Finite size scaling and first order phase transition in a
modified XY-model

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Abstract
Monte Carlo simulation has been performed in a two-dimensional modified XY-
model first proposed by Domany et.al [E. Domany, M. Schick and R. H. Swendsen,
Phys. Rev. Lett. 52, 1535 (1984)]. The cluster algorithm of Wolff has been used
and multiple histogram reweighting is performed. The first order scaling behavior of
the quantities like specific heat, order parameter susceptibility and free energy barrier
are found to be obeyed accurately. While the lowest order correlation function was
found to decay to zero at long distance just above the transition, the next higher order
correlation function shows a non-zero plateau.

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1 Introduction

More than two decades ago Domany et.al [1] proposed a generalization of the two-dimensional
XY- model where the shape of the usual $\cos \theta$ type potential could be modified with the

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help of a single parameter. The two-dimensional spins located at the sites of a square lattice interact with the nearest neighbors through a potential

\[ V(\theta_{ij}) = 2 \left[ 1 - \left( \cos^2 \frac{\theta_{ij}}{2} \right)^{p^2} \right] \]

where \( \theta_{ij} \) is the angle between the spins and \( p^2 \) is a parameter used to alter the shape of the potential. For \( p^2 = 1 \) the potential reproduces the conventional XY-model while for larger values of \( p^2 \) the potential well becomes narrower. The conventional two-dimensional XY model does not possess any true long range order which is ruled out by the Mermin Wagner theorem. However a continuous quasi-long-range-order-disorder transition resulting from the unbinding of topological defects [2, 3] is known to occur in this system and the order parameter correlation function is characterized by a slow algebraic decay instead of the fast exponential decay observed in a disordered system and this is referred to as the Kosterlitz-Thouless (KT) transition in literature. Domany et.al [1] performed Monte Carlo (MC) simulation and observed that as the potential well gets narrower with the increase in the parameter \( p^2 \), the continuous transition gets converted into a first order phase transition and for \( p^2 = 50 \) the transition is very sharp as is manifested by a huge peak in the specific heat. This phenomenon is in apparent contradiction with the prediction of the renormalization group theory according to which systems in the same universal class (having same symmetry of the order parameter and same lattice dimensionality) should exhibit the same type of phase transition with identical values of critical exponents.

The generalized XY-model of Eqn.1 has been analyzed by a number of authors [4, 5] using the renormalization approach of the Migdal-Kadanoff type. These investigators were of the opinion that the transition in the generalized XY-model appears to be first order in nature because the MC simulation of Domany et.al [1] and Himbergen [6] were carried out on relatively small lattices and for large system sizes the usual KT transition is expected to occur. Nearly a decade later, Mila [7] using the same sort of renormalization group analysis arrived at a similar conclusion. Lastly, using the same line of approach, Garel et.al [8] put forward a different type of interpretation of the above mentioned RG analysis and were of the view that the transition is indeed first order.

Minnhagen [9, 10, 11] has carried out a detailed study of the behavior of the phase transition exhibited by a 2-D Coulomb gas, which very well describes the characteristics of a 2-D system consisting of vortex-antivortex pairs. It was demonstrated that the KT behavior
is obtainable in a 2-D Coulomb gas only at low particle densities. For higher particle densities the charge unbinding transition was shown to be first order. Also a new gas-liquid like critical point was found in the 2-D Coulomb gas — the first order line in the temperature-particle density plane ends at a critical point. The KT transition line, obtainable at lower densities was seen to join smoothly with the first order line at a temperature slightly lower than the critical point. Jonsson, Minnhagen and Nylen [12] performed MC simulation in a 2-D XY-model with a modified potential, which essentially is equivalent to that of Eqn.(1) and established a new critical point. They determined the critical exponents for the system and interpreted the transition to be of the vortex unbinding type.

van Enter and Shlosman [13] presented a rigorous proof that various SO(n)-invariant n-vector models which have a deep and narrow potential well, would exhibit a first order transition. The model represented by Eqn.(1) is a member of this general class of systems. These authors based their proof on the so called method of reflection positivity, a technique borrowed from the field theory and used in statistical mechanics. van Enter and Shlosman argued that in spite of the order parameter in 2-D n-vector model being predicted to vanish by the Mermin-Wagner theorem, long range order prevails in the system via higher order correlation functions. More recently, S. Ota and S. B. Ota [14] have performed MC simulation of the modified XY-model using microcanonical ensemble and have identified a first order phase transition in the system.

The present article describes MC simulation of the 2-D modified XY-model where computations have been performed on systems of reasonably large size and finite size scaling rules for first order phase transition have been tested on the results of the simulation. The motivation is to resolve the question on the nature of the phase transition in this model and the contradictions among the views put forward by different investigators for the last quarter of a century as has been summed up above. Our observation is that the transition is indeed first order for a large value of the parameter $p^2$ (we have used $p^2 = 50$) as all finite size scaling rules are nicely obeyed. We however have made no attempt to investigate the existence of the critical point in this model or to determine the critical exponents as has been done by Jonsson et.al [12] in relatively small systems. Among other observables we have computed the spin-spin angular correlation functions of different orders. We observe that while the lowest order correlation function decays to zero, the next higher order corre-
lation function has a finite plateau which is in accordance with statement of van Enter and Sholsman [13].

Another interesting aspect of our work is the application of the Wolff cluster algorithm [15] to simulate the model. It has been pointed out by a numbers of workers [1, 16] that the two-dimensional model is difficult to simulate using the conventional single spin flip Metropolis algorithm [17]. To increase the reliability of the results we have used the multiple histogram reweighting, due to Ferrenberg and Swendsen [18] along with the Lee and Kosterlitz’s method [19] of finite size scaling for a first order phase transition.

2 The definition of the thermodynamic quantities related to the model

The Monte-Carlo simulation was carried out on a square lattice of dimension $L \times L$ with the two-dimensional spins located at each site and interacting with the nearest neighbors via the Hamiltonian

$$H = \sum_{\langle ij \rangle} 2 \left[ 1 - \left( \cos^2 \frac{\theta_{ij}}{2} \right)^2 \right]$$

(2)

The specific heat at a dimensionless temperature $T$ is related to the energy fluctuation

$$C_v = \frac{\langle (H^2) - \langle H \rangle^2 \rangle}{NT^2}$$

(3)

where $N$ is the number of spins. The conventional long range order parameter is given by

$$\langle P_1 \rangle = \langle \cos \theta \rangle$$

(4)

where $\theta$ is the angle that a spin makes with the preferred direction of orientation and the average is over the entire sample. The next higher rank order parameter is defined as

$$\langle P_2 \rangle = \frac{1}{2} \langle 3\cos^2 \theta - 1 \rangle$$

(5)

The order parameter susceptibility is defined in terms of the fluctuations of the order parameter $\langle P_1 \rangle$

$$\chi = \frac{\langle (P_2^2) - \langle P_1 \rangle^2 \rangle}{T^2}$$

(6)
The first rank pair correlation coefficient is defined as
\[ G_1(r) = \langle \cos \theta_{ij} \rangle_r \tag{7} \]
where \( i \) and \( j \) are two spins separated by a distance \( r \). The second rank pair correlation coefficient is defined as
\[ G_2(r) = \langle P_2(\cos \theta_{ij}) \rangle_r \tag{8} \]

3  The computational details

In this section we briefly describe the Wolff cluster algorithm, the Ferrenberg-Swendsen multiple histogram reweighting technique and the Lee-Kosterlitz finite size scaling for first order phase transition. The Monte-Carlo(MC) simulations were performed on square lattices of size \( L^2 \) for \( L = 16, 32, 64, 96, 128, 160 \) and 192. We have used Wolff’s cluster flip algorithm, the essential steps of which are as follows.

(1) A random unit vector \( \vec{r} \) is taken and a spin flip \( \vec{\sigma}_x \rightarrow \vec{\sigma}'_x \) is defined as

\[ \vec{\sigma}'_x = \vec{\sigma}_x - 2 (\vec{\sigma}_x, \vec{r}) \vec{r} \tag{9} \]

(2) Bonds \((x, y)\) of the lattice are activated with a probability

\[ P(x, y) = 1 - \exp \left( \min \{0, \beta S_7\} \right) \tag{10} \]

where,

\[
\begin{align*}
S_7 &= S_6 - S_5 \\
S_6 &= 2 \left( \frac{1 + S_1}{2} \right)^{p^2} \\
S_5 &= 2(S_4)^{p^2} \\
S_4 &= \frac{(1 + (S_1 - 2S_2S_3))}{2} \\
S_3 &= (\vec{\sigma}_y, \vec{r}) \\
S_2 &= (\vec{\sigma}'_x, \vec{r}) \\
S_1 &= (\vec{\sigma}'_x, \vec{\sigma}_y)
\end{align*}
\]

This process leads to the formation of a cluster on the lattice.
(3) All spins in a cluster are now flipped according to $\vec{\sigma}_x \rightarrow \vec{\sigma}'_x$

We have calculated the thermodynamic quantities using multiple histogram reweighting technique of Ferrenberg and Swendsen [18], which is briefly described below. The partition function of the system is given by

$$Z(\beta) = \sum_E \rho(E) \exp[-\beta E]$$  \hspace{1cm} (11)

where $\rho(E)$ is the density of states, $\beta = 1/T$ (the Boltzmann constant has been set equal to unity) and $E$ is the energy of the system. In the histogram reweighting method, energy histograms are generated at a number of temperatures $\beta_i$ with $i = 1, 2, \ldots, R$ and $N_i(E)$ is the histogram count for the $i^{th}$ temperature. We denote by $n_i$ the total number of configurations generated in the $i^{th}$ simulation, i.e, $n_i = \sum_E N_i(E)$. According to references [18] and [20], the best estimate of the density of states, obtained after histogram reweighting, is given by

$$\rho(E) = \frac{\sum_{i=1}^{R} g_i^{-1} N_i(E)}{\sum_{j=1}^{R} n_j g_j^{-1} Z_j^{-1} \exp[-\beta_j E]}$$  \hspace{1cm} (12)

where, $g_i = 1 + 2\tau_i$, $\tau_i$ being the auto-correlation time for energy at the $i^{th}$ temperature. Substituting eqn.(13) in eqn.(12) gives us a self consistent equation for the partition function at any temperature $\beta$:

$$Z(\beta) = \sum_E \frac{\sum_{i} g_i^{-1} N_i(E) \exp[-\beta E]}{\sum_{j} g_j^{-1} n_j Z_j^{-1} \exp[-\beta_j E]}$$  \hspace{1cm} (13)

One can also carry out the computation in terms of the probability instead of the partition function. The unnormalized probability for an energy $E$ in the $k^{th}$ simulation is given by

$$p_k(E) = \rho(E) \exp[-\beta_k E]$$  \hspace{1cm} (14)

i.e.,

$$Z(\beta_k) = \sum_E p_k(E)$$  \hspace{1cm} (15)

The free energy at the temperature $\beta_k$ is

$$f_k = -\frac{1}{\beta_k} \ln Z(\beta_k)$$  \hspace{1cm} (16)
\[
\exp(-\beta f) = \sum_E p_k(E) = Z(\beta)
\]

(17)

In place of eqn.(14) we get a self consistent equation for the reweighted probability,

\[
p_k(E) = \frac{\sum_i g_i^{-1} N_i(E) \exp[-\beta E]}{\sum_j g_j^{-1} n_j \exp[\beta (f_j - E)]}
\]

(18)

The best estimate of the energy or any other observable \(Q\) is given by \[20\]

\[
\langle Q \rangle = \frac{1}{Z(\beta)} \sum_{i,s} g_i^{-1} Q_{is} \exp[-\beta E_{is}]
\]

(19)

where \(Q_{is}\) is the histogram count of the observable \(Q\) in the state \(s\) obtained during the \(i^{th}\) simulation and \(E_{is}\) is the total energy of such a state. The factors \(g_k\) now correspond to the observable \(Q\). Lee and Kosterlitz \[19\] proposed a convenient method for the determination of the order of the phase transition which can be applied to systems having linear dimension less than the correlation length. For a temperature driven first order transition in a finite system of volume \(L^d\) with periodic boundary condition one needs to compute the histogram count of the energy distribution denoted by \(N(E; \beta, L)\). The \(p^2 = 50\) model has a characteristic double peak structure for \(N(E; \beta, L)\) in the neighborhood of the transition temperature. The two peaks of \(N\) at \(E_1(L)\) and \(E_2(L)\) corresponding respectively to the ordered and disordered phases are separated by a minimum at \(E_m(L)\). A free-energy-like quantity is defined as

\[
A(E; \beta, L, \mathcal{N}) = -\ln N(E; \beta, L)
\]

(20)

where \(\mathcal{N}\) is the number of configurations generated. The quantity \(A(E; \beta, L, \mathcal{N})\) differs from the free energy \(F(E; \beta, L)\) by a temperature and \(\mathcal{N}\) dependent additive quantity. A bulk free energy barrier can therefore be defined as

\[
\Delta F(L) = A(E_m; \beta, L, \mathcal{N}) - A(E_1; \beta, L, \mathcal{N})
\]

(21)

It may be noted that at the transition temperature, \(A(E_1; \beta, L, \mathcal{N}) = A(E_2; \beta, L, \mathcal{N})\) and \(\Delta F\) is independent of \(\mathcal{N}\). For a continuous transition \(\Delta F(L)\) is independent of \(L\) and for a temperature driven first order transition it is an increasing function of \(L\), even when \(L\) is
smaller than the correlation length, $\xi$, prevailing at the system at the transition temperature. If one is in a region where $L$ is much greater than $\xi$, then $\Delta F$ obeys the scaling relation [19]

$$\Delta F \sim L^{d-1}$$  \hspace{1cm} (22)

Clearly, the temperature at which the double-well structure of $A$ has two equally deep minima gives a precise estimation of the transition temperature.

## 4 Results and discussion

Square lattices of linear dimension $L$ ranging from 16 to 192 were simulated and for each lattice simulations were performed at 9 to 13 temperatures in the neighborhood of the transition to record the histograms for energy. In Table 1 we have depicted for each lattice size and temperature the technical quantities of interest. These include the number of Wolff clusters generated ($n_c$), the percentage of average cluster size in units of lattice size for each temperature $\langle c \rangle$, the number of equivalent Monte Carlo sweeps (MCS) and the energy auto-correlation time $\tau_e$. The number of configurations generated ranges from about $10^8$ to $10^9$. In Fig.1 we have plotted the percentage of average cluster size in units of the lattice size $\langle c \rangle$ against temperature for $L = 128$. It is clear that the average cluster size for a given lattice, decreases with increase in temperature and there is a sharp fall at the transition. The maximum cluster size in units of the lattice size is about 84.4% (for $L = 16$) and is seen to decrease with increase in the system size. The auto-correlation time, which was calculated by the method proposed by Madras and Sokal [21], is seen to increase rapidly with the increase in lattice size and possesses a sharp maximum at the transition temperature. The logarithm of the peak value of the energy auto-correlation time has been plotted against $L$ in Fig.2. We find empirically a scaling rule, $\ln \tau_e \sim L^\phi$ where $\phi = 3.05$. The behavior of the order parameter correlation time $\tau_o$ is found to be similar in nature as that of $\tau_e$.

The energy histograms obtained for $L = 128$ are shown in Fig.3. For this lattice, simulations were performed at 13 temperatures ranging from 1.0000 to 1.0175. This temperature range is rather small and were chosen to bracket the transition temperature. This diagram shows that there is an energy range where almost no sampling takes place for any temperature and there are dual peaked histograms at a number of temperatures where sampling takes place with one peak in the ordered phase and the other in the disordered phase. The
existence of these dual peaked histograms is a signature of a first order phase transition where two phases can coexist at a given temperature.

The error in estimating the reweighted probability \( p_k(Q) \) from the raw histograms is given by

\[
\delta p_k (Q) = \frac{1}{\left[ \sum_{n=1}^{R} g_n^{-1}(q)N_n(q) \right]^{1/2} p_k (Q)}
\]  

and this can be estimated directly from the histogram counts. The percentage error in
Figure 3: The histograms for $E$, the average energy per particle generated for the $128 \times 128$ lattice for the $p^2 = 50$ model at the 13 temperatures indicated.

Figure 4: The average energy per particle $E$ plotted against dimensionless temperature $T$ for different lattice sizes. For clarity error bars are shown only for $L = 16, 160$ and $192$.

The reweighted probability for energy in the lattice $L = 192$ is about 0.74% where the raw histograms have peaks in the ordered phase. In the intermediate energy range where little sampling takes place for any choice of temperature the error is evidently large and this cannot be significantly reduced by any realistic effort.

Fig. 4 shows the temperature variation of the energy for a number of lattices, as is obtained by applying histogram reweighting technique. From the energy histograms, we
have calculated the free energy like quantity $A$, defined as $A(E; \beta, L, N) = -\ln N(E; \beta, L)$ where $N(E; \beta, L)$ is the histogram count of the energy distribution. The free energy barrier $\Delta F(L)$ was evaluated and in Fig.5 we have plotted $\Delta F$ against $L$ where a good linear fit has been obtained. This is a direct verification of the scaling rule $\Delta F \sim L^{d-1}$ of Lee and Kosterlitz [19] since the lattice dimensionality $d = 2$ in this model. We further note that the scaling relation is well obeyed down to $L = 16$ which happens to be of the order of the correlation length, $\xi$ for the system, as one can estimate from the relation $\Delta F(\xi) \approx 1$ [19].

The specific heat $C_v$ was obtained from the energy fluctuation and Fig.6 shows its temperature variation. It is evident that the peak height of $C_v$ grows rapidly at the transition. From Fig.7 where the maxima of $C_v$ are plotted it is clear that the standard scaling rules $C_v \sim L^d$ for first order transition [22] are accurately obeyed in this model.

We have also tested the the finite size scaling relation

$$T_c(L) - T_c(\infty) \sim L^{-d}$$

which is valid for a first order phase transition [22]. $T_c(\infty)$ represents the thermodynamic limit of the transition temperature $T_c$. We have estimated the transition temperature in two ways — $T_c^{C_v}$ is the estimate of $T_c$ obtained from the peak position of the specific heat $C_v$ and $T_c^F$ represents the transition temperature obtained from the fine tuning of the free energy vs energy curve to obtain two equally deep minima. In Fig.8 the transition temperatures thus obtained have been plotted against $L^{-2}$. It is seen that the linear fits are
Figure 6: The specific heat $C_v$ plotted against temperature $T$ for different lattice sizes. For clarity only the above lattice sizes are shown and the error bars have been indicated for two lattice size.

Figure 7: The peak heights of $C_v$ plotted against $L^2$ with the linear fit represented by the straight line. The error bars for most points are smaller than the dimensions of the symbols used for plotting.

good within statistical errors and the thermodynamic limit of the transition temperature is $1.00897 \pm 6 \times 10^{-5}$, within which the two linear fits are seen to converge.

The pair correlation functions $G_1(r)$ and $G_2(r)$ were calculated for temperatures $T = 1.0081, 1.0085, 1.0092$ and $1.0095$ for $L = 128$ and are shown in Fig. 9 and 10. The first two of these temperatures are less than the transition temperature for this lattice while
Figure 8: The transition temperature $T_c$ obtained from (a) specific heat peak position and (b) fine tuning of free energy curve plotted against $L^{-2}$ along with the respective linear fits. The intercept on the Y-axis is $1.00897 \pm 6 \times 10^{-5}$.

Figure 9: The plots of the pair correlation function $G_1(r)$ against $r$ for the $128 \times 128$ lattice for the temperatures indicated. The curves are plotted for $r$ ranging up to $L/2$.

the other two temperatures are in the disordered phase. The curves have been fitted to a power law $G_i(r) = a_i r^{-b_i} + f_i$ for $i = 1$ and 2. It may be noted that the parameter $f$ is the asymptotic value of the pair correlation function. We observe that while the first rank correlation function $G_1(r)$ decays to zero at the two higher temperatures ($f_1 = 0$), this is not the case for the higher rank correlation function $G_2(r)$ ($f_2 \sim 0.22$). In other words, while the lowest rank correlation among the spins vanishes just above transition, the next higher rank correlation continues to persist.
Figure 10: The plots of the pair correlation function $G_2(r)$ against $r$ for the $128 \times 128$ lattice for the temperatures indicated. The curves are plotted for $r$ ranging up to $L/2$.

5 Conclusions

The simulations in the two dimensional modified XY-model presented in this communication show that all the first order finite size scaling rules are obeyed. Computation has been performed in system size up to $192 \times 192$ which may be considered to be reasonably large for the purpose of arriving at a conclusion regarding the behavior of the model. We are inclined to conclude that the model exhibits a first order phase transition. This is in agreement with the views of some of the earlier investigators including Domany et.al [1] and van Enter and Shlosman [13]. The existence of a quasi-long-range-order-disorder transition observed in the 2-D XY-model is known to be due to vortex-antivortex unbinding (KT transition). In absence of the role played by the vortices, one would not observe any order-disorder transition in the XY-model in accordance with the Mermin-Wagner theorem. In the class of models we have investigated the role played by the vortices changes qualitatively with change in $p^2$ (which increases the non-linearity of the potential well) as has been seen in the early work of Himbergen [6]. Also we have seen that the number of vortex pairs grows rapidly with the increase in $p^2$ [23]. Qualitatively, one may therefore think that the modified XY-model for large values of $p^2$, behaves like a dense defect system and gives rise to a first order phase transition as has been predicted by Minnahagen [9, 10, 11].

A similar change in the nature of phase transition has been observed to occur in a two-dimensional Lebwohl-Lasher model and a modified version of it [24]. The potentials in these
two models are \(-P_2(\cos \theta)\) and \(-P_4(\cos \theta)\) respectively, the latter having a greater amount of non-linearity. Although both models are in the same universality class, it was observed that while the \(-P_2(\cos \theta)\) potential leads to a continuous transition, the modified model with \(-P_4(\cos \theta)\) potential exhibits a strong first order phase transition. It has also been noticed that the suppression of the defects in these models leads to a total disappearance of the phase transitions \[25\].

We mention another point before ending this section. This is the performance of Wolff cluster algorithm which turned out to be very convenient to simulate the model. Conventional algorithms, as we have seen, does not work well in this model. Our earlier attempt \[16\] using the recently developed Wang-Landau (WL) algorithm \[26\] which directly determines the density of states of a system is also not a good choice for simulating this model. The main problem while using the WL algorithm is that configurations near the minimum energy take a very long time to be sampled during the random walk and it becomes impractical to simulate continuous models of even moderate size because of the huge CPU time that becomes necessary. Among other things, a great virtue of the Wolff algorithm is that it does not contain any adjustable parameter even while simulating a continuous model.

Besides using the Wolff algorithm for the simulation we have used the Ferrenberg-Swendsen multiple histogram reweighting technique and the finite size scaling rules of Lee and Kosterlitz. We conclude by noting that a combination of these computational tools till now provides a very efficient and accurate method of analyzing results obtained in an unknown system.

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Table 1: $T$ is the dimensionless temperature, $L$ is the lattice size, $n_c$ is the number of Wolff clusters, which varies from $1.1 \times 10^8$ to $10^9$ with lattice sizes, $(c)$ is the average cluster size as percent of the lattice size, MCS is the number of equivalent Monte Carlo sweeps in units of $10^8$ and $\tau_c$ is the auto-correlation time for energy (in units of Wolff clusters).

| $L = 192$ | $T$ | $n_c$ | $MCS$ | $\tau_c$ |
|-----------|-----|-------|-------|---------|
|           | 1.0025 | 1.0050 | 1.0075 | 1.0085 | 1.0087 | 1.0089 | 1.0090 | 1.0091 | 1.0093 | 1.0100 | 1.0112 | 1.0125 |
|           | $10^8$ | $10^9$ | $10^8$ | $10^8$ | $10^8$ | $10^8$ | $10^8$ | $10^8$ | $10^8$ | $10^8$ | $10^8$ | $10^8$ |
|           | 67 | 64 | 60 | 56 | 56 | 50 | 5 | 2 | 0.59 | 0.34 | 0.21 | 0.16 |
| $MCS$ | 6.71 | 6.46 | 6.04 | 5.67 | 5.60 | 5.06 | 0.586 | 0.233 | 0.059 | 0.034 | 0.021 | 0.016 |
| $\tau_c$ | 239 | 349 | 808 | 2522 | 4342 | 211246 | 1802195 | 1194159 | 82892 | 57193 | 55714 | 53209 |

| $L = 160$ | $T$ | $n_c$ | $MCS$ | $\tau_c$ |
|-----------|-----|-------|-------|---------|
|           | 1.0025 | 1.0050 | 1.0075 | 1.0087 | 1.0090 | 1.0093 | 1.0100 | 1.0112 | 1.0125 |
|           | $10^8$ | $10^9$ | $10^8$ | $10^8$ | $10^8$ | $10^8$ | $10^8$ | $10^8$ | $10^8$ |
|           | 69 | 65 | 60 | 56 | 58 | 41 | 9 | 1 | 0.76 | 0.36 | 0.25 | 0.19 |
| $MCS$ | 6.74 | 6.50 | 6.08 | 5.60 | 1.81 | 0.09 | 0.049 | 0.031 | 0.023 |
| $\tau_c$ | 239 | 354 | 788 | 3873 | 185157 | 54589 | 44409 | 37398 | 39685 |

| $L = 128$ | $T$ | $n_c$ | $MCS$ | $\tau_c$ |
|-----------|-----|-------|-------|---------|
|           | 1.0000 | 1.0025 | 1.0050 | 1.0075 | 1.0080 | 1.0085 | 1.0090 | 1.0093 | 1.0100 | 1.0125 | 1.0150 | 1.0175 |
|           | $9 \times 10^9$ | $9 \times 10^9$ | $9 \times 10^8$ | $9 \times 10^8$ | $9 \times 10^8$ | $9 \times 10^8$ | $9 \times 10^8$ | $9 \times 10^8$ | $9 \times 10^8$ |
|           | 70 | 67 | 65 | 62 | 60 | 58 | 47 | 20 | 1 |
| $MCS$ | 6.30 | 6.14 | 5.93 | 5.58 | 5.45 | 5.23 | 4.25 | 1.86 | 1.33 |
| $\tau_c$ | 185 | 242 | 344 | 780 | 1111 | 1906 | 838017 | 84172 | 33708 |
| $\pi$ | 27202 | 24802 | 21925 | 20478 |

| $L = 64$ | $T$ | $n_c$ | $MCS$ | $\tau_c$ |
|-----------|-----|-------|-------|---------|
|           | 1.0000 | 1.0025 | 1.0050 | 1.0075 | 1.0081 | 1.0087 | 1.0093 | 1.0100 | 1.0125 | 1.0150 | 1.0175 | 1.0200 |
|           | $8 \times 10^8$ | $8 \times 10^8$ | $8 \times 10^8$ | $8 \times 10^8$ | $8 \times 10^8$ | $8 \times 10^8$ | $8 \times 10^8$ | $8 \times 10^8$ | $8 \times 10^8$ |
|           | 70 | 69 | 66 | 63 | 61 | 56 | 43 | 15 | 1 |
| $MCS$ | 5.66 | 5.52 | 5.34 | 5.04 | 4.92 | 4.55 | 3.46 | 1.27 | 0.11 |
| $\tau_c$ | 181 | 229 | 319 | 977 | 2451 | 3720 | 49156 | 249144 | 136940 |
| $\pi$ | 20637 |

| $L = 32$ | $T$ | $n_c$ | $MCS$ | $\tau_c$ |
|-----------|-----|-------|-------|---------|
|           | 0.9900 | 1.0000 | 1.0050 | 1.0075 | 1.0100 | 1.0112 | 1.0125 | 1.0137 | 1.0150 | 1.0200 | 1.0300 | 1.0400 |
|           | $1.7 \times 10^9$ | $1.7 \times 10^9$ | $1.7 \times 10^8$ | $1.7 \times 10^8$ | $1.7 \times 10^8$ | $1.7 \times 10^8$ | $1.7 \times 10^8$ | $1.7 \times 10^8$ | $1.7 \times 10^8$ |
|           | 76 | 72 | 68 | 65 | 52 | 39 | 23 | 11 | 7 |
| $MCS$ | 1.29 | 1.23 | 1.16 | 1.10 | 0.88 | 0.67 | 0.39 | 0.19 | 0.11 |
| $\tau_c$ | 110 | 170 | 561 | 2149 | 7488 | 8420 | 7941 | 6152 | 4070 |
| $\pi$ | 1556 | 1355 | 1290 |

| $L = 16$ | $T$ | $n_c$ | $MCS$ | $\tau_c$ |
|-----------|-----|-------|-------|---------|
|           | 0.9500 | 0.9750 | 1.0000 | 1.0062 | 1.0125 | 1.0188 | 1.0219 | 1.0250 | 1.0312 | 1.0375 | 1.0500 | 1.0800 | 1.1000 |
|           | $1.1 \times 10^8$ | $1.1 \times 10^8$ | $1.1 \times 10^8$ | $1.1 \times 10^8$ | $1.1 \times 10^8$ | $1.1 \times 10^8$ | $1.1 \times 10^8$ | $1.1 \times 10^8$ | $1.1 \times 10^8$ |
|           | 84 | 80 | 74 | 66 | 57 | 38 | 25 | 17 | 8 |
| $MCS$ | 0.93 | 0.889 | 0.816 | 0.734 | 0.631 | 0.425 | 0.275 | 0.197 | 0.094 |
| $\tau_c$ | 73 | 82 | 269 | 657 | 1226 | 1593 | 1560 | 1259 | 736 |
| $\pi$ | 507 | 332 | 319 | 281 |