COMPUTATIONAL METHODS
TERM PROJECT

MONTE CARLO SIMULATION OF 2D-MAGNETIC MATERIALS

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INTRODUCTION

Classical mechanics, a completely deterministic theory, provides second order PDEs in state space or first order PDEs in phase space. For deterministic prediction of time evolution of an N particle system in 3D space, a total of 6N PDEs(Hamilton's equations of motion) will be needed. While studying the properties and associated phenomena of different materials, no matter how simplistic the constructed Hamiltonian is, 6N PDEs are still required. In most cases, these can't be solved analytically. A vast library of numerical schemes for solving PDEs exists but to characterize the experimentally observed emergent phenomena, a large number of particles are needed to be considered and that makes it hugely compute and memory intensive to be numerically solved. Also the observed emergent phenomena like phase transition or variation of specific heat are portrayed by algebraically or statistically reduced physical quantities. These phenomena can't directly be shown by some unique phase space trajectory alone. With these problems as motivation, to study condensed matter systems where the *'more is different'* picture appears in its full glory, statistical mechanics is deployed. In this project, statistical mechanical study of 2D-ferromagnetic materials is done using 2 different models for the Hamiltonian- Ising and XY. The numerical scheme that will be used falls under the class of Monte Carlo schemes. Unlike numerical simulation of PDEs, where the states are computed at discrete times by re-formulating a calculus problem as an algebraic one; most Monte Carlo schemes, as a core feature, sample the state space based on probability distributions derived from statistical mechanical arguments. In this project, the Metropolis scheme, that works on the similar principle, was used to study the system in a range of temperatures.

CANONICAL ENSEMBLE AND THE METROPOLIS ALGORITHM

Consider a system with a large number of particles(thermodynamic limit) in thermal equilibrium with an energy reservoir at a temperature T. If μ is the phase space vector(called the microstate) of the system and $H(\mu)$ is the Hamiltonian function then the probability(or probability density in case the microstates form a continuous space) that the system equilibriates at the microstate μ is[Kar07b]:

$$p_T(\mu) = \frac{e^{-\beta H(\mu)}}{Z(T)} \tag{1}$$

Where β is $1/k_B T$ and $Z(T)$, the partition function is written as the normalization factor:

$$Z(T) = \sum_{\mu} e^{-\beta H(\mu)} \tag{2}$$

The analytic form for $Z(T)$ would provide us with all the statistically derived quantities and associated phenomena, but in most cases this is not derivable. To numerically compute $Z(T)$, a naive way would be to randomly sample(uniformly distributed) a large number of microstates and compute $Z(T)$(knowing that generating the set of all possible microstates isn't feasible since it grows exponentially with the size of the system). This method would provide $Z(T)$ up to a good approximation but only at sufficiently high temperatures(low values of β). At moderate or low temperatures, the distribution of Eq(1) is fairly exponential and a uniform sampling would throw μ's that have negligible contribution to $Z(T)$. A way out from this is to work with relative probabilities rather than absolute ones to eliminate the use of $Z(T)$. And this is the seed to the Metropolis algorithm. To develop the physical intuition behind the algorithm, consider a system in contact with a reservoir while being initial at any random state. Now the variables of the state keep changing with time due to their conjugate momenta, just like thermal motion of atoms, spin flips or rotation in materials, transitions between atomic or molecular states etc. So it is reasonable to model time evolution of states as a Markov Chain. Labeling the discrete microstates with i, P_i their associated probability and $W_{i\rightarrow j}$ as the transition probability from state i to state j, we get the master equation[Sta06]:

$$\frac{\mathrm{d}P_i}{\mathrm{d}t} = \sum_{j\neq i} (W_{j\rightarrow i} P_j - W_{i\rightarrow j} P_i) \tag{3}$$

Now any random initial state is possible for the system to equilibriate to in the canonical ensemble. Its probability will be given by Eq(1). So if the Markov chain is in equilibrium, the condition of detailed balance holds:

$$W_{j\rightarrow i} P_j = W_{i\rightarrow j} P_i \tag{4}$$

If start with any initial random state(system's equilibrium state) then the ratio of transition probabilities after using Eq(1) becomes:

$$\frac{W_{i\rightarrow j}}{W_{j\rightarrow i}} = e^{-\beta(E_j - E_i)} \tag{5}$$

This roughly translates to the probability of transition $i \rightarrow j$ and it can be used for the numerical generation of Markov chain of states using the following algorithm:

1. Randomly initialize a state
2. Choose a state variable
3. Change its value by a random amount from a chosen set
4. Calculate the change in energy associated to that change ΔE
5. If $\Delta E < 0$ then execute the change, otherwise execute it with a probability of $e^{-\beta \Delta E}$
6. repeat the procedure with another state variable

By the construct of the algorithm, the chain will converge towards states with lesser energy while the disorder will be tuned by β, since for lesser values of β, the probability for a change in state variable is higher. Iterating the algorithm steps 2 to 6 for a sufficient number of times, we converge towards the most probable equilibrium state according to Eq(1).

ISING MODEL

Consider a 2D grid of spin-1/2 particles with the spin-exchange interaction according to the Heisenberg Model:

$$H = -2J \sum_{<ij>} \mathbf{S_i} \cdot \mathbf{S_j} \tag{6}$$

Where J is the exchange integral and **S** is the 2-spinor. In the simplification where the spinors are constrained to point either up or down, reliable in the case where a magnetic field is applied perpendicular to the 2D grid, we get the Hamiltonian:

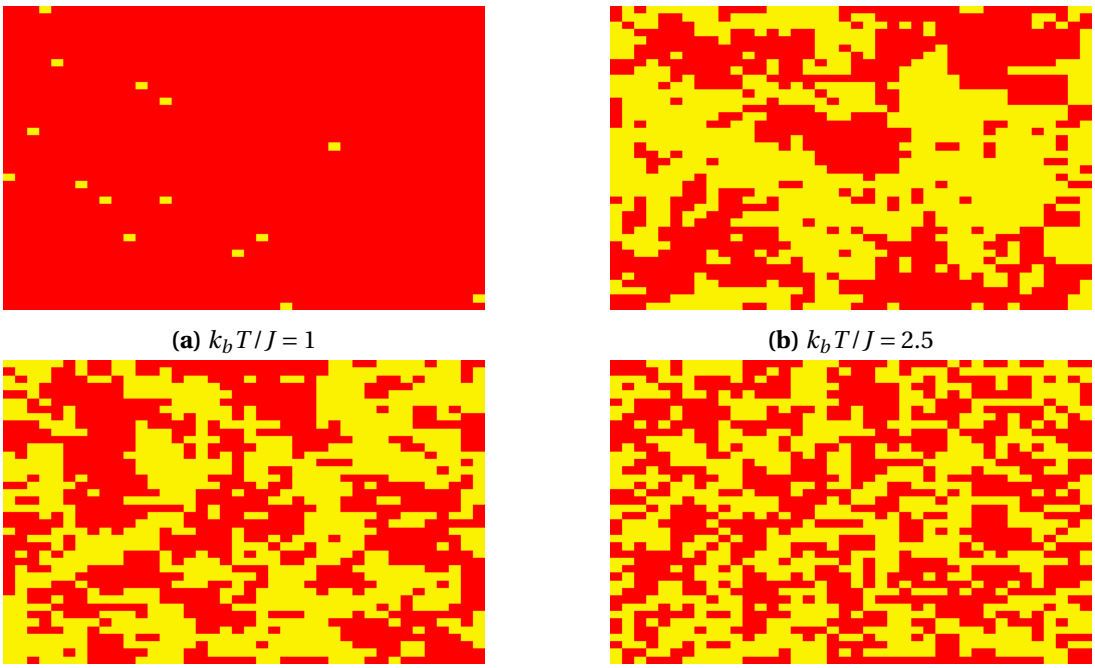
$$H = -J \sum_{<ij>} S_i S_j \tag{7}$$

Where S is 1 or -1 and $< i\, j >$ means the set of neighbouring particles. This is the 2D Ising model. For ferromagnetic materials $J > 0$ and hence the neighbouring particles are statistically preferred to be aligned in the same direction because that reduces the energy. To simulate the Ising model using Metropolis algorithm we make the following substitutions to it:

1. Randomly initialize a N×N matrix-S with values 1 and -1.

2. For every element compute $\Delta E = 2J\sum_{<ij>} S_i S_j$ including periodic boundary conditions
3. If $\Delta E < 0$ then flip the spin at the index, else flip it with the probability $e^{-\beta\Delta E}$

Simulating a 40×40 grid at different values of $k_B T/J$ i.e different temperatures we get the following equilibriums after 1000 iterations each:

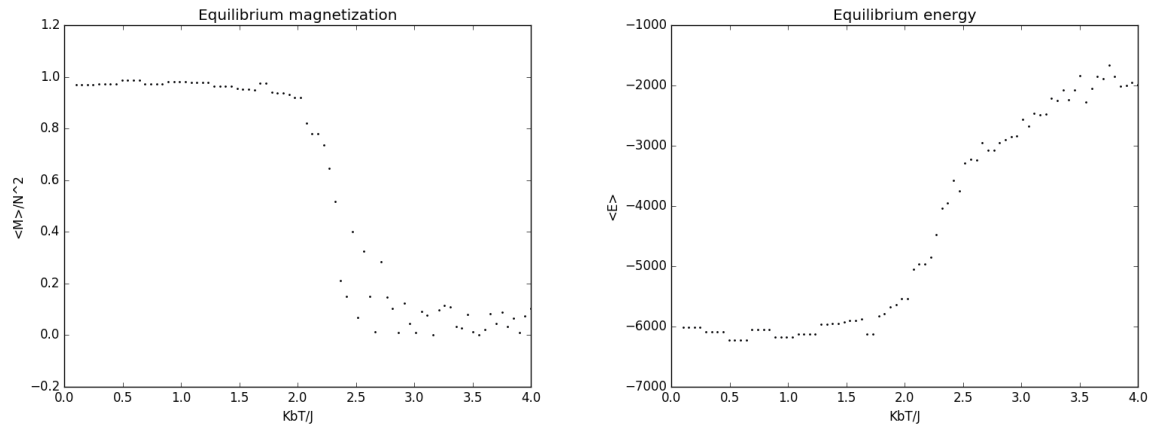


(a) $k_b T/J = 1$ **(b)** $k_b T/J = 2.5$

(c) $k_b T/J = 3$ **(d)** $k_b T/J = 5$

Figure 1: Equilibrium states of 2D-Ising model at different temperatures. Red pixels correspond to particles with spin up, though in no-field condition both are equivalent

From the results it can be seen that at low temperatures their is long range order in spin while the direction remains to be arbitrary. This shows that at low temperatures, when the Metropolis algorithm is run, transitions to higher energy states is negligibly favoured. In 1000 iterations, each particle is switched to a lower energy spin for about 500 times and the rest of the times it was left unchanged. This lead to a formation of domains of large sizes in the material and hence spontaneous magnetization is seen by ferromagnetic materials at low temperatures. As the temperature increases, so does the disorder and at higher temperatures the domains completely randomize with close to 0 net contribution to the magnetization. To study this transition in more detail, the simulation was ran for a larger set of temperatures, over paralleled cores(since 1000 iterations of 1600 particles is compute intensive) and the results obtained were as follows:



(a) Average Magnetization **(b)** Total energy

Figure 2: Order parameters' variation with temperature

A phase transition is observed in the result as predicted by analytical results(2D-Ising being one of the very few models to have analytical results). Relatively large variations in the order parameters is also seen in the higher temperatures which shall shrink is the number of iterations is increased considerably. Here parallel processing was used for simulation for different temperatures and that of different regions of the grid at the same temperature was avoided. This is because parallel generation of pseudo random numbers for separate spatial regions might induce unwanted long range correlations.

2D-XY Model

Again for a 2D grid of spin-1/2 particles if the spinors are constrained to lie in the plane of grid(conventionally xy plane), then the Hamiltonian following the Heisenberg model becomes:

$$H = -J \sum_{<ij>} cos(\theta_i - \theta_j) \tag{8}$$

And this substitutes in the algorithm as:

1. Randomly initialize a N×N matrix-S with values in range $(0, 2\pi)$
2. Choose an angle $\delta\theta$ in range $(-10°, 10°)$
3. For every element compute $\Delta E = 2J\sum_{<ij>} cos(\theta_i + \delta\theta - \theta_j)$including periodic boundary conditions

4. If $\Delta E < 0$ then change the spin at the index by $\delta\theta$, else change it with the probability $e^{-\beta\Delta E}$

Simulating a 30×30 grid at different temperatures, we get the spin configurations shown in Figure(3). Here we again observe that as the temperature increases, the spins tend to randomize and hence loosing spontaneous magnetization. Another feature that is prevalent in the 2D-XY model is that in low and moderate temperatures, the spins though misaligned, if we draw out integral curves considering the spins to represent a vector field, the curves tend to loop(which might be clear if we view the fields in a 2-Torus manifold since periodic boundary conditions have been imposed). These loops are called vortices and these are topologically stable configurations since the spins are parallelly aligned to the neighbouring ones and a threshold of energy is needed to break it. This unbinding of vortices is characterized by the Kosterlitz-Thoules transition[Kar07a]. Unlike the 2D-Ising model, there isn't any sharp phase-transition in magnetization observed. The following computed plot show this:

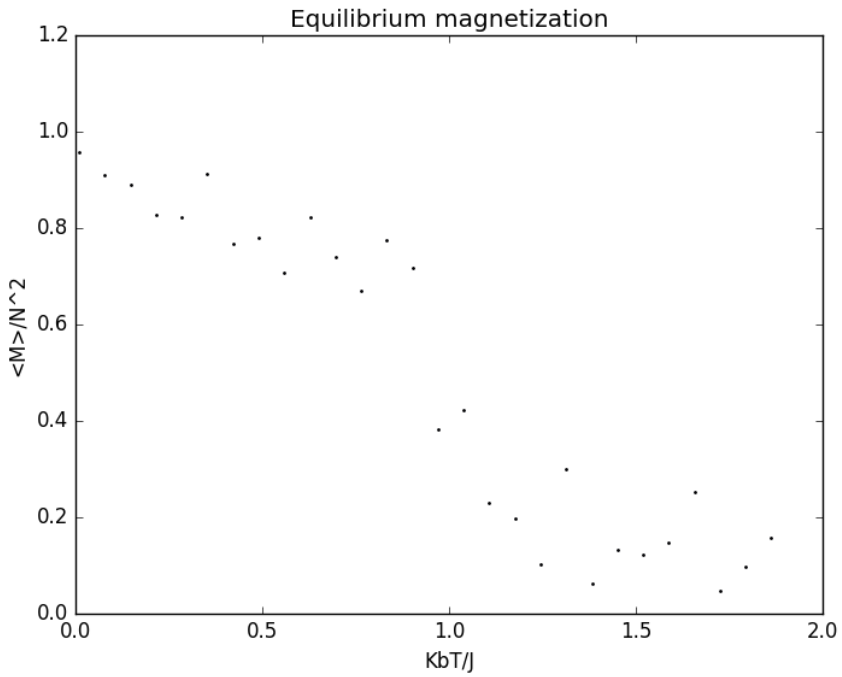
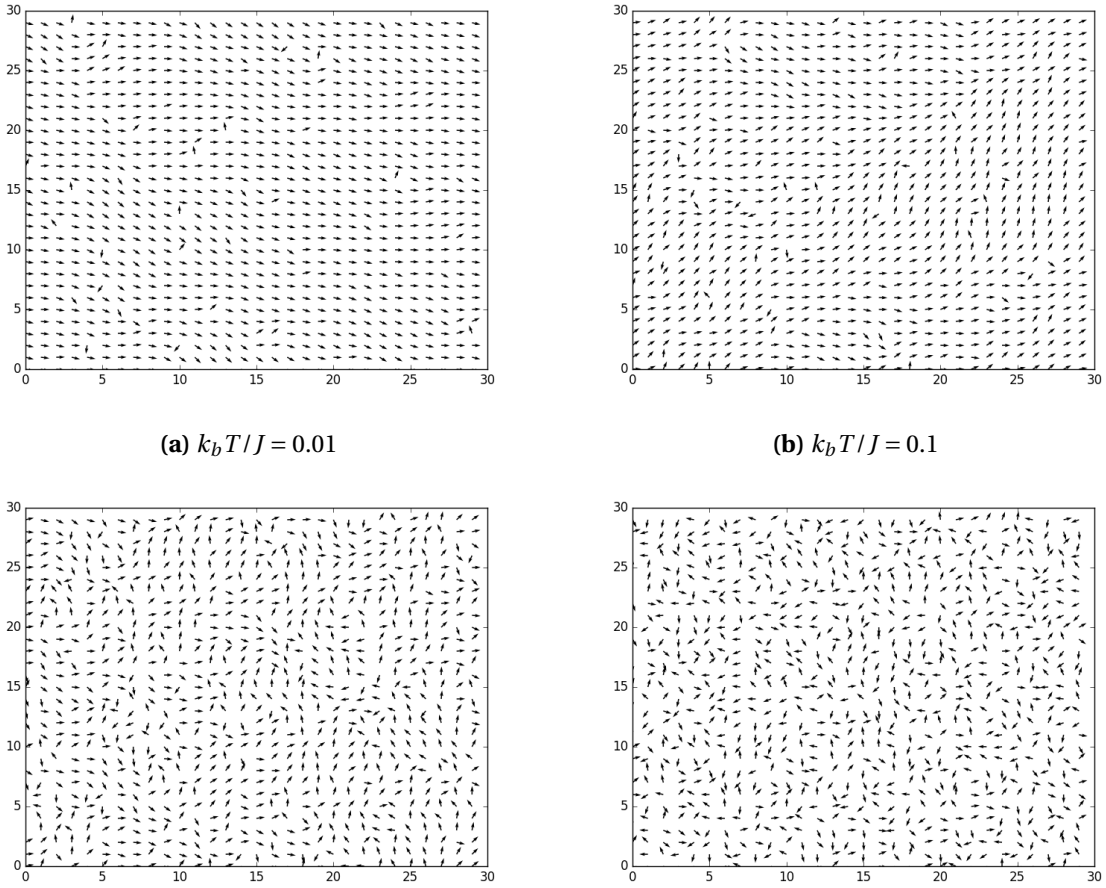


Figure 3: Change in magnetization with increasing temperature in 2D-XY model

For the same number of iteration, the variation in magnetization is more than 2D-Ising model because w.r.t a change $\delta\theta$ in any range like $(-10°, 10°)$, the Hamiltonian gets multiple local minimas and this adds an extra layer of disorder.



(a) $k_bT/J = 0.01$ **(b)** $k_bT/J = 0.1$

(c) $k_bT/J = 1$ **(d)** $k_bT/J = 2$

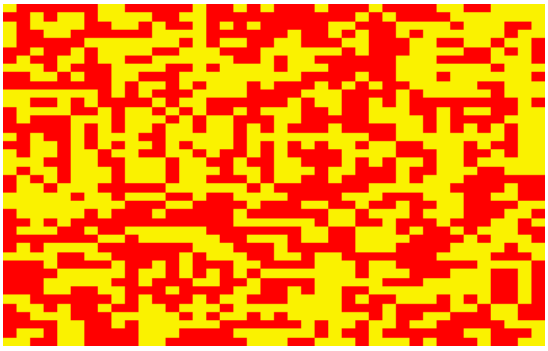
Figure 4: Equilibrium states of 2D-XY model at different temperatures.

PARAMAGNETISM

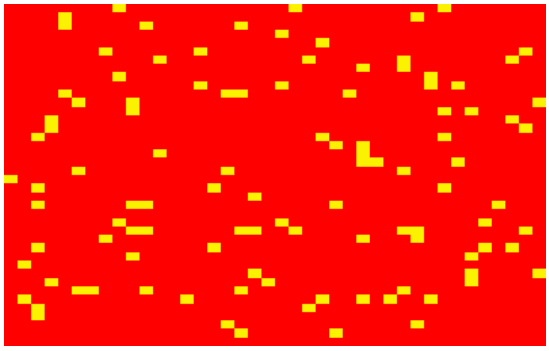
The phenomenon of paramagnetism can be explained using the same models used till now with a slight change in the Hamiltonian that now a quantity h proportional to the external magnetic field strength appears:

$$H = -hS_i - J \sum_{<ij>} S_i S_j \tag{9}$$

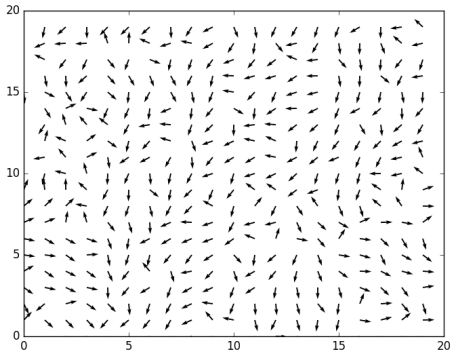
But what separates these materials from ferromagnets is the relatively very low value of J which results to J/k_BT attaining very low values at moderate temperatures leading to disorder and hence no significant spontaneous magnetisation. Following are the simulation of 2D-paramagnets(low value of J) in the presence and absence of field h at the same temperatures:



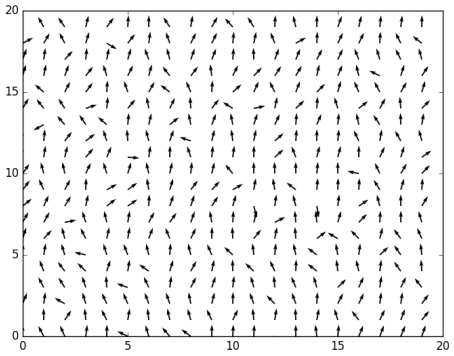
(a) 2D-Ising at no-field



(b) 2D-Ising with outward pointing field



(c) 2D-XY in no-field



(d) 2D-XY with upward pointing field

Figure 5: Paramagnetic materials attaining order, hence magnetization in the presence of external magnetic field

CONCLUSION

When the time evolution is described using deterministic PDEs, the numerical integration schemes can be used. Those methods can be deployed in systems of high dimensions but that would require large memory, long time horizon to reach the equilibrium and will be sensitive to time discretization. In contrast statistical mechanical description of the same systems provide a window to use Monte Carlo schemes like the Metropolis algorithm where the system can directly be studied feasibly in the equilibrium region while no explicit use of time discretization comes into the picture. Metropolis algorithm was used to successfully explain the phase transitions in ferromagnetic materials and also the induced magnetization in paramagnetic material using the 2D-Ising and XY model.

Bibliography

[Sta06] Dietrich Stauffer. *A Guide to Monte Carlo Simulations in Statistical Physics. By.* 2006.

[Kar07a] Mehran Kardar. *Statistical physics of fields.* Cambridge University Press, 2007.

[Kar07b] Mehran Kardar. *Statistical physics of particles.* Cambridge University Press, 2007.