Particle Methods Homework 1 – Metehan Dündar

A) Determination of the Critical Temperature Tc

The theoretical critical temperature for the 2D Ising model on a square lattice with coupling J = 1 and Boltzmann constant kB = 1 is given by $T_c \approx 2.269$.

In our simulations for different lattice sizes (L = 5, 10, and 15), the following observations were made:

- For temperatures below approximately T = 2.2, the absolute magnetization $\langle |M| \rangle$ remains close to 1, indicating a strongly ordered phase.
- As the temperature increases from T = 2.1 to T = 2.4, a marked decrease in $\langle |M| \rangle$ is observed, together with an increase in energy per spin.
- This behavior indicates that the phase transition occurs in the range $T \approx 2.2$–2.3.

Thus, from both theoretical and numerical perspectives, we confirm that the critical temperature is approximately $T_c \approx 2.27$.

B) Dependence on System Size L

Simulations were performed for lattices of sizes L = 5, 10, and 15. The main findings related to the system size are as follows:

Magnetization $\langle |M| \rangle$

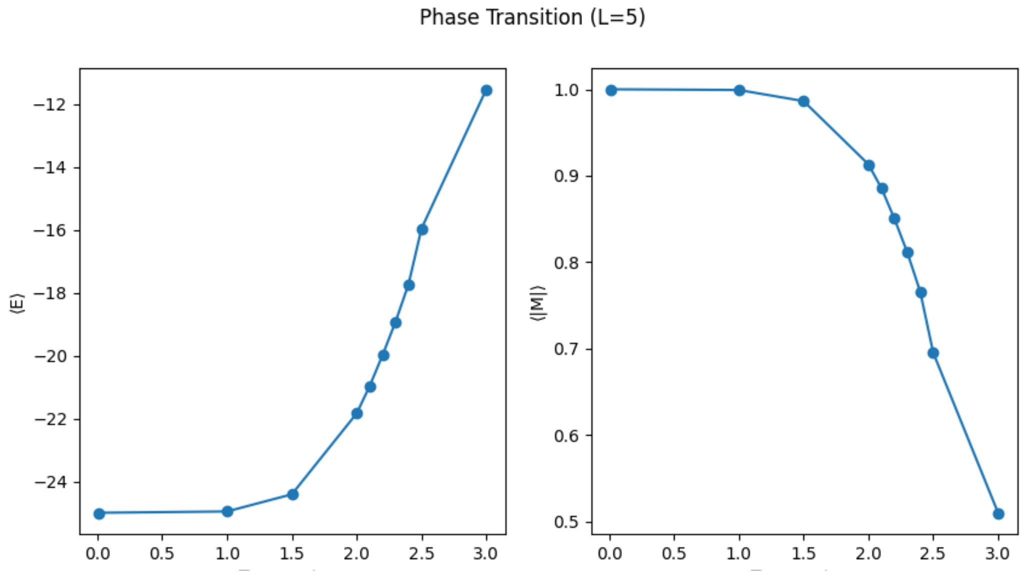
- **Low Temperatures ($T \ll T_c$)**:
  All lattice sizes exhibit $\langle |M| \rangle \approx 1$. This indicates that the spins are nearly all aligned in the ordered phase.
- **Near the Critical Region ($T \approx T_c$)**:
  Finite-size effects become significant.
  - In smaller systems (L=5), the magnetization decreases more gradually as T increases.
  - In larger systems (L=10 and L=15), the drop in $\langle |M| \rangle$ is sharper.

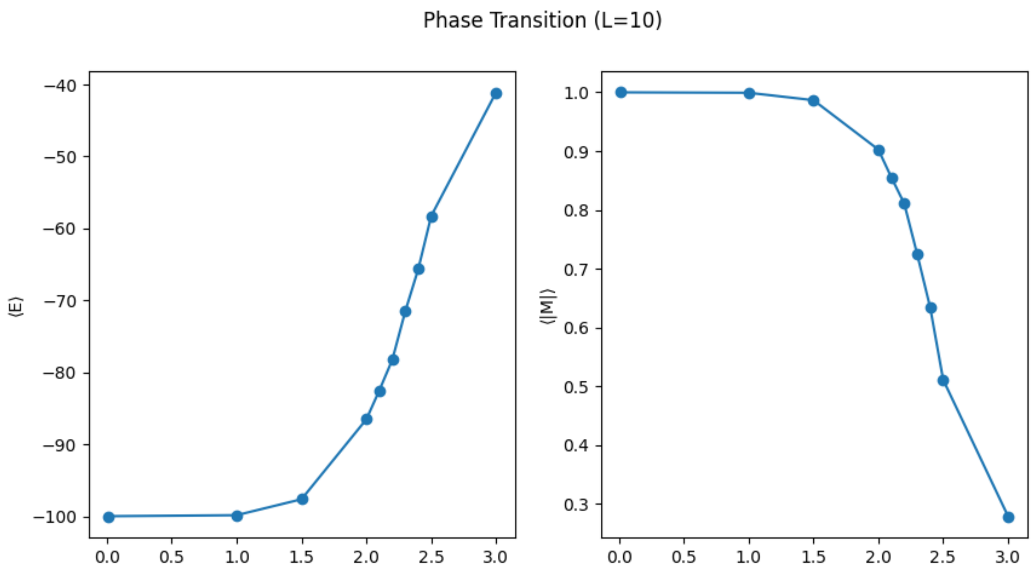
  These observations suggest that as the system size increases, the phase transition becomes more pronounced and the finite-size rounding diminishes.

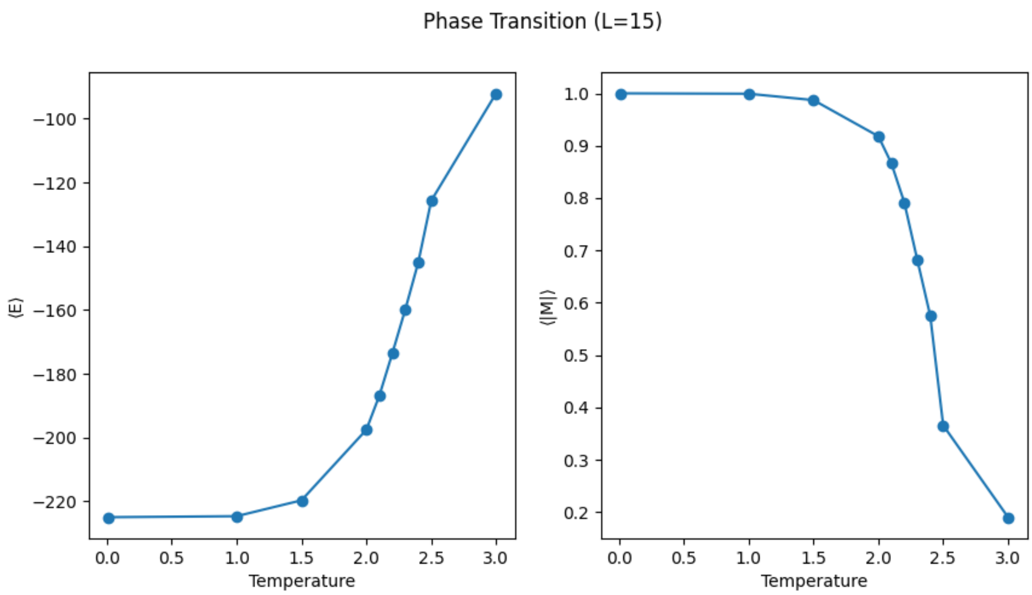
Energy $\langle E \rangle$

- The energy scales with the number of spins. By normalizing the total energy by the number of spins (L×L), we obtain comparable energy per spin values across different lattice sizes.
- The energy per spin changes more rapidly near the critical temperature, and larger systems show a steeper variation in energy around Tc.

In summary, increasing the lattice size leads to a sharper manifestation of the phase transition, with larger systems displaying more pronounced decreases in ⟨|M|⟩ and a steeper change in energy near Tc.







C) Time Evolution of Magnetization for T<Tc

The attached time series plot (for a small system, L=5, at T=2.2) reveals the following behavior:

- **Magnetization Fluctuations**:
  The magnetization M exhibits large fluctuations and shows spontaneous sign flips between values near +1and −1. This indicates that, even though the system is below the critical temperature where long-range order is expected, finite-size effects allow the entire lattice to reverse its magnetization.
- **Finite-Size Effects**:
  For small systems, thermal fluctuations are strong enough to overcome the energy barrier separating the two ordered states, resulting in the observed magnetization sign flips. In larger systems, while local domains may fluctuate, it becomes increasingly unlikely for the entire system's magnetization to switch spontaneously when T is well below Tc.

These observations confirm that for small lattices at temperatures below Tc, the magnetization can undergo spontaneous coherent flips due to the enhanced impact of thermal fluctuations.