Information and Order Parameters in the Gauge Ising Model.

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One of the main methods to study many body problem in numerical Physics is Monte Carlo simulation. Traditionally, in Condensed Matter Physics people have studied different thermodynamic quantities and their temperature dependence. Big part of these studies is finding phase transitions. Standard method that is used to find such a phase transition, which is usually named "critical point", is to study order parameter behavior. Problem is that for many systems it is not known or does not exist. At the same time Monte Carlo simulation behaves different in the regions with qualitatively different physical properties. In this work I am studying Ising Gauge model, it's thermodynamic properties and compare it to the Information theory properties that were obtained from the dynamics of the simulation. Further I study how excess entropy can be used as a natural order parameter to find the phase transition temperature.

I. INTRODUCTION

People use Monte Carlo simulations to find numerical solutions for the problems that can not be solved analytically. Main problem is that phase space grows exponentially and summation that is used to find the partition function can be obtained only in several cases, where symmetries of the problem can help in some way. Power of the Monte Carlo simulation is that it does not explore all of the phase space, but only it's small subspace in which states have significant probability. Temperature is one of the parameters of the simulations so it looks natural to guess that dynamics of the simulation will depends on the temperature. And this is indeed the case. Much less trivial fact is that simulation goes different in different physical regions. For example big problem of the simulations is "critical slowing down", meaning simulations explores the phase space very slowly in the vicinity of the critical point. Thus there is interesting correlation between physics of the problem and nature of the simulation and goal of this project is to get some insight in this correlation.

In this work I will use methods that are developed in the Natural computation and Information theory to analyze the dynamics of the the Monte Carlo simulations for the 3 dimensional Ising Gauge theory.

Model is described by the Hamiltonian:

$$H = -J \sum_{\langle i,j,k,l \rangle} S_i S_j S_k S_l \tag{1}$$

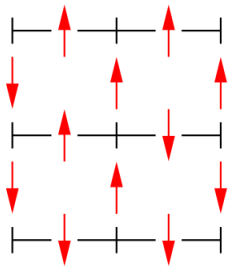

FIG. 1: Red arrows - spins that are represented in the Hamiltonian as $S_i = \pm 1$ values

Where $S_i = \pm 1$ and sum is over the plaquets of the cubic lattice with periodic boundary conditions. See Fig. 1. This model has local gauge symmetry which makes it impossible to use any local quantity as an order parameter to find phase transition temperature. But at the same time this model can be mapped on the $2d$ Ising model that can be solved analytically. And from this solution we know the exact value of the critical temperature $T_c = 1.3157$. See work[1].

For a given set of the input parameters (lattice size in 3 dimensions: (n_x, n_y, n_z), temperature T) at each step simulation either moves to the next state or stays in the same state. We can say that at each step we observe some quantity, some observable. And this observable will be main object of the following analysis.

II. SET UP.

Monte Carlo algorithm that generates the data.

A. Update algorithm.

One local lattice update:

1. Calculate energy for the current state E_{old}
2. Consider flipping random spin.
3. Calculate energy for the state with flipped spin E_{new}
4. Do this flip with probability $p = \frac{1}{1+e^{(E_{new}-E_{old})/T}}$

This local update is repeated $(n_x n_y n_z d)$ times so that on average each spin is tried to be flipped once, where $d = 3$, because I work with 3 dimensional lattice.

One lattice update will be done after we tried to flip on average each spin of the lattice, i.e. One lattice update = $dn_x n_y n_z \times$ local update.

First I do 10000 lattice updates without taking any measurements. This moves system to the thermal equilibrium. After this I do 4000 lattice updates, measuring energy at the end of each try of the spin flip. And this leads to the $3^4 \times 4000 = 324000$ measurements.

B. Parameters of the simulation.

Measurements that I do during simulation allow me to find thermodynamic quantities using following identities:

$$E = \frac{1}{n_x n_y n_z d} \langle E_i \rangle \tag{2}$$

$$C = \frac{1}{(n_x n_y n_z)^2} \frac{\langle E_i^2 \rangle - \langle E_i \rangle^2}{T^2} \tag{3}$$

$$S(T) = S(0) + \frac{E(T)}{T} + \int_{\infty}^{1/T} \frac{dE}{T} \tag{4}$$

To do the Natural computations analysis I needed to choose what will be my measurement alphabet. Algorithm complexity grows exponentially with the alphabet size, so I was forced to choose minimal non trivial alphabet size – 2. I think there are different ways to choose it but in this work I was doing it in such a way:

- We go to the next state(we flip spin) $\Longrightarrow 1$
- We stay in the same state(we do not flip spin) $\Longrightarrow 0$

Thus we obtain

$$\ldots 1111011110001100000000101010011011011011011 \ldots$$

This series of 1 and 0 presumably looses all information about the energy, magnetization, etc(For example all changes in the energy as $-8, -4, 4, 8$ give you same number 1 in this time series), but it will keep dynamics of the simulation.

To infer ϵ-machines I used Bayesian inference with $[1, 2]$ state systems.

For some temperatures I do several simulations with different random number seeds and in this case results are averaged to get smaller errorbars.

III. THERMODYNAMIC RESULTS

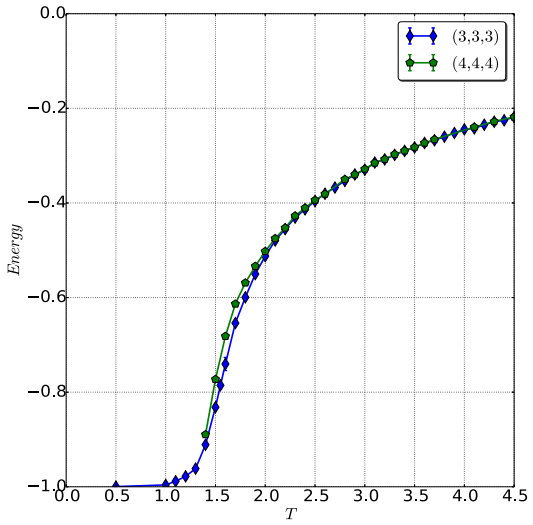

FIG. 2: Energy versus temperature for 10000 thermal and 4000 measurement sweeps for the cubic lattice with shape $(3, 3, 3)$.

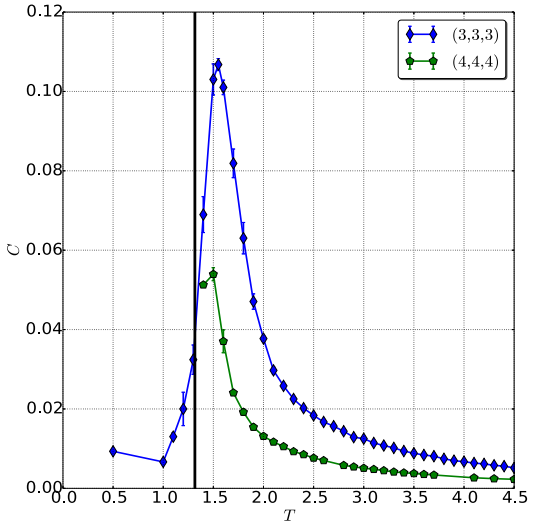

FIG. 3: Specific heat versus temperature for 10000 thermal and 4000 measurement sweeps for the cubic lattice with shape $(3, 3, 3)$. Black vertical line - critical temperature value.

IV. INFORMATION THEORY RESULTS.

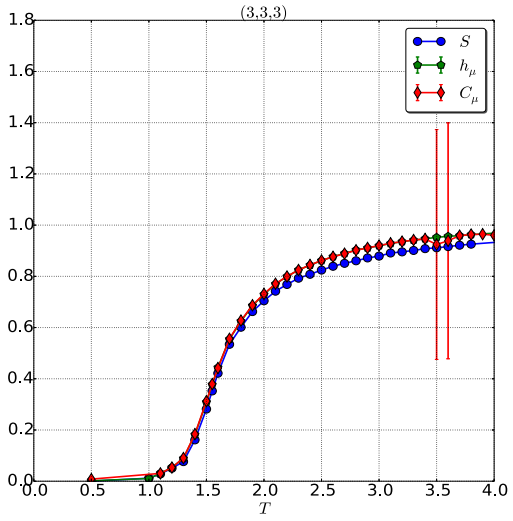

FIG. 4: Thermodynamic entropy S, entropy rate h_μ and statistical complexity C_μ versus temperature for 10000 thermal and 4000 measurement sweeps for the cubic lattice with shape $(3, 3, 3)$.After preforming numerical integration entropy curve was shifted that it's value will be equal to zero when $T \to 0$ and after this scaled that it will be equal 1 at $T \to \infty$

As we can see h_μ and C_μ coincide and what is remarkable they are very close to the thermodynamic entropy S, which was obtained using numerical integration.

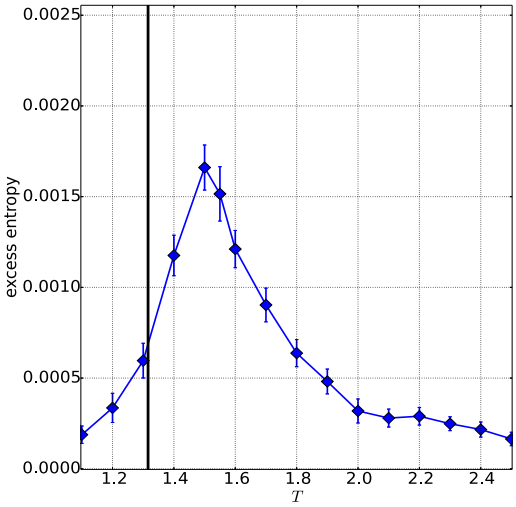

FIG. 5: Excess entropy versus temperature for 10000 thermal and 4000 measurement sweeps for the cubic lattice with shape $(3, 3, 3)$. Black vertical line - critical temperature value.

It looks like peak in the excess entropy is at the same position as a specific heat peak, so may be this excess entropy singularity is at least as good signature of the critical point as the specific heat peak.

V. CONCLUSION.

This statements can be a bit powerful, but still:

- Entropy rate h_μ and statistical complexity C_μ of the Monte Carlo simulation are equal to the thermodynamic entropy of system that this Monte Carlo simulates.
- Excess entropy can be used as a natural order parameter to find phase transition temperature.

VI. QUESTIONS THAT ARE RAISED BY THIS WORK.

- How does these results will change if we will work with larger systems?
- Are results of this work is just an accident or they will hold for other systems also?
- Will excess entropy that worked here for the second order phase transition will work that well for the first order or KT transition?
- Does this approach work only for spin systems or it will also work for the fermionic/bosonic systems?
- Is the method an improvement? Eg for some known phase transition can one get some interesting observables (Tc, exponents,...) to higher accuracy or with less computer time?
- Is there a model where we do not know whether there is a phase transition or not that we can try?
- Is this useful for the sign problem in some way?

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[1] Kogut, John B. "An introduction to lattice gauge theory and spin systems." Reviews of Modern Physics 51.4 (1979): 659.