Computer simulation of two continuous spin models using Wang-Landau-Transition-Matrix Monte Carlo Algorithm

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Abstract
Monte Carlo simulation using a combination of Wang Landau (WL) and Transition Matrix (TM) Monte Carlo algorithms to simulate two lattice spin models with continuous energy is described. One of the models, the one-dimensional Lebwohl-Lasher model has an exact solution and we have used this to test the performance of the mixed algorithm (WLTM). The other system we have worked on is the two dimensional XY-model. The purpose of the present work is to test the performance of the WLTM algorithm in continuous models and to suggest methods for obtaining best results in such systems using this algorithm.

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1 Introduction

The Metropolis algorithm [1], proposed more than half a century ago has proved to be a very important and useful tool in Monte Carlo (MC) simulation, for the prediction of

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equilibrium thermodynamic properties of a large variety of systems. In this method one generates a large number of microscopic states of a system according to their canonical probabilities and the averages of different observables are calculated directly. However, problems crop up in the neighbourhood of a critical point, where due to critical slowing down it becomes rather difficult to overcome the large correlation time problem and get reliable results. Also for simulating systems with difficult potential energy landscapes as in proteins, spin-glasses etc, simulation using Metropolis algorithm results in trapping of the random walker in a potential energy minimum resulting in rather inefficient sampling.

During the last couple of decades or so a number of MC algorithms have been proposed which are designed to overcome the shortcomings of the Metropolis algorithm. To deal with the critical slowing down in a discrete spin model a cluster algorithm was proposed by Swendsen and Wang, while the Wolff cluster algorithm has proved to be an important tool for simulating continuous spin models. The multiple histogram reweighting technique of Ferrenberg and Swendsen emerged as a very useful method of improving the results obtainable from MC simulations in general.

Instead of tracing out the historical development of the MC algorithms, detailed discussion of most of which may be found in recent books like Newman and Berkema and Landau and Binder, we mention two algorithms which are of particular relevance to the subject of this communication. One of these is the Transition Matrix Monte Carlo (TMMC) algorithm developed by Oliveria et al and subsequently generalized by Wang and co-workers. The other algorithm, which was developed by Wang and Landau and goes by their name (WL), has drawn wide attention of researchers since its inception. Both of these methods determine the density of states (DOS) of a system as a function of one or more macroscopic observables like energy, order parameter, correlation function etc. A knowledge of the DOS enables one to determine the partition function or the averages of other thermodynamic quantities by the usual Boltzmann reweighting procedure. Both TMMC and WL algorithms depend on broad sampling of the phase space and are easy to implement. While the WL algorithm
is capable of an efficient sampling of the phase space, the TMMC method gives more accurate estimates of the DOS and this improves with longer MC runs. Shell and co-workers in 2003 \cite{13} proposed an algorithm which combines the TMMC and WL algorithms in an efficient way so as to make best use of the benefits of each algorithm. The new algorithm, known as the Wang Landau Transition Matrix (WLTM) Monte Carlo algorithm, uses the WL sampling scheme along with the TMMC method so as to result in an algorithm which is both efficient and accurate. The method was tested by Shell et. al \cite{13} in two dimensional Ising model and a Lenard-Jones fluid which suggests that the method is capable of handling both discrete and continuous systems.

In this communication we have performed elaborate WL and WLTM simulation of two continuous spin models. Continuous models are understandably more laborious and difficult subjects of MC simulation and need special considerations regarding the choice of certain parameters — a problem one does not encounter while simulating a discrete model. The aim of this paper is to critically judge the performance of WL and WLTM methods in continuous systems. We have investigated the manner in which the performance of the WLTM algorithm in particular could be improved in such systems. We have chosen i) the one dimensional Lebwohl-Lasher (1-d LL) model \cite{23} and ii) the two dimensional XY (2-d XY) model for this purpose. The reason for the choice of the former is that the model is exactly solvable \cite{24} and hence one can compare the performance of the WLTM algorithm with the exact results. This is analogous to the practice where the results of a new MC algorithm is being compared with the exact results on a 2d Ising model. For the XY-model, where the exact partition function is not available, we have compared our results with the results of the conventional Metropolis simulation.

The scheme of the presentation is as follows. The WL, TMMC and WLTM algorithms are briefly described in the next section. In section 3 we have described the models we have worked upon. Computational details appear next and is followed by the results we have obtained.
2 The different algorithms

2.1 The Wang Landau algorithm

In a system where the energy can take up continuous values, discretization of the energy range is necessary to label the macrostates of a system. The allowed energy range is divided into a number of bins, and the mean energy of the $I^{th}$ bin is taken as $E_I$. The WL algorithm directly determines the density of states (DOS) of the system as a function of $E_I$ which is precisely the number of microscopic configurations which have energy lying in the range which corresponds to the $I^{th}$ bin. This therefore is just the degeneracy factor which is denoted by $\Omega(I)$ and it is natural to consider bin-widths which are sufficiently small. Of course one can perform WL simulation to determine the DOS as a function of quantities other than energy like, say, the order parameter, correlation function etc. Also, a determination of DOS (more precisely, joint density of states, JDOS) as a function of two variables is possible and is necessary in many situations \cite{25, 26, 27, 28}.

For a macroscopic system, $\Omega(I)$ is a large number, and it is convenient to work with its logarithm, $g(I) = \ln \Omega(I)$. At the beginning of the simulation one has no knowledge of the $g(I)$’s — these are therefore set equal to zero for all values of $I$ and the algorithm generates the DOS profile, which progressively becomes closer to the actual DOS of the system, by an iterative process, which is briefly outlined below. Since the DOS is independent of temperature, and contains complete information about the system, the task is to determine it (or the JDOS, if necessary) as accurately as possible. The rest of the work, which involves the determination of the partition function $Z$ or other thermodynamic quantities at any temperature is done in a simple and straightforward manner by the standard Boltzmann reweighting procedure.

The implementation of the WL algorithm is done in the following manner. One starts with some microscopic configuration and a random walk is generated by rotating the spins (one at a time, in our case). Thus starting from a microstate $i$ one generates another state $j$. The probability with which the transition $i \rightarrow j$ is accepted is given by,

$$P(i, j) = \min \left( \frac{\Omega(I)}{\Omega(J)}, 1 \right)$$  

(1)
where \( i \in I \) and \( j \in J \) relates the microstates with the corresponding macrosates. Thus the probability of acceptance is inversely proportional to the current value of the DOS. In the event of the new state being accepted one makes the following modifications:

\[
g(J) \rightarrow g(J) + \ln f \tag{2a}
\]

\[
\text{and} \quad H(J) \rightarrow H(J) + 1 \tag{2b}
\]

Here \( H(I) \) represents the histogram count of the \( I^{th} \) bin and, \( f \) is a modification factor whose initial value is greater than 1 (in our case we started with \( \ln f = 1 \)). In case the probability test (1) fails, the changes given in equation (2) are made to the bin labelled by \( I \) instead of \( J \). This procedure is continued till the histogram becomes sufficiently flat, which may be say 90%. This means that the histogram count \( H(I) \) for each value of \( I \) is at least 90% of the average \( \left( \sum_{I=1}^{M} H(I) \right) / M \), where \( M \) is the number of bins. When this condition is fulfilled, one iteration is said to be complete. One then resets the \( H(I) \)’s to zero for each value of \( I \), changes \( \ln f \rightarrow \ln f / 2 \) (or in some other way) and starts a fresh iteration using the \( g(I) \)’s which have been generated in the previous iteration. Iterations are continued with the DOS steadily approaching the true DOS profile, till \( \ln f \) is sufficiently small. We have stopped the process when \( \ln f \) is as small as \( 10^{-9} \). The error which is present in the density of states has been predicted to be proportional to \( \sqrt{\ln f} \) as is apparent from the theoretical work of Zhou and Bhatt [29]. This has been tested for a number of discrete and continuous models and the prediction has been found to be correct [30, 31].

### 2.2 The Transition Matrix Monte Carlo algorithm

The TMMC algorithm also directly evaluates the DOS of a system and was first proposed by Oliveria et al. [18] in the year 1996. Let \( I \) and \( J \) be the labels of two macrostates and \( i \) and \( j \) represent the set of all microstates which correspond to the states \( I \) and \( J \) respectively. The probabilities for the transitions \( i \rightarrow j \) and \( I \rightarrow J \) are written as \( t(i,j) \) and \( T(I,J) \) respectively. Both these quantities must satisfy the following conditions:

\[
\sum_j t(i,j) = 1, \quad t(i,j) \geq 0 \tag{3a}
\]
The two types of transition probabilities are related in a simple manner. If $\Omega(I)$ and $\Omega(J)$ are the DOS’s corresponding to the macrostates $I$ and $J$, then one can write,

$$ T(I, J) = \frac{1}{\Omega(I)} \sum_{i \in I} \sum_{j \in J} t(i, j) $$

(4)

If $T(J, I)$ is the reverse transition probability i.e. for the $J \rightarrow I$ transition, then from eqn (4) it follows that,

$$ \frac{T(I, J)}{T(J, I)} = \frac{\Omega(J)}{\Omega(I)} \frac{\sum_{i \in I} \sum_{j \in J} t(i, j)}{\sum_{j \in J} \sum_{i \in I} t(j, i)} $$

(5)

The transitions like $i \rightarrow j$ etc. are effected in a MC simulation by random walk in the configuration space and in lattice-spin models, and are constituted by spin flips (in discrete model) or spin rotations (in continuous models). The process of transition $i \rightarrow j$ is actually composed of two parts: i) the transition being proposed and ii) it being accepted. If we represent by $a(i, j)$, the probability of proposing the transition $i \rightarrow j$ and by $P(i, j)$, the probability of this being accepted then we can write,

$$ t(i, j) = a(i, j)P(i, j) $$

(6)

The probability $a(i, j)$ depends on the type of MC move used while the quantity $P(i, j)$ has the flexibility of being chosen. If one considers an infinite temperature then $P(i, j) = 1$ for all states $i$ and $j$. This can easily be seen to be correct by considering a Metropolis dynamics at infinite temperature (then $P(i, j)$ would simply be the ratio of the Boltzmann factors of the two states). Therefore combining equations (5) and (6) for the temperature $T = \infty$, we can write,

$$ \frac{T_\infty(I, J)}{T_\infty(J, I)} = \frac{\Omega(J)}{\Omega(I)} \frac{\sum_{i \in I} \sum_{j \in J} a(i, j)}{\sum_{j \in J} \sum_{i \in I} a(j, i)} $$

(7)

where $T_\infty(I, J)$ represents the infinite temperature transition probability. It may be noted that the DOS’s which appear in the r.h.s. of equation (7) remain unchanged for these are not dependent on temperature. For random walk in the configuration space involving
symmetric moves, like single spin flip or rotation, as we have done, \( a(i, j) = a(j, i) \) and equation (7) can be simplified to,

\[
\frac{T_{\infty}(I, J)}{T_{\infty}(J, I)} = \frac{\Omega(J)}{\Omega(I)}
\]  

(8)

This equation indicates that one can calculate the DOS from a knowledge of the infinite temperature transition probabilities. The procedure for this is to keep a record of a transition matrix, called the C-matrix, \( C(I, J) \) for all proposals \( I \rightarrow J \), during the random walk. One starts the simulation with \( C(I, J) = 0 \) for all \( I, J \) and updates the matrix by

\[
C(I, J) \rightarrow C(I, J) + 1
\]

(9)

for each proposal \( I \rightarrow J \). Once the construction of the C-matrix is started it is never zeroed during the simulation. So the current estimate of the infinite temperature transition probability \( \tilde{T}_{\infty} \) is given by,

\[
\tilde{T}_{\infty}(I, J) = \frac{C(I, J)}{\sum_{K} C(I, K)}
\]

(10)

where the sum extends over all \( K \) for which the \( I \rightarrow K \) transition can occur. Of course, the C-matrix element, connecting states between which a transition can never be proposed is always zero. Finally with the knowledge of \( \tilde{T}_{\infty}(I, J) \) one can estimate the DOS \( \Omega \) from equation (8) and this is possible at any stage of the simulation. However, equation (8) leads to an over specified condition for the purpose of determining the \( \Omega \)'s as, for a given initial state \( I \), a number of possible states \( J \) can be proposed and each such pair \((I, J)\) satisfies equation (8) leading to a number of equations for determining \( \Omega(I) \), say. One can then, for the best estimate of \( \Omega(I) \), make a multi-variable optimization as has been described in [12, 13]. For most simulations however, it is adequate only to consider transitions involving \( I, J \) which are neighbouring states. In the TMMC algorithm, in order to ensure that the random walker visits all macrostates in the region of interest, a uniform ensemble, where all macrostates are equally probable is considered. The probability of occurrence of a given microstate \( i \) is then inversely proportional to the number of microstates which are associated with the macrostate \( I \), where \( i \in I \). So the
probability of acceptance of a move \( i \rightarrow j \) is given by,

\[
P(i, j) = \min \left( \frac{\Omega(I)}{\Omega(J)}, 1 \right)
\]  
(11)

Since the density of states are not known a priori, the above acceptance criterion is implemented by using equation (8) for the ratio of the density of states:

\[
P(i, j) = \min \left( \frac{\tilde{T}_{\infty}(J, I)}{\tilde{T}_{\infty}(I, J)}, 1 \right)
\]  
(12)

It may be noted that in the above mentioned procedure one does not actually use the strict acceptance criterion for all proposed moves. This does not lead to any self contradiction in what has been stated in the arguments leading to equation (12). This is because the manner in which one constructs the C-matrix, from which the estimate of the infinite-T transition probability is generated via equation (10), is independent of the actual acceptance probability used and depends only on the configurations which are being proposed. The errors in the TMMC simulation for different models have been described in detailed in the work of Wang and Swendsen [12]. However, the TMMC algorithm suffers from a number of drawbacks. The most important of these is that the convergence of the density of states in this method is not guaranteed and consequently the method is inefficient in terms of the computer time necessary.

### 2.3 The Wang Landau-Transition Matrix Monte Carlo algorithm

In the WLTM algorithm, first proposed by Shell and co-workers [13] one efficiently combines the WL and TM Monte Carlo methods. Here one uses the original acceptance criterion given by equation (11) and the density of states and a histogram count are updated via equation (2). Along with this, a C-matrix, which is never zeroed, is constructed and this may start at a suitable stage of the simulation process (as is elaborated in section (5) below). The DOS available from the C-matrix via the infinite-T transition probability (equations (10) and (8)) is used to replace the DOS which is generated by the WL-algorithm. This we call the ‘refreshing’ of the DOS and is done after each
iteration. The result of amalgamating the WL and TM algorithms is to yield a two fold advantage: \(i\) better sampling of states due to the WL algorithm and \(ii\) improvement in the accuracy of DOS as a result of the TMMC algorithm.

3 The models used in the present work

3.1 The 1-d Lebwohl-Lasher model

In this model one considers a linear-array of three dimensional spins interacting with nearest neighbours (nn) via a potential,

\[ V_{ij} = -P_2(\cos \theta_{ij}) \]  

where \(P_2\) is the second Legendre Polynomial and \(\theta_{ij}\) is the angle between the nearest neighbour spins \(i, j\). Periodic boundary conditions are used. This model represents an one-dimensional nematic liquid crystal. The 3-d Lebwohl-Lasher (LL) model is a lattice version of a 3-d nematic, described in the mean field approximation by the Mair-Saupe theory \[32\], and exhibits an orientational order-disorder transition. The 1-d LL model has been simulated by \[33\] and has also been solved exactly by Vuillermot and Romero \[24\] using a group theoretic method. As is to be expected in a low-dimensional model with nn interaction, the 1-d LL model does not exhibit any finite temperature phase transition. The results obtained in \[24\] are quoted below. The partition function \(Z_N(\tilde{K})\) for the \(N\) particle system is given by,

\[ Z_N(\tilde{K}) = \tilde{K}^N \exp[\frac{2}{3} N \tilde{K}] D^N(\tilde{K}^{\frac{1}{2}}) \]  

where \(\tilde{K} = \frac{3}{2T}\) is a dimensionless quantity. \(D\) is the Dawson function given by,

\[ D(x) = \exp(-x^2) \int_0^x \exp(u^2) \, du \]  

(15)

The dimensionless internal energy \(U_N(\tilde{K})\), entropy \(S_N(\tilde{K})\) and the specific heat \(C_N(\tilde{K})\) are given by,

\[ \frac{2U_N(\tilde{K})}{N} = 1 + \frac{3\tilde{K}^{-1}}{2} - \frac{3}{2} \tilde{K}^{-\frac{1}{2}} D^{-1}(\tilde{K}^{\frac{1}{2}}). \]  

(16)
\[
\frac{S_N(\tilde{K})}{N} = \frac{1}{2} + \tilde{K} - \frac{1}{2} \tilde{K}^{1/2} D^{-1}(\tilde{K}^{1/2}) + \ln[\tilde{K}^{-1/2} D(\tilde{K}^{1/2})]. 
\] (17)

\[
\frac{2C_N(\tilde{K})}{N} = 1 - \tilde{K}^{1/2}\left[\frac{\tilde{K}^{-1}}{2} - 1\right] D^{-1}(\tilde{K}^{1/2}) - \frac{1}{2} \tilde{K} D^{-2}(\tilde{K}^{1/2}).
\] (18)

3.2 The 2-d XY model

In this model planar spins placed at the sites of a planar square lattice interact with nearest neighbours via a potential,

\[
V(\theta_{ij}) = 2\left\{1 - [\cos^2(\theta_{ij}/2)]\right\}
\] (19)

where \(\theta_{ij}\) is the angle between the nearest neighbours \(i, j\). [This particular form of the interaction, rather than the more conventional \(-\cos(\theta_{ij})\) form, was chosen by Domany et. al \[34\] to enable them to modify the shape of the potential easily, which led to what is now known as the modified XY-model \]. The XY-model is known to exhibit a quasi-long-range-order disorder transition which is mediated by unbinding of topological defects as has been described in the seminal work of Kosterlitz and Thoules \[35, 36\]. The XY-model has also been the subject of extensive MC simulation over last few decades and some of the recent results may be found in \[37\].

4 Computational details:

In the 1-d LL model the configurations of the system are stored in terms of the direction cosines of the spins, i.e. a set of three numbers \((l_1, l_2, l_3)\) describe the orientation of each spin. The simulation is started with a random configuration of the spins. To generate a new configuration, one spin at a time is randomly selected and a move \(l_i \rightarrow l_i + p \ast r_i\) (for \(i=1, 2, 3\)) is effected where \(r_i\) is a uniformly generated random number between -1 and +1. To preserve the unit magnitude of the spins, the normalization condition \(l_1^2 + l_2^2 + l_3^2 = 1\) is always applied. In the 2-d XY-model, two direction cosines are needed to describe the orientation of each spin. In the 1-d LL model, for a chain of length \(L\) (in
units of the lattice spacing), the energy of the system can have any value between \(-L\) to \(L/2\) while for the 2-d XY-model of linear dimension \(L\) the system energy lies between 0 and \(4L^2\). In order to apply the WL or WLTM algorithm we have restricted the random walk in the energy space from \(-L\) to 0 and from 0 to \(2L^2\) for the 1-d and 2-d models respectively (actually a small energy band near the ground state was also excluded as is explained below), and this energy range was divided into a number of bins, each having a width \(d_e\). At the beginning of the simulation, we set all \(g(I)\)’s to zero. Starting from a microstate \(i\), the random generation of configurations by the above mentioned procedure leads to a new state \(j\) being proposed. The probability of acceptance of this state is given by \(P(i,j)\) in equation (1). It may be noted that, there is always a possibility that \(j\) and \(i\) represent the microstates belonging to the same macrostate — in that case the move is always accepted. The random walk is continued until the histogram reaches 90% flatness. With the knowledge of the C-matrix which has accumulated in the process, we calculate the current DOS and use it to refresh the previous DOS. This completes one iteration, following which, we reduce the modification factor \(lnf \rightarrow lnf/2\), reset the histogram counts to zero and start a new random walk cycle. It is important to note that the C-matrix is never reset to zero and hence it stores the entire history of the moves proposed in the simulation process.

The iterations are continued till the factor \(lnf\) gets reduced to \(10^{-9}\). The WLTM algorithm has the flexibility in that, it is possible to refresh the DOS from the accumulated C-matrix at any stage. It is even possible to refresh at the very end when all the iterations have been completed. This therefore amounts to doing pure WL simulation along with keeping a record of the C-matrix which is used only at the end to refresh the DOS. The dependence of the accuracy of the results resulting from refreshing the DOS at different stages is described in the following section.
5 Results and discussion

5.1 The 1-d LL model:

We have simulated the 1-d model for system sizes $L = 80, 160$ and $220$ and the minimum of the energy range over which random walk has been carried out were -79, -158, -218 respectively, the upper limit being 0 in each case. The small cut in the energy near the ground state had to be made since it takes a prohibitively long time to fill these states. Moves which take the system energy outside the specified range are rejected and the C-matrix is updated as $C(I, I) \rightarrow C(I, I) + 1$ where the index $I$ labels the initial state. The energy bin-width was chosen to be $d_e = 0.1$ in all cases and the parameter $p$, defined

![Figure 1: $g(E)$, the logarithm of the density of states in the 1-d LL model for the three system sizes are plotted against energy per particle in the energy range of interest.](image)

in the previous section, was also chosen to be 0.1. As the bin-width is made narrower, the number of microstates which correspond to a particular bin gets reduced. Ideally, $d_e$ should be as small as possible for better discretization, but this is limited by computational difficulties in its implementation. Choosing a very small bin-width increases the
number of bins proportionately and the book-keeping work becomes difficult. Problems arise both with CPU time as well as with available computer memory and this becomes severe particularly for a large lattice size. Optimization of these considerations resulted in our choice of the bin width.

The parameter $p$ determines the amplitude of a rotation which is given to a spin at

![Diagram showing percentage error in lnZ against temperature for different cases of the 1-d LL model.](image)

**Figure 2:** Percentage error in the logarithm of partition function ($\ln Z$) is plotted against temperature for the 1-d LL model. Errors are plotted for the different cases where the construction of C-matrix is started at different stages of simulation. The meaning of the symbol $\lambda$ is described in the text. Percentage error in $\ln Z$ obtained from the WL algorithm with 90% flatness criterion is also shown in the figure.

the time of generating new configurations. Too small a value of $p$ leads to the configuration being trapped in the same bin and a large value results in visits always outside the starting bin. Actually, while simulating a continuous spin system using WL or WLTM algorithm, a proper choice of the parameters $d_e$ and $p$ is particularly important. Clearly the two parameters are interrelated and our choice of $p = 0.1$ for the particular value of $d_e = 0.1$ was based on the consideration that about 50% of the attempted moves go
outside the starting bin so that care is taken of microstates in the initial bin as well as its neighbours \[13\]. This approach, besides ensuring a uniform sampling, also optimizes the CPU time.

Figure 3: Percentage error in $\ln Z$ is plotted against temperature for three lattice sizes 80, 160 and 220. The results are for the parameter $\lambda = \lambda_2$.

We have used the histogram flatness criterion to determine when an iteration with a given modification factor $f$ is to be terminated. This condition, although it increases the CPU time enormously, was found to be necessary for minimizing the errors in the observables. Shell et al \[13\] while prescribing the WLTM algorithm suggested that a single visit to each macrostate should be enough to determine where to terminate an iteration. We have observed that while this works reasonably well for a model with a discrete energy spectrum \[38\], in a system with continuous energy spectrum, as is ours, a single visit criterion fails to work. This is however not surprising in view of the fact that when discretization is achieved by a certain choice of the energy bin-width, the multiplicity of states associated with each bin (for any choice of bin-width) is generally much greater
than that for an energy level in a discrete system of comparable size.

Figure 4: Percentage error in \( \ln Z \) is plotted against temperature for three lattice sizes 80, 160 and 220. The results are for the parameter \( \lambda = \lambda_2 \).

In figure 1 we have shown the plots of \( g(E) \), the logarithm of the DOS against the energy per spin for three system sizes. Figure 2 is a plot of the error in \( \ln Z \), \( Z \) being the partition function) and a comparison has been made with the exact results of [24]. Here we have presented the results of simulation where the construction of the C-matrix was started at different stages of iteration. We denote by \( \lambda_c \) a preassigned number and when the current value of \( \ln f \) becomes just less than \( \lambda_c \), the construction of the C-matrix is started. For instance, the graph for \( \lambda_c = \lambda_2 = 10^{-2} \) shows the error in \( \ln Z \) obtained in the simulation in which the construction of the C-matrix was started when \( \ln f \) becomes just less than \( 10^{-2} \). Following this the simulation was continued till \( \ln f \) reaches \( 10^{-9} \), with the usual procedure of DOS refreshing along with the condition of 90% histogram flatness. It is clear from the figure that in order to get the best result, a compromise is to be made in getting the most useful C-matrix. If it is constructed from the very beginning of the
Figure 5: The variation of energy per particle in the 1-d LL model is plotted against temperature (solid line) for $L = 220$ and $\lambda_0$. Exact results available for the system are also plotted in the same graph and are indicated by '+' symbol. In the inset, the percentage error $\epsilon(E)$ in energy is compared with exact results.
Figure 6: Specific heat per particle for the $L = 220$ 1-d LL model is plotted against temperature for $\lambda = \lambda_0$. The '+' symbol indicates the exact results for the system. The percentage error in the $C_v$ in comparison with the exact results is shown in the inset.
simulation while the DOS profile is far away from being a realistic representation of the actual one, the errors which accumulate in the C-data lead to large error. Again when the construction begins at a stage too late, some important information of the simulation process is lost resulting again in increase in errors. In particular, figure 2 shows that the error for $\lambda_2$ is significantly smaller than that for $\lambda_0$. Also shown in figure 2 is the error in $\ln Z$ for pure WL simulation with the condition of 90% histogram flatness imposed. It is clear from the diagram that it is possible to achieve better accuracy with the WLTM algorithm. However the gain in the accuracy seems to be only marginal and that too is at an appreciable increase in the CPU time involved.

In figure 3 is shown the error in $\ln Z$ for the three lattice sizes, achieved with the WLTM algorithm and C-matrix updating corresponding to $\lambda_2$. Since the theoretical estimate of $\ln Z$ [24] is for the thermodynamic limit, it is natural to expect that the error should decrease with the increase in system size. In figure 4, we have compared the WLTM results

![Graph](image)

**Figure 7:** The variation of entropy per particle with temperature for $L = 220$ 1-d LL model for $\lambda = \lambda_0$ is shown. Exact results are also plotted and the error in entropy obtained in comparison with the exact result is shown in the inset.
obtained with the 90% flatness method with those obtained with the 'single visit per bin' condition imposed. It is clear that the latter leads to a huge error in the density of states and hence in the partition function and is not usable in a continuous model. In figure 5, 6 and 7 we have plotted the energy, specific heat and entropy against temperature for \(L=220\) for \(\lambda_0\)-simulation and the results have been compared with the exact values of these observables obtained from the exact results [24]. In the inset in each figure we have also shown the corresponding errors in these parameters obtained in comparison with the exact results.

5.2 The 2-d XY model

In this model simulations were carried out for lattice sizes 10 \(\times\) 10 and 20 \(\times\) 20 and the corresponding minimum of the energy range were chosen to be 3 for each. Histogram flatness was restricted to 80% in all WL and WLTM simulations. In addition to the already mentioned cut in the energy range, for the 20 \(\times\) 20 system, in order to save CPU time, we had to relax the condition for histogram flatness check for the first 500 bins. The XY-model and the phase transition it exhibits have been worked out in detail in references [35, 36]. However it is not possible to compare the results of our simulation in the XY-model for the DOS or partition function, with the exact results for this model, as we have done for the 1-d LL model, because such exact results for this model are not available. We therefore present here a comparison of our WL and WLTM results with those obtained from simulation using the conventional Metropolis algorithm, which is known to work satisfactorily for this model [37]. To increase the reliability of our results, we have performed 20 independent simulations for each of the Metropolis, WL and WLTM method and have averaged the respective results. In the Metropolis simulation the averaging was done directly over the observables while in the other two cases, the DOS was averaged before it was used to obtain the observables.

Regarding the choice of energy bin-width \(d_e\) and the parameter \(p\), the considerations as were applied to the 1-d LL model, were taken into account. Unless otherwise stated, we
Figure 8: The average energy per particle for the XY-model is plotted (a) against temperature for $10 \times 10$ and $20 \times 20$ lattice sizes, obtained using three MC methods namely, WLTM, WL and M (Metropolis). These results correspond to the $\lambda_2$ case and all results are obtained by taking averages over 20 independent simulations. Similar plots for the specific heat per particle against temperature are shown in (b).
have used $d_e = 0.1$ and $p = 0.1$ in this model too. This led us to work with a large number of bins, namely 8000, for the $20 \times 20$ lattice.

In figures 8(a) and 8(b) we have shown the variation of the average energy, $E$ and the specific heat, $C_v$ respectively with the temperature for the $10 \times 10$ and $20 \times 20$ lattices, obtained with the WL, WLTM and Metropolis algorithms. This diagram and all the following diagrams, depicting the results of the XY-model, represent the results of 20 independent simulations for each of the algorithms used. As the plots shown in figure 8 do not clearly reveal the errors in the different simulations, we present these in detail in figure 9. The percentage errors presented in figures 9 to 12 have been obtained by comparing the results of simulations with that obtained by using the Metropolis algorithm. Figure 9(a) shows the errors in energy for the $10 \times 10$ lattice obtained for the pure WL simulation and the WLTM simulation for three different starting points of the C-matrix. Figure 9(b) shows the same for the specific heat $C_v$. For the energy curve, WLTM simulation with $\lambda_2$ seems to be the best choice where the error is $\sim 0.1\%$. In the specific heat curve, where the errors are slightly greater, as is to be expected for this being a fluctuations quantity, simulations with $\lambda_1$ and $\lambda_2$ have comparable errors. It is clear from these diagrams that the choice of $\lambda_0$ for the commencement of the C-matrix leads to larger errors in the WLTM simulation. Figures 10(a) and 10(b) are the plots of the errors in energy and specific heat for the $20 \times 20$ lattice. These diagrams clearly reveal that the errors in the pure WL algorithm are greater than those for the WLTM algorithm and for the latter, the performance of the $\lambda_0$ simulation is worst. In figure 11 we have shown the errors in specific heat $C_v$ for different choices of the bin width $d_e$, other conditions remaining the same. As is perhaps to be expected, the smaller bin-width $d_e = 0.05$ gives best results while the choice $d_e = 0.2$ is the worst. These results are for the $\lambda_0$ simulation. Figure 12 demonstrates that the $\lambda_0$ simulation with $d_e = 0.05$ and the $\lambda_1$ simulation for $d_e = 0.1$ leads to comparable errors in $C_v$. 
Figure 9: This figure (a) shows the errors in energy for the XY-model for 10 × 10 lattice obtained from WL simulation and WLT M simulation for three different starting points $\lambda_0, \lambda_1, \lambda_2$ of the C-matrix. The errors have been calculated by comparing the results of simulations with that obtained by using the Metropolis algorithm. The straight line segments are guide to the eyes. Similar plots for the specific heat per particle against temperature are shown in figure (b).
Figure 10: Plots are same as those in Figure 9 for the $20 \times 20$ lattice sizes.
Figure 11: The errors in specific heat $C_v$, for the different choices of the bin width keeping other parameters fixed, are plotted against temperature.

Figure 12: A comparison of the errors of $\lambda_0$ simulation with bin width $d_e = 0.05$ and the $\lambda_1$ simulation with bin width $d_e = 0.1$. 

6 Conclusion

We have presented results of extensive MC simulations using WL and WLTM algorithms in two continuous lattice spin models. Simulation of continuous models needs a choice of two parameters, a bin-width $d_e$ (for energy) and $p$, which determines the amplitude of the rotation to be imparted to the spins. We are of the opinion that while the bin-width should be as small as possible, depending on the computer resources available, the parameter determining the amplitude of spin rotation should be chosen in such a way that, of the proposed moves during the random walk, about 50% should take the random walker out of the starting macrostate to a neighbouring one. In the simulation of a model involving continuous macroscopic variables, these two parameters critically determine the accuracy of the results, while no such considerations are needed for simulating a discrete model.

Our work on the two continuous models show that it is possible to obtain results of better accuracy with the WLTM algorithm than that is obtainable from the WL algorithm. For this purpose, one must be careful about the starting point for the construction of the C-matrix. While this matrix should contain as much information as possible regarding the transitions proposed, care must be taken not to include information about the proposed moves which are generated very early in the simulation, when the profile of the DOS is just in a formative stage. We had also to make an improvisation in the WLTM algorithm regarding the question of convergence of the DOS. The 'single visit to each macrostate' criterion, which saves a lot of CPU time and was proposed by Shell et. al in their original work [13], though adequate for a discrete model, seems to result in poor accuracy of the results for a continuous model. So we had to retain the condition for the flatness check of the histogram as is used in the original version of the WL algorithm. This of course results in a significant increase in the CPU time.

We end this section with a few comments. We are of the opinion that the gain in accuracy over the WL algorithm which can be achieved using the WLTM algorithm, with a choice of various parameters as well as the commencement point of the C-matrix, done in the most judicious way, is not significant. This too is possible only at the cost of a huge
increase in CPU time. We would also point out that simulating a continuous model of a reasonably large size using the WLTM algorithm, leads to the requirement of a vast amount of computer memory (RAM) and it would be an almost impossible task if one needs to determine a joint density of state by performing a two-dimensional random walk (including quantities like order parameter, correlation function etc. besides energy) in a system of a reasonably large size. It may also be added that for this purpose, the WL algorithm has also proved to be inadequate [26, 31].

We are of the view that in order to simulate a continuous model of large size, the more than a decade old method of multiple histogram reweighting, proposed by Ferrenberg and Swendsen [16, 39] still seems to be the best choice. In addition, if one is dealing with a system not exhibiting a temperature induced first order phase transition, the Wolff cluster algorithm [15] is useful for reducing critical slowing down. Examples of such work, to name a few, may be found in [40, 41, 42, 43, 44]. The methods like WL, TM or WLTM which directly determine the DOS do not seem to be a suitable choice for these jobs, unless of course one uses a computer code for parallel processing using OPENMP or MPI [45].

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References

[1] N. Metropolis, A. W. Rosenbluth, A. H. Teller and E. Teller, J. Chem. Phys. 21 (1953) 1087.
[2] M. E. J. Newman and G. T. Barkema, Monte Carlo Methods in Statistical Physics, Clarendon Press, Oxford (1999).

[3] R. G. Ghulghazaryan, S. Hayryan and C. Hu, J. Comput. Chem 28 (2007) 715.

[4] F. Wang and D. P. Landau, Phys. Rev. Lett. 86 (2001) 2050; F. Wang and D. P. Landau, Phys. Rev. E 64 (2001) 056101.

[5] C. Yamaguchi and Y. Okabe, J. Phys. A 34 (2001) 8781.

[6] J. D. Muñoz and H. J. Herrmann, Comp. Phys. Commu. 121-122 (1999) 13.

[7] N. Rathore and J. J. de Pablo, J. Chem. Phys. 124 (2002) 7225.

[8] T. S. Jain and J. J. de Pablo, J. Chem. Phys. 116 (2002) 7238.

[9] D. Jayasri, V. S. S. Sastry and K. P. N. Murthy, Phys. Rev. E. 72 (2005) 036702.

[10] Q. Yan and J. J. de Pablo, Phys. Rev. Lett. 90 (2003) 035701.

[11] J. R. Errington, J. Chem. Phys. 118 (2003) 9915

[12] J. S. Wang and R. H. Swendsen, J. Stat. Phys. 106 (2001) 245.

[13] M. S. Shell, P. G. Debenedetti and A. Z. Panagiotopoulos, J. Chem. Phys, 119 (2003) 9406.

[14] R. H. Swendsen and J. S. Wang, Phys. Rev. Lett. 58 (1987) 86.

[15] U. Wolff, Phys. Rev. Lett. 62 (1989) 361.

[16] A. M. Ferrenberg and R. H. Swendsen, Phys. Rev. Lett. 63 (1989) 1195.

[17] D. Landau and K. Binder, A Guide to Monte Carlo Simulations in Statistical Physics, CUP (2005).

[18] P. M. C. de Oliveria, T. J. P. Penna and H. J. Hermann Braz. J. Phys. 26 (1996) 677; P. M. C. de Oliveria, Eur. Phys. J. B. 6 (1998) 111.
[19] M. S. Shell, P. G. Debenedetti and A. Z. Panagiotopoulos, Phys. Rev. E 66 (2002) 056703.

[20] Q. Yan, R. Faller and J. J. de Pablo, J. Chem. Phys. 116 (2002) 8745.

[21] D. P. Landau, S. Tsai and M. Exler, Am. J. Phys. 72 (2004) 1294.

[22] J. Xu and H. Ma, Phys. Rev. E 75 (2007) 041115.

[23] P. A. Lebwohl and G. Lasher, Phys. Rev. A 6 (1972) 426.

[24] P. A. Vuillermot and M. V. Romerio, J. Phys. C 6 (1973) 2922; P. A. Vuillermot and M. V. Romerio, Commun. Math. Phys. 41 (1975) 281.

[25] A. Tröster and C. Dellago, Phys. Rev. E 71 (2005) 066705.

[26] K. Mukhopadhyay, N. Ghoshal, S. K. Roy, Physics Letters A, 372 (2008) 3369.

[27] C. Zhou, T. C. Schulthess, S. Torbrügge and D. P. Landau, Phys. Rev. Lett. 96 (2006) 120201.

[28] P. Poulain, F. Calvo, R. Antoine, M. Broyer, Ph. Dugourd, Phys. Rev. E 73 (2006) 056704

[29] C. Zhou and R. N. Bhatt, Phys. Rev. E 72 (2005) 025701.

[30] H. K. Lee, Y. Okabe and D. P. Landau, Compt. Phys. Commu., 175 (2006) 36.

[31] S. Sinha and S. K. Roy, arXiv: 0711.1031v2.

[32] W. Maier and A. Saupe, Z. Natureforsch. A 13 (1958) 564; W. Maier and A. Saupe, Z. Natureforsch. A 14 (1959) 882; W. Maier and A. Saupe, Z. Natureforsch. A 15 (1960) 287.

[33] C. Chiccoli, P. Pasini, C. Zannoni, Liq. Cryst. 3 (1988) 363.

[34] E. Domany, M. Schick and R. H. Swendsen, Phys. Rev. Lett. 52 (1984) 1535.

[35] J. M. Kosterlitz and D. J. Thouless, J. Phys. C: Solid State Phys, 6 (1973) 1181.
[36] J. M. Kosterlitz, J. Phys. C: Solid State Phys., 7 (1974) 1046.

[37] P. Olsson, Phys. Rev. B 52 (1995) 4511; P. Olsson, Phys. Rev. B 52 (1995) 4526; J. Maucourt and D. R. Grempel, Phys. Rev. B 56 (1997) 2572; P. Archambault, S. T. Bramwell et al, J. Applied Phys. 83 (1998) 7234; G. Palma, T. Mayer and R. Labbe, Phys. Rev. E 66 (2002) 026108.

[38] D. Bhowmik, A. Chakraborty, S. K. Roy, to be published.

[39] A. M. Ferrenberg and R. H. Swendsen, Phys. Rev. Lett. 61 (1988) 2635.

[40] E. Mondal and S. K. Roy, Phys. Lett. A 312 (2003) 397.

[41] Z. Zhang, O. G. Mouritsen, M. J. Zuckermann, Phys. Rev. E 48 (1993) 2842.

[42] H. Kunz and G. Zumbach, Phys. Rev. B 46 (1992) 662.

[43] A. Pal and S. K. Roy, Phys. Rev. E 67 (2003) 011705.

[44] A. Pal and S. K. Roy, Phys. Rev. E 69 (2004) 021709.

[45] L. Zhan, Comp. Phys. Comm. 179 (2008) 339