Stochastic Dynamics and Phase Transitions: A Study of Random Walks and the Ising Model

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1 Introduction

This project will explore two important topics in statistical physics: the modeling of diffusion through random walks and the study of thermodynamic behavior using the 2D Ising model with the Metropolis algorithm. These models help us understand various complex phenomena, like particle motion and phase transitions.

2 Random walk

2.1 Theory

As always, a few theoretical concepts should be discussed, specifically the first and second of Fick's laws.

Fick's first law: Movement of particles from high to low concentration (diffusive flux) is directly proportional to the particle's concentration gradient.

$$J = -D\nabla\rho \tag{1}$$

Fick's second law: Describes how the concentration of particles evolves over time due to diffusion.

$$\frac{\partial\rho}{\partial t} = D\nabla^2\rho \tag{2}$$

where J the flux, ρ the concentration (or number density) and D the diffusion constant.

Fick's laws and the concept of random walk are connected through the statistical behavior of particles undergoing Brownian motion. On a microscopic level, particles take random steps in space, each independent of the last. Over many steps, the probability distribution of their positions approaches the solution of the diffusion equation.

The key quantity calculated in this exercise is the mean squared displacement $\langle R^2\rangle$ of a random walker, which grows linearly with time in a continuous limit (2D case):

$$\langle R^2\rangle = 4Dt \tag{3}$$

2.2 Implementation

Time to get a little more practical. The model I created simulates sequential steps of unit length in random directions on the XY plane (i.e., in 2D), with each step independent of the last. The particle starts at the origin and takes N steps, represented as:

$$(\Delta x_1, \Delta y_1), (\Delta x_2, \Delta y_2), (\Delta x_3, \Delta y_3), \ldots, (\Delta x_N, \Delta y_N)$$

It can be shown that the root-mean-square (RMS) distance from the origin after N steps is proportional to the square root of N:

$$R_{\text{rms}} = \sqrt{\langle R^2 \rangle} \approx \sqrt{N} \tag{4}$$

For 1000 steps and 10 trials, here are the steps taken:

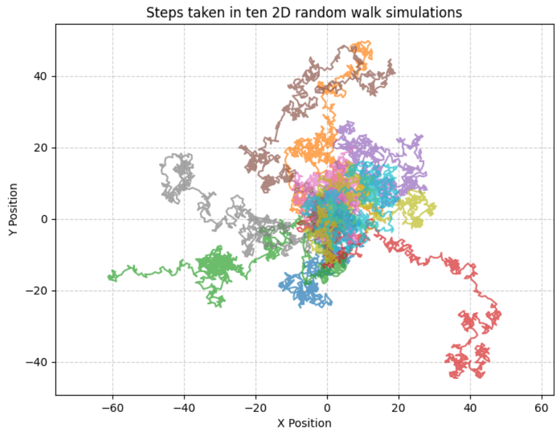

Figure 1: A thousand steps taken in ten 2D random walk simulations.

A few notes about this: the infinitesimal displacements have been normalized to ensure that each step has unit length. To calculate the root mean square (RMS) distance, the following equation was used:

$$R_{RMS}^2 = \langle R^2 \rangle = \frac{1}{M} \sum_{m=1}^{M} R_m^2 \tag{5}$$

This resulted in the following plot:

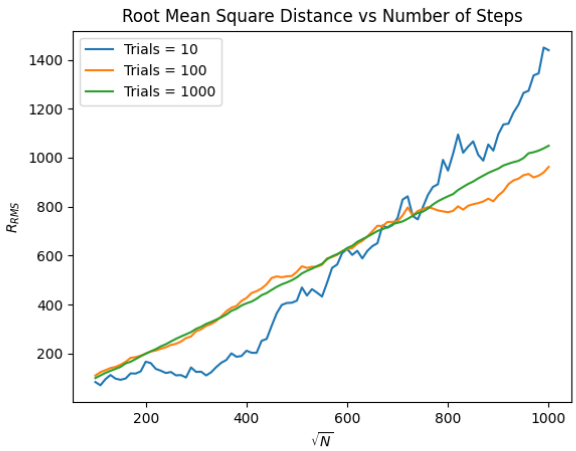

Figure 2: RMS distance from origin vs the $\sqrt{N}$ calculated from 10, 10^2 and 10^3 random walks.

As expected, the more trials we do, the smoother the curve becomes and the closer it follows the ideal linear trend. With just 10 trials, the curve fluctuates a lot, while with 1000 trials, it is nearly a straight line, confirming eq. 5.

3 The Ising Model

3.1 Theory

As in the previous section, I will begin by discussing a few key points about the Ising model.

From basic theory, we know that ferromagnetic materials can retain permanent magnetization even without an external field, as the spins tend to align and create a net magnetic moment. This magnetization weakens with increasing temperature and vanishes above the Curie Temperature (T_c), where the thermal fluctuations overcome the effects of the quantum mechanical exchange interaction.

I will focus on the 2D model, where spins are arranged on a $N \times N$ lattice and labeled as S_{ij}, with i and j denoting spatial indices. In the code, a single-index notation S_k will be used instead. Spins can be either **"up"** ($S_k = +1$) or **"down"** ($S_k = -1$) and the Hamiltonian is given by:

$$H = -\frac{1}{2} J \sum_a \sum_\beta S_a S_\beta - B \sum_a S_a \tag{6}$$

with J being the exchange constant and B the external magnetic field.

For information about the Metropolis algorithm, visit the wiki (Metropolis Algorithm).

The thermodynamic quantities that will be calculated are the following:

$$\langle E \rangle = \frac{1}{n_{tot}} \sum_{i=1,n_{tot}} H_i \tag{7}$$

$$c = \frac{\partial \langle E \rangle}{\partial T} = \frac{1}{k_B T^2} \left(\langle E^2 \rangle - \langle E \rangle^2 \right) = \frac{1}{k_B T^2} \,\mathrm{var}(E) \tag{8}$$

$$\langle M \rangle = \frac{1}{n_{\mathrm{tot}}} \sum_{i=1,n_{tot}} M_i, \quad M_i = \sum_k S_k \tag{9}$$

$$\chi = \frac{\partial \langle M \rangle}{\partial B} = \frac{1}{k_B T} \left(\langle M^2 \rangle - \langle M \rangle^2 \right) = \frac{1}{k_B T} \,\mathrm{var}(M) \tag{10}$$

Lastly, there is thermalization. Thermalization is the process by which a system evolves from an initial, often artificial, non-equilibrium state to thermal equilibrium, where physical observables stabilize. I will be using the "cold start", where all spins are initially aligned, requiring sufficient thermalization time before analysis.

A cold start begins from the ground state with all spins aligned, while a hot start begins with spins randomly arranged. Since the system is allowed to thermalize fully, the choice of initial condition should not affect the final results, so only the cold start is used.

3.2 Case 1: J = 1 and B = 0

The first case that I will study is the case of $J = 1$ (ferromagnetic) without an external magnetic field ($B = 0$). By running the Monte Carlo simulation, the results are the following:

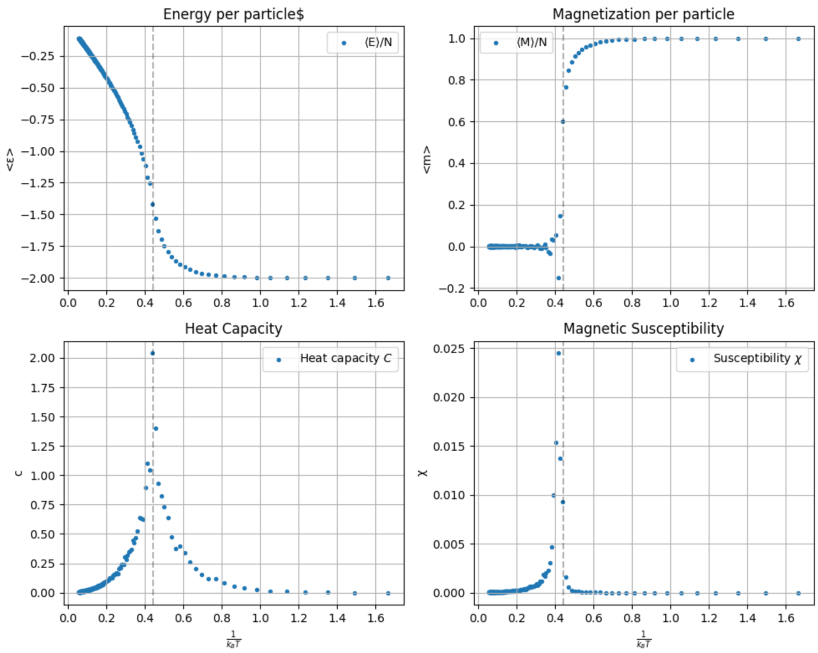

Figure 3: Plots of the thermodynamic quantities vs $\frac{1}{k_BT}$ for Case 1.

It is important to note that each plot is shown as a function of $\frac{1}{k_BT}$, rather than k_BT.

Starting with the energy plot: in general, as the temperature of a system increases, so does the energy. Since the plots are in terms of $\frac{1}{k_BT}$ (which decreases as temperature increases), the observed trend, energy decreasing with increasing $\frac{1}{k_BT}$, is consistent with our expectations.

For magnetization, at high temperatures (low $\frac{1}{k_BT}$), thermal fluctuations disrupt the alignment of magnetic moments (spins), leading to a disordered phase with no net magnetization. As the temperature decreases, thermal energy becomes insufficient to overcome spin interactions, and the spins begin to align, resulting in a nonzero magnetization.

The sudden spike near $\frac{1}{k_BT} \approx 0.4406$ (or $T \approx 2.269$) corresponds to the system reaching the Curie Temperature, which as described in the Theory section, spontaneous magnetization vanishes.

Using Onsager's exact solution, the Curie temperature for the 2D Ising model can be calculated as follows:"

$$\frac{J}{k_BT_C} = \frac{1}{2}ln(1+\sqrt{2}) \approx 0.4406868 \tag{11}$$

From the plots, the Curie Temperature can be estimated by locating the temperature corresponding to the peak of the heat capacity and magnetic susceptibility. As the system approaches T_C, the fluctuations in magnetization increase, causing the susceptibility peaks **sharply**, indicating the transition from ferromagnetic to a paramagnetic state. A similar behavior is expected in the heat capacity plot, for almost the same reasons.

The magnetic susceptibility plot shows a peak at $T_C = 2.417$, and the heat capacity one at $T_C = 2.227$, both of which are in great agreement with the theoretical value!

3.3 Case 2: J = 1 and B = 1

This is the second case where $J = 1$ (ferromagnetic) but with an external magnetic field ($B = 1$).
Again, by repeating the process:

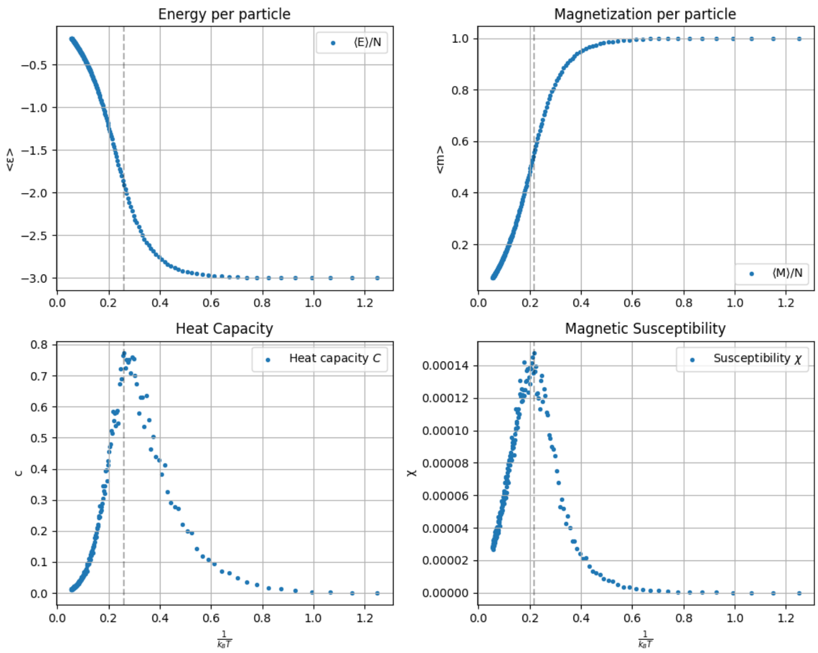

Figure 4: Plots of the thermodynamic quantities vs $\frac{1}{k_B T}$ for Case 2.

It is important to mention that with the presence of an external magnetic field, it breaks the spin-flip symmetry of the model, making it much more difficult to solve analytically, so no comparison to the value we could expect theoretically is given.

Starting with the energy plot again: the same tendency is observed as before, but this time the Curie Temperature appears to be higher than in the first case (again, I should highlight that the plot is in regard to $\frac{1}{k_B T}$). This shift in T_C is likely due to the external magnetic field, which favors the alignment of spins in its direction, lowering the system's energy compared to the $B = 0$ case. As expected, the system reaches a lower energy state due to this alignment.

Regarding magnetization, the same tendency is observed, but no other comments about it can be made.

As explained earlier, the Curie Temperature can only be determined numerically due to the presence of the external field. The magnetic susceptibility plot shows a peak at $T_C = 4.599$, and the heat capacity one at $T_C = 3.839$. This time the values appear to differ more than they did in the previous section

Additionally, compared to the results that we got for $B = 0$, regarding the heat capacity and the magnetic susceptibility plots, applying an external magnetic field to the ferromagnetic system smoothens and shifts the peaks in heat capacity and magnetic susceptibility to higher temperatures, suggesting a crossover from a sharp to a smoother phase transition.

3.4 Spin configuration plots for Case 1 and Case 2

These are the spin configuration maps for $J = 1$ $B = 0$ and $B = 1$:

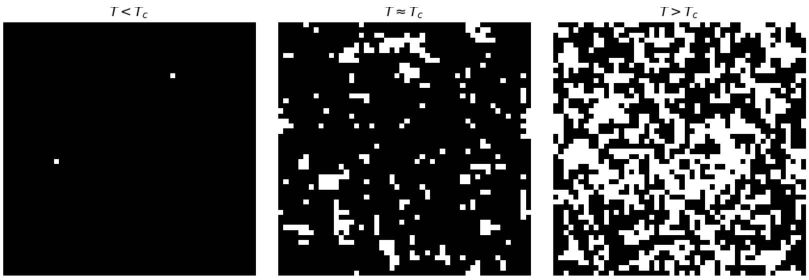

Figure 5: Spin configuration map for $J = 1$ $B = 0$.

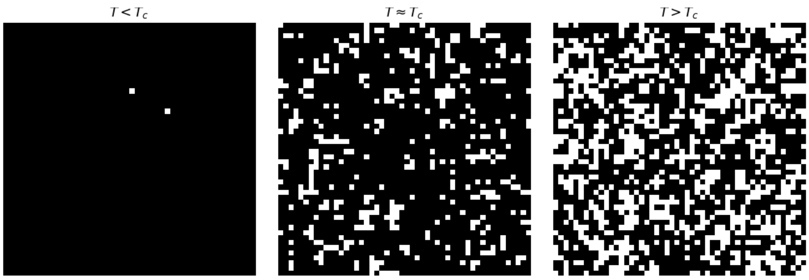

Figure 6: Spin configuration map for $J = 1$ $B = 1$.

1. **Left panel:** $T < T_c$
   All the spins are aligned in the same direction in the system. Thermal fluctuations are weak and insufficient to disrupt the ferromagnetic ordering.

2. **Middle panel:** $T \approx T_c$
   Near the Curie Temperature, the system is in a transition state and the spin configuration begins to become disordered. The system shows no clear long-range order, indicating the switch from the ferromagnetic state to the paramagnetic. The thermal energy is almost sufficient to neutralize the tendency of the spins to align.

3. **Right panel:** $T > T_c$
   At higher temperatures, the thermal energy becomes sufficient to disrupt spin alignment entirely. The system enters a highly disordered state, and as it can be seen in the plot, roughly half of the spins have different alignment relative to the others.

3.5 Case 3: What would happen if J = 1 and B = -1

What could we expect to happen if we reverse the applied external magnetic field? Well the magnetic field directly affects the magnetization of the material. By keeping the value of the magnetic field the same but just reversing its direction, the only thing that is expected to happen is the spins will align in the opposite direction to $B = 1$, and thus mirroring the magnetization curve.

So I would expect that the Curie Temperature would be the same as the second case.