

FYS3150 Computational Physics - Project 4

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Using the Metropolis algorithm to study a system of coupled paramagnets, the Ising model. Derived exact solutions of expectation values for a 2 by 2 lattice and found the algorithm to make accurate predictions to the third decimal in 10^6 Monte Carlo cycles. Further, looked at a 20 by 20 lattice and found a link between the equilibration time and the temperature of the system. Lastly, tried to observe the phase transition, and replicate the result produced by Onsager [1], observed the expected behavior qualitatively, but failed to extract numbers.

INTRODUCTION

In this report, we will look at the Ising model, a model describing locally coupled paramagnets and how this model can be studied numerically using the Metropolis Monte Carlo algorithm, which in short emulates the time-development of the system using statistics and random numbers.

The model has analytic solutions for a 2-Dimensional lattice, which will be used as a way of testing the code. These analytic predictions include expectation values for the 2×2 lattice, as well as the critical temperature, when the system undergoes a phase transition which in the thermodynamic limit where $L \rightarrow \infty$ was first derived analytically by Onsager [1]

The programs accompanying this report were written in python, and can be found on my github https://github.com/nicholaskarlsen/FYS3150/tree/master/Project_4.

THEORY, ALGORITHMS AND METHODS

The Ising Model

The Ising model aims to model a lattice of magnetic dipoles, and can be thought of as an extension to the ideal paramagnet, by looking at the 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 and makes predictions of phase transitions for dimensions greater than one.

The lattice energy in a system described by the Ising model with no external fields is given by Eqn. 1, where $s_i \in \{-1, 1\}$ and J is a coupling constant, within which is contained type of the coupling. For this project we will look at $J = 1$, which corresponds to a ferromagnetic coupling.

$$E = -J \sum_{\langle kl \rangle} s_k s_l \quad (1)$$

In this sum, the notation $\langle kl \rangle$ 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.

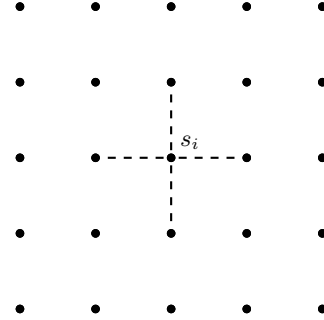


FIG. 1: Section of a 2D lattice, where each spin-site is represented by a dot. In the Ising model, spin-site i will only interact with its directly neighboring spin-sites, indicated by dotted lines in this diagram

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.

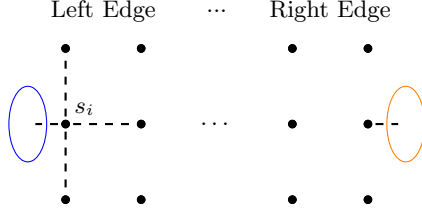


FIG. 2: Spin-site i , located at the left edge of the lattice interacting with its direct neighbors, as well as the spin site on the opposite edge of the lattice

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

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

However, the magnetization, is quite unstable and will frequently oscillate about 0 in the region of temperatures which will be studied, as seen in Fig. 3, a select result from one of the simulations to be discussed later. As such, we will instead look at the absolute value of the net magnetization, as it will provide more stable results that are easier to interpret.

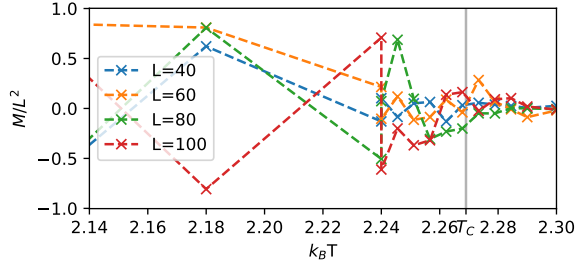


FIG. 3: Net magnetization as a function of temperature, simulated with $2 \cdot 10^6$ Monte Carlo cycles

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 state at temperature¹

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

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

$$Z = \sum_s e^{-\beta E_s} \quad (3)$$

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

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

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

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

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 susceptibility², χ , is calculated from $\sigma_{|\mathcal{M}|}^2$ [2]

$$\chi = \frac{\sigma_{|\mathcal{M}|}^2}{k_B T} \quad (6)$$

For more details on the Ising model, or Boltzmann statistics refer to Schroeder [3, Ch 6, 8.2], Hjorth-Jensen [2], or similar texts on the topic.

Analytic solution of 2×2 Lattice

Consider now a 2×2 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

$$E = -J \sum_{\langle kl \rangle} s_{kl} = -J(2s_1s_2 + 2s_1s_3 + 2s_2s_4 + 2s_3s_4) \quad (7)$$

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

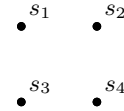


FIG. 4: A 2×2 lattice of spin-sites

¹ Contained within β in this notation

² Using the absolute magnetization to compute χ , in line with the problem text for 4e

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 degenerate³. The different micro-states and their degeneracies are summed up in table I from Hjorth-Jensen [2]

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 from Eqn. 3 that the partition function for the system will take the following form

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

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 [3, Ch 6.2]

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

Similarly, the expectation value of E^2 is computed easily by another expression found in Schroeder [3, Ch 6.2]

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

From this, we can compute the variance of E

$$\sigma_E^2 = \langle E^2 \rangle - \langle E \rangle^2 \quad (11)$$

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

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

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

We can then compute the variance of the absolute net magnetization

$$\sigma_{|\mathcal{M}|}^2 = \langle |\mathcal{M}|^2 \rangle - \langle |\mathcal{M}| \rangle^2 \quad (14)$$

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

In table II we have the analytic results for the 2×2 lattice for $T = 1$ in units where $J = 1$, $k_B = 1$.

TABLE II: Analytic values for $T = 1$

$\langle E \rangle / L^2$	-1.99598209
$\langle \mathcal{M} \rangle / L^2$	0.9986607
C_V / L^2	0.03208233
χ / L^2	0.00401074

Phase Transitions

As mentioned in the introduction, the 2-Dimensional Ising model was solved in the thermodynamic limit by Onsager [1]. Which predicts a phase-transition for a lattice of size $L \rightarrow \infty$ at curie temperature $T_C \approx 2.269$ in our dimensionless units [4].

This temperature, is related to a finitely sized lattice by the following [4]

$$T_C(L) - T_C(L = \infty) = aL^{-1/\nu} \quad (15)$$

Where a is a constant of proportionality, and ν is a number related to the correlation length of the system [4], which is set to 1 for this project.

A simple property that will change after the phase transition, that is when $T > T_C$, is that a ferromagnet will no longer exhibit spontaneous magnetization. As such, the magnetization will go to 0 when $T \geq T_C$ when there is no external field present.

For more, see Hjorth-Jensen [2].

The Metropolis Algorithm

The metropolis algorithm is a type of Monte Carlo simulation, that is an algorithm where the system is sampled in a random way. The metropolis algorithm belongs to a family of Markov Chain Monte carol methods which simulate the time-evolution of stochastic systems.

³ Two micro-states corresponds to the same observable macro-state.

Specifically, for our system we pick L^2 spin-sites in the lattice for each Monte Carlo cycle, or sweep of the lattice. For each sample, we then perform the metropolis algorithm, which qualitatively evaluates the current state of the system, then evaluates the system if the spin of the current spin-site were to change. The likeliest state of the system is then chosen, and the energy and magnetization of the system is updated accordingly.

Or more precisely

1. For each Monte Carlo cycle, sample L^2 random spin-sites.
2. Compute the change in energy ΔE due to flipping the spin
3. If $\Delta E \leq 0$, set this as the new state of the system, and sample a new state.
4. Else, If $\Delta E < 0$ compute $w = e^{-\beta \Delta E}$, If $w \geq r$, where r is a random number in the interval $[0, 1)$, accept the flipped state, and sample a new one.
5. If neither of the prior two statements are true, the system remains in its current state and a new sample is chosen.

Afterwards, the expectation values are computed from the sums of all the states divided by the number of Monte Carlo cycles.

Further, because computing w is expensive, this algorithm is effectivized by pre-computing the possible energy changes of the system of which there are only 5, as shown in Hjorth-Jensen [2].

RESULTS AND DISCUSSIONS

Testing algorithm, L=2

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 shown⁴ in Fig. 7. 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.

⁴ Had some issues with figure placements, and no time to redo the report in something simpler to deal with than Revtex, so please excuse the poor placement of the larger figures.

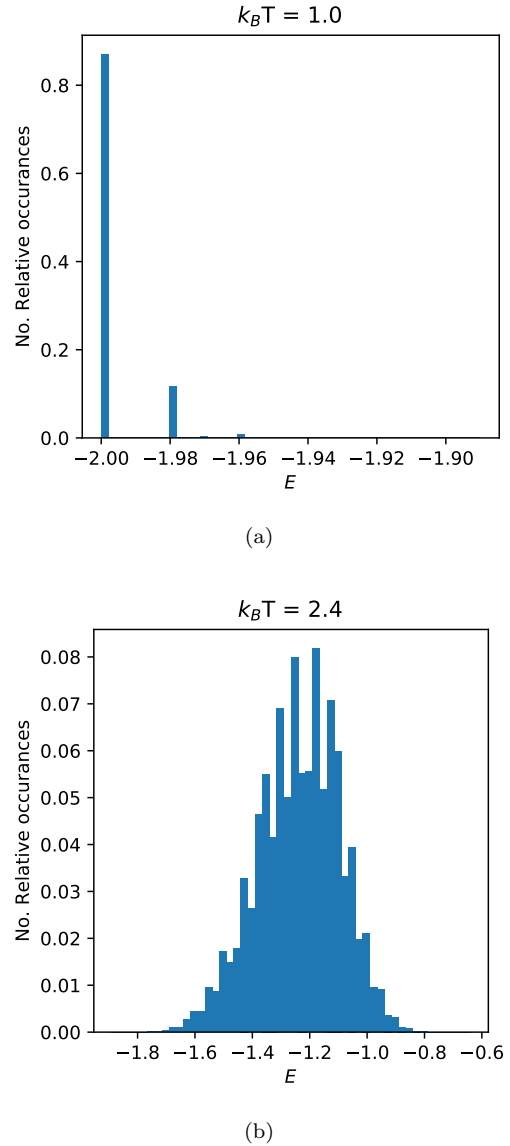


FIG. 6: Normalized histograms showing the relative no. occurrences of each energy in an equilibration time of 10^3 Monte Carlo cycles for $T = \{1, 2.4\}$.

Further investigations of the Ising model

Then, moving on to a larger, 20×20 lattice we see in Fig. 5 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 see that the acceptance rate for the initially disordered 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 ordered 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 disordered, 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.

Now, we look at the distribution of energy in these systems given an equilibration time of 10^3 Monte Carlo cycles, giving the system time to reach a steady-state. From Fig. 6 we see that the system at $T = 1$ is very thinly distributed, corresponding to a small variance. As we move on to $T = 2.4$, we see the energy of the system increasing and become more widely spread throughout a number of states, corresponding to a larger variance, and by extension, an increase in its heat capacity, as expected because $C_V \propto T^{-2}$.

Phase transitions

Finally, we look at Fig. 8, where we have simulated with $2 \cdot 10^6$ Monte Carlo cycles each for lattices of size $L \in \{40, 60, 80, 100\}$ for temperatures $T \in [2, 2.3]$. Note that temperatures $T < 2.14$ are omitted from the figure as there was no interesting behavior observed in this region. I first performed a rough sweep of 6 evenly placed temperatures in the range $T \in [2, 2.3]$, then another fine sweep in the region close to T_C of 10 points for $T \in [2.2, 2.3]$.

Here, we observe traits indicative of a phase transition happening, and as the lattice size increases, this seems to tend toward the theoretical $T_C(L = \infty)$ as we expect from Eqn. 15, however, from these lattice sizes one can at best claim that T_C exists somewhere in the range between $\sim 2.24, 2.3$ as it is difficult to approximate the critical temperature $T_C(L)$, from the resolution and accuracy of the data plotted in this figure.

CONCLUSIONS

We have seen how the metropolis algorithm can be used to study the Ising model numerically, and how it can successfully replicate theoretical results predicted by this model. We have further seen how the results produced by the algorithm will vary on a per-run basis, and that one can minimize this fluctuation by increasing the number of Monte Carlo cycles. Found indications a phase transitions, and by extension the Curie temperature to a precision of ~ 0.1 , but this result could be improved by running the algorithm for larger sizes, which could become feasible to compute if i were to parallelize the code to utilize multiple cores on my CPU, or perhaps my GPU. Sadly, development time was much more costly compared

to runtime⁵ when working on this project, so i did not prioritize reducing the runtime by parallelization.

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- [1] L. Onsager, *Phys. Rev.* **65**, 117 (1944).
 - [2] M. Hjorth-Jensen, "Computational physics lectures: Statistical physics and the ising model," (2017).
 - [3] D. V. Schroeder, *An Introduction to Thermal Physics*, 1st ed. (Pearson, 1999).
 - [4] M. Hjorth-Jensen, "Studies of phase transitions in magnetic systems, fys3150 project 4." (2018).

⁵ The scripts were ran overnight

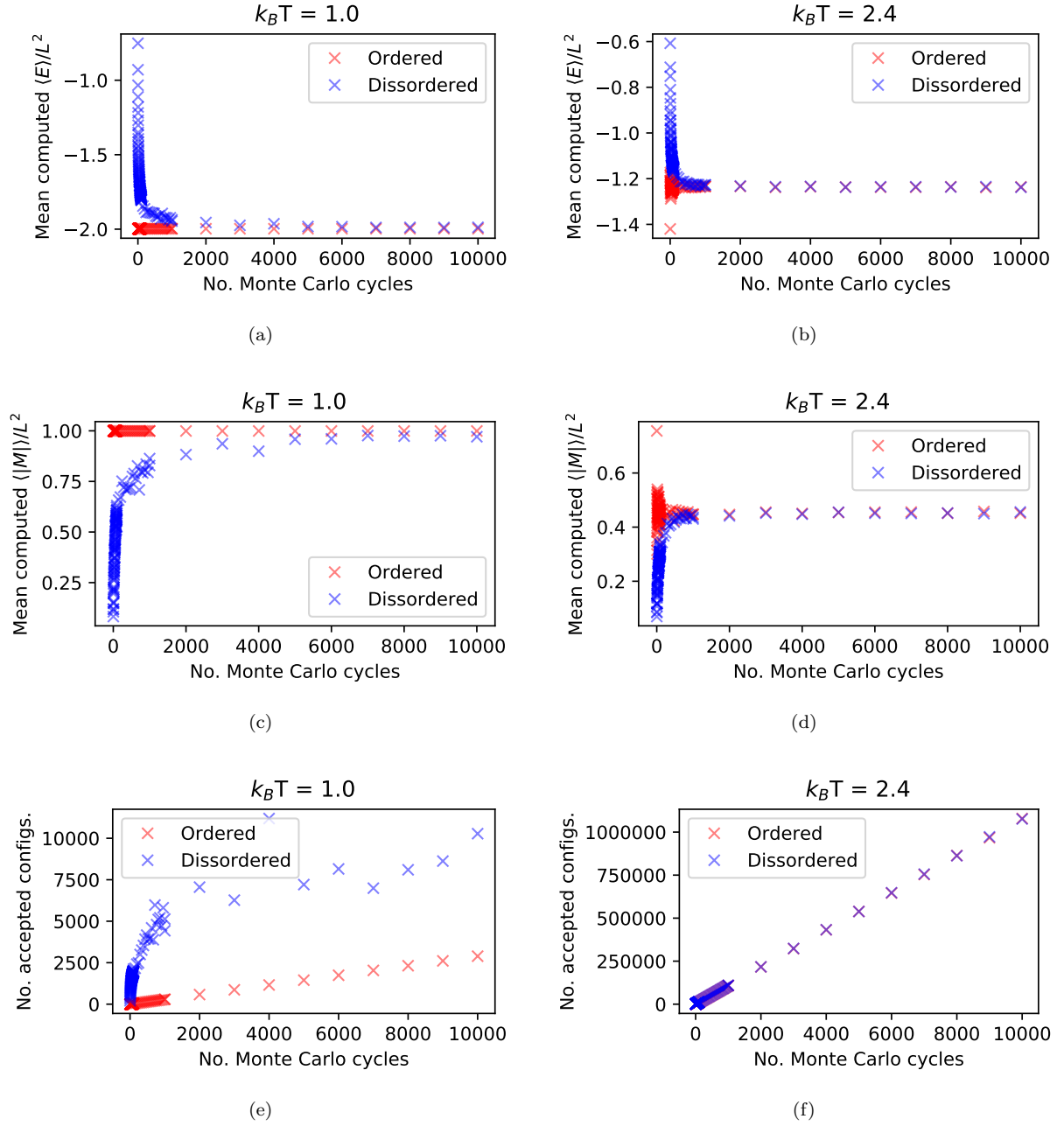


FIG. 5: Expectation values computed for different numbers of Monte Carlo cycles for an ordered initial state of spin-ups and random initial state, different for each computed expectation value.

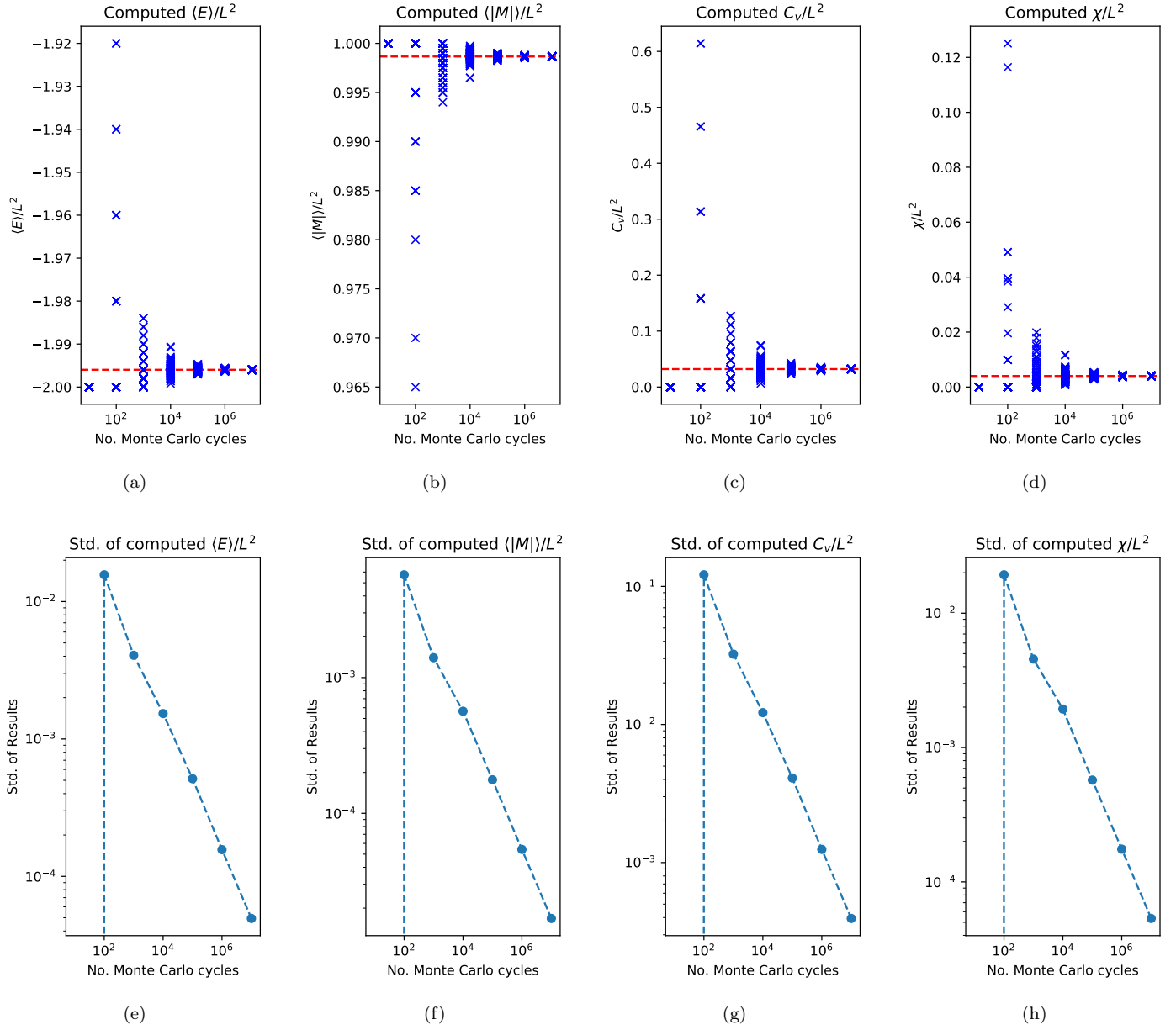
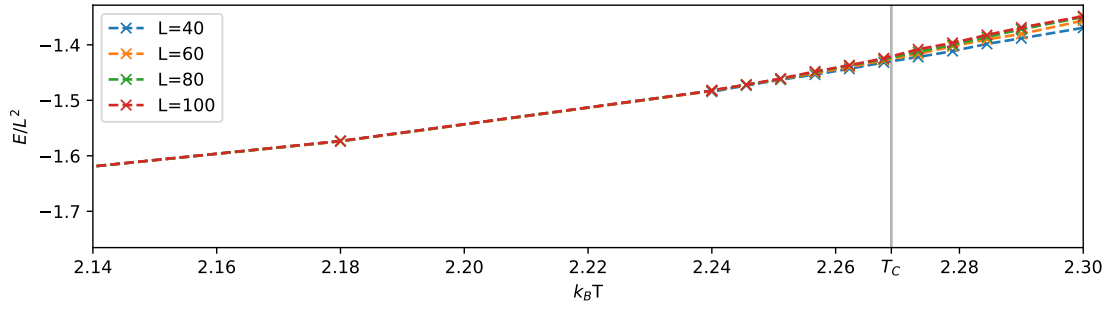
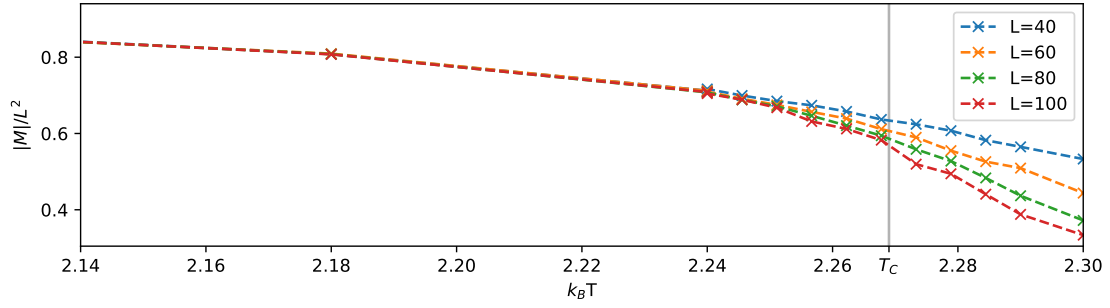


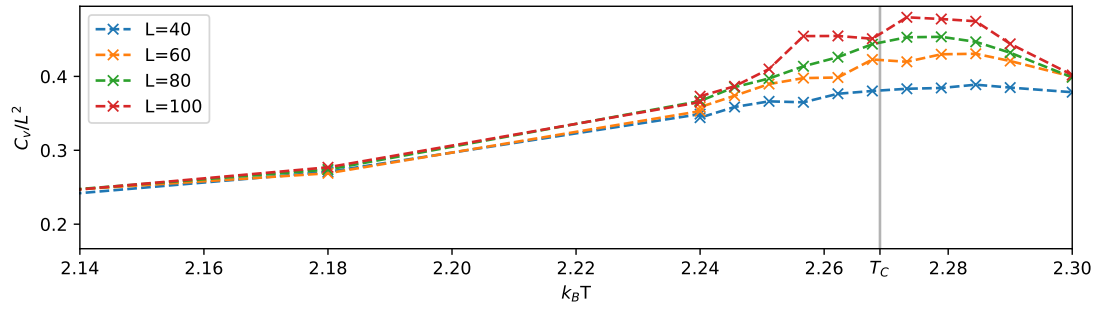
FIG. 7: (a-d) Computed results from running the algorithm 100 times per number of Monte Carlo cycles for select expectation values with an ordered initial state of a 2×2 lattice of spin ups at $k_B T = 1$, where the theoretical value is indicated by the dashed red line. (e-h) The standard deviation (Std.) of the computed results.



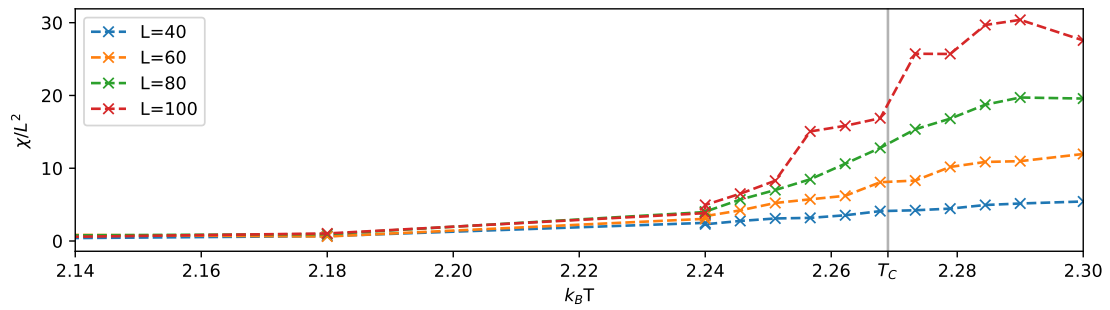
(a)



(b)



(c)



(d)

FIG. 8: Expectation values computed from $2 \cdot 10^6$ Monte Carlo cycles for $T \in [2, 2.3]$