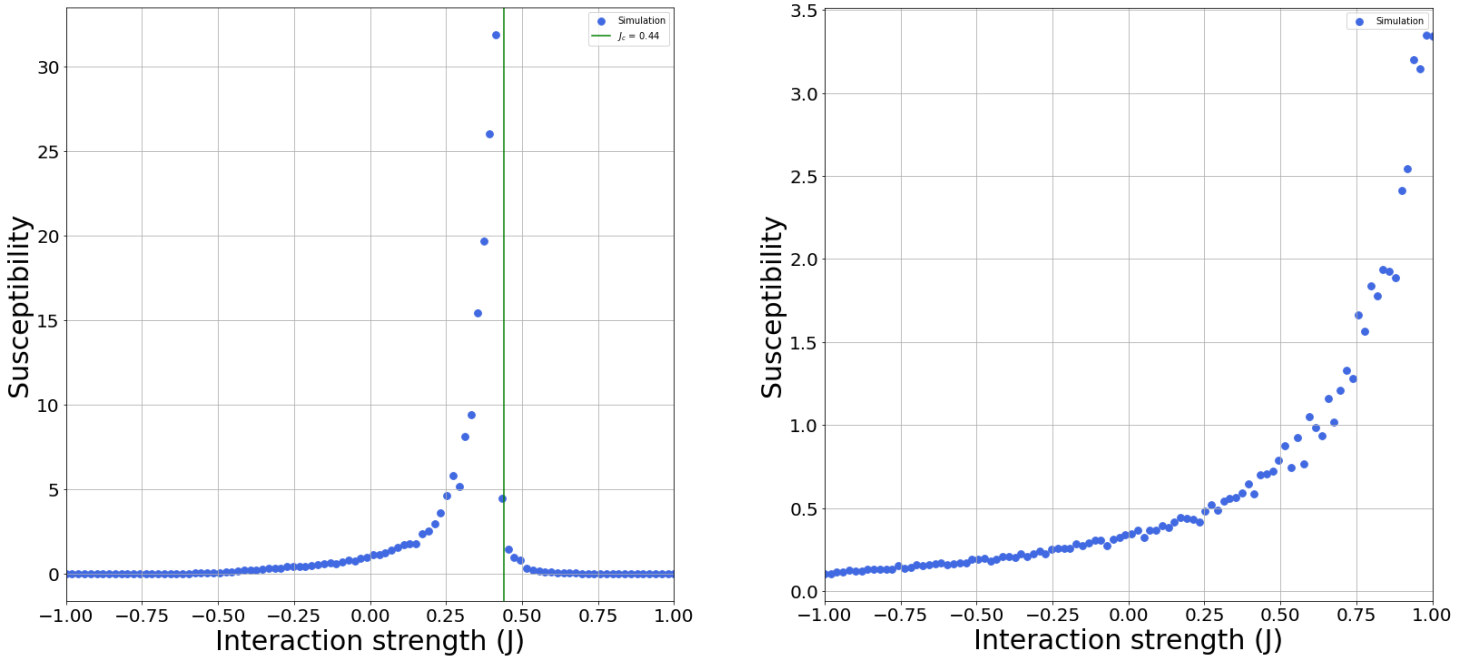


Figure: The left image ($T = 1 < T_c$) and the right image ($T = 3 > T_c$)

- The $< E >$ per spin and specific heat capacity graphs are symmetric as before in 1D case.
- Ferromagnetic phase exists only when $T < T_c$. The simulation obeys the other form of following relation, $T_c = 2.269J$ as

$$J_c = 0.44T$$

By J_c, we mean that the value of computed quantity peaks there for a particular temperature (T).

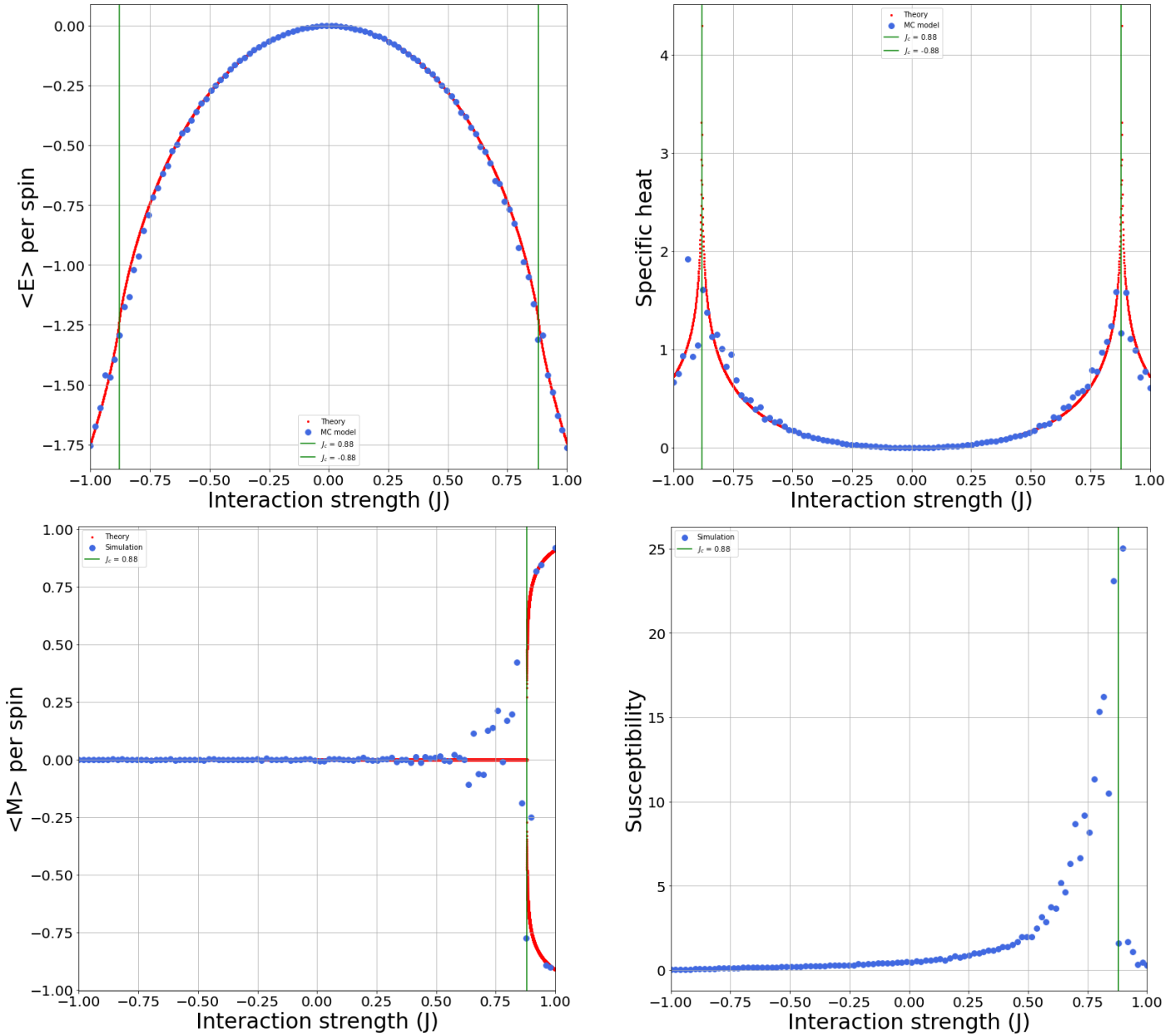


Figure: $T = 2 \approx T_c = 2.269$ for all graphs. Only here ferromagnetic nature emerges suddenly at $J \approx 1$. ($Jc = 0.44 * 2.269 \approx 1$)

Here the phase of system is described below,

- When $J < 0 \rightarrow$**(antiferromagnetic)**, always independent of temperature value. Here The $< M >$ per spin is zero and susceptibility is very small positive value (nearly zero).
- When $J > 0$ and $T \leq T_c$, then J_c can be computed from $\boxed{J_c = 0.44\,T}$, for $J \in [0, 1]$
- $J \in [0, J_c) \rightarrow$ **(paramagnetic)**. Here $< M >$ per spin is zero and Susceptibility increases from zero and peaks at J_c.
- $J > J_c \rightarrow$ **(ferromagnetic)**. Here $< M >$ per spin has two stable values $+1$ and -1. Susceptibility becomes zero.
- $J \in [0, 1]$ and $T > T_c \rightarrow$ **(paramagnetic)**. No paramagnetic to ferromagnetic phase transition occurs.

3D model - Temperature response

The 3D NN Ising model has **no existing analytical solution**. So the system can be studied only using simulation techniques. So MCMC technique is applied to simulate the system.

The relation Between J and T could be established but now only on the pure basis of simulation results, which we got is,

$$T_c = 4.43J$$

and the other relation when studying the J response is

$$J_c = 0.23T$$

But the actual relation up to 2 digit accuracy is $\boxed{T_c = 4.51J}$, which is comparable.

The error we got is statistical in nature because the lattice simulated is very small $N = 10$ and the no of MC time steps allowed to equiliberate (1000) isn't adequate. This is due to the limited computing power we have at the moment.

Other than the above mentioned points the characteristics of 3D NN ising model is same as that of 2D NN ising model discussed before.

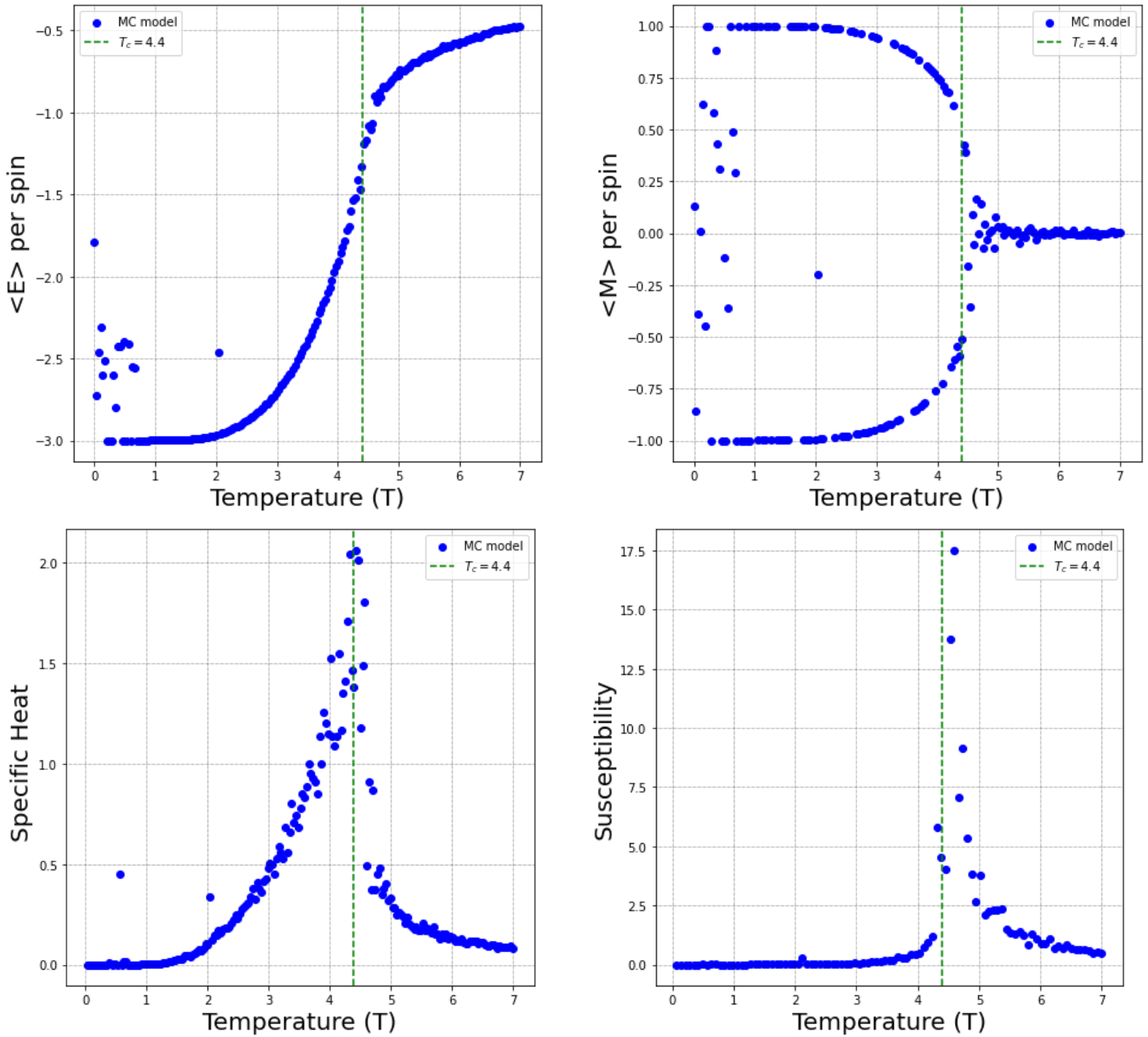


Figure: $J = 1$, Temperature response of 3D NN model.

3D model - interaction strength response

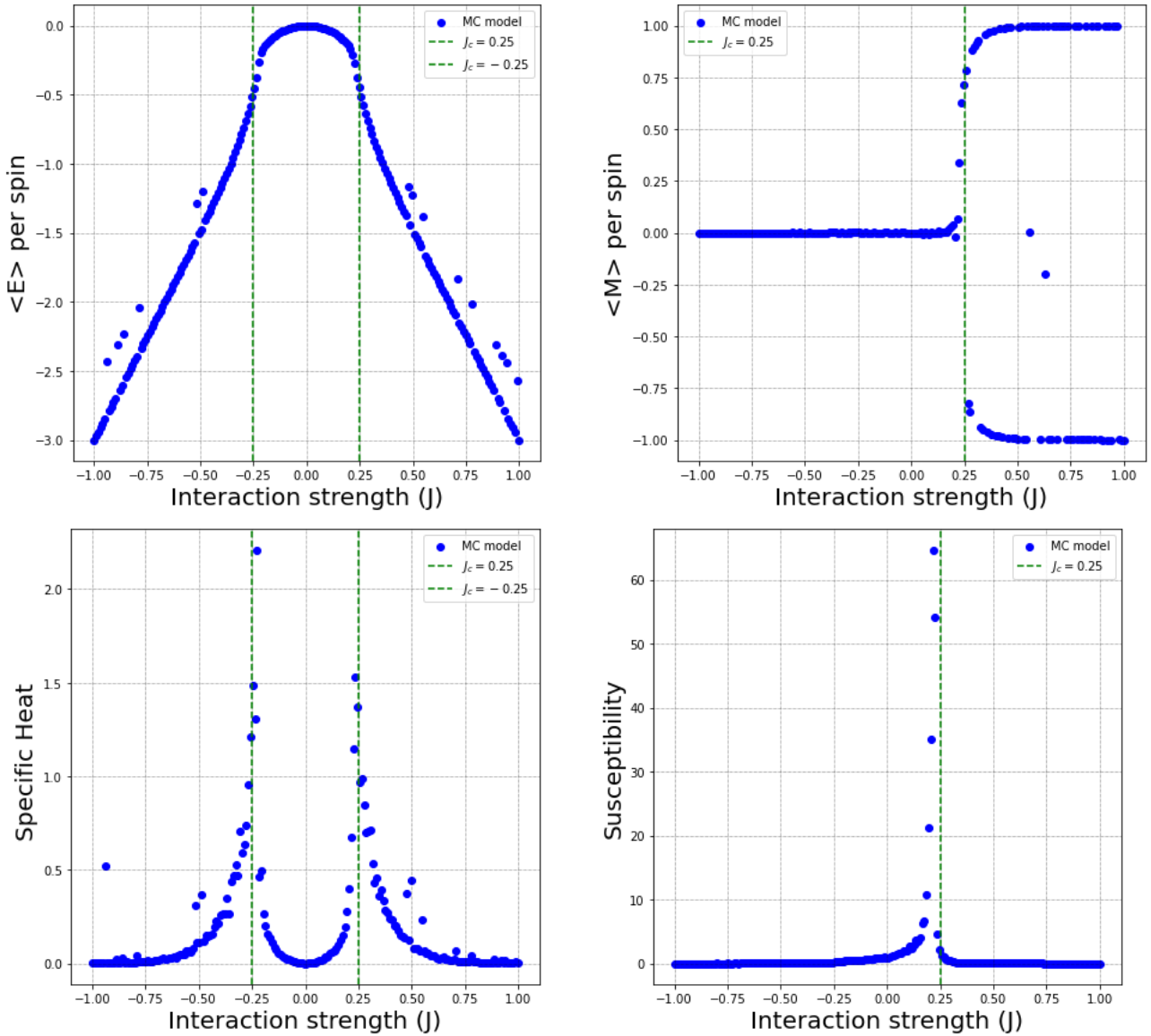


Figure: $T = 1 < T_c$, for all graphs. J response of 3D NN model.

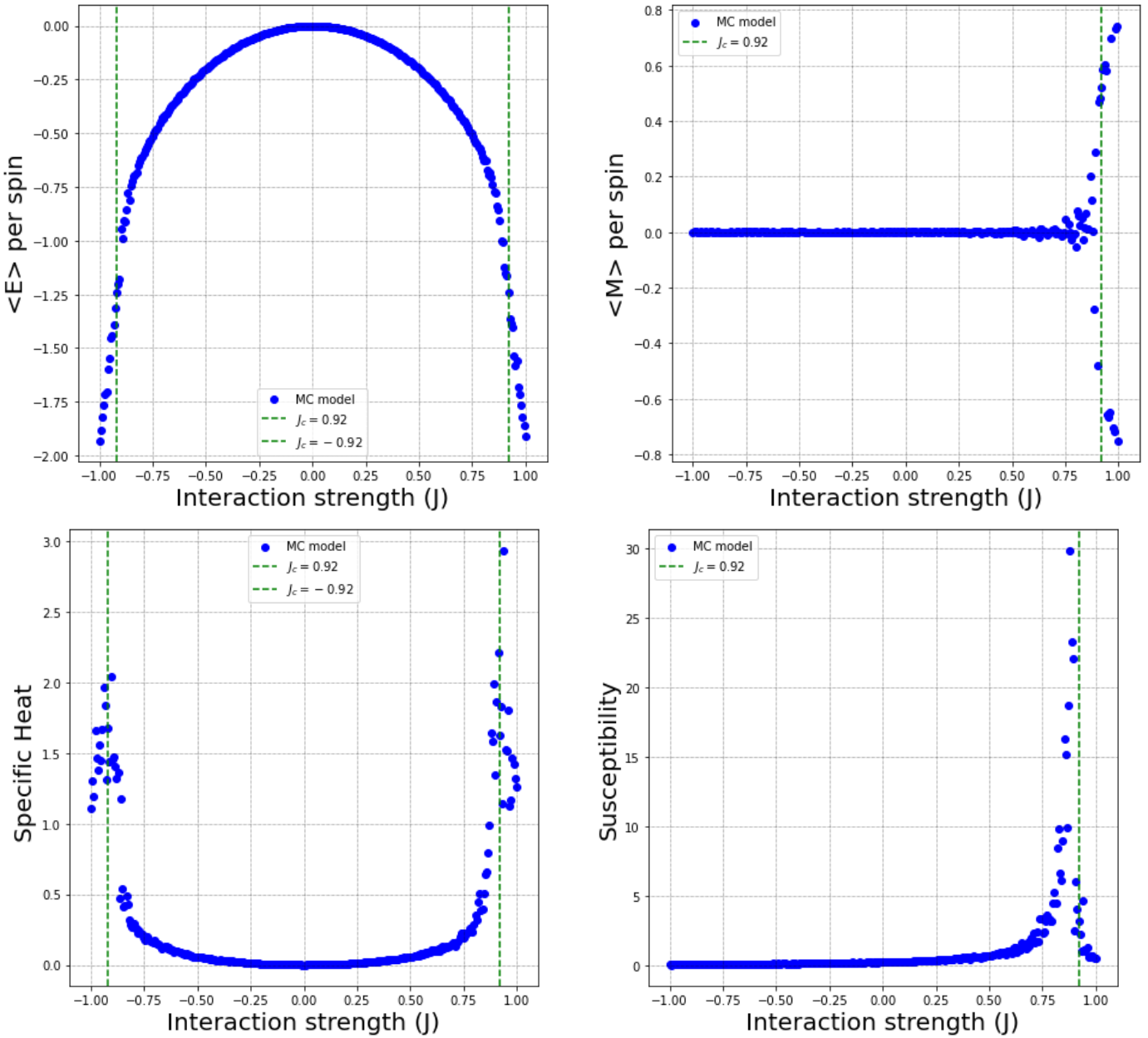


Figure: $T = 4 \approx T_c = 4.51$, for all graphs. J response of 3D NN model.

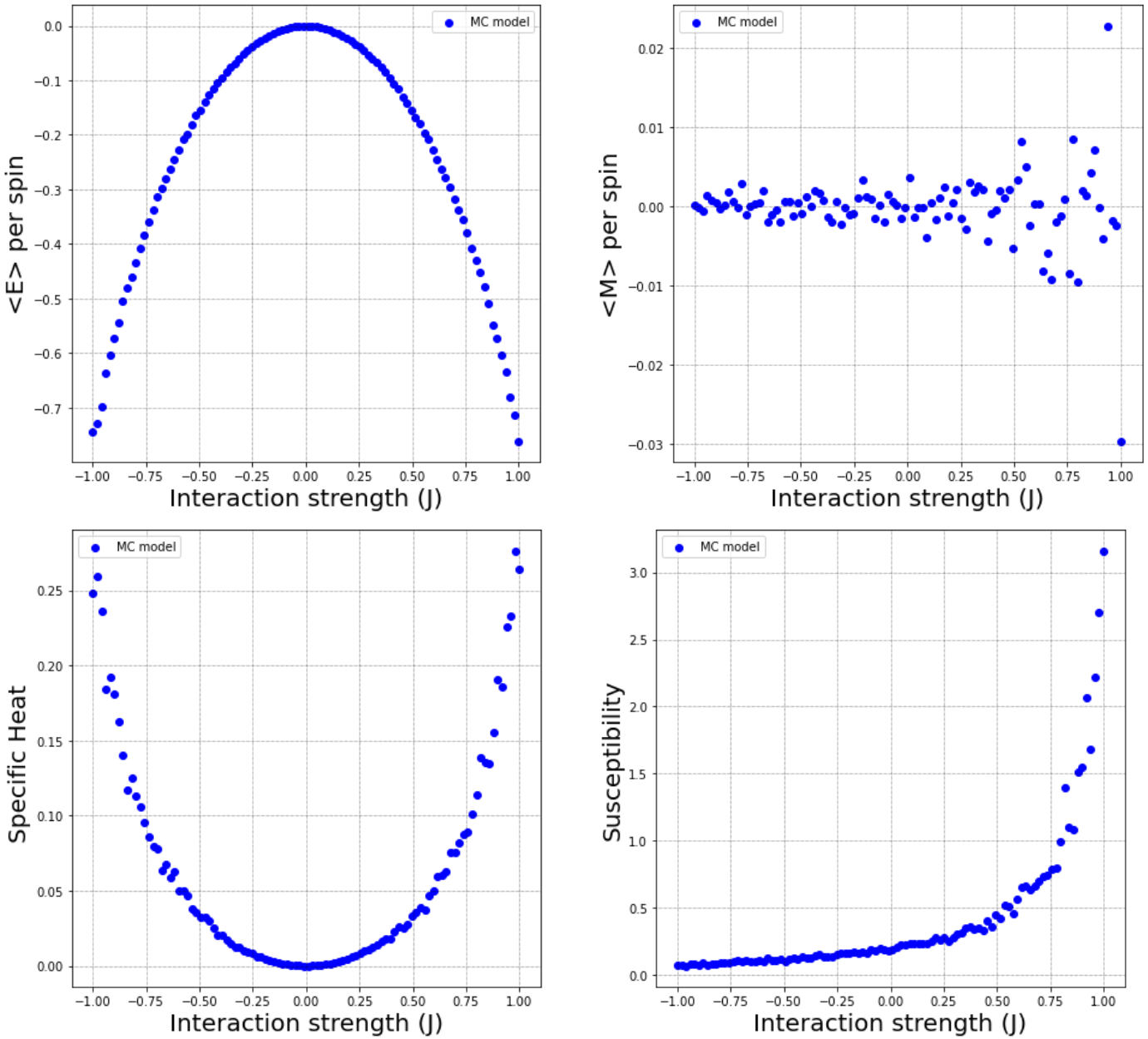


Figure: $T = 5 > T_c$, for all graphs. J response of 3D NN model (no ferromagnetic phase). Graphical characteristics is like 1D NN model.

2D ising model with NNN interaction

This model also has no analytical solution. The same 2D ising model as before (with $J_1, J_2 > 0$) in a square lattice of $10x10 = 100$ lattice points is studied with the next nearest neighbour interaction.
Hamiltonian studied:

$$\mathcal{H} = -J_1 \sum_{NN} S_i S_j - J_2 \sum_{NNN} S_i S_k \tag{15}$$

- J_1 and J_2 are the interaction strengths for NN and NNN interactions respectively.
- J_1 and J_2 are assumed to be related by the following equation,

$$J_2 = rJ_1 \tag{16}$$

This system is simulated using the MCMC algorithm for different r values as the temperature varies and the results were analysied.

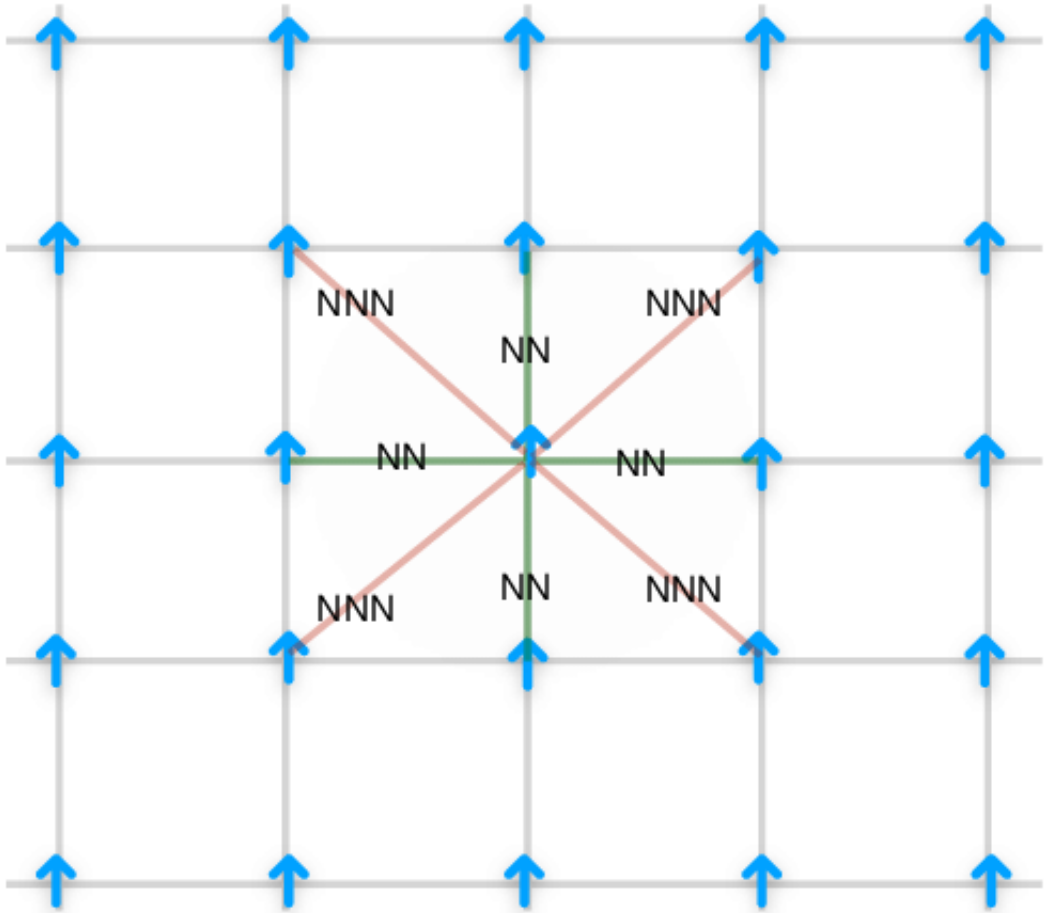


Figure: Interactions associated with any individual spin

Periodic boundary condition is chosen for the simulation.

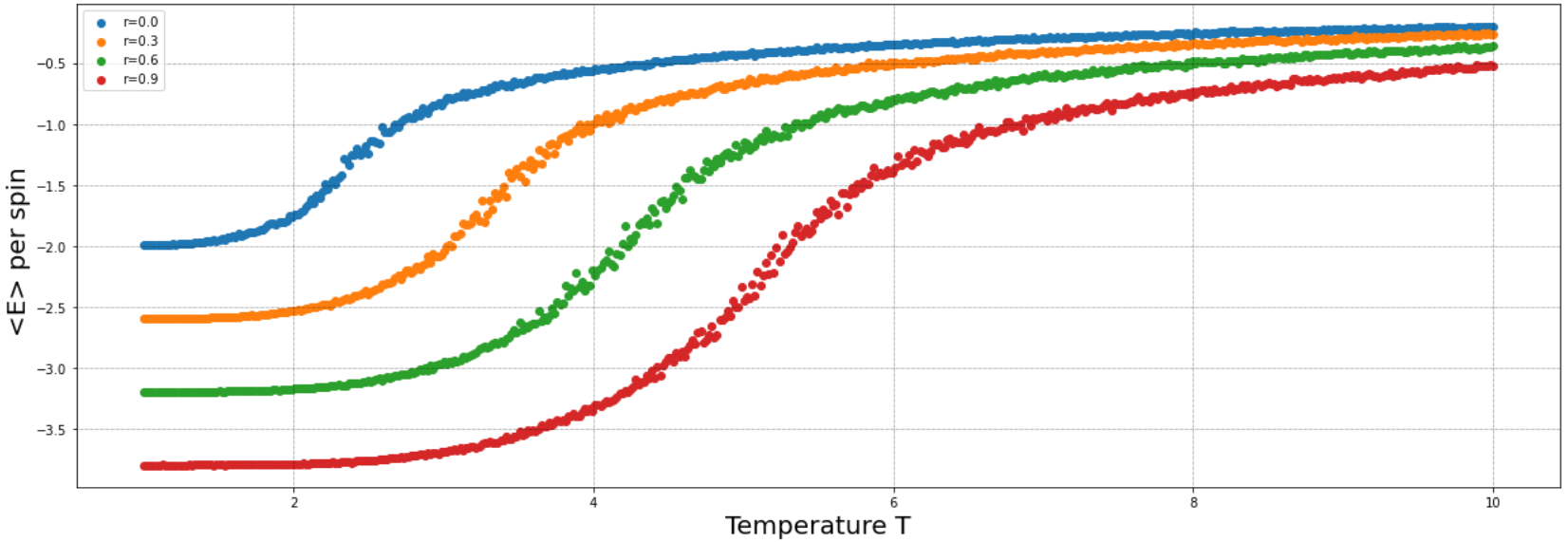


Figure: $< E >$ Vs T, $N = 10$, $J_1 = 1$

- The blue curve is the model with no NNN interaction. It has the lowest energy as -2 units.
- The lower most energy decreases more when there is strong NNN interaction. But the nature of curve remains the same. The lowest value of energy is obeying the following relation, as NNN contribution changes,

$$< E_{ground} >= -2 - (2 * r) units \tag{17}$$

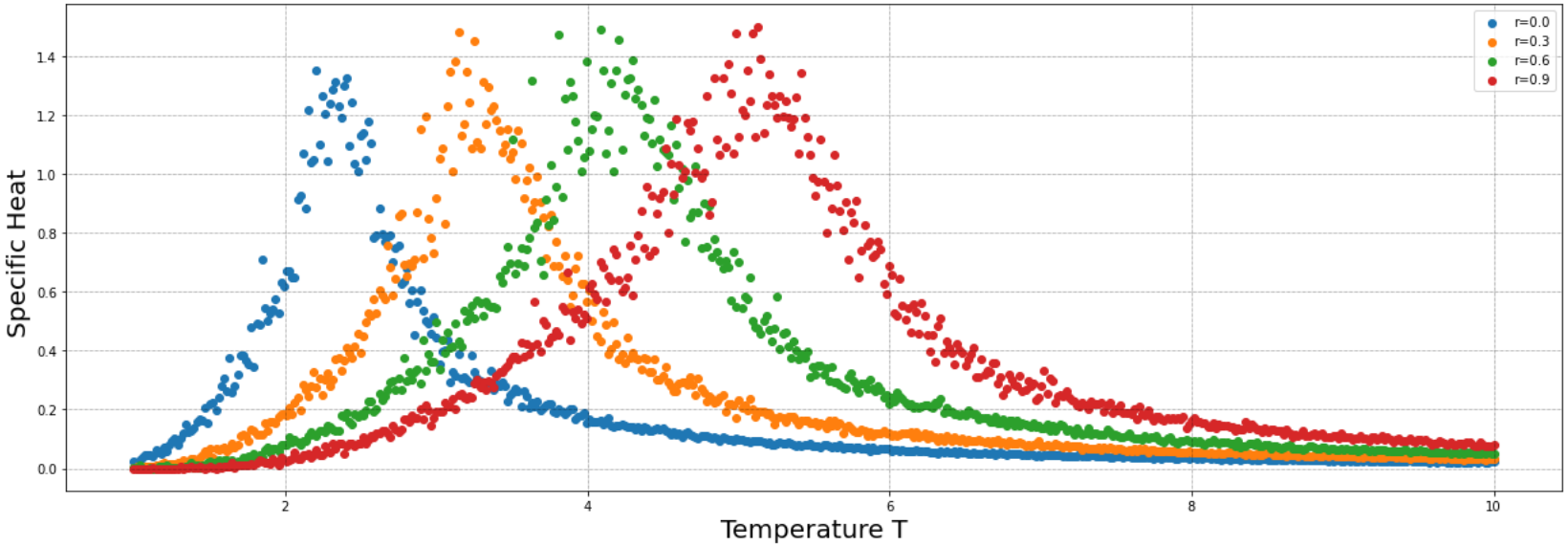


Figure: Specific heat Vs T, $N = 10$, $J_1 = 1$

- The max value of specific heat don't change much because the system studied is the same $10x10$ lattice.
- The NNN interaction increases the critical temperature value.

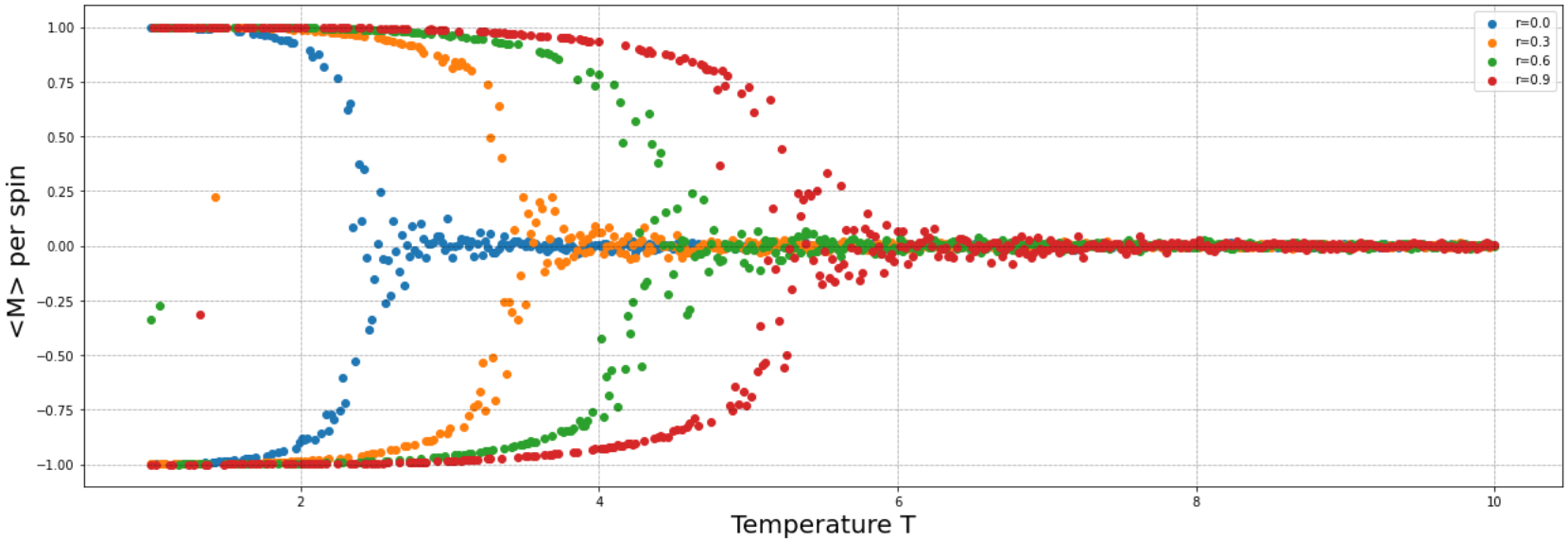


Figure: $< M >$ Vs T, $N = 10$, $J_1 = 1$

- This graph also confirms the increase of critical temperature as the NNN contribution increases.
- This means that spin flipping requires more energy than the regular 2D ising model (NN). So to change the phase of the system from ferromagnetic to paramagnetic phase, more internal energy is needed. Hence critical temperature increases.

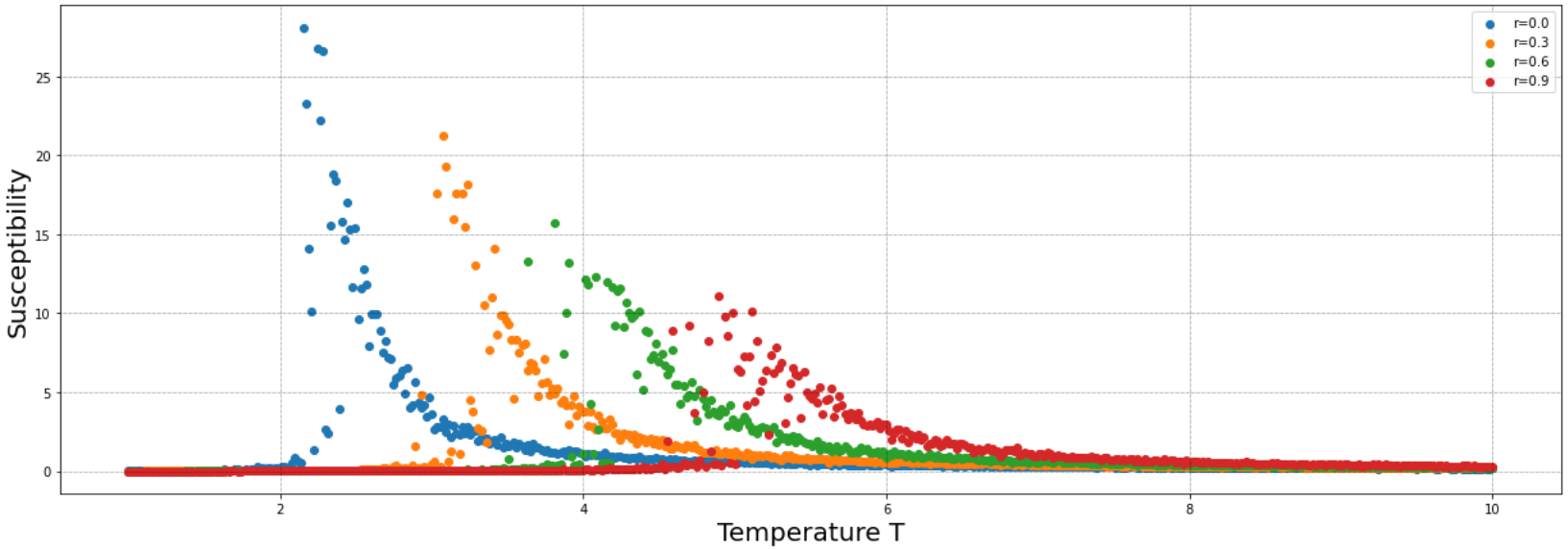


Figure: X Vs T, $N = 10$, $J_1 = 1$

- The maximum value of susceptibility decreases as NNN contribution increases.
- The NNN interaction makes it more energy consuming for any randomly chosen spin to flip. This is reflected in the susceptibility (the ability to get magnetised) curve as above mentioned.

3D model with NNN interaction

3D model with next nearest neighbour interaction is considered (with $J_1, J_2 > 0$). A cubic lattice of 10 x 10 x 10 = 1000 lattice points is simulated using MCMC algorithm. 1000 MC steps are used for thermalisation and the quantities are averaged over 1000 MC steps after thermalisation. Results are similar to 2D NNN model.

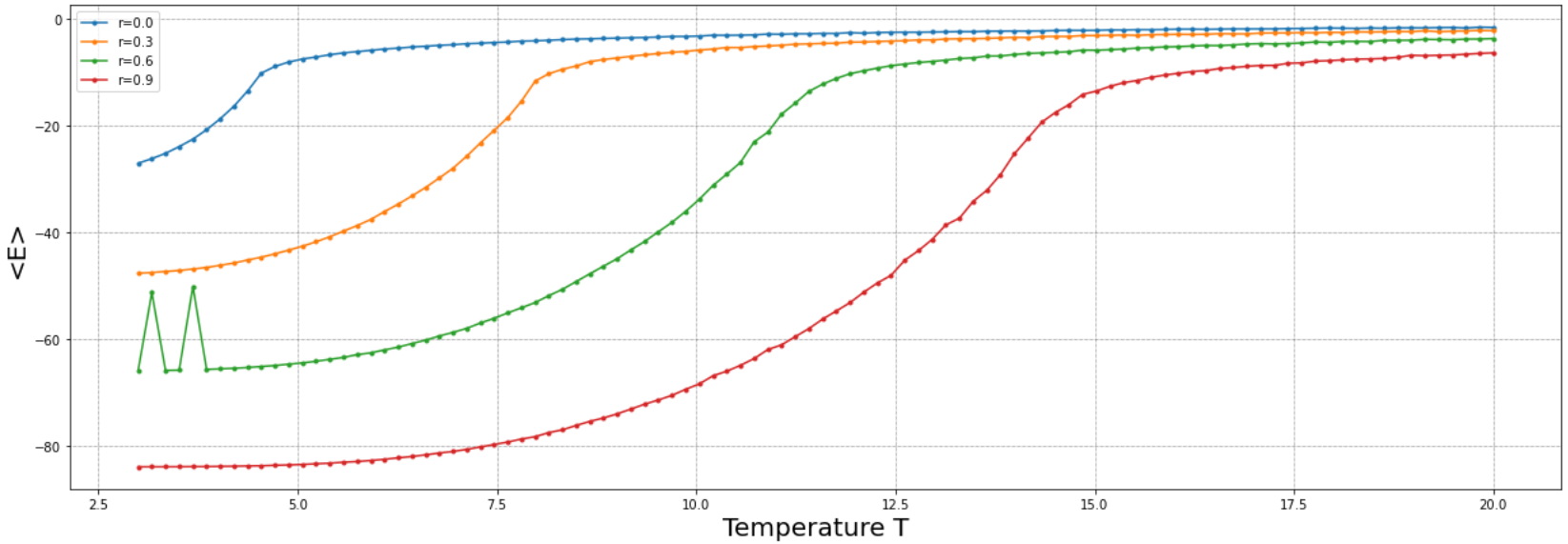


Figure: $< E >$ VS T, N=10, J_1=1

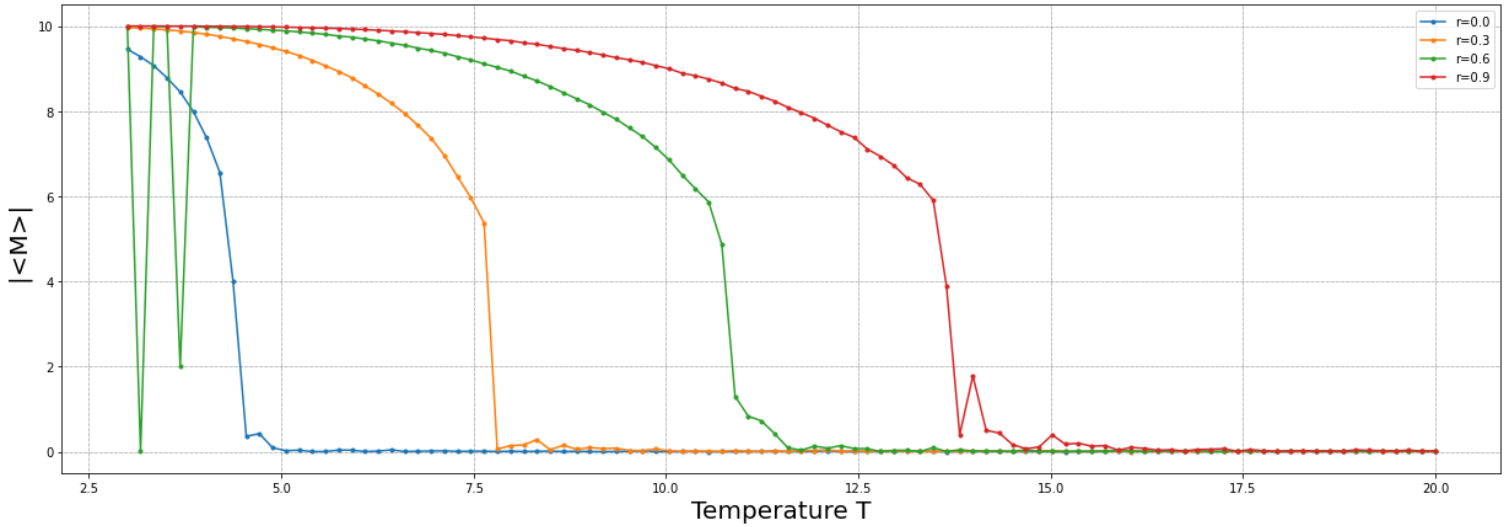


Figure: $< M >$ Vs T, N=10, J_1=1

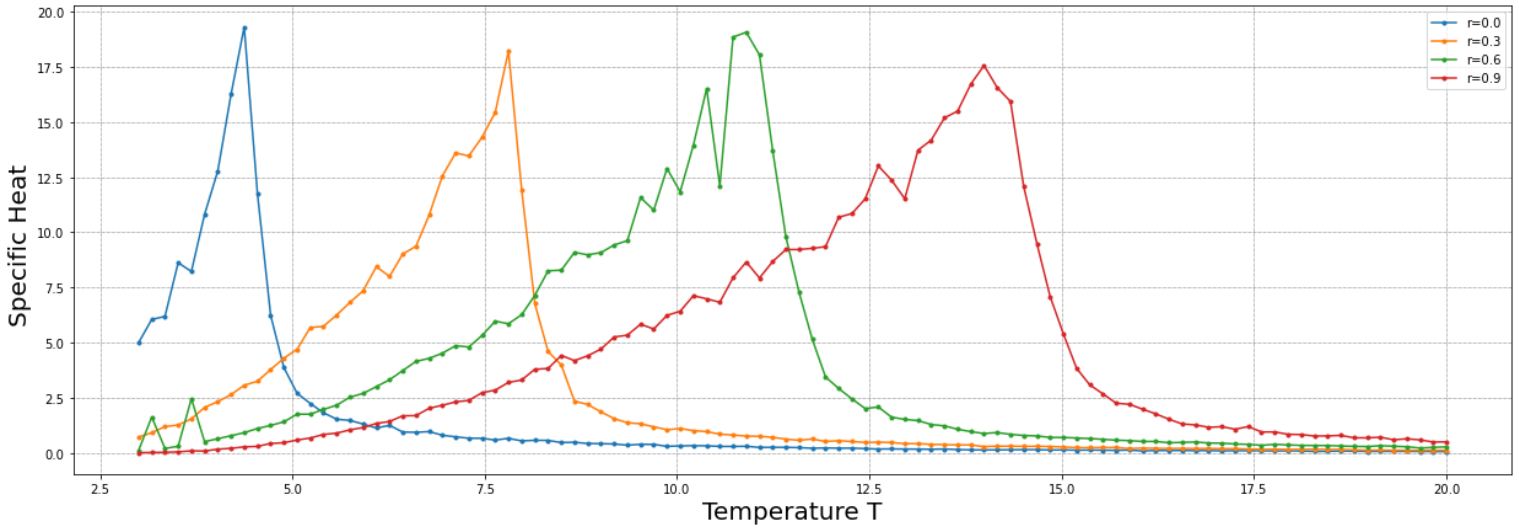


Figure: C Vs T, N=10, J_1=1

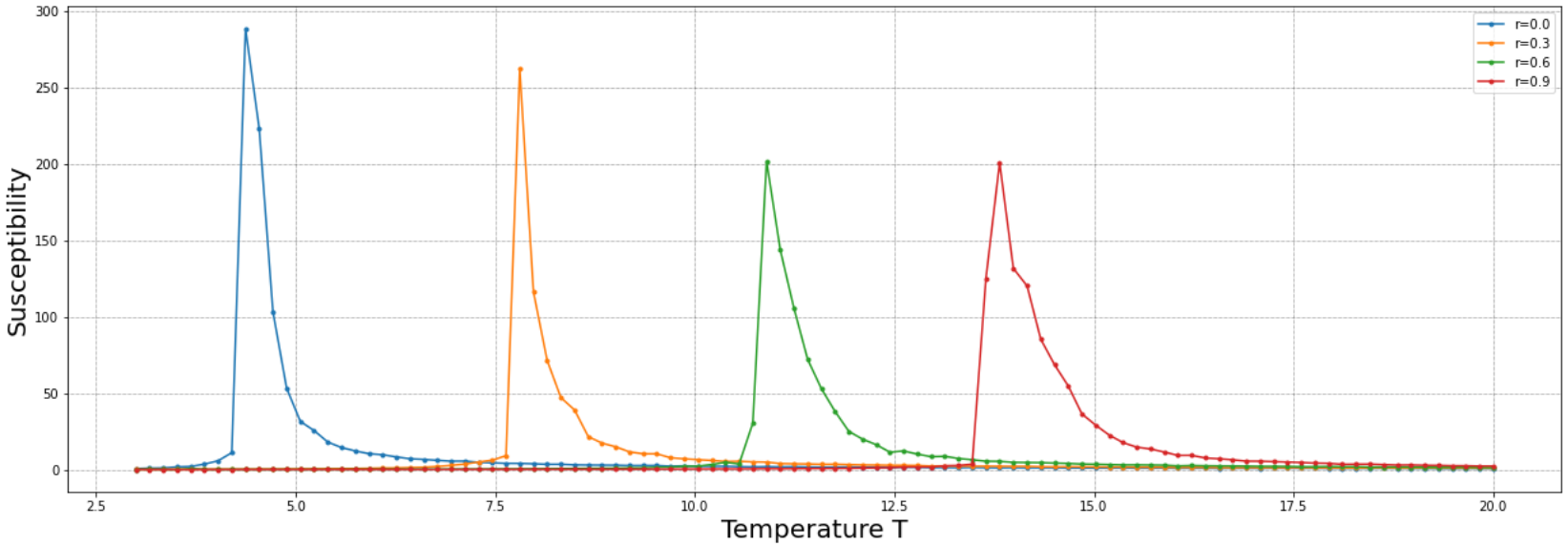


Figure: X Vs T, N=10, J_1=1

Binder's cumulant

The Binder's cumulant is an observation tool for estimating the critical point. For different sizes of the lattices , the average magnetization curve always passes through a fixed point, which coincides with the critical point. It is a fourth order cumulant related to kurtosis. It is defined as,

$$U = 1 - \frac{< M^4 >}{3 < M^2 >^2} = \begin{cases} 2/3 & ; T < T_c \\ U_B & ; T = T_c \\ 0 & ; T > T_c \end{cases}$$

where, U_B is the same value taken by Binder's cumulant of different lattice sizes at T_c.

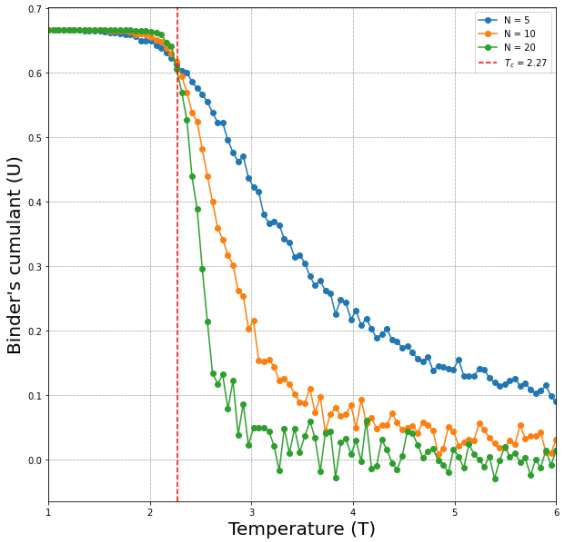


Figure: $T_c \approx 2.27$, identified from above graph for 2D NN model

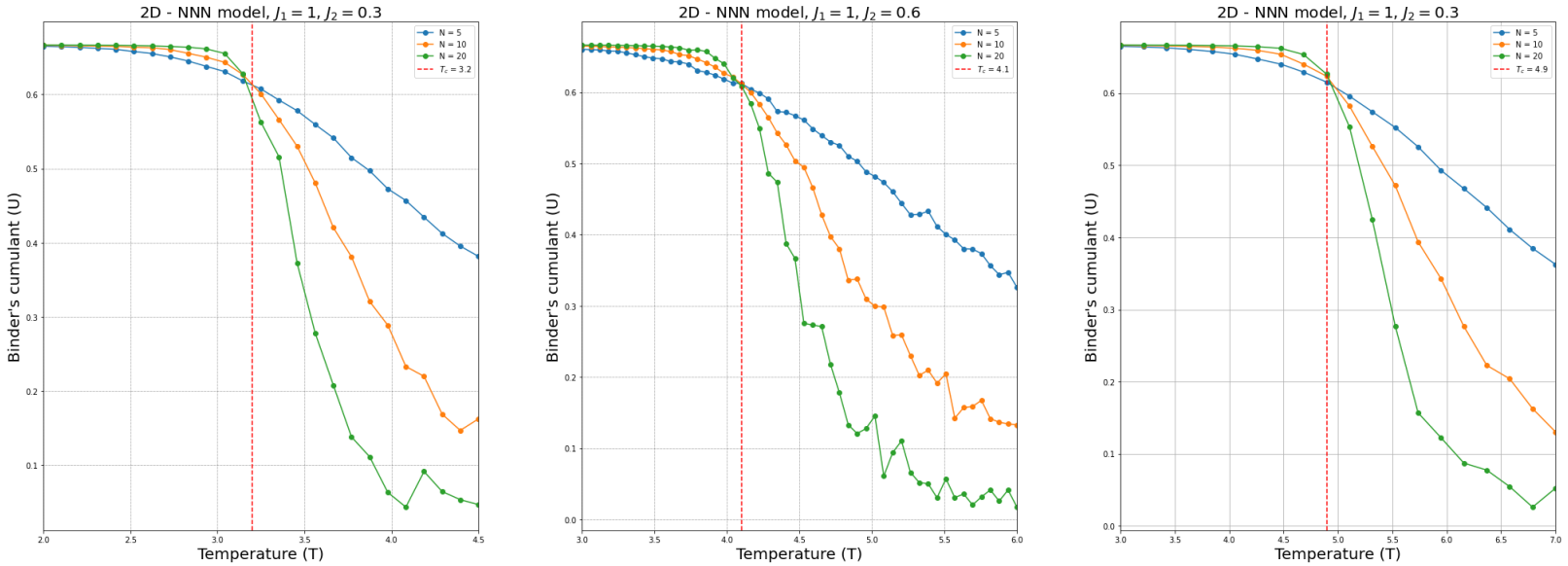


Figure: Critical values identified from above graphs for 2D NNN models

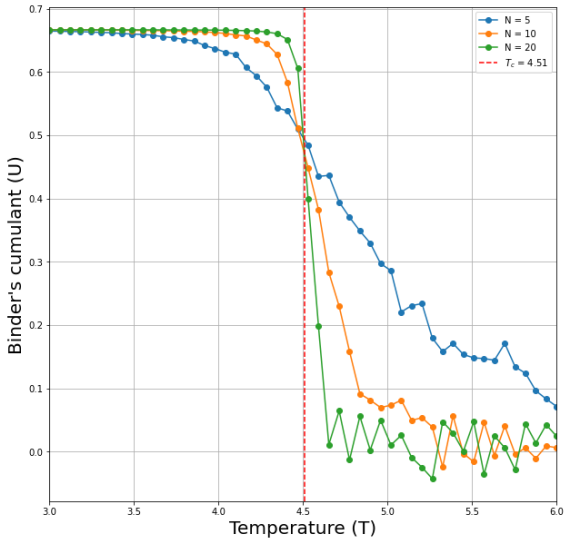


Figure: $T_c \approx 4.51$, identified from above graph for 3D NN model

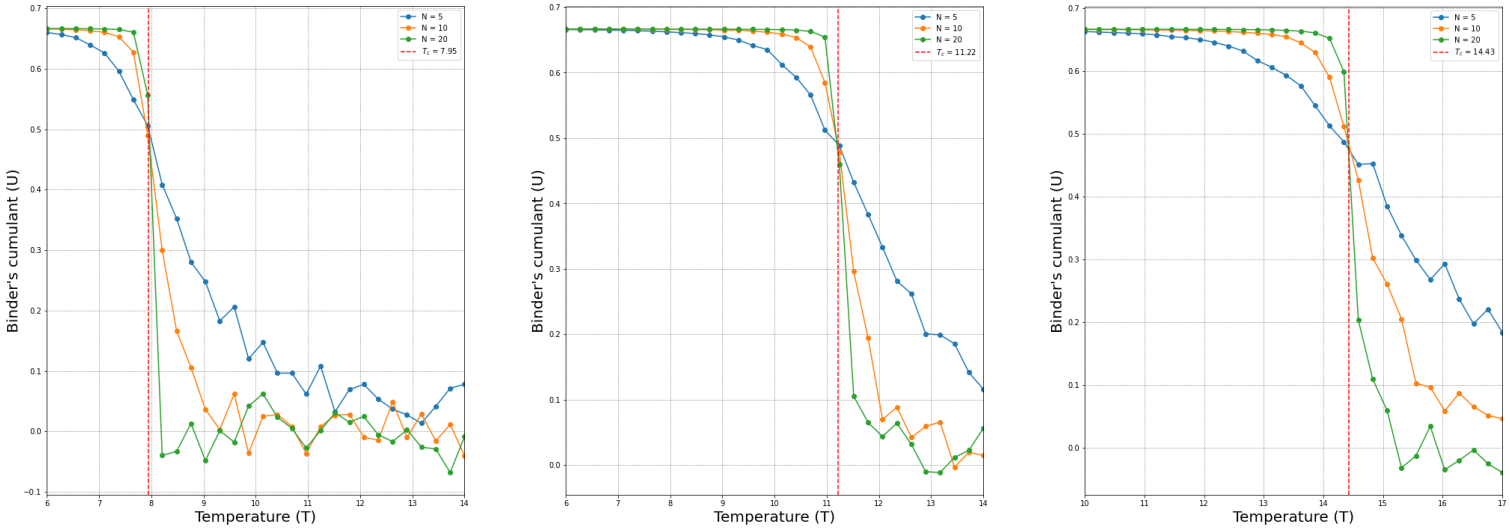


Figure: 3D NNN models for $J_2 = 0.3, 0.6, 0.9$ respectively.

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