PROJ 201

Computational Simulation of a Order-Disorder Phase Transition Project

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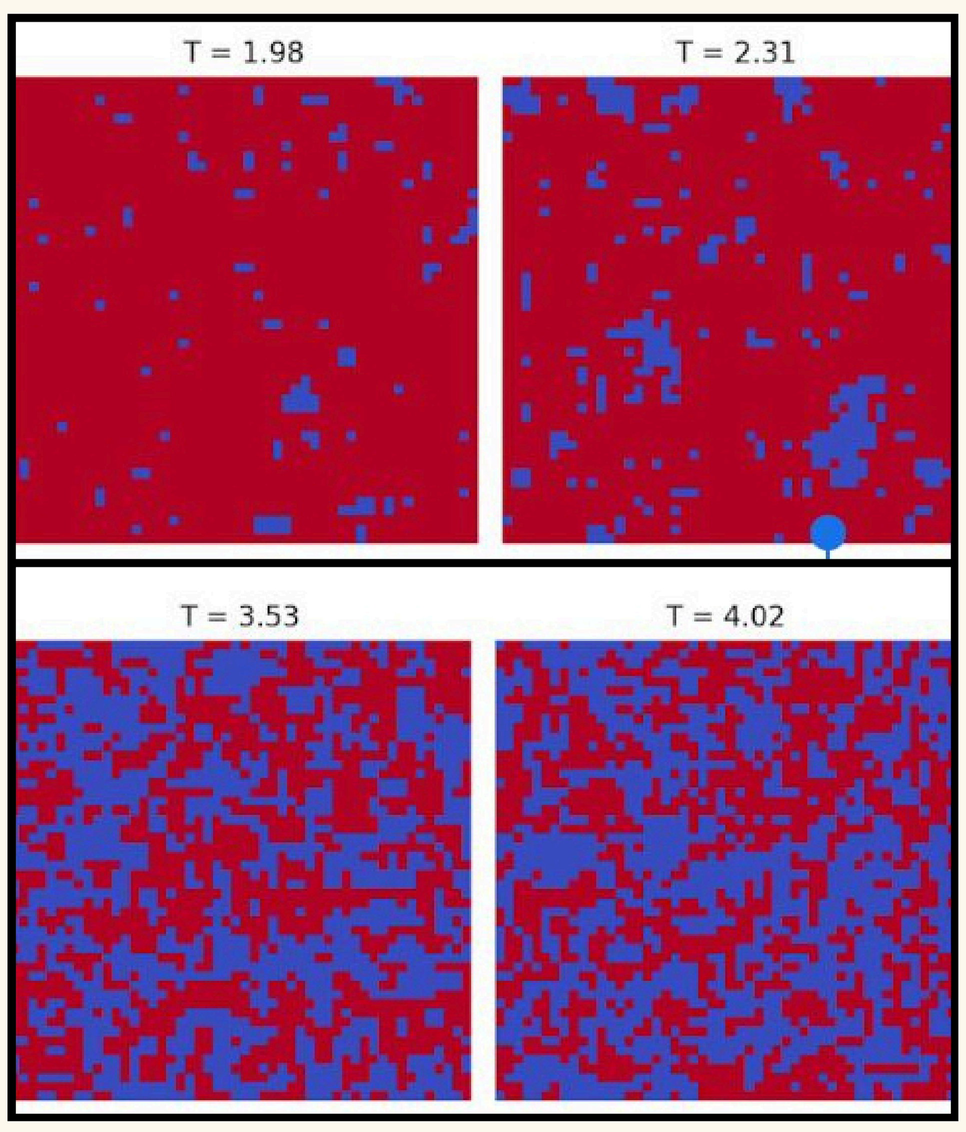
Monte-Carlo Experiment

A **Monte Carlo experiment** is a computational technique that uses **random sampling** to estimate numerical results for problems that may be deterministic in nature. It relies on repeated random trials to model complex systems and approximate solutions.

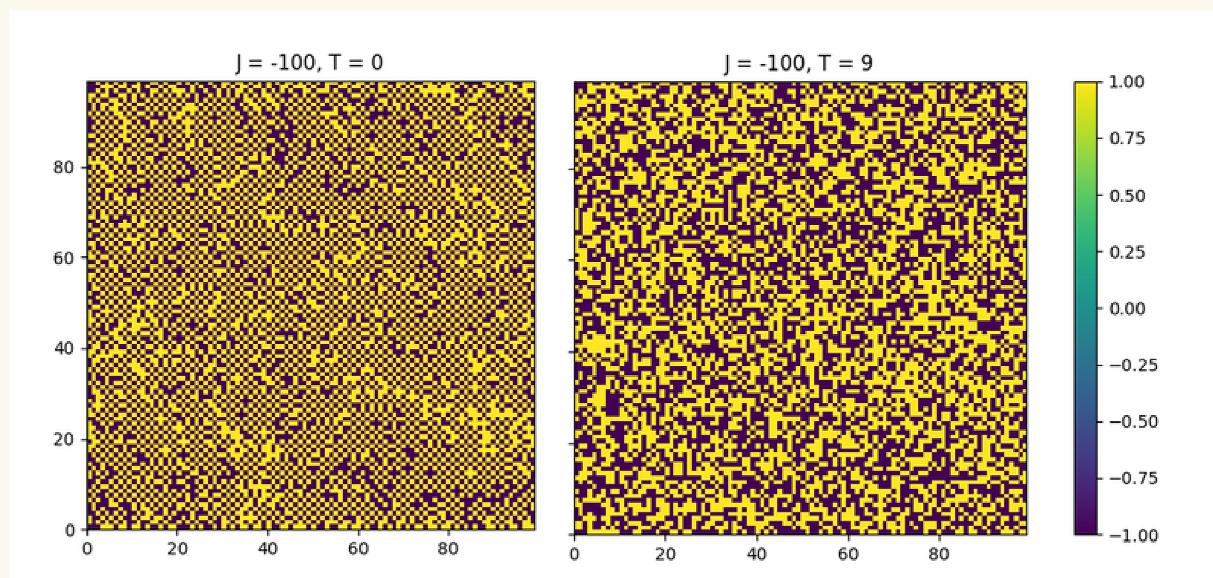


Ising Model & Phase Transitions

The **Ising model** is a mathematical model used in statistical physics to describe **ferromagnetism** in materials. It provides an excellent framework for **simulating order-disorder phase transitions**, particularly near a critical temperature. The Ising model exhibits rich behavior and is widely studied in the context of phase transitions, critical phenomena, and lattice-based systems.

Phase transitions in Monte Carlo experiments are studied by sampling system configurations as parameters (e.g., temperature) vary. Key indicators include sudden energy changes, peaks in specific heat, or susceptibility near critical points.

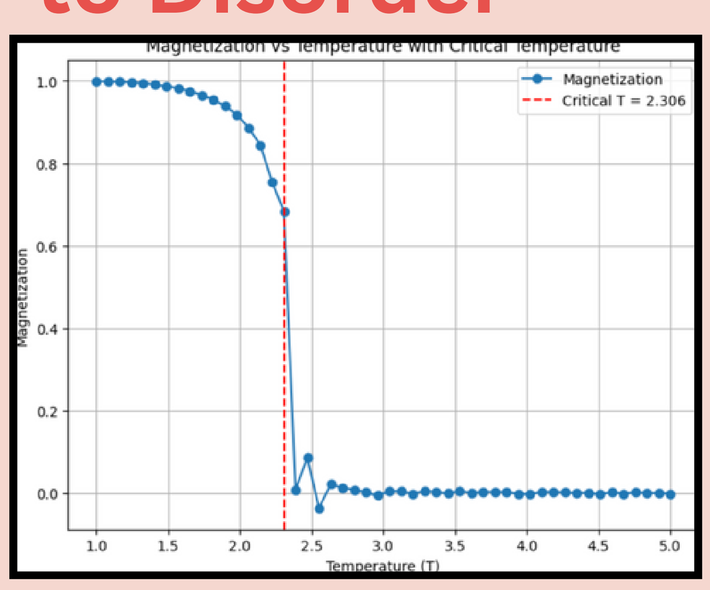
Simulation Of Order to Disorder With Negative J



At lower temperatures, spins align in an antiferromagnetic order, forming a checkerboard pattern of alternating spins to minimize energy. Total magnetization is nearly zero due to an equal number of +1+1 and −1−1 spins, reflecting a low-energy, ordered structure.

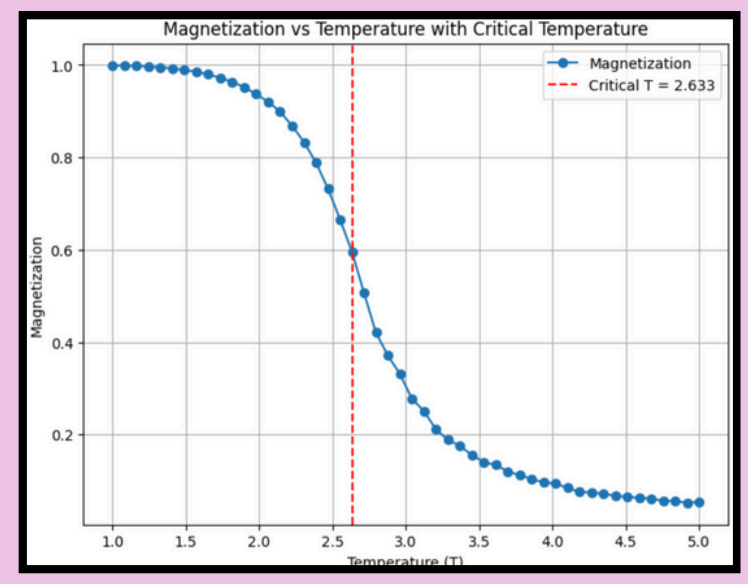
At high temperatures, thermal fluctuations dominate, destroying the antiferromagnetic order. Spins become randomly distributed with no pattern, leading to high entropy and total magnetization close to zero as the net magnetic moment cancels out.

Simulation Of Order to Disorder



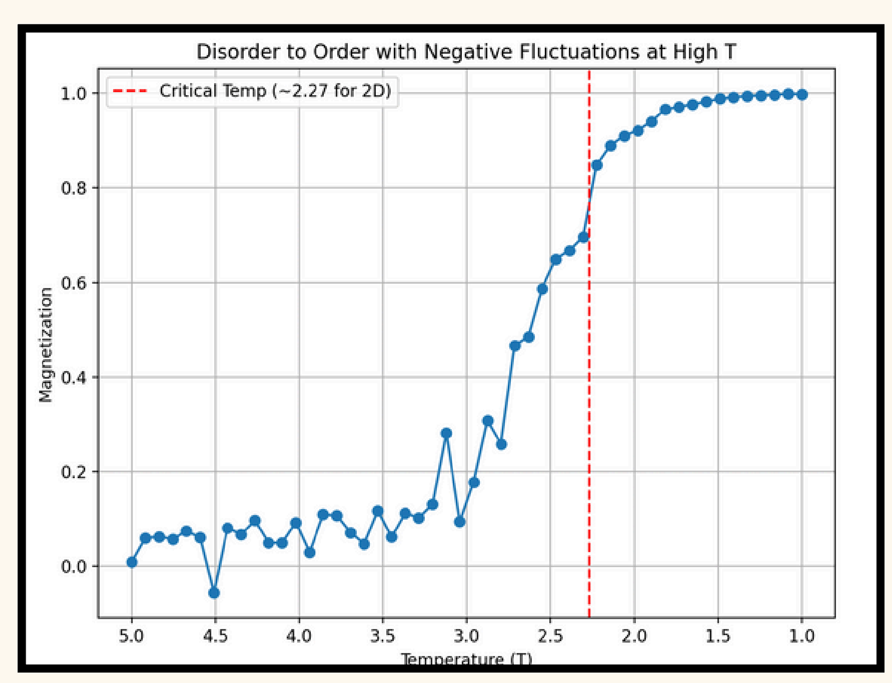
This **2D Ising model simulation** shows how magnetization changes with temperature. **At low temperatures**, spins align, producing near-maximal magnetization. **As temperature rises**, thermal fluctuations weaken this order. N**ear the critical temperature (around 2.31)**, magnetization drops sharply, marking a phase transition from ferromagnetic to paramagnetic behavior. **Above this temperature**, magnetization averages near zero, reflecting a disordered, high-energy state.

Simulation Of Order to Disorder with External Bias



This 2D Ising simulation shows the transition from order to disorder with a higher number of steps per temperature (10,000) and an averaged measure over the last 2,000 steps, reducing fluctuations. An external bias (h = 0.1) further shifts equilibrium magnetization. As temperature rises to around T_c, the carefully averaged data still reveal a sharp drop in magnetization, marking the phase transition. Above this critical point, the system's fluctuations are significantly smoothed, and the spins settle into a disordered, low-magnetization state.

Simulation of Disorder to Order



A disorder-to-order plot shows **how a system transitions to an ordered state as it cools**. **At high temperatures**, spins are random (disordered), but **as the temperature drops below the critical point** TcTc, spins align, and magnetization increases sharply, indicating the system's shift to an ordered phase.