Read the general-instructions page before beginning this problem.

Historical introduction

The Ising model is an important model of magnetic phenomena in materials. Proposed by Wilhelm Lenz in 1920, it was solved completely in one dimension by Ernst Ising in 1925. For discrete spins arranged in a given geometry in any dimension, the system energy is described by pair interactions between spins, which have only two possible orientations, and each spin's interaction with an external magnetic field. Ising's solution did not predict the phase transition by which a ferromagnet becomes paramagnetic above a critical temperature. This appeared only in 1944, when Lars Onsager solved the two-dimensional model without magnetic fields. The model therefore studies material properties near a phase transition, such as magnetization and heat capacity. Its simplicity and success have also led to applications in other phenomena where pair interactions produce collective effects.

Ising model

This experiment explores simulations of a two-dimensional Ising model on an $N \times N$ square lattice. Each cell contains a spin representing a magnetic moment pointing up or down, with value $+1$ or -1 respectively. Each spin interacts only with the applied external magnetic field and its nearest neighbours: four neighbours on the square lattice. We impose periodic boundary conditions, so each boundary spin interacts with the spin on the opposite boundary [1].

Materials in an external magnetic field include two groups: paramagnets and ferromagnets. Both have spins aligning with the field, but only ferromagnets can retain magnetization after it is removed. Only ferromagnets have significant spin interactions forming magnetic domains; the Ising model represents paramagnets by neglecting the neighbour-interaction term. Temperature disrupts order. Above a critical temperature, a ferromagnetic system behaves as a paramagnet.

About the simulator

The OIbF 2021 academic committee created a spin simulator at `https://app.graxaim.org/oibf/2021/page/slsim_r/1?title=` . It runs in the web browser of a computer, smartphone or tablet. This section introduces its parameters for simulating paramagnets and ferromagnets on a two-dimensional Ising lattice. The program is called SLSIM (`Spin Lattice Simulator`); its interface appears in Figure 1.

The interface has the following fields of interest:

A) System type: choose a paramagnetic or ferromagnetic material.

B) Initial state: choose random, all spins up (up), or all spins down (down).

C) Size: select the lattice size. Only an integer N is accepted.

D) Reinitialize button: clears the previous realization and resets the system. Use it whenever changing the spin-lattice size.

[1] Applies to both top/bottom and left/right boundaries.

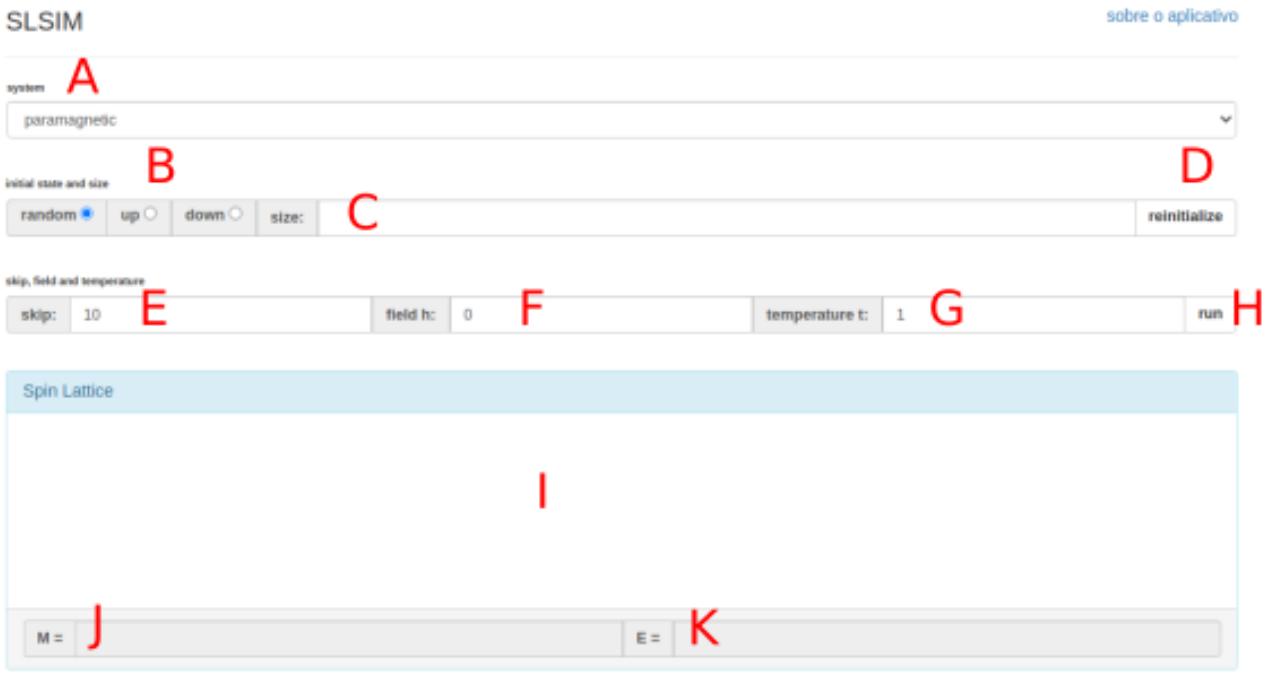


Figure 1: Interface of the square-spin-lattice simulator.

E) skip field: the system's time parameter, always an integer. When skip $= T$, the simulator attempts TN^2 spin flips. This avoids repeatedly pressing run to approach equilibrium.

F) Field H: a dimensionless magnetic-field-strength parameter, taking positive or negative real values. Positive values correspond to the upward direction.

G) Temperature t: a dimensionless temperature parameter, taking positive real values.

H) run button: attempts spin flips according to the interface settings. Pressing run once with skip=10 is statistically equivalent to pressing it ten times with skip=1.

I) Display of the last simulated lattice: blue circles are up spins and red circles down spins.

J) Total lattice magnetization, in units of an electron's magnetic moment. It is the number of up spins N_+ minus down spins N_-: $M = N_+ - N_-$.

K) Total energy calculated from the last simulated spin configuration.

The square lattice has dimension $N \times N$. The square lattice ranges from 1×1 ($N^2 = 1$ cell) to 64×64 ($N^2 = 4096$ cells). Larger lattices require more computation time. Total magnetization M and energy E vary with lattice size, whereas magnetization per cell $m = M/N^2$ and energy per cell $e = E/N^2$ are size-independent.

Repeated runs with the same parameters give spin configurations fluctuating about a mean, because the simulation is stochastic. As an example, consider the total magnetization M of a 64×64 lattice in field $2H_0$ at temperature

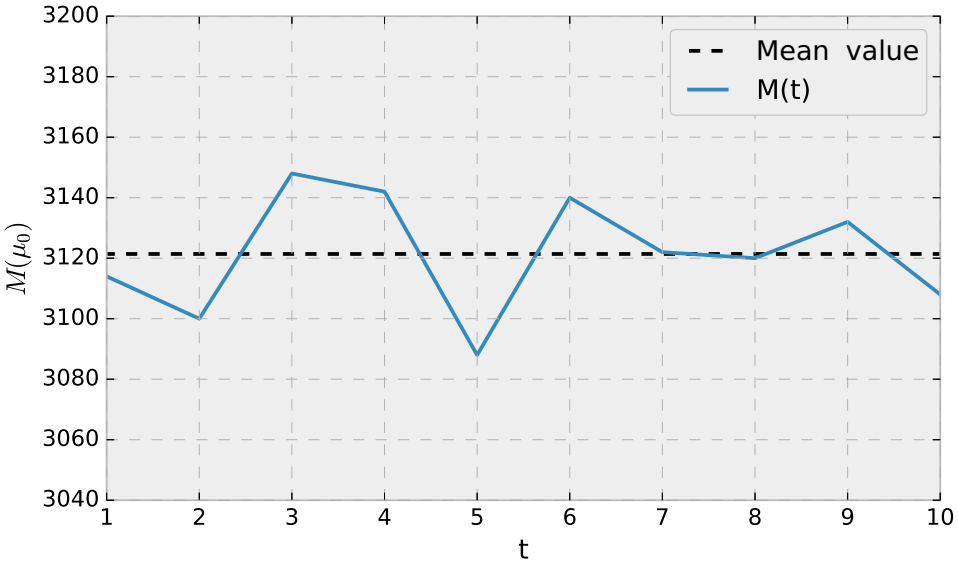


Figure 2: Magnetization of a 64×64 lattice in field $2H_0$ and temperature $T = 2T_0$ for different realizations (solid line). The dashed line is the mean of ten runs.

$T = 2T_0$ for different realizations, as in Figure 2. Use the spread between runs to estimate measurement uncertainty.

Notice: every requested measurement must use **at least ten runs**. **Always report the mean with its estimated uncertainty.** All later experimental results require an error estimate, except A1 and B of part 2, where error analysis is unnecessary.

Study of paramagnetic materials (7 points)

Part A — free spins (2,0 points)

First study spins in an ideal paramagnet without a magnetic field H. Each spin then has a 50% probability of pointing up or down.

Magnetization M is the difference between up-spin number N_+ and down-spin number N_-. Since it depends on lattice size $N \times N$, study magnetization per cell $m = M/N^2$.

Whenever a measurement is requested, report its mean and estimated uncertainty.

A.1 Run the system several times and examine total magnetization M. Is it always zero? Briefly discuss your observations. 0,5pt

A.2 Measure m for the paramagnet without magnetic field. Tabulate individual runs, the mean and estimated uncertainty. 1,0pt

A.3 Investigate how the measurement uncertainty changes as system size $N \times N$ increases. 0,5pt

Part B — determining magnetic susceptibility (5,0 points)

In a linear system the material's magnetic susceptibility χ_m^0 is defined by

$$\vec{M} = \chi_m^0 \vec{H}. \tag{1}$$

Real materials do not always obey this linear relation. Define a differential magnetic susceptibility $\chi_m(H)$ in such cases as

$$\chi_m(H) = \lim_{\Delta H \to 0} \frac{\Delta M}{\Delta H}, \tag{2}$$

Geometrically this is the slope of the tangent to M (or m) plotted against H.

B.1 Plot magnetization per cell m against applied field H at temperature $t = 2$. Use at least ten different field values, lattice 15×15 and $skip = 20$. 2,5pt

B.2 Under what conditions may the paramagnet be treated as linear? 0,5pt

B.3 Determine χ_m^0 at zero field ($H = 0$) and temperature $t = 2$. 2,0pt

Study of ferromagnetic materials (13 points)

To model a ferromagnet include interactions between nearby spins. Here only immediate neighbours interact: each spin interacts with its four neighbours on the square lattice. The simulator performs the calculations.

Part C — effect of temperature on magnetization (5,0 points)

C.1 Start with all spins up and temperature $t = 0,1$. Evolve the system and verify that magnetization persists even at zero field. Describe the procedure and data supporting your conclusion. Use lattice 16×16 and $skip = 10$. 0,5pt

C.2 Evolve the system while slowly increasing temperature, with fixed field $h = 0,5$ and all spins initially up. Does the material always retain the permanent magnetization observed at $t = 1,8$? Discuss. Use lattice 16×16 and $skip = 1000$. 1,0pt

C.3 Use a paramagnet with the final settings from the preceding part. Record temperature and measure magnetization M and total energy E, keeping the same lattice size, skip, external field and temperature. 1,5pt

C.4 Changing the previous system from paramagnetic to ferromagnetic automatically recalculates energy including neighbouring-spin interactions. Give the interaction contribution E_{in} and external-field contribution E_{ext} to the total energy measured above, with uncertainties. 2,0pt

Part D — magnetic hysteresis (3,0 points)

Magnetic materials often exhibit hysteresis. This explains why magnetization induced in materials such as iron by strong fields persists after the fields are removed.

A unique relation between field H and magnetization M cannot then be established. Instantaneous $M(t)$ depends on both $H(t)$ and previous values $H(t')$ for $t' < t$. Figure 3 gives an experimental hysteresis curve.

At point 1 most spins point up; at point 2 most point down.

Magnetization $M_{12}(H)$ along $1 \to 2$ differs from $M_{21}(H)$ along $2 \to 1$, as shown. Other (H, M) pairs result from different time-dependent fields $H(t)$.

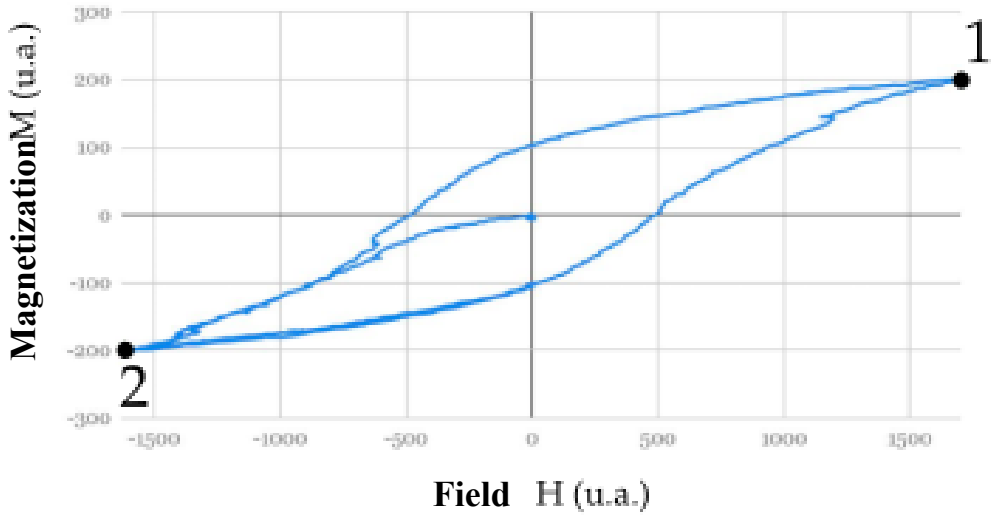


Figure 3: An experimental $M \times H$ hysteresis curve. Axes use arbitrary units. Points 1 and 2 are saturation regions with most spins up and down respectively.

D.1 Plot m against H for hysteresis path $1 \to 2 \to 1$ at temperature $t = 0,5$. Vary the field as appropriate. Use lattice 16×16 and $skip = 1500$. A rectangular curve, unlike the example, is acceptable. 3,0pt

Part E — phase transitions (5,0 points)

Investigate the system's phase transition. Theoretically this Ising model has a *second-order* transition, with abrupt changes in quantities including magnetization, susceptibility and heat capacity. Such abruptness occurs only in infinite systems; our finite system has a more gradual transition.

Like familiar transitions such as water freezing, it is described by a critical temperature t_C. For water–ice at normal pressure, $t_C = 0°\text{C}$. A transition is already suggested by comparing low and high t: at low t almost all spins align; at high t their directions are distributed approximately uniformly.

Find the Ising critical temperature by measuring magnetization against temperature at zero field, $H = 0$.

Below t_C the model is *order*ed, with most spins aligned; above t_C it is *disorder*ed and spins take either direction. Observe this in the simulated lattice or in the magnitude of magnetization per cell, $|m(t)|$.

Use $N = 20$ and $skip = 5000$ in this section.

E.1 From the qualitative descriptions of order and disorder, find $t_{\min}$ and $t_{\max}$ satisfying $t_{\min} \leq t_C \leq t_{\max}$ and $t_{\max} - t_{\min} \leq 1$. 1,5pt

Within that temperature interval, analyse magnetization

per cell more precisely.

E.2 Plot $|m(t)|$ against temperature from $t_{\min}$ to $t_{\max}$. 2,5pt

In an infinite system, critical temperature t_C is the lowest temperature t at which $|m(t)| = 0$. Here, as the preceding graph shows, the magnitude of magnetization per cell never reaches 0. Therefore, define the critical temperature in the finite system as the temperature t where the graph of $|m(t)|$ changes concavity.

E.3 Using this discussion, estimate critical temperature t_C. 1,0pt