2024 OPhO Experimental Exam: Ising Model of Ferromagnetism

August 30 - September 1

Introduction

Paramagnetic materials have atoms with permanent magnetic dipoles, but point in random directions unless aligned by an external magnetic field. On the other hand, magnetic dipoles in ferromagnetic materials align with neighboring dipoles and can have a significant magnetization even without an external field.

Iron is one common example of a material that is ferromagnetic at room temperature. Other materials undergo a phase transition, where they are paramagnetic at higher temperatures, but become ferromagnetic below a certain temperature (the Curie temperature, T_c).

In this experiment, we will use the Ising Model and a Monte Carlo simulation to compute and examine the properties of this phase transition.

The Ising Model is a simple approximation for ferromagnetism. We take a 2D lattice of atoms and assume that each dipole points either up ($s_i = 1$) or down ($s_i = -1$) along the same axis. Then we run the Monte Carlo simulation, which uses the following algorithm:

1. Start with a 2D grid of size $L \times L$, where each site represents a spin that can be either $+1$ or -1. The initial configuration is randomly assigned.

2. Energy Calculation: For each spin at position (i, j), calculate the change in energy (ΔE) if the spin is flipped. This is done by considering the interaction of the spin with its nearest neighbors. The energy change ΔE (in the absence of an external field) is given by:
$$\Delta E = 2J \times \text{spin} \times \left(\sum_{\text{neighbors}} \text{spin} \right)$$
where J is the interaction strength.

3. For each Monte Carlo step:
   - Randomly select a spin in the grid.
   - Calculate the energy change ΔE if this spin were to be flipped.
   - If $\Delta E < 0$, flip the spin.
   - If $\Delta E \geq 0$, flip the spin with probability $e^{-\Delta E/k_B T}$, where T is the temperature and k_B is the Boltzmann constant.

4. Repeat the spin-flipping process for a set number of steps, allowing the system to reach equilibrium.

5. The final configuration of the grid after the simulation, representing the state of the system at temperature T.

Phase Transition [25pts]

For the following questions, include the figure with uncertainty if applicable, your reasoning, and any graphs if used.

a) Find the value of T_c and explain what criteria you used. **[6pts]**

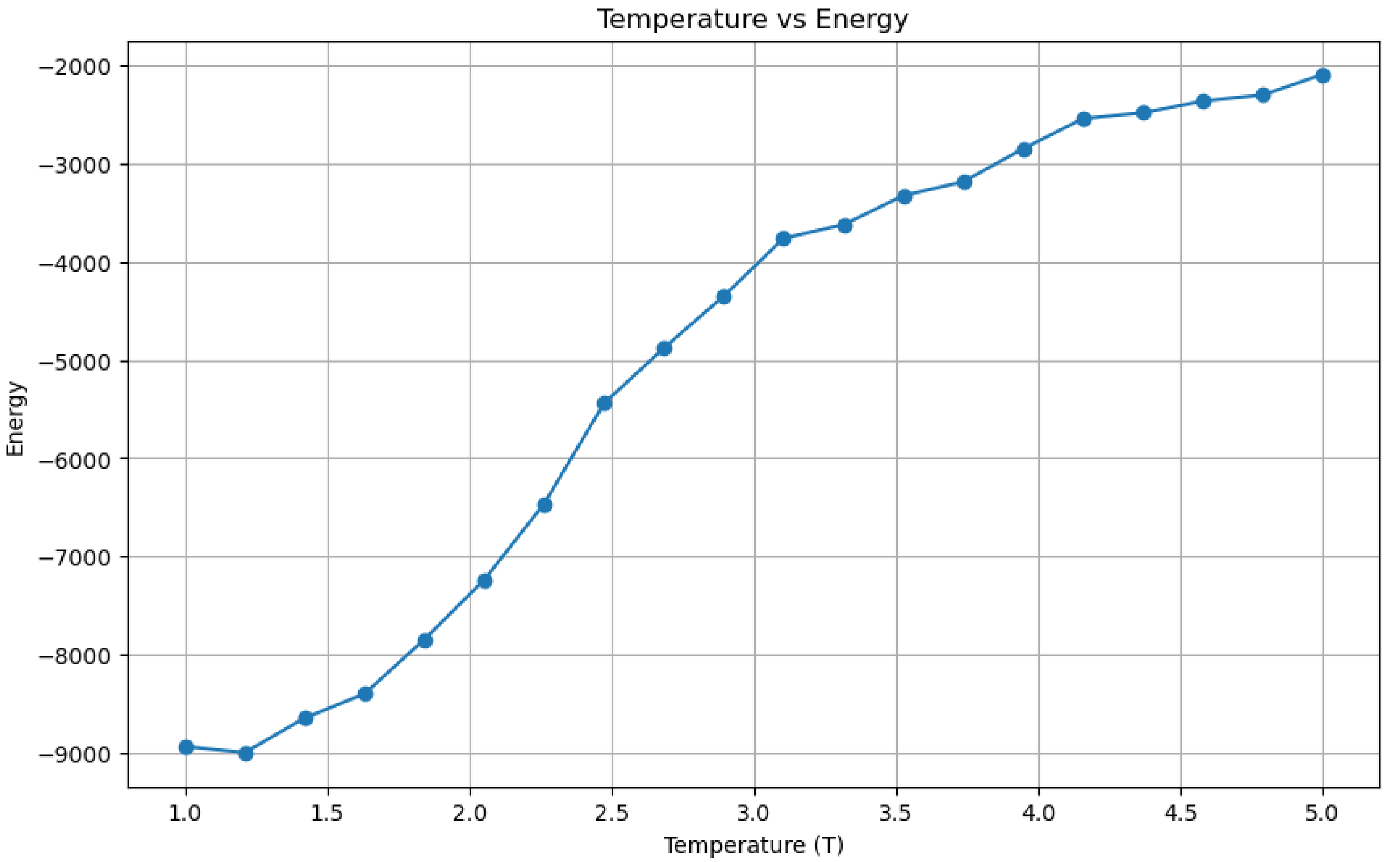
Solution Needs:

1. **[2pts]** Set $B = 0$, vary T and plot measures.
2. **[3pts]** Measures of switching from ferromagnetism to paramagnetism:
   (a) Transition of average magnetization oscillates between -1, 1 to tapering at 0.
   (b) Inflection point of absolute value of magnetization.
   (c) Transition between ~ 0 energy to increasing energy.
3. **[1pts]** Final Answer: $T_c \in [2.269 \pm 0.5]$ **AND** one of the above is scored.

b) Keeping the external magnetic field constant, plot the energy E of the system as a function of temperature. [4pts]

Solution Needs:

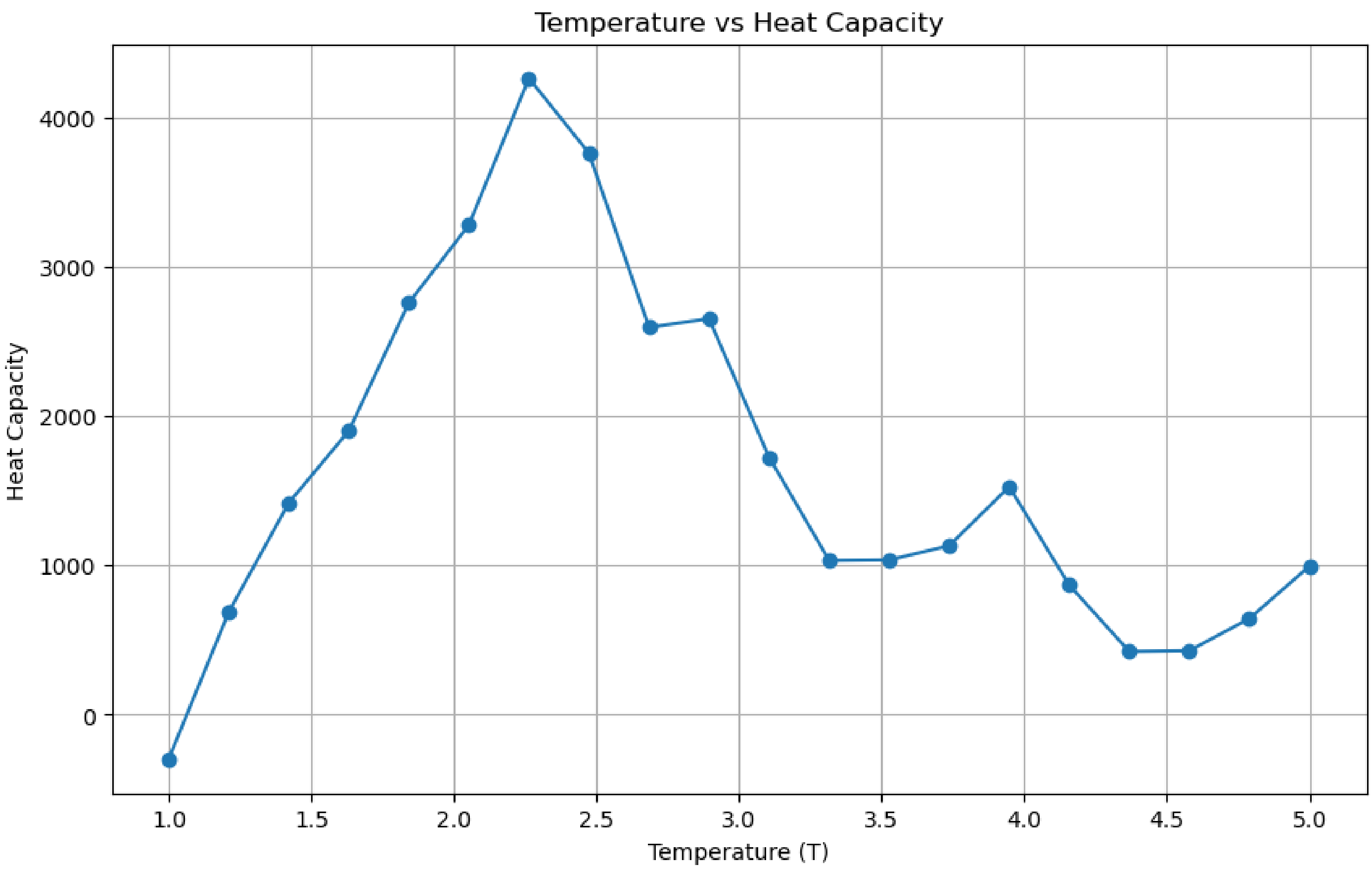
1. [1pts] Correct energy Hamiltonian.
2. [2pts] Write code/use method to calculate E.
3. [1pts] Plot T vs. E. Look smth like this:



c) Plot the heat capacity C of the system as a function of temperature. What are its maximum and minimum values? A phase transition is first order in temperature if the energy is discontinuous, second order if the energy is continuous but its first derivative is discontinuous, etc. What is the order of the phase transition here? **[5pts]**

Solution Needs:

1. **[1pts]** Note $C = \frac{\mathrm{d}E}{\mathrm{d}t}$.
2. **[3pts]** Write code/use method to calculate C and plot C vs. T. Look smth like this:



3. **[1pts]** Conclude 2nd Order Phase transition.

Consider the net magnetization $M = \mu \sum_{i=1}^{N} s_i$ of the system.

d) At temperatures slightly below T_c, M can be approximated as $M = \alpha|T_c - T|^\beta$. Find values for α and β. **[6pts]**

Solution Needs:

1. **[3pts]** Plot $\ln(M)$ vs. $\ln(|T_c - T|)$ or equivalent.
2. **[2pts]** Fit linear line either via code or fitting.
3. **[1pts]** Conclude $\beta \in (\frac{1}{8} \pm 0.05)$ **AND** equivalent steps to above were followed.

e) Set $T = T_c$. Plot how the net magnetization reacts as B is varied. Qualitatively, what do you observe? What happens if $T < T_c$? **[4pts]**

Solution Needs:

1. **[2pts]** Plot M vs. B and make observation.
2. **[2pts]** Plot M vs. B varying both T, B. Observations may vary.