MSN 514 - Computational Methods for Material Science and Complex Systems

Homework 07

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I. INTRODUCTION

Magnetic materials show complex behavior when subjected to changes in temperature and external magnetic fields. A widely used model to study these phenomena is the Ising model, which simplifies magnetic interactions by representing each atomic spin as a discrete variable $S_i = \pm 1$. In a two-dimensional square lattice, the Ising Hamiltonian with periodic boundary conditions is given by

$$E = -J \sum_{\langle i,j \rangle} S_i S_j \; - \; B \sum_i S_i, \tag{1}$$

where J is the coupling constant, B represents the external magnetic field, and the notation $\langle i, j \rangle$ indicates that the sum is over nearest neighbor pairs.

A. Magnetization and Misalignment

In the ferromagnetic case ($J > 0$), the system tends to align all spins parallel, leading to a nonzero average magnetization

$$m = \frac{1}{N} \sum_i S_i, \tag{2}$$

where N is the total number of spins. At low temperatures, thermal fluctuations are minimal and m remains close to 1 (assuming an initially ordered state).

For antiferromagnetic systems ($J < 0$), the natural ground state is an alternating (checkerboard) arrangement of spins. In order to quantify this ordering, we define the *misalignment* (or staggered magnetization) as

$$n = \frac{1}{N} \sum_{x,y} f(x, y)\, S_{x,y}, \tag{3}$$

with

$$f(x, y) = \begin{cases} +1, & \text{if } (x + y) \text{ is even,} \\ -1, & \text{if } (x + y) \text{ is odd.} \end{cases}$$

In an ideal antiferromagnetic state, n approaches 1, indicating perfect checkerboard order, while the standard magnetization m remains near zero.

B. Monte Carlo Simulation and Numba Optimization

The Metropolis algorithm, a Monte Carlo method (widely used in AI and RL approaches), is used to sample configurations from the Boltzmann distribution. In each sweep of the simulation, a spin is randomly chosen and a flip is accepted with a probability

$$P(\Delta E) = \begin{cases} 1, & \Delta E < 0, \\ \exp\left(-\frac{\Delta E}{k_B T}\right), & \Delta E \geq 0, \end{cases} \tag{4}$$

where ΔE is the energy change due to the flip, T is the temperature, and k_B is the Boltzmann constant (often set to 1 in reduced units).

Given the large number of spin updates required for a lattice of size 100×100, computational efficiency is critical. In our implementation, the `numba` library is employed to compile performance-critical functions (e.g., the spin-update function) to machine code, yielding significant speed-ups compared to pure Python execution (reducing runtime from approximately 25 minutes to 2 minutes).

C. Objective of the Study

The goal of this work is to simulate both ferromagnetic ($J = +1$) and antiferromagnetic ($J = -1$) systems under varying temperatures and external magnetic fields ($B = 0, 0.5, 1, 1.5$). By analyzing the temperature dependence of the order parameters m and n, we aim to:

1. Examine how thermal fluctuations drive the phase transition from an ordered to a disordered state.

2. Understand the influence of an external magnetic field on the stability of spin ordering.

3. Compare the behavior of ferromagnetic and antiferromagnetic phases using appropriate order parameters.

II. RESULTS

A. Ferromagnetic Case ($J = +1$)

For the ferromagnetic simulation, the system is initialized in a uniform state with all spins set to +1. Figure 1 displays the magnetization m as a function of temperature T for different external field strengths. At low temperatures, m remains nearly 1, reflecting a highly ordered state. However, as the temperature increases, thermal fluctuations cause a rapid decline in m, signifying the onset of a phase transition. The effect of an external field is clearly visible; higher field strengths help to sustain the magnetization even as the system approaches the critical temperature.

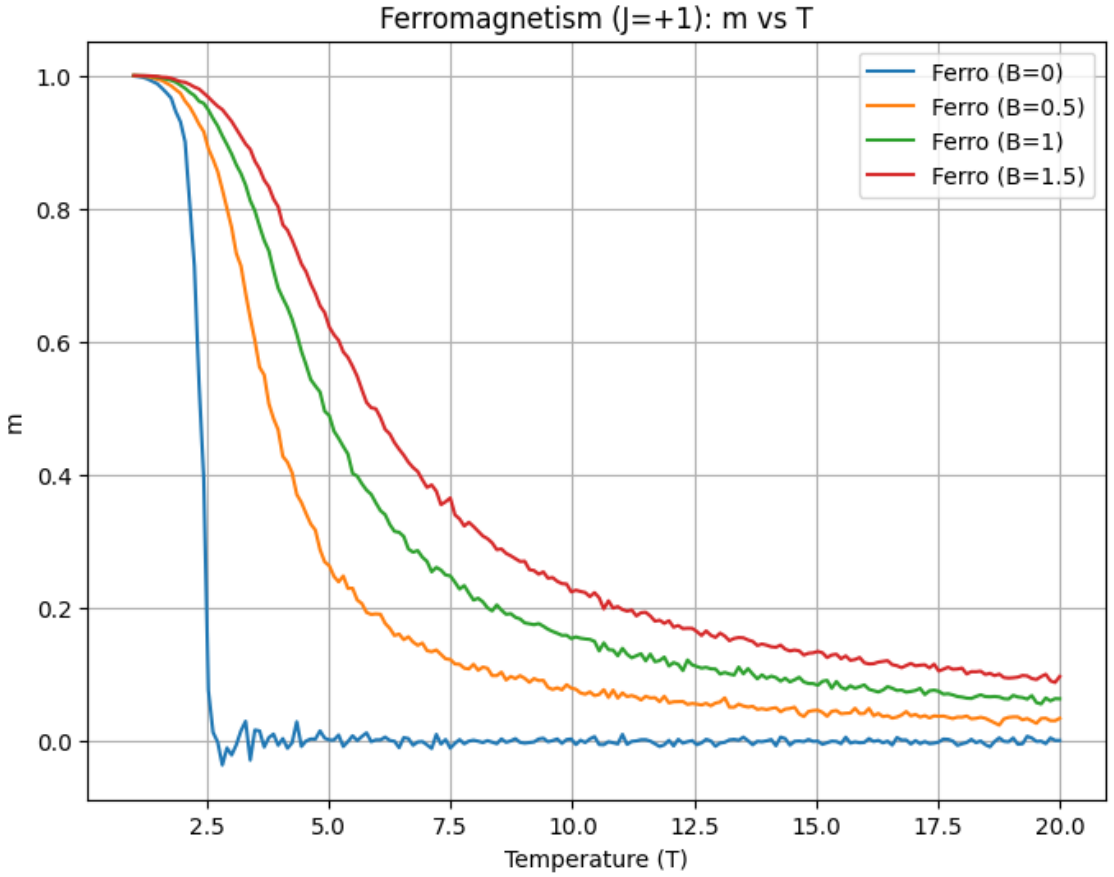

FIG. 1. Ferromagnetism ($J = +1$): Temperature dependence of magnetization m for $B = 0, 0.5, 1, 1.5$.

In contrast, when the system is initialized with a checkerboard pattern (via the built-in function for generating a control matrix), the misalignment n is computed. Figure 2 shows

that n remains low over the entire temperature range, as expected, because a ferromagnetic system does not naturally support a staggered order. The near-zero values of n corroborate the strong alignment of spins, regardless of the external field.

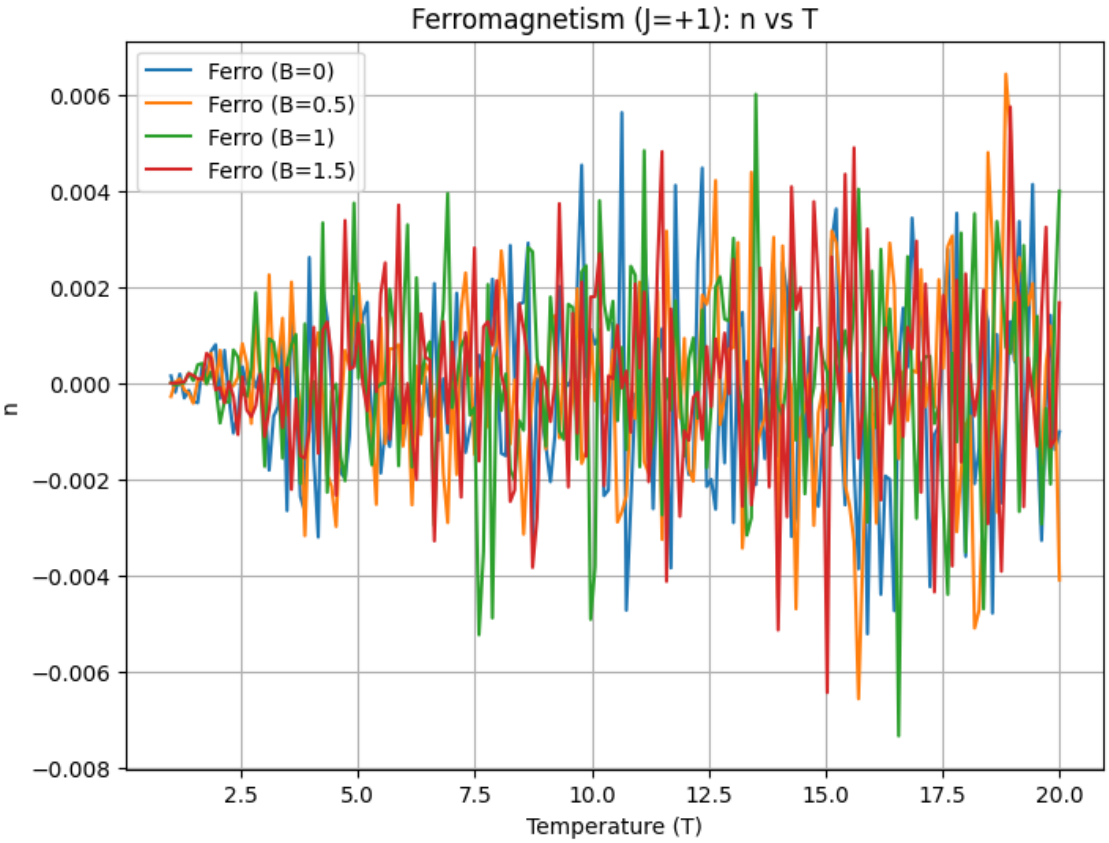

FIG. 2. Ferromagnetism ($J = +1$): Temperature dependence of misalignment n for $B = 0, 0.5, 1, 1.5$.

B. Antiferromagnetic Case ($J = -1$)

For the antiferromagnetic scenario, the system is initialized with a checkerboard configuration to reflect the ground state of antiparallel spin alignment. Figure 3 presents the staggered magnetization n as a function of temperature. At low temperatures, n is close to 1, indicating a nearly perfect checkerboard ordering. As the temperature rises, the influence of thermal fluctuations disrupts this order, leading to a decrease in n. Furthermore, an external magnetic field accelerates this decay, as it competes with the natural antiferromagnetic ordering.

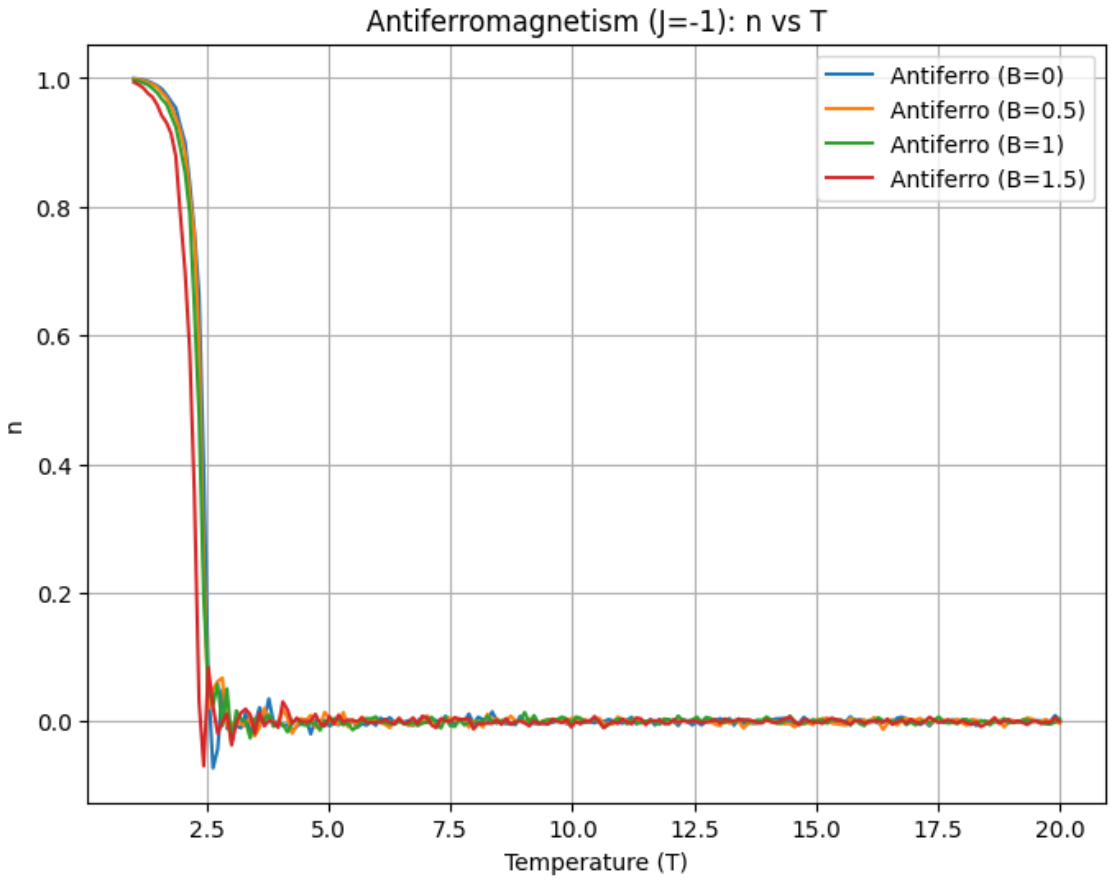

FIG. 3. Antiferromagnetism ($J = -1$): Temperature dependence of misalignment n for $B = 0, 0.5, 1, 1.5$.

In addition, when the antiferromagnetic simulation starts from a uniform state, the computed magnetization m (see Figure 4) initially exhibits non-zero values. However, as the simulation progresses and the system tends towards an alternating pattern, m decreases toward zero. This behavior demonstrates that while the external field tends to align the spins (thereby increasing m), the intrinsic antiferromagnetic interactions (due to $J = -1$) favor a zero net magnetization.

C. Discussion

The simulation results highlight several key physical insights:

- **Phase Transition:** In ferromagnetic systems, a sharp decline in m as T increases indicates a phase transition from an ordered to a disordered state. This is characteristic

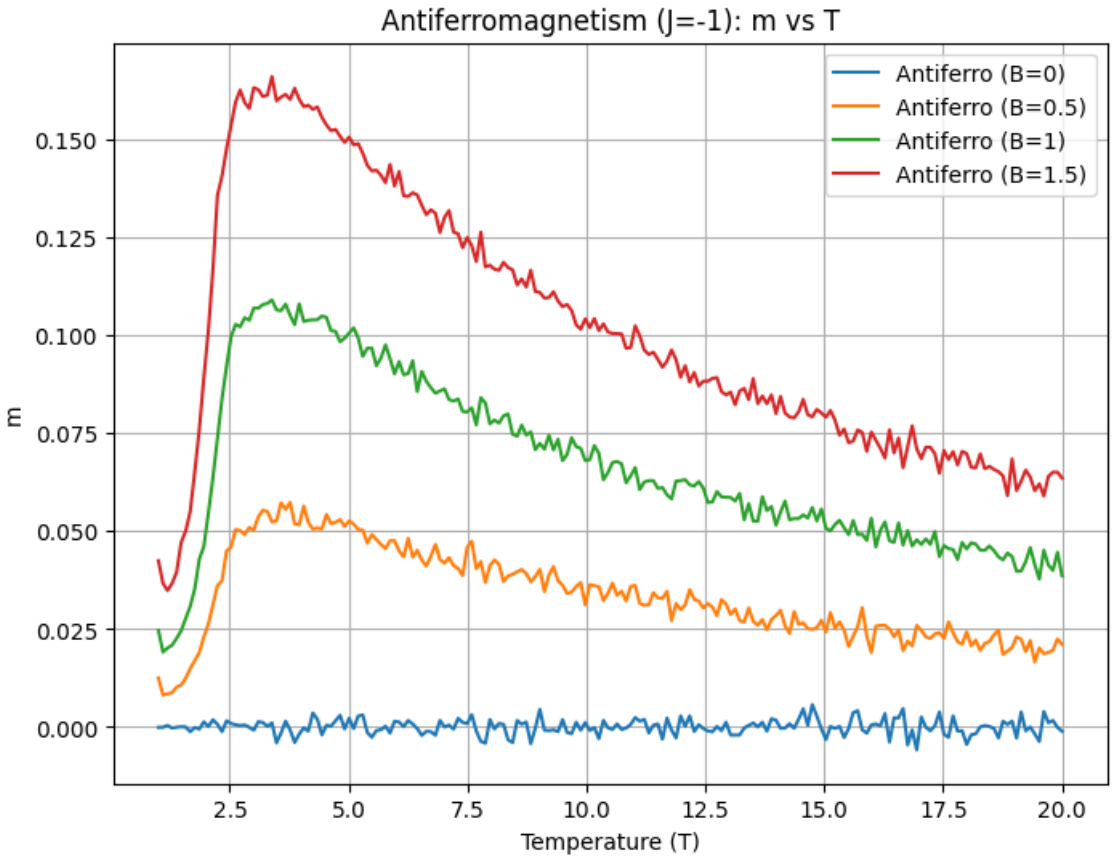

FIG. 4. Antiferromagnetism ($J = -1$): Temperature dependence of magnetization m for $B = 0, 0.5, 1, 1.5$.

of the Ising model, where a critical temperature T_c marks the onset of spontaneous magnetization loss.

- **Role of External Field:** An increasing external field B tends to stabilize the ordered phase by energetically favoring aligned spins. This effect is visible in both ferromagnetic and antiferromagnetic simulations, although the influence is more pronounced in ferromagnetic systems.

- **Order Parameters:** The use of distinct order parameters m and n is crucial for differentiating between ferromagnetic and antiferromagnetic order. While m effectively captures the uniform alignment in ferromagnets, n quantifies the alternating pattern inherent to antiferromagnets.

- **Sharp Transition at $T = 0$:** It should be noted that in antiferromagnetic systems,

the m vs. T plot, and in ferromagnetic systems, the n vs. T plot, do not exhibit a sharp transition from values near 1 to 0 as $T \to 0$. This is because these order parameters are not the most appropriate measures of ordering for their respective systems. In antiferromagnets, the staggered magnetization n is the correct order parameter, and in ferromagnets, the uniform magnetization m captures the phase transition more clearly. Using the non-ideal order parameter tends to smooth out the transition, leading to a gradual change rather than a sharp drop.

- **Computational Efficiency:** The implementation leverages the `numba` library to accelerate the Metropolis sweeps. By compiling the critical update routines to machine code, the simulation runs significantly faster, enabling the exploration of large parameter spaces (e.g., extensive temperature ranges and multiple field strengths).

The mathematical formulation of the Metropolis acceptance criterion (Equation 4) and the definitions of m and n (Equations 2 and 3) provide a rigorous framework for understanding the system's behavior. The observed trends in the simulation not only validate theoretical predictions but also demonstrate the impact of thermal fluctuations and external perturbations on magnetic order.

III. CONCLUSION

In this study, we implemented a Monte Carlo simulation of the two-dimensional Ising model to investigate both ferromagnetic ($J = +1$) and antiferromagnetic ($J = -1$) phases under varying temperatures and external magnetic fields. Our simulations show that:

- Ferromagnetic systems maintain high magnetization m at low temperatures, with a rapid decline near the critical temperature. The external magnetic field reinforces the aligned state, delaying the onset of disorder.

- Antiferromagnetic systems exhibit high staggered magnetization n at low temperatures, indicative of the checkerboard order. As temperature increases, thermal agitation disrupts this order, leading to a decrease in n; external fields further destabilize the antiferromagnetic arrangement.

- The distinct behaviors of m and n underscore the necessity of employing appropriate order parameters when studying different magnetic interactions. In particular, the lack of a sharp transition in the antiferromagnetic m vs. T plot and the ferromagnetic n vs. T plot highlights that these parameters do not accurately capture the ordering phenomena in their respective systems.

- The use of `numba` for JIT compilation significantly improves computational performance, making it feasible to perform extensive simulations on large lattices.

Overall, the simulation results confirm the theoretical predictions of the Ising model and provide insight into the complex interplay between temperature, external fields, and magnetic ordering. These findings contribute to a deeper understanding of phase transitions in magnetic systems and demonstrate the efficacy of computational methods in studying complex physical phenomena.
