Computational study of 2D Ising Model

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October 23, 2025

Objective

1. To study how energy per spin, magnetization per spin, specific heat, and susceptibility change as a function of temperature.
2. To study the effects of topology on the lattice behavior.
3. Extracting critical exponents via finite-size scaling and estimation of critical temperature.

The Ising Model – A Fundamental Framework in Statistical Physics

What Is It?

A mathematical model to study **magnetism** and **phase transitions** in materials.

- Spins $s_i = \pm 1$ on a lattice.
- Hamiltonian:

$$H = -J \sum_{\langle i,j \rangle} s_i s_j - h \sum_i s_i$$

  - J: Interaction strength between neighbouring spins
  - h: External magnetic field

Behavior

- Ferromagnetic $(J > 0)$: Spins align
- Antiferromagnetic $(J < 0)$: Spins anti-align
- **Phase Transition** in 2D
  - Above T_c: Disordered (paramagnetic)
  - Below T_c: Ordered (ferromagnetic)
- We take a 2D lattice of size $L \times L$ with random spins (± 1).

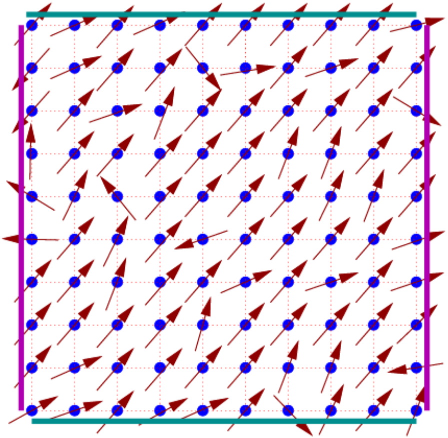


Figure: 2D square lattice with random spin orientation.

Thermodynamic quantities

The Hamiltonian for 2D ising model in absence of external magnetic field is

$$H = -J \sum_{\langle i,j \rangle} s_i s_j$$

1. Energy :

$$E = -J \sum_{\langle i,j \rangle} s_i s_j$$

2. Magnetization :

$$M = \frac{1}{N} \sum_{i} s_i$$

3. Specific heat:

$$C_v = \frac{1}{NT^2} (< E^2 > - < E >^2)$$

1. Magnetic susceptibility :

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

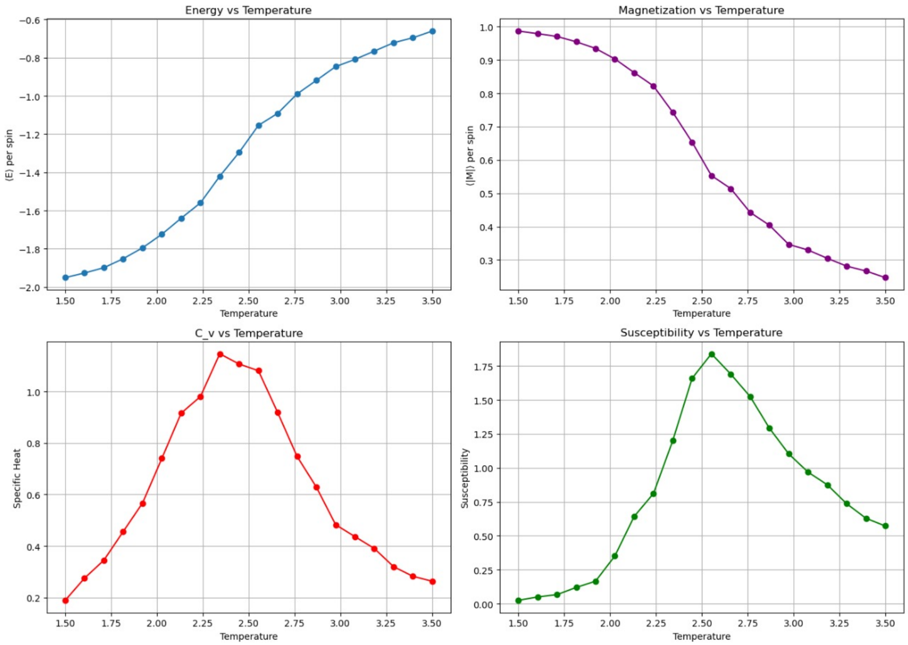
Metropolis Algorithm

1. Pick a random spin: Choose the lattice site (i, j) at random.
2. Calculate the energy change ΔE if the spin is flipped:

$$\Delta E = E_{\text{new}} - E_{\text{old}} = -J(-s_{ij}) \sum_{\text{nn}} s_{\text{nn}} - \left[-J s_{ij} \sum_{\text{nn}} s_{\text{nn}} \right]$$

$$\Delta E = 2J \; s_{i,j} (s_{i+1,j} + s_{i-1,j} + s_{i,j+1} + s_{i,j-1})$$

3. Step 3: Decide whether to flip or not flip
   - If $\Delta E \leq 0$:
     Flip the spin
   - If $\Delta E > 0$:
     Flip with the probability $P = exp(\frac{-\Delta E}{KT})$
4. Step 4: Repeat this for the desired Monte Carlo steps.


Energy vs Temperature
⟨E⟩ per spin
Temperature
Magnetization vs Temperature
⟨|M|⟩ per spin
Temperature
C_v vs Temperature
Specific Heat
Temperature
Susceptibility vs Temperature
Susceptibility
Temperature

Effects of topology on the lattice behaviour I

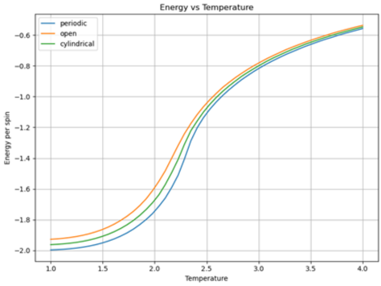
1. Periodic boundary conditions:
    - The lattice "wraps around" like a torus.
    - The left edge is connected to the right edge, and the top is connected to the bottom.
    - Mimics an infinite system by eliminating boundary effects.
    - Every site has 4 neighbours, no matter its position.
    - Most commonly used in simulations to approximate bulk behaviour.
2. Open boundary conditions:
    - The lattice edges are not connected: If a neighbour is outside the grid, it is ignored (or treated as zero).
    - Models a finite, isolated patch of spins.

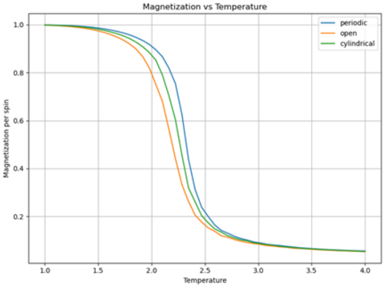
Effects of topology on the lattice behaviour II

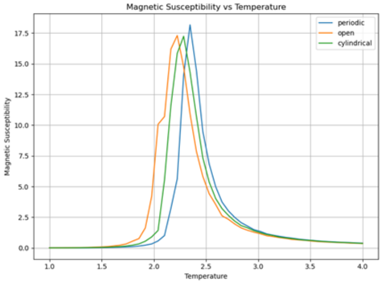
- Edge spins have fewer neighbours, making alignment less favourable at the boundaries.
- Leads to edge effects: surface spins behave differently than interior ones.

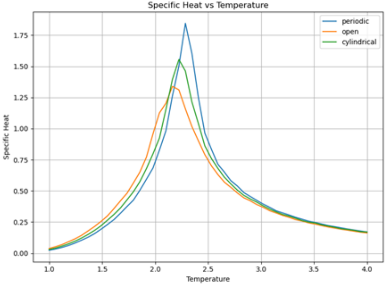
3. Cylindrical boundary conditions:
   - Like rolling the lattice into a cylinder: Wrap in one direction (usually vertical) and leave the other direction open (horizontal).
   - Vertical neighbours use periodic wrapping, and horizontal neighbours are treated as open (only valid if they fall within bounds).
   - Edge effects are intermediate between open and periodic.

Plots


Energy vs Temperature
periodic
open
cylindrical
Energy per spin
Temperature


Magnetization vs Temperature
periodic
open
cylindrical
Magnetization per spin
Temperature


Magnetic Susceptibility vs Temperature
periodic
open
cylindrical
Magnetic Susceptibility
Temperature


Specific Heat vs Temperature
periodic
open
cylindrical
Specific Heat
Temperature

Behaviour at different boundaries

Magnetization behaviour at Boundary:

1. Periodic: Minimizes edge effects, producing the clearest and sharpest phase transition.
2. More spin disorder near boundaries reduces net magnetization slightly and can smooth the transition.
3. Cylindrical: Behaves between open and periodic. Some boundary symmetry is preserved.

Behaviour at different boundaries

Energy behaviour at Boundary:

1. Periodic: Yield slightly lower ground-state energy due to maximized spin interactions.
2. Open: Edge effects slightly alter energy levels due to fewer neighbours.
3. Cylindrical: Intermediate behaviour between open and periodic boundary conditions.

Behaviour at different boundaries

Specific heat behaviour at Boundary:

1. Periodic: Exhibits the sharpest and highest peak, reflecting the most accurate bulk behaviour.
2. Open: Broader and lower peak due to increased surface effects and reduced interactions at edges.
3. Cylindrical: Intermediate behaviour, with one direction preserving periodicity.

Behaviour at different boundaries

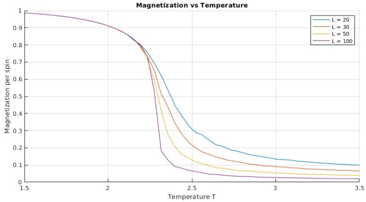
Magnetic susceptibility behaviour at Boundary:

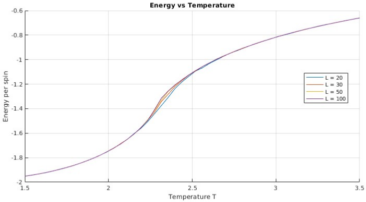
1. Periodic: Produces a sharp, high peak—indicating strong magnetic response near the transition.
2. Open: Reduced overall susceptibility, and a smoother peak, due to less cooperative spin alignment at the edges.
3. Cylindrical: Intermediate behaviour between open and periodic cases.

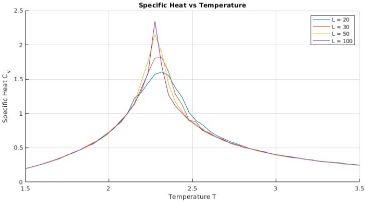
Finite Size Scaling

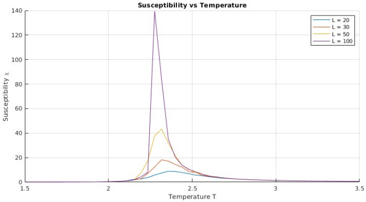
- In theory, the phase transition occurs only in infinite systems, i.e. L$\to \infty$.
- We simulate Ising model on a finite lattice of size L x L, so the transitions are smoothened out.
- **Finite Size Scaling** is a technique to extract infinite system behaviour from finite system simulations.

Plots of physical quantities at different L









The estimated critical temperature is T_c= 2.3163

Power Law Scaling and Critical Exponents

- $\zeta \sim |T - T_c|^{-\nu}$
- $M \sim |T - T_c|^{\beta}$
- $\chi \sim |T - T_c|^{-\gamma}$
- $C_v \sim |T - T_c|^{-\alpha}$

where, ν, β, γ, α are the critical exponents.

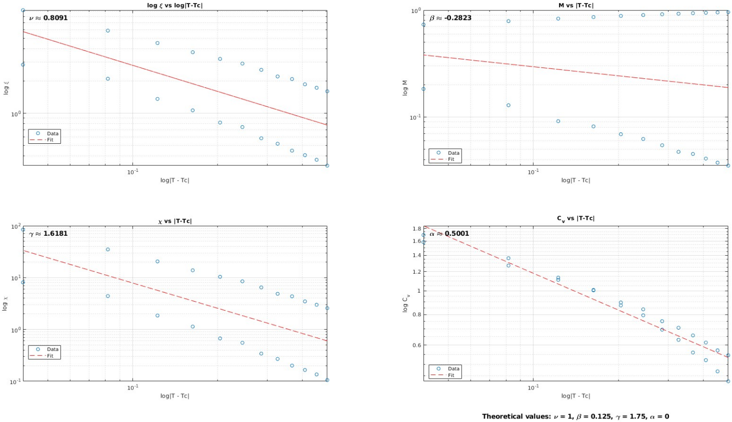
Critical exponents describe how physical quantities diverge or vanish as a system approaches a critical point.

At the critical point T $= T_c$, the system becomes scale invariant because the correlation length ζ, becomes infinite at T_c.

That means:

- No single length scale dominates
- Small and large clusters behave similarly

log-log plots to find critical exponents



Here, there are two points for one $log|T - T_c|$ value. This is because the value of T is approaching the critical temperature from both the sides.

Limitations of Power Law Fits in Simulations

- Power law behaviour is strictly valid exactly at T_c.
- Simulation is done in the region near T_c.
- Near T_c, correction to scaling terms are included.
- Singularity isn't pure power law scaling, but include logarithmic corrections.

How Finite-Size Scaling Overcomes Power-Law Limitations

1. **Exploiting Size Dependence**
2. **Scaling Form:**

$$Q(L,T) = L^p f(x), \tag{1}$$

   where, Q(T,L) is the physical quantity of interest, p is a scaling dimension related to the critical exponent of Q, f(x) is the scaling function, where the scaling variable x $= L^{\frac{1}{\nu}} |T - T_c|$.

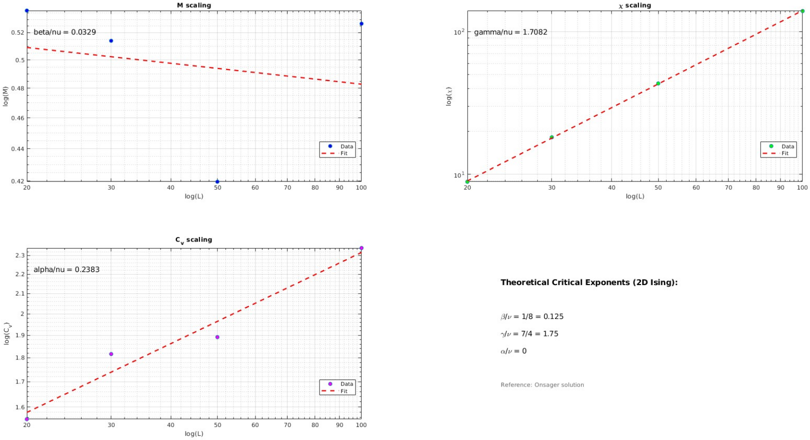
3. **Extracting Exponents from Scaling**

FSS Hypothesis

The FSS hypothesis at $T = T_c$ states:

1. Magnetization: $M \sim L^{-\beta/\nu}$
2. Susceptibility: $\chi \sim L^{\gamma/\nu}$
3. Specific Heat: $C_v \sim L^{\alpha/\nu}$

Visualizing Finite-Size Scaling



Conclusion

- Fitting simulation data using simple power laws near the critical temperature T_c can provide a rough estimate of critical behaviour.
- However, such fits are prone to inaccuracies due to:
  - Finite-size effects,
  - Corrections to scaling near T_c,
  - Logarithmic or non-power-law deviations from ideal scaling.
- Finite-Size Scaling offers a more robust and accurate framework by:
  - Systematically analyzing dependence of observables on system size L,
  - Exploiting universal scaling relations predicted by the theory of critical phenomena,
  - Allowing precise extraction of critical exponents.
- Therefore, FSS is essential for the reliable characterization of critical behaviour in finite systems.