PHY905 Project 4 - Ising Model

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(Dated: April 16, 2017)

Background: A fairly accurate model of the solar system can be achieved with the use of newtonian mechanics. However, this leads to many coupled differential equations which are difficult to solve analytically.
Purpose: The goal of this work is to solve the Ising model in two dimensions to probe the properties of phase transitions in magnetic materials.
Method: We use the Metropolis algorithm to generate the possible spin configurations on the lattice and the Grand Canonical ensemble to analyze the statistical physics at play.
Results: We find the the Euler method is unstable even in the binary Earth-Sun system, and causes non-conservation of both energy and angular momentum. In contrast, the velocity Verlet method is found to be very stable and enforces conservation of energy and angular momentum.
Conclusions: Our results demonstrate both the importance of an effective differential equation solver, and that the sun (due to its large mass) essentially controls all of the dynamics of the other bodies in the system.

I. INTRODUCTION

While there are many types of magnetism in physics, the strongest and most common type one encounters in everyday life is ferromagnetism, in which a metal, such as iron or cobalt, becomes permanently magnetized when exposed to a magnetic field. This phenomenon is initiated by a quantum mechanical interaction which causes the spins of unpaired electrons to align, acting against the thermodynamic tendency to randomize the spins.

One of the most common ways to analyze magnetism is the Ising model, in which the magnetic material is treated as a lattice of atomic spins which interact with each of their nearest neighbors. In this model, at low temperatures the system exhibits spontaneous magnetization wherein the average magnetization is nonzero. As the temperature increases the system undergoes a second order phase transition at a specific temperature, known as the critical temperature. In a second order phase transition the two phases on either side of the transition are identical and the transition manifests as a discontinuity in the derivative of the energy, which is different from a first order transition (such as evaporation) in which the two different phases coexist at the critical temperature and the transition manifests as a discontinuity of the energy.

In this work, we implement the metropolis algorithm with the ising model in two dimensions in order to study phase transitions of magnetic systems. Calculations of the average energy, heat capacity, average magnetization and the susceptibility are performed and compared to the expected values for a small system. In addition, the behavior of these quantities as a function of temperature is analyzed in order to extract the critical temperature of the phase transition. Finally, the performance of the metropolis algorithm is analyzed. In Sections II and III, the necessary theory and implementation of the algorithms are described. In Section IV the performance and accuracy of the code are analyzed. Finally, in Section V we give a summary and our conclusions.

II. THEORY

In this work we will use the Canonical ensemble, where the probability of a given state i is given by the Boltzman distribution (with the Boltzman constant set to one):

$$P_i(T) = \frac{e^{-E_i/T}}{Z} \tag{1}$$

where Z is the partition function given by the following sum over all possible states:

$$Z = \sum_i e^{-E_i/T}. \tag{2}$$

The energy of a particular microstate is given by:

$$E = -J \sum_{\langle kl \rangle} s_k s_l - B \sum_k s_k \tag{3}$$

where J is a coupling constant, B is the external magnetic field and $s_{k,l}$ are the spins. In this work, the coupling constant is taken to be one and there is no external magnetic field.

For a simple 2x2 lattice the possible states are given in Table I and the partition function is given by:

$$Z = 2e^{8/T} + 2e^{-8/T} + 12. \tag{4}$$

Number of spins up	Degeneracy	E_i	M_i
4	1	-8	4
3	4	0	2
2	4	0	0
2	2	8	0
1	4	0	-2
0	1	-8	-4

TABLE I: Energy and magnetization of all possible spin configurations for a 2x2 lattice.

Similarly the average energy and average squared energy are given by:

$$\langle E\rangle = \sum_i E_i e^{-E_i/T} = -16e^{8/T} + 16e^{-8/T} \quad (5)$$

$$\langle E^2\rangle = \sum_i E_i^2 e^{-E_i/T} = 128e^{8/T} + 128e^{-8/T}. \quad (6)$$

From these quantities we can calculate the energy variance, which is related to the heat capacity by:

$$C_V = \frac{1}{T^2}\left(\langle E^2\rangle - \langle E\rangle^2\right)$$
$$= \frac{1}{T^2}\left(128e^{-8/T} - 128e^{8/T} + 512\right) \quad (7)$$

Similarly, one can calculate the average magnetization, average square magnetization, and the magnetic susceptibility as:

$$\langle |M|\rangle = \sum_i |M_i| e^{-E_i/T} = 8e^{8/T} + 8 \quad (8)$$

$$\langle M^2\rangle = \sum_i M_i^2 e^{-E_i/T} = 32e^{8/T} + 32 \quad (9)$$

$$\chi = \frac{1}{T}\left(\langle M^2\rangle - \langle |M|\rangle^2\right) = \frac{1}{T}\left(-96e^{8/T} - 32\right). \quad (10)$$

In the Canonical ensemble the important potential is the Helmholtz free energy, which is given by:

$$F = -TlnZ. \quad (11)$$

The average energy and heat capacity can then also be related to the first derivative of the Hemlholtz energy as: ******THESE EQNS NEED TO BE FIXED LATER***

$$\langle E\rangle = T^2\left(\frac{\partial lnZ}{\partial T}\right)_{V,N} \quad (12)$$

$$C_V = -\frac{1}{T^2}\frac{\partial^2(TlnZ)}{\partial T^2} \quad (13)$$

As discussed in Section I, the phase transition will manifest as a discontinuity in the derivative of the energy (thus the heat capacity). However, near the critical temperature (T_C), the dependance of several physical quantities on temperature can be expressed using the following power laws:

$$\langle M(T)\rangle \sim (T - T_C)^\beta \quad (14)$$

$$C_V(T) \sim |T_C - T|^{-\alpha} \quad (15)$$

$$\chi(T) \sim |T_C - T|^{-\gamma} \quad (16)$$

where the exponents are given by $\beta = 1/8$, $\alpha = 0$, and $\gamma = -7/4$.

III. METHODS

For an NxN lattice, the number of spin configurations is given by 2^{N^2}. From Equations 5-10, we see that in order to calculate the various physical quantities of interest, we must sum over all possible microstates, however this is not trivial to perform computationally. To solve this problem we use the Metropolis algorithm [**?**] to generate a new configuration from the previous one.

In the Metropolis algorithm, we pick a random spin and determine the change in energy of the system when the spin is flipped. If that energy is less than the previous energy we accept the transition, if not then we calculate the value $w = e^{\Delta E/T}$ and generate a random number, r. If the random number is less than w, then the move is also accepted. This constitutes one Monte Carlo cycle, and is repeated until some maximum number of cycles has been achieved that presumably ensures all configurations have been tested.

As the lattice in our calculations is of dimension N^2 rather than infinite, there will be edge spins which have fewer neighbors than the rest. To get around this we will use periodic boundary condititons, where for example the top left spin's "top" neighbor is the bottom left spin etc.

In addition, the lack of an infinite lattice means the behavior near the critical temperature will be modified from Equations 13-15, namely:

$$\langle M(T)\rangle \sim N^{-\beta/\nu} \quad (17)$$

$$C_V(T) \sim N^{\alpha/\nu} \quad (18)$$

$$\chi(T) \sim N^{\gamma/\nu} \quad (19)$$

where ν is defined by the relationship between the infinite critical temperature and the calculated critical temperature:

$$T_C(N) - T_C(N=\infty) \sim aN^{-1/\nu} \quad (20)$$

where a is a constant.

IV. RESULTS

We first aim to ensure the algorithm is working as expected by comparing the output for a 2x2 lattice to Equations 5-10. The number of Monte Carlo (MC) cycles needed for 0.1% agreement is given in Table II.

In addition, we want to explore the equilibration time for the average energy and magnetization. To view this, we plot each quantity as a function of the number of

Quantity	Error (%)	MC cycles
$\langle E\rangle$	0.004	5000
$\langle E^2\rangle$	0.09	900
C_V		
$\langle \|M\|\rangle$	0.09	6000
$\langle \|M^2\|\rangle$	0.089	3000
χ		

TABLE II: Energy and magnetization of all possible spin configurations for a 2x2 lattice.

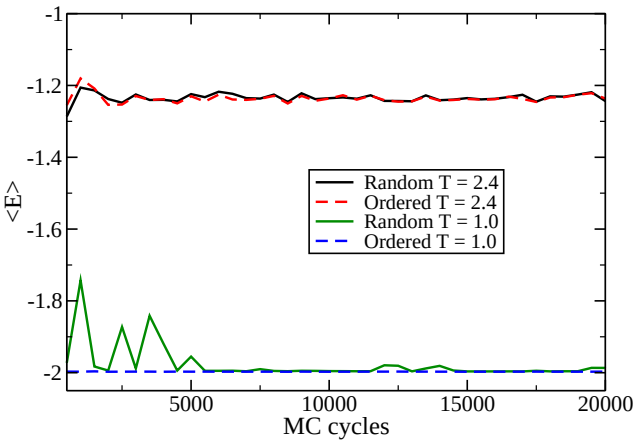

FIG. 1: Average energy as a function of the number of Monte Carlo cycles.

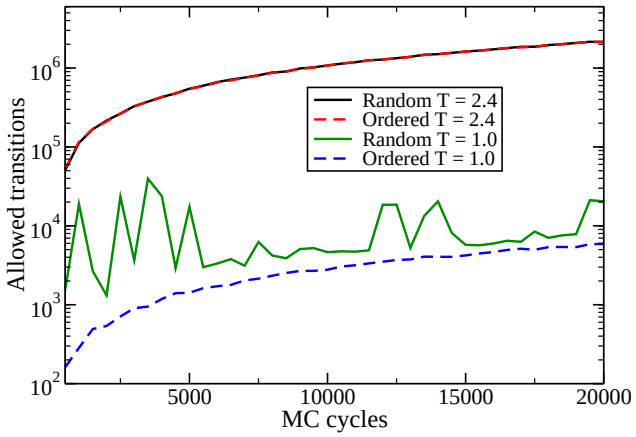

FIG. 3: Number of allowed transitions as a function of the number of Monte Carlo cycles.

Monte Carlo cycles. For comparison, we start with all the spins aligned or the spins aligned randomly. These are shown in Figures 1 and 2 respectively where the black(green) solid curve corresponds to the initially random configuration and the red(blue) dashed curve corresponds to the initial configuration with all spins up at T = 2.4 (1.0). In each figure we see that at the lower temperature, equilibrium is almost immediately reached for the ordered configuration, while it takes roughly 5000 MC cycles for the random configuration. In contrast, at the higher temperature the time to equilibrium seems to be independent of the initial configuration as both take roughly 2000 MC cycles.

Next, we investigate the number of accepted transitions as a function of the number of MC cycles in Figure 3 and as a fucntion of temperature in Figure 4. In Figure 3 we again see that for the higher temperature that the performance is almost independent of the initial configuration, while the random configuration allows more transitions than the ordered configuration for small numbers of MC cycles. In Figure 4 the black solid line corresponds to XXXX.

V. CONCLUSIONS

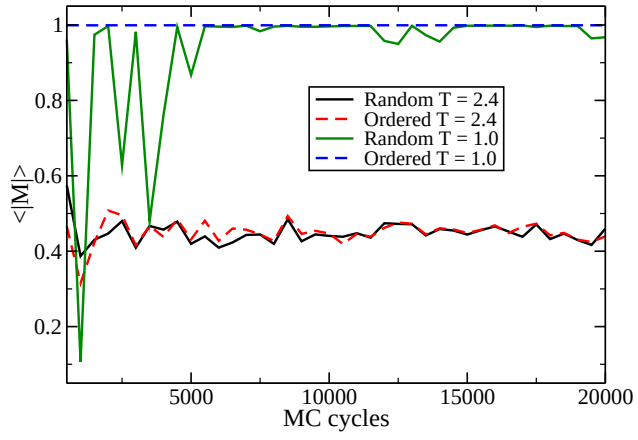

FIG. 2: Average magnetization as a function of the number of Monte Carlo cycles.

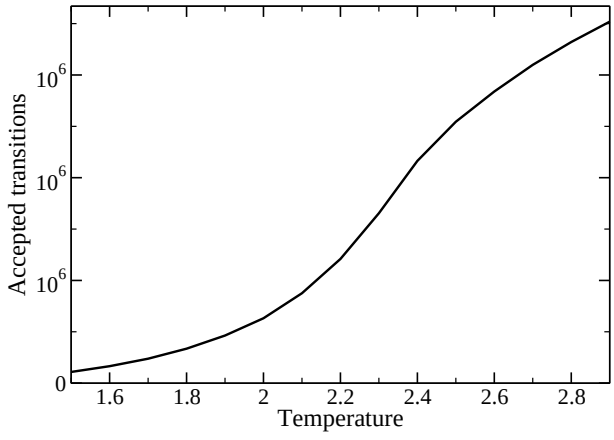

FIG. 4: Number of allowed transitions as a function of temperature for 20000 MC cycles

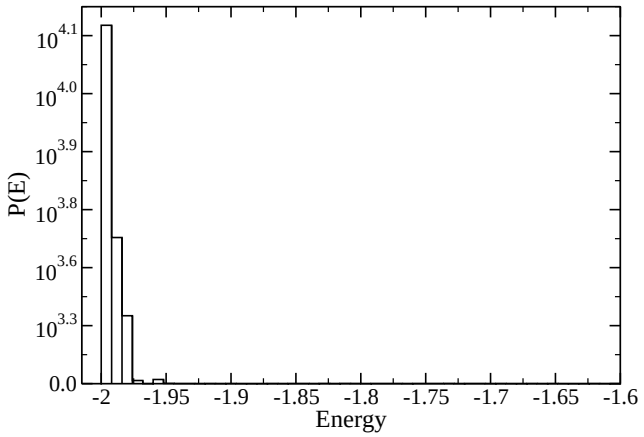

FIG. 5: Energy probability distribution for 20000 MC cycles at T = 1.0

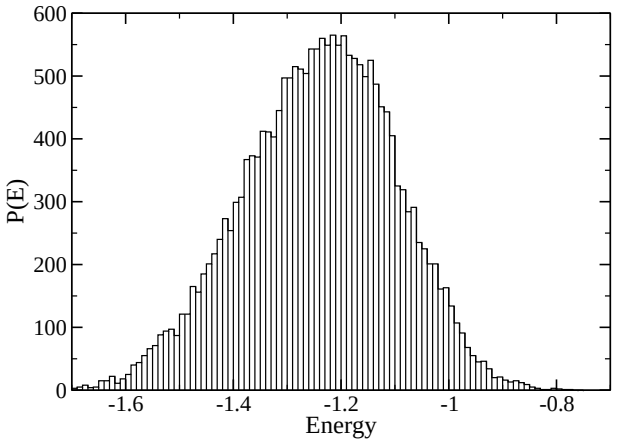

FIG. 6: Energy probability distribution for 20000 MC cycles at T = 2.4