Monte Carlo of 2D Ising Model

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Reduced units: $\hat{\beta} = \beta J$, $k_B = 1, \hat{\mathcal{H}} = \mathcal{H}/J$

- Initialise the LxL lattice configuration $S = \{s_{ij}\}_{i,j\in[L]}$.
- Choose random point (i, j) and compute ΔE_{ij} corresponding to flipping that spin.

$$\Delta E_{ij} = \mathcal{H}(\tilde{S}) - \mathcal{H}(S) = J\left(s_{i,j}\left(s_{i+1,j} + s_{i-1,j} + s_{i,j+1} + s_{i,j-1}\right)\right)$$

- Make decision to flip $(s_{ij} \rightarrow -s_{ij})$ with transition probability,

$$W = \begin{cases} 1 & \Delta E_{ij} < 0 \\ e^{-\beta \Delta E_{ij}} & \Delta E_{ij} > 0 \end{cases}$$

To mimic infinite system, periodic boundary conditions are applied in both the directions. For 1D chain it is equivalent to lattice points on circle and for 2D lattice it is equivalent to points on Torus topologically. In this work, I have taken interaction strength $J = 1$.

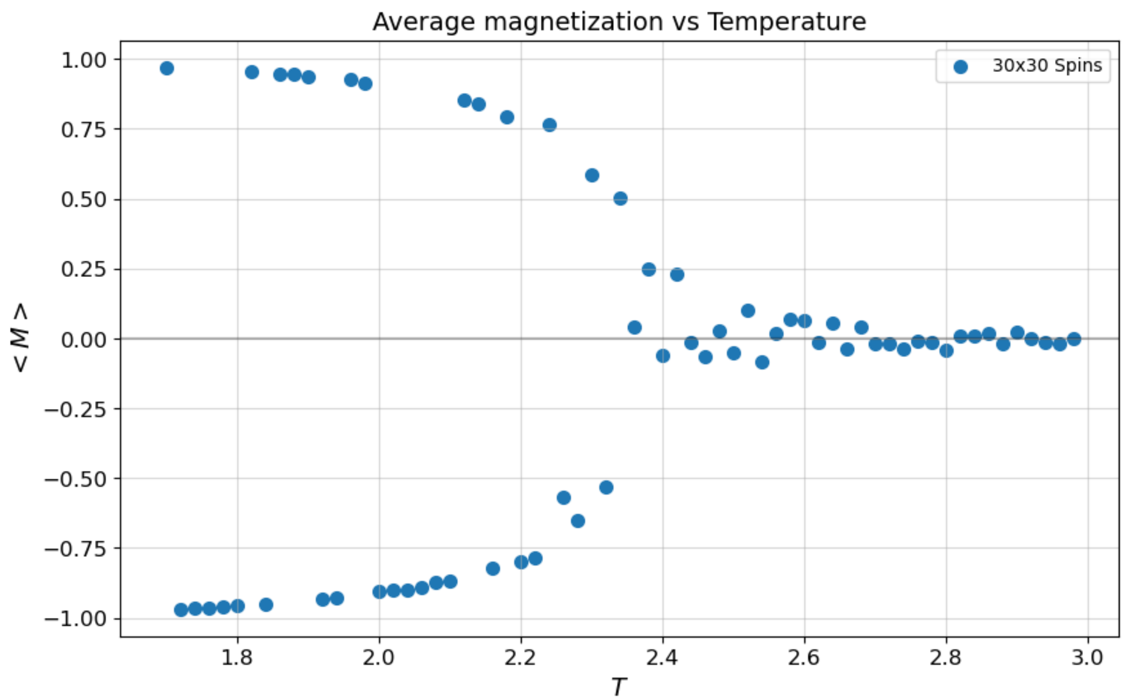
1 Average Magnetization

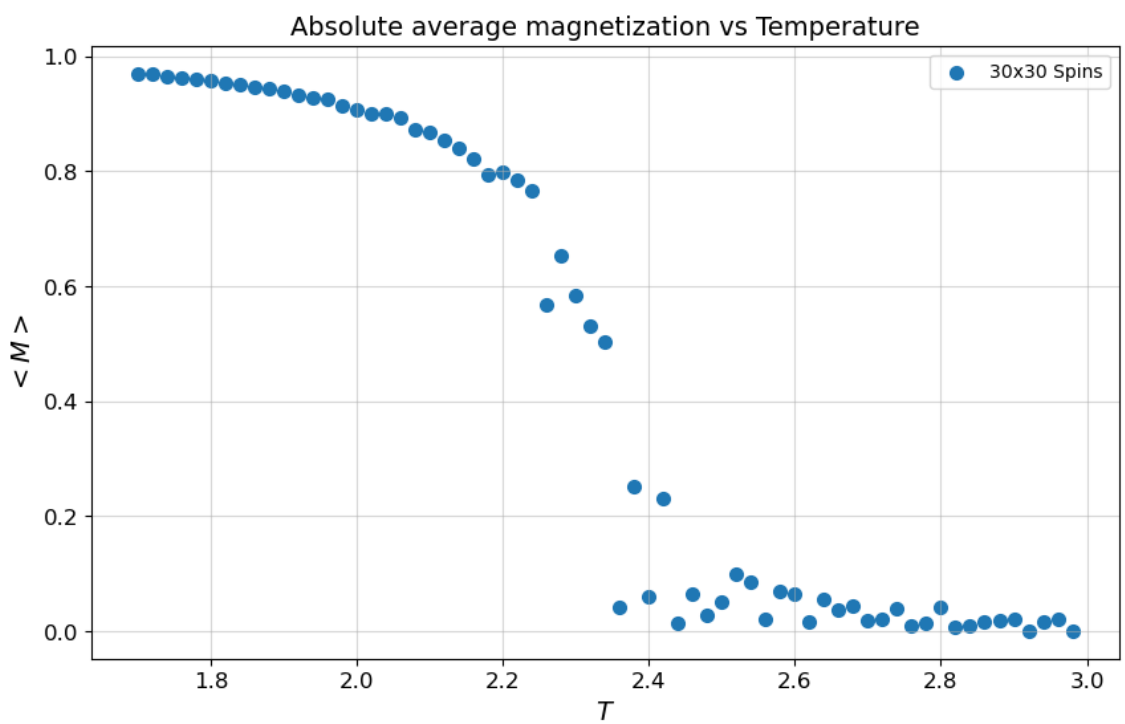
$$\langle M \rangle = \sum_S M(S) e^{-\beta \mathcal{H}(S)}/Z = \sum_S M(S) \frac{e^{-\beta \mathcal{H}(S)}}{Z}$$

where $Z = \sum_S e^{-\beta \mathcal{H}(S)}$ and $M(S) = \sum_{ij} s_{ij}$

$$\implies \sum_S M(S) Pr(S) \simeq \frac{1}{N_{mc}} \sum_{n=1}^{N_{mc}} M_n$$

where $M_n = \frac{1}{L^2} \sum_{ij} s_{ij}$ and N_{mc} = Number of Monte Carlo samples.

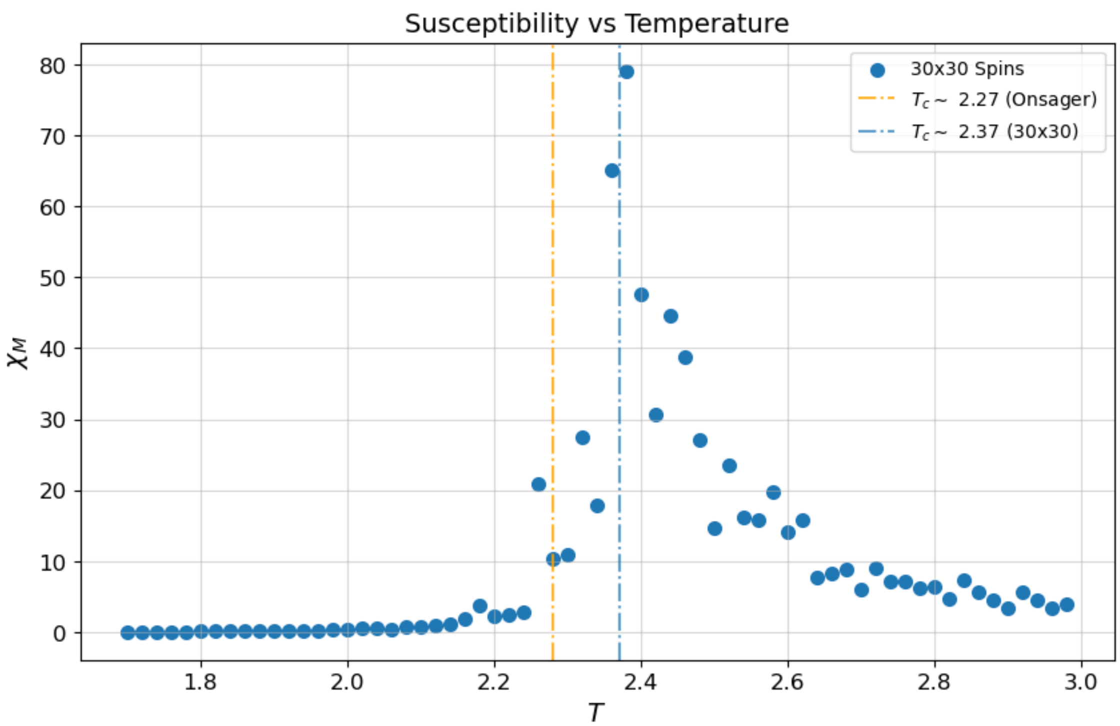

Average magnetization vs Temperature
30x30 Spins
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
< M >
1.8
2.0
2.2
2.4
2.6
2.8
3.0
T


Absolute average magnetization vs Temperature
30x30 Spins
1.0
0.8
0.6
0.4
0.2
0.0
< M >
1.8
2.0
2.2
2.4
2.6
2.8
3.0
T

2 Magnetic susceptibility: χ

$$\chi_M = \frac{\beta}{L^2}\left(\langle M^2\rangle - \langle M\rangle^2\right)$$

where $\langle M\rangle$ and $\langle M^2\rangle$ are calculated like previous section.



At T_c (critical temperature), the magnetic susceptibility goes to infinity.

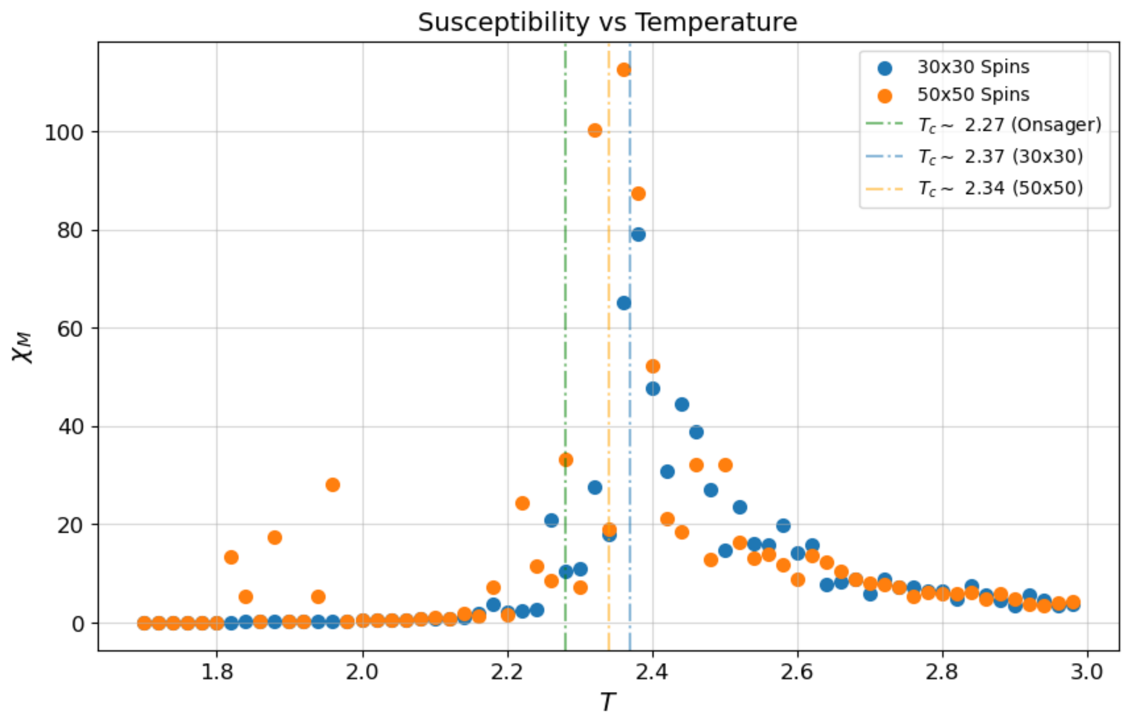
$$\chi_M \sim \frac{1}{|T - T_c|^\gamma}$$

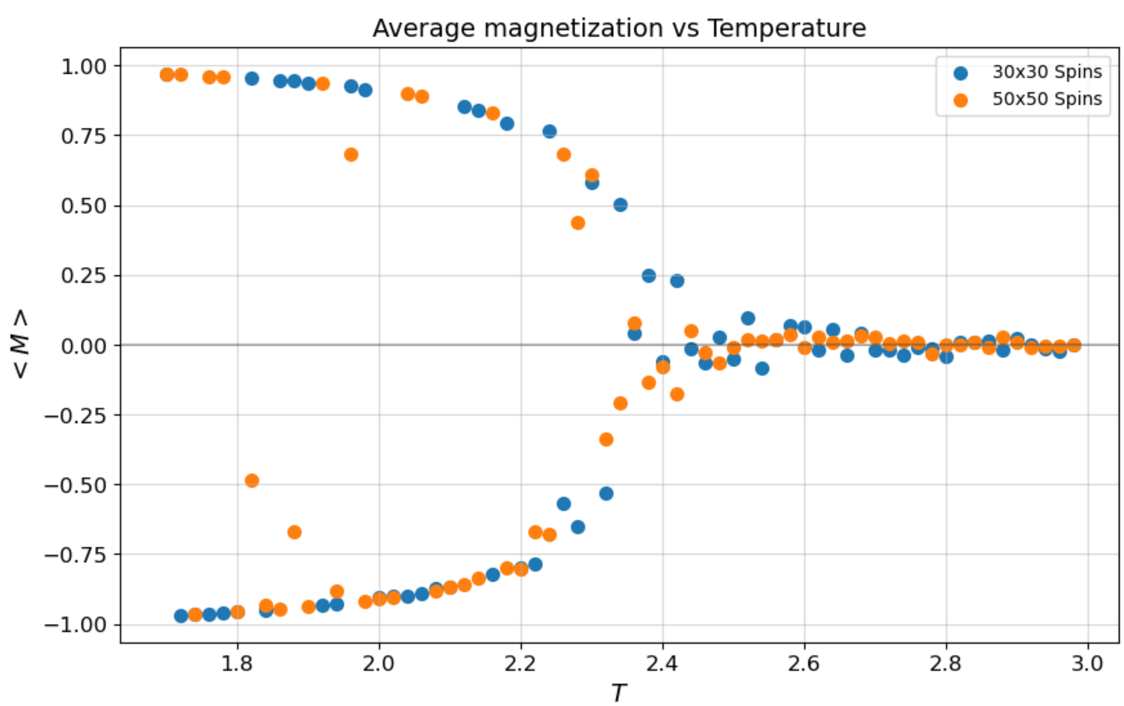
But due to the finite size of the simulation, $\chi < \infty$. We can approximately infer critical temperature where the χ takes a large value. Exact solution to T_c for 2D Ising model was derived by Onsager $T_c = \frac{2}{\ln(1+\sqrt{2})} \simeq 2.269185$ $(J = 1, k_B = 1)$. In simulation I have calculated T_c as the average of temperatures where the maximum two χ occurs.

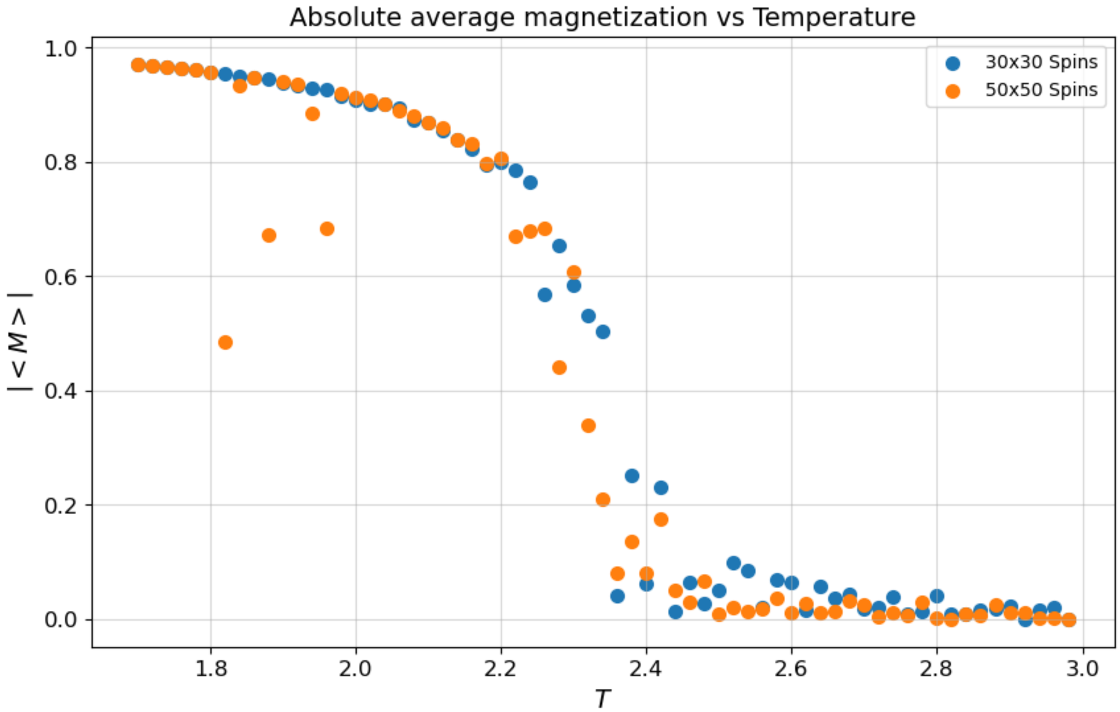
3 System size dependence

$$\Gamma(r) = \frac{1}{r^p} e^{-\frac{r}{\zeta}}, \quad \zeta \sim |T - T_c|^{-\nu}, \quad T \to T_c \implies \Gamma(r) = \frac{1}{r^p}$$

Length correlation function decays in power law instead of exponential $\implies$ we have long range correlation. Thus the system with large length gives better estimate of T_c.


Susceptibility vs Temperature
30x30 Spins
50x50 Spins
$T_c \sim$ 2.27 (Onsager)
$T_c \sim$ 2.37 (30x30)
$T_c \sim$ 2.34 (50x50)
χ_M
T


Average magnetization vs Temperature
30x30 Spins
50x50 Spins
$< M >$
T



Although the periodic boundary condition used to mimic infinite system, this approximation breaks down for small L at critical phenomenon. Due to periodic boundary $s_{i+L,j} = s_{i,j}$, $s_{i,j+L} = s_{i,j}$ and due to the power law decay, the L must be chosen large enough to ensure $\Gamma(r) \sim \frac{1}{L^p} \rightarrow 0$.