FYS3150 Computational Physics - Project 4

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Using the Metropolis algorithm to study a system of weakly coupled paramagnets, the Ising model. Derived exact solutions of expectation values for a 2x2 lattice and found that the required $\sim 10^5$ Monte-Carlo cycles to consistent results with $\sigma \sim 10^{-3}$.

INTRODUCTION

THEORY, ALGORITHMS AND METHODS

The Ising Model

In its simplest case, a paramagnet is described as a lattice of noninteracting dipole moments, each in a state up or down. Where the energy of the system is proportional to the sum of the spins, up or down of each noninteracting constituent.

The Ising model is a natural extension to this, by adding local interaction between directly neighboring spins (See fig. 1), such that the energy of the system is instead proportional to the sum of the interactions of all coupled spins, which gives a more accurate description of the system compared to the simple case of an ideal paramagnet.

Or more precisely, the energy is given by Eqn. 1, where $s_i \in \{-1, 1\}$ and J is a coupling constant.

$$E = -J \sum_{<kl>} s_k s_l \tag{1}$$

In this sum, the notation $< kl >$ means that we take the sum over each coupling $s_k s_l$. Consider again Fig.1. The contribution, ϵ_i, to the total energy due the interactions at spin-site i is the sum of its interactions, $\epsilon_i = s_i(s_\uparrow + s_\downarrow + s_\leftarrow + s_\rightarrow)$ where the arrows denote the spin-site directly neighboring site i in the direction of the arrow. Now wish to compute the energy contribution due to the interactions at the spin-site left of site i. In this case, the interaction between it, and spin-site i has already been computed, and must not be counted again.

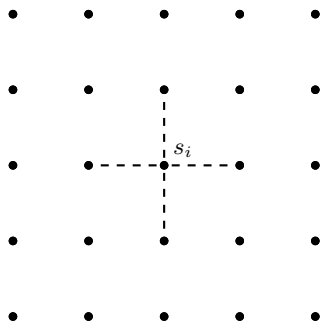

FIG. 1: Section of a 2D lattice, where each spin-site is represented by a dot. In the Ising model, spin-site i will only interact with its directly neighbouring spin-sites, connected by dotted lines in this diagram

Further, in this project the lattice will be treated as pseudo-continuous where any spin-sites located at an edge, will also interact with the spin-site on the opposing edge, illustrated in Fig. 2, which strictly speaking constitutes having periodic boundary conditions. If instead we had fixed boundary conditions, there would simply be no such across-lattice interactions, and spin-sites located at the edges would then only interact with 3 other spin-sites (2 in the case of corner sites) in the 2D case.

Much simpler, the net magnetization, $\mathcal{M}$, of the system is taken as the sum over all spins

$$\mathcal{M} = \sum_i s_i$$

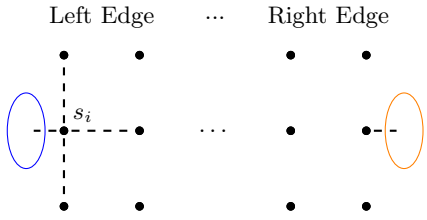

FIG. 2: Spin-site i, located at the left edge of the lattice interacting with its direct neighbors, as well as the spin site on the opposite edge of the lattice

Boltzmann Statistics

From this model we can derive many thermodynamic quantities by the use of Boltzmann statistics, where we

have the probability of the system being in some specific macro-state[1] at temperature[2]

$$\mathcal{P}(E_s) = \frac{1}{Z} e^{-\beta E_s} \tag{2}$$

With $\beta \equiv \frac{1}{k_B T}$, the thermodynamic beta and Z, the partition function, acting as a normalization factor given by

$$Z = \sum_s e^{-\beta E_s} \tag{3}$$

From this, the expectation value of some quantity X, with micro-states X_s can be computed by

$$\langle X \rangle = \sum_s X_s \mathcal{P}(E_s) = \frac{1}{Z} \sum_s X_s e^{-\beta E_s} \tag{4}$$

Using this, we can compute the specific heat capacity, C_V by computing the expectation values of E, E^2 [1], related by the following expression

$$C_V = \frac{\langle E^2 \rangle - \langle E \rangle^2}{k_B T^2} \tag{5}$$

Where $\langle X^2 \rangle - \langle X \rangle^2$ is recognized as the variance of a set of randomly distributed quantities, σ_X^2.

In a similar fashion, the magnetic susceptibility[3], χ, is calculated from $\sigma^2_{|M|}$ [1]

$$\chi = \frac{\sigma^2_{|\mathcal{M}|}}{k_B T} \tag{6}$$

For more details on the Ising model, or Boltzmann statistics refer to Schroeder [2, Ch 6, 8.2], Hjorth-Jensen [1], or similar introductory texts on the topic.

Analytic solution of 2x2 Lattice

Consider now a 2x2 lattice, each with spin ± 1. The energy of the system for a particular micro-state is given by Eqn. 1, so for a 2×2 lattice we have

$$E = -J \sum_{<kl>} s_{kl} = -J(2s_1 s_2 + 2s_1 s_3 + 2s_2 s_4 + 2s_3 s_4) \tag{7}$$

The multiplicity, that is number of possible combinations of micro-states for a system consisting of 4 spins is $2^4 = 16$.

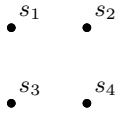

FIG. 3: A 2×2 lattice of spin-sites

If we first consider the micro-state in which all the spins are in parallel, we get energy $E = -8J$. Thus, this particular macro-state is at least 2-fold degenerate[4]. The different micro-states and their degeneracies are summed up in table I from Hjorth-Jensen [1]

TABLE I: Possible configurations of 2x2 lattice

No. spin up	Degeneracy	E	$\mathcal{M}$
4	1	-8J	4
3	4	0	2
2	4	0	0
2	2	8J	0
1	4	0	-2
0	1	-8J	-4

See that there are only 3 distinct energy macro-states, $E = -8J, 0, 8J$ corresponding to $2, 12$ and 2 of the possible micro-states respectively.

It is then easy to see that the partition function for the system will take the following form

$$Z = 2e^{+8J\beta} + 2e^{-8J\beta} + 12 = 4\cosh(8J\beta) + 12 \tag{8}$$

From this, we derive analytic values for $\langle E \rangle, \langle |\mathcal{M}| \rangle, C_V$ and χ.

First, compute the expectation value of the energy using an alternate, simpler expression from Schroeder [2, Ch 6.2]

$$\langle E \rangle = -\frac{1}{Z} \frac{\partial}{\partial \beta} Z = -\frac{8J \sinh(8J\beta)}{\cosh(8J\beta) + 3} \tag{9}$$

Similarly, the expectation value of E^2 is computed easily by another expression found in Schroeder [2, Ch 6.2]

$$\langle E^2 \rangle = -\frac{1}{Z} \frac{\partial^2}{\partial \beta^2} Z = \frac{64J^2 \cosh(8J\beta)}{\cosh(8J\beta) + 3} \tag{10}$$

From this, we compute the variance of E

$$\sigma_E^2 = \langle E^2 \rangle - \langle E \rangle^2 = \frac{64J^2}{\cosh(8J\beta) + 3} \tag{11}$$

[1] Macroscopic states being characterized by their energy, meaning i could just as well have written "... the probability of the system having some speciffic energy"

[2] Contained within β in this notation

[3] Using the absolute magnetization to compute χ, in line with the problem text for 4e

[4] Two micro-states corresponds to the same observable macrso-state.

With which we can compute C_V using Eqn. 5. Compute expectation values of $|\mathcal{M}|, |\mathcal{M}|^2$ using Eqn. 4 and Table I

$$\begin{aligned}\langle|\mathcal{M}|\rangle &= \frac{1}{Z}\sum_s |\mathcal{M}_s| e^{-\beta E_s} \\ &= \frac{8e^{8J\beta} + 16e^0}{Z} = \frac{2e^{8J\beta}+4}{\cosh(8J\beta)+3}\end{aligned} \tag{12}$$

$$\begin{aligned}\langle|\mathcal{M}|^2\rangle &= \frac{1}{Z}\sum_s |\mathcal{M}_s|^2 e^{-\beta E_s} \\ &= \frac{1}{Z}\left(16e^{8J} + 32e^0\right) = \frac{4e^{8J\beta}+8}{\cosh(8J\beta)+3}\end{aligned} \tag{13}$$

We then compute the variance of the net magnetization

$$\begin{aligned}\sigma^2_{\mathcal{M}} &= \langle|\mathcal{M}|^2\rangle - \langle|\mathcal{M}|\rangle^2 \\ &= \frac{1}{\cosh(8J\beta)+3}\left(4e^{8J\beta} + 8 - \frac{4e^{16J\beta}+16}{\cosh(8J\beta)+3}\right)\end{aligned} \tag{14}$$

Which can be used to compute the magnetic susceptibility using Eqn 6.

The Metropolis Algorithm

Metropolis Algorithm

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1 Initialize State
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RESULTS AND DISCUSSIONS

In order to test the functionality, and consistency of the algorithm a 2×2 lattice with an initial state of all spin-ups was simulated 100 times each for a range of Monte-Carlo cycles. The results for which are shown in Fig. 5. If we disregard the results for $N = 10$ Monte-carlo cycles, we see that the standard deviation of the output seems shrink in an approximately linear fashion with the logarithm of the number of Monte-Carlo cycles. In particular, we see that for 10^6 monte-carlo cycles we have a standard deviation of $\sim 10^{-4}$ meaning the algorithm outputs values consistent to the third decimal, and matches the theoretical result.

Then, moving on to a larger, 20×20 lattice we see in Fig. 4 the expectation values for a selection of different number of Monte Carlo cycles, where for each number of Monte-carlo cycles, the algorithm is ran 100 times and averaged for both $T = 1$ and $T = 2.4$. For $T = 1$, we se that the acceptance rate for the initially dissordered states are on average much greater in the region of > 2000 monte-carlo cycles, but seems to smooth out towards a similar rate for the initially orderd state, which follows a uniform rate. On the other hand, for $T = 2.4$, a more energetic system, the acceptance rate is similar for both the dissordered, and ordered system all throughout, and is far greater than for $T = 1$.

This is reflected in the mean energy and magnetization as well, which converge towards similar values at a greater rate for $T = 2.4$. This suggests that there is a link between the equilibration time of the algorithm and the temperature of the system, which for $T = 2.4$ seems to be ~ 1000 Monte Carlo cycles.

CONCLUSIONS

[1] M. Hjorth-Jensen, "Computational physics lectures: Statistical physics and the ising model," (2017).

[2] D. V. Schroeder, *An Introduction to Thermal Physics*, 1st ed. (Pearson, 1999).

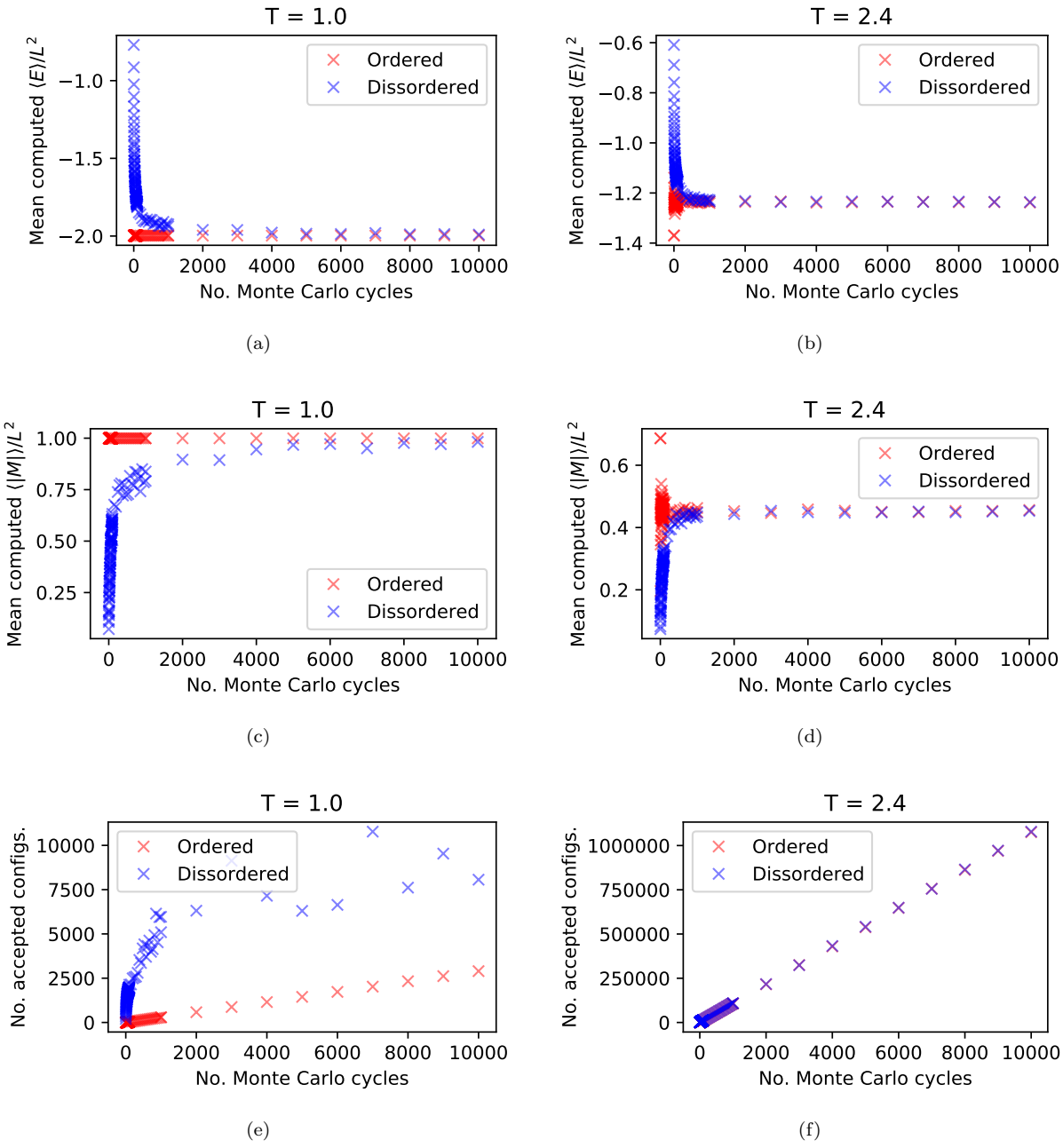


FIG. 4: Expectation values computed for different numbers of Monte Carlo cycles for an ordered initial state of spin-ups and random initial state, different for each computed expectation value.

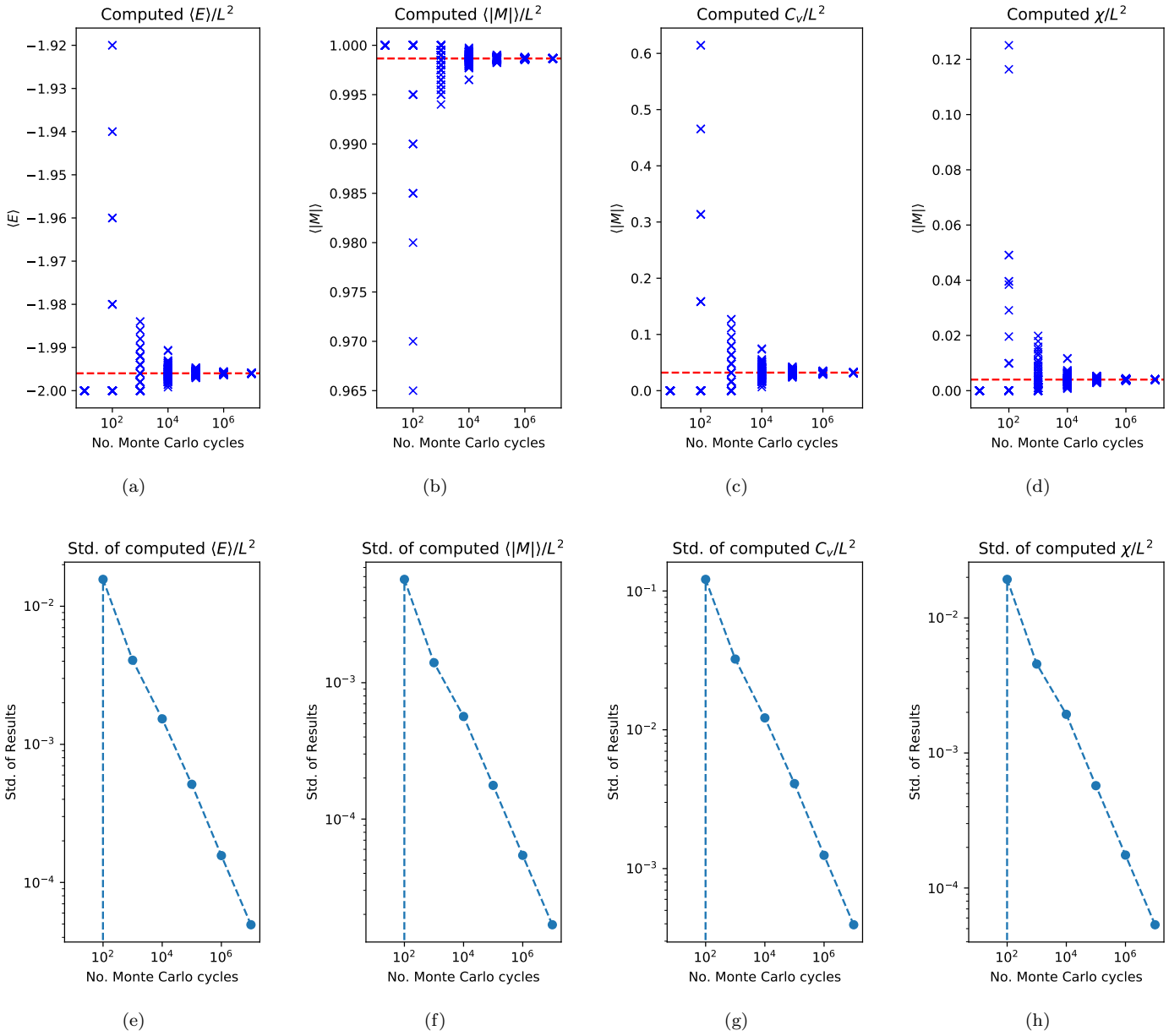
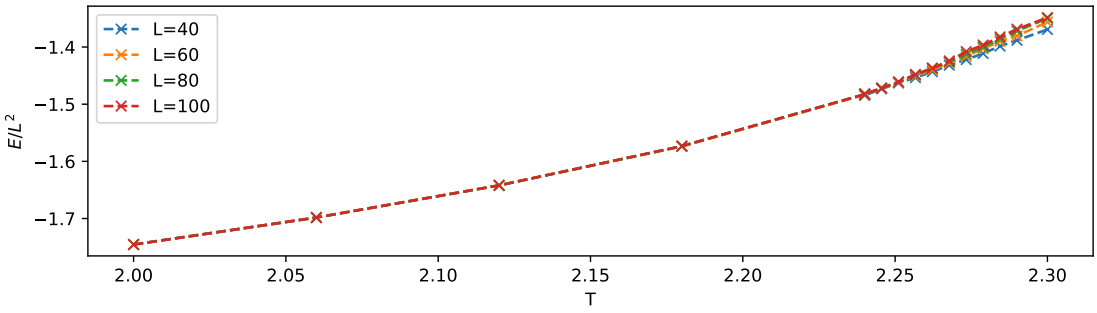
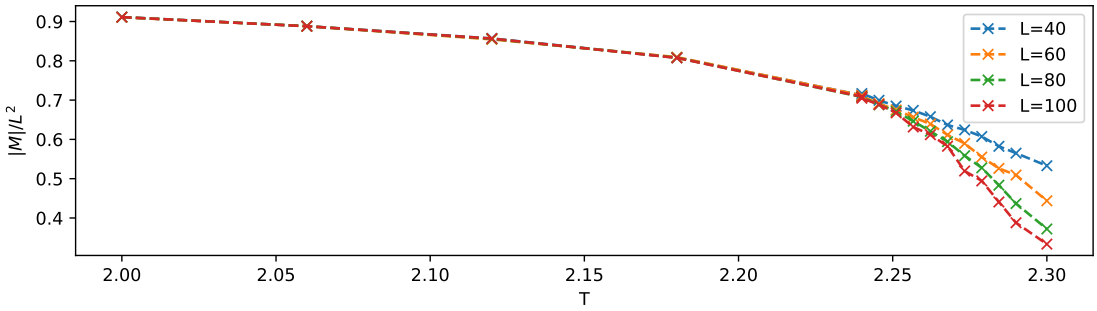


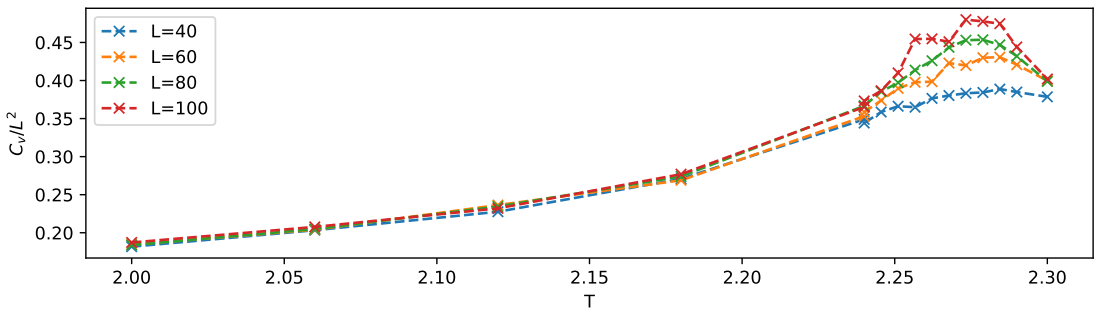
FIG. 5: (a-d) Computed results from running the algorithm 100 times per number of monte-carlo cycles for select expectation values with an ordered initial state of a 2x2 lattice of spin ups, where the theoretical value is indicated by the dashed red line. (e-h) The standard deviation (Std.) of the computed results.



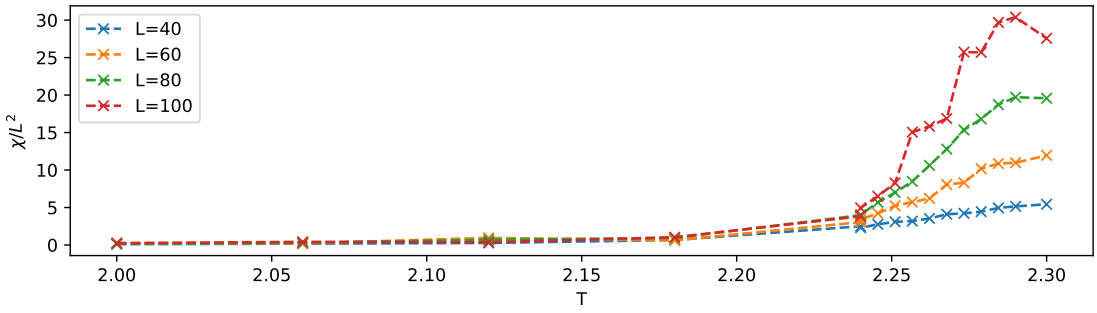
(a)



(b)



(c)



(d)

FIG. 6: Expectation values computed from $2 \cdot 10^6$ Monte Carlo cycles for $T \in [2, 2.3]$