Ising Model with non-reciprocal coupling: Studying flocking in active systems

Numerical Techniques Term Paper

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Abstract

Effective interactions that violate Newton's third law of action-reaction symmetry are common in systems where interactions are mediated by a non-equilibrium environment. Extensive Monte Carlo simulations are carried out on a two-dimensional Ising model, where the interactions are modified non-reciprocally. We demonstrate that the critical temperature decreases as the non-reciprocity increases and this decrease depends only on the magnitude of non-reciprocity. Further, travelling spin waves due to the local fluctuations in magnetisation are observed which are related to flocking behaviour in active systeems.

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1 Introduction

In many of the complex systems, the interactions between the particles are mediated by the environment. For example, motile bacteria modify their activity based on the local concentration of autoinducer molecules, which is termed as quorum sensing. This quorum sensing changes the effective interactions between the motile bacteria. Another example is active systems, such as bird flocks, with a visual perception. One major implication of non-reciprocal interactions is that these systems do not obey detailed balance and time reversal symmetry, thereby driving the system out of equilibrium. This results in the emergence of new features such as time-dependent states and oscillatory dynamics leading to self-propelling bands or dynamic micropatterns. These non-reciprocal interactions and the nonequilibrium dynamics generated by them play a significant role in the structure and dynamics of active particles, animal groups, social systems. Currently, these systems, motivated by the effect of non-reciprocal interactions, have become a focus of growing research interest. In general, the non-reciprocal interactions are non-Hamiltonian and most of the classical statistical mechanics formalism cannot be applied to systems with non-reciprocal interactions. Recently, there have been a large number of numerical and theoretical investigations to understand the effects of non reciprocal interactions on the phase behaviour and dynamics of such non-equilibrium systems. It has been shown that the interplay between non-reciprocal enhancement of fluctuations and many-body effects leads to time-dependent phases which can be viewed as dynamical restorations of spontaneously broken continuous symmetry. The interplay between self-propulsion and non-reciprocity induces a chaotic chasing band phase. Another interesting observation about these time-dependent phases is that these systems can give rise to stable travelling waves. In this work, we introduce an Ising model with nonreciprocal interactions and carry out detailed Monte Carlo investigations on the model.

2 Monte Carlo Metropolis Algorithm

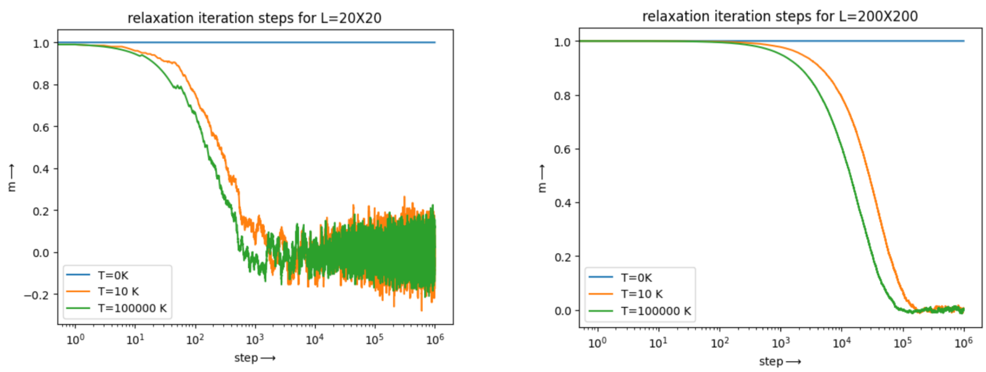
The Monte Carlo Metropolis algorithm is commonly used in computational physics and statistical mechanics, offering a powerful tool for simulating complex systems governed by stochastic processes. Its inception in the mid-20th century by Metropolis et al. heralded a paradigm shift, enabling scientists to tackle intricate problems that were previously intractable through analytical means.

At its core, the Monte Carlo Metropolis algorithm leverages the principles of Markov chain Monte Carlo (MCMC) methods to sample from probability distributions, particularly those associated with equilibrium states of physical systems. It embodies the spirit of exploration and exploitation by iteratively proposing new states based on a transition probability and accepting or rejecting these moves according to a defined acceptance criterion. By constructing a Markov chain whose stationary distribution corresponds to the desired probability distribution, the algorithm circumvents the need for explicit enumeration of all possible states, thereby sidestepping the notorious curse of dimensionality.

Key to the algorithm's success is the balance it strikes between exploration and exploitation. Through the acceptance criterion, which often involves the Metropolis-Hastings ratio, proposed moves that lead to a decrease in energy or an increase in probability are accepted with a certain probability, thereby preventing the chain from getting trapped in local energy minima or probability maxima. Here however we must keep in mind not get stuck at a local minima far from ground state, as it may lead to dynamic freezing at that point since the probability of exploration is infinitesimally smaller farther from ground state.

3 Approach to the problem

We start with a LxL lattice implemented as a array, initialize with one. We take up spin to be 1 and down spin to -1. We sweep the model through 100 steps of temperature between 10^{-5}K to 10 K. We carry out the sweep for different temperature parallely and employ the metropolis algorithm to randomly choose a spin to flip and calculate the change in energy of spin dE. And then we take a random number between [0,1) from a uniform distribution and compare it with $e^{-\frac{dE}{T}}$ if it is less than the latter we flip the spin else keep it to be the same. This allows even unlikely steps to be accessed and finally reach a good ground state.



(a) Relaxation of 20x20 lattice system

(b) Relaxation of 200x200 lattice system

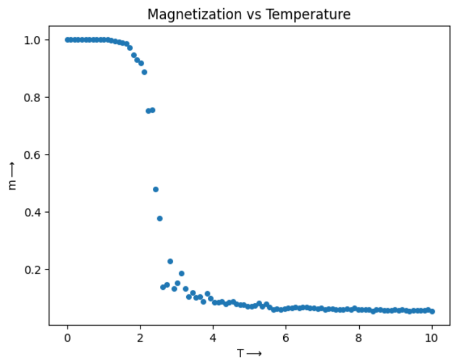
Figure 1: Steps required for relaxation

The fluctuations we see for the 20x20 lattice is due to the non-equilibrium nature of system so it oscillates about a mean value. We however see that these fluctuations are diminished in a 200x200 lattice system. But due to computational efficiency we use small lattice sizes. We carry out $L^2 \times 1000$ metropolis steps. After which we calculate properties like Magnetization, Energy, Specific Heat and Susceptibility and at the end of which we average over last 10,000 steps to diminish the fluctuations. This completes a Markov chain for a given size, Δ and temperature. We do this for all temperature steps and store the data in csv file. We repeat this many times computing 77 such markov chains stored in csv files for data retrieval. While retrieving data we mean out the chains and display the plots and calculate required values.

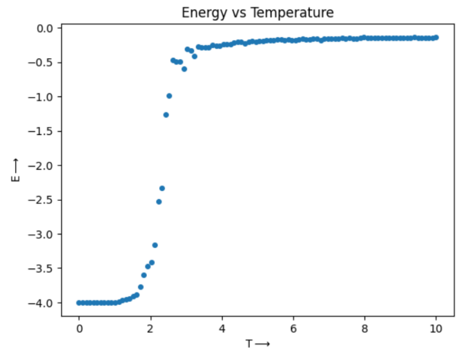
4 Results

4.1 Thermodynamic Properties

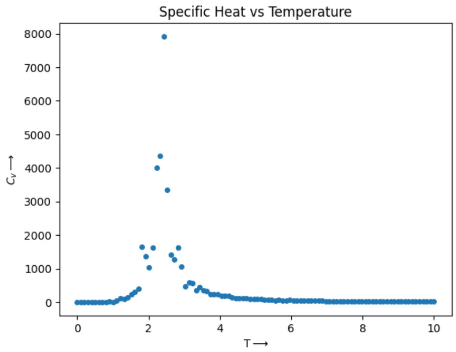
We find out the thermodynamic properties plot for a 18X18 lattice with $\Delta = 0$ and we find the usual ising model plot.



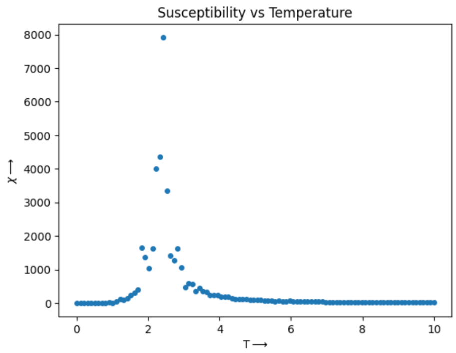
(a) Magnetization vs Temperature plot



(b) Energy vs Temperature plot



(c) Specific Heat vs Temperature plot



(d) Susceptibility vs Temperature plot

4.2 Curve Fitting and finding T_c

We try to find the critical temperature at which the phase transition occurs to do so we tried to find the maximum height index of specific heat plot but it did not give a good estimate due to large fluctuation about the critical temperature. So we could try to fit that plot to find the T_c but and easier fit was found to be magnetization plot which we fitted with a re-scaled and constant shifted fermi-dirac distribution function(which does not shifts the T_c),

$$\frac{A}{e^{B.(T-T_c)}+1}+C$$

this provide a really good fitting and esitimate of critical temperature, the value B can also be associated with the "temperature" of fermi distribution here equivalently proportianal to size of the system.

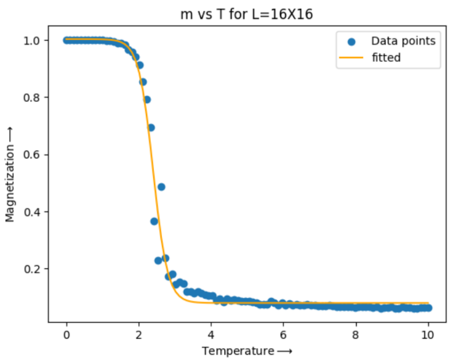


Figure 2: Fitting of data

4.3 Dependence of T_c with Δ

We from stored csv file and subsequent curve fit of magnetization find the T_c for different Δ values and plot them. From perturbation theory we expect that the first order term will cancel and hence forth only Δ^2 term remains and hence we expect a parabolic nature to the curve. We get the same nature and fit the data points and find T_c at T=0K which come out to be 2.353049K.

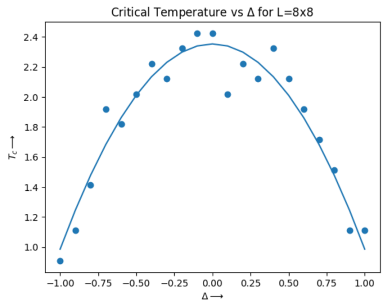


Figure 3: T_c vs Δ

4.4 Finite size scaling

We from stored csv file find how the T_c change for $\Delta = 0.0$ with the size of the system we find the plot of T_c with $\frac{1}{size}$ and the extrapolate the data we see at $size$ = inf T_c comes out to be 2.249823584K. We see with increasing size the model tends to a finite temperature to a correct estimate of critical temperature and hence we conclude the validity.

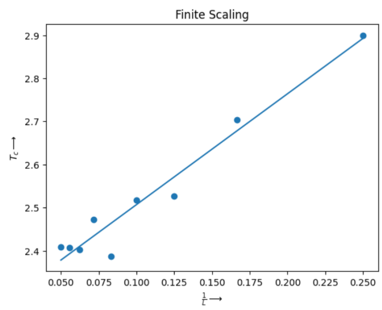
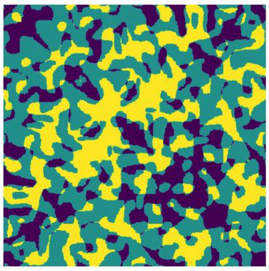


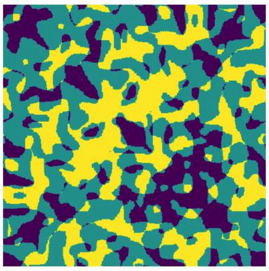
Figure 4: Finite Scaling

4.5 Flocking and Dynamics of clusters

We see the metropolis step of isotropic coupling at temperature a little above critical temperature where we see find clusters of spin.

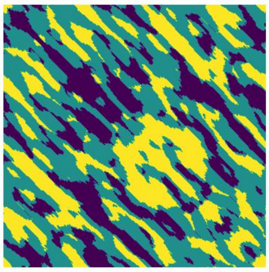


(a) 30M-th metropolis step

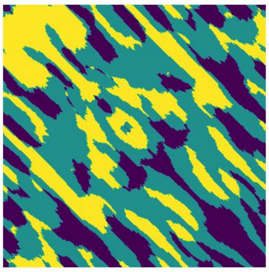


(b) 40M-th metropolis step

We see that the clusters do not move with time(steps) thus not dynamic. We however see something interesting in different coupling, we see a bit about critical temperature we find clusters of spin which is equivalent to grouping of active systems and due to the anisotropic coupling the clusters move together at that.



(c) 179M-th metropolis step



(d) 335M-th metropolis step