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Wang-Landau Algorithm and its Implementation for the Determination of Joint Density of States in Continuous Spin Models

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1. Introduction

The Metropolis algorithm (Metropolis et al., 1953) developed more than half a century ago has been extensively used to simulate a wide variety of problems of interest in statistical physics. The method is based on importance sampling and directly generates the equilibrium configurations in the canonical distribution of a system. Thus Monte Carlo (MC) simulations using the Metropolis algorithm are carried out at a number of closely spaced temperatures and the observables are calculated by taking the configurational averages over the states generated by the algorithm. The method does not directly lead to an evaluation of the entropy or density of states of a system.

Although the Metropolis algorithm, which is rather simple to implement in a computer, is still being widely used it suffers from a number of notable drawbacks. In case of a system having a first order phase transition, the random walker in the Metropolis algorithm gets trapped in metastable states, thus leading to long runs which mostly result in inaccurate results. Also in the case of systems exhibiting a second order phase transition, critical slowing down reduces the efficiency of the algorithm to a large extent. To overcome such problems, for a spin system other algorithms have been developed and the Swendsen-Wang algorithm (Swendsen & Wang, 1987) was an important step in this direction. Wolff cluster algorithm (Wolff, 1989) which was developed later has proved to be very important in reducing critical slowing down in continuous spin systems. Using these algorithms, accurate estimation of thermodynamic quantities has become possible using the histogram reweighting technique which was developed by Ferrenberg and Swendsen in 1988 (Ferrenberg & Swendsen, 1988). This works equally well for systems exhibiting both first order and second order phase transitions.

The above mentioned algorithms and the data analysis techniques depend on the generation of configurations of a system at different temperatures. For a few decades after standard

Monte Carlo simulation began following the publication of the Metropolis approach, there existed no method which directly or indirectly evaluates the partition function of a system. A knowledge of the partition function (as a function of temperature) would lead to a straight forward evaluation of most thermodynamic quantities of interest and would prove to be very attractive.

The partition function of a system can easily be evaluated if the density of states $\Omega(E)$ of a system for a given energy E in known. The density of states is a quantity independent of temperature and depends on the number of configurations which a system possesses for a given energy. The partition function can be written as

$$Z(\beta) = \sum_E \Omega(E) e^{-\beta E} \tag{1}$$

where $\beta = 1/K_B T$, T being the temperature and K_B the Boltzmann factor. It may be noted that $\Omega(E)$, although called the density of states (DOS) is actually the number of states or simply the degeneracy factor of a state of the system with energy E. The above relationship therefore shows that once we have a knowledge of $\Omega(E)$, the partition function at any temperature can easily be evaluated simply by Boltzmann reweighting. Without going into the history of development of Monte Carlo techniques which leads to the determination of the density of states (since such material may be found in books like Newman and Barkema (Newman & Barkema, 1999) or Binder and Landau (Landau & Binder, 2000)) we name two techniques which have been proposed in the past one decades or so. These are the Transition Matrix Monte Carlo method (TMMC) and the Wang-Landau algorithm (WL). The TMMC method, first proposed by de Oliveria et al. in 1996, makes use of a book keeping of all transitions between the microstates of a system as a random walk is performed in the energy space and the transition probabilities are used to give an accurate estimation of the density of states.

The subject of this chapter is to discuss the other method, the Wang-Landau algorithm, first proposed in 2001 (Wang & Landau, 2001). This has since attracted a wide attention of researchers and have been applied to a large variety of systems. In the original work Wang and Landau applied this method to simulate discrete spin systems showing first order (Pott's model (Wu, 1982)) as well as second order (two-dimensional Ising model (Onsager, 1944)) phase transitions. Also a system having rough energy landscape, like the Edwards-Anderson model (Edwards & Anderson, 1975) of three-dimensional spin glass, which is rather difficult to be simulated using conventional Monte Carlo algorithms, was simulated using the WL algorithm.

The WL algorithm, to be discussed in detail in the following section, is an iterative scheme where during each iteration an histogram of the energy distribution is generated during a random walk in the energy space. Starting from no knowledge of the density of states of a system, one gradually builds up the profile of the density of states by forcing the random walker to make more visits to those energy regions where the density of states is smaller. The method is based on the generation of a flat histogram for each iteration. A small number, called the modification factor is used to build up the DOS profile during each iteration and as the process goes on this modification factor is made smaller and smaller thus making finer adjustments to the value of the DOS.

In the original work of Wang and Landau application of the algorithm only to discrete spin systems were discussed. Also the random walk performed was one-dimensional – only in the energy space. The statistical average of an observable which is directly related to energy is thus given by

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$$\langle f(E,\beta) \rangle = \frac{\sum_E f(E)\Omega(E)e^{-\beta E}}{\sum_E \Omega(E)e^{-\beta E}} \qquad (2)$$

However if one intends to determine quantities (ϕ) like the order parameter, correlation function etc., which are not directly related to energy, a two dimensional random walk in the $E - \phi$ space needs to be performed. Consequently the DOS will also be a function of two variables – energy E and the other observable ϕ. This is generally called the joint density of states (JDOS) and is denoted by $\Omega(E,\phi)$. The ensemble average of any function of ϕ is obtained from the relation:

$$\langle f(\phi,\beta) \rangle = \frac{\sum_E \sum_\phi f(\phi)\Omega(E,\phi)e^{-\beta E}}{\sum_E \sum_\phi \Omega(E,\phi)e^{-\beta E}} \qquad (3)$$

Apart from the necessity of generating JDOS, another modification of the original WL algorithm needs to be done even when simulating spin systems. Systems like the XY-, Heisenberg- and the Lebwohl-Lasher (LL) (Lebwohl & Lasher, 1972) models are examples of lattice spin models which have a continuous energy spectrum. It is possible to generate both DOS and JDOS in such system using WL algorithm. The basic algorithm remains the same but one discretizes the energy values by dividing the energy range of interest into narrow bins. In the case of a two-dimensional random walk both the E-space and ϕ- space are discretized. Thus in the most general case we need to handle the generation of JDOS in a continuous lattice-spin model. This is the subject matter of this chapter (Mukhopadhyay et al., 2008). One can of course apply the WL algorithm to systems other than lattice-spin models but we shall not go into this. With a knowledge of simulating JDOS in continuous spin systems it is straight forward to apply the algorithm to simulate any other system of interest.

In the following section we discuss the WL algorithm and how one can implement this for a discrete spin system. Next we discuss the one-dimensional LL model and this is followed by a section where the technique for handling a continuous model is discussed. This model is chosen because it is the only continuous spin model (although not exhibiting a phase transition) which has an exact solution (Vuillermot & Romerio, 1973; 1975) and thus will allow us to check the accuracy of the results of our simulation. We have also applied the model to a two-dimensional XY model – known to exhibit the Kosterlitz-Thouless (Kosterlitz & Thouless, 1973; Kosterlitz, 1974) phase transition mediated by topological defects. We have compared our results obtained from one-dimensional random walk for the XY model with those obtained from the standard Metropolis algorithm to check the accuracy of our simulation. Results obtained from the simulated JDOS are also presented for this model.

We conclude this section with an important comment, nowhere in their original paper Wang and Landau discussed why the DOS obtained using their algorithm should be the true value of the DOS of a system. The question of convergence of the DOS obtained by the iterative process is also skipped. However, some authors have dealt with this question in more recent papers and we, in a concluding section, will discuss briefly this aspect of the WL algorithm.

2. The Wang Landau algorithm

Using an iterative scheme the WL method determines the density of states $\Omega(E)$ of a system as a function of energy E. In this method random walk in discrete energy space of a spin system is performed by flipping spins in a random manner. A random walker without any bias tends to visit regions of energy where $\Omega(E)$ is greater. In order to produce a "flat

histogram", the WL algorithm visits states with a probability which is inversely proportional to $\Omega(E)$(instead of sampling with the Boltzmann weights $e^{-\beta E}$ used in the conventional Metropolis like algorithms). However, since the density of states $\Omega(E)$ is not known *a priori* all $\Omega(E)$s are set equal to a common constant value, say 1 at the beginning of a simulation. At every step of the random walk $\Omega(E)$ is modified by a multiplicative factor $f > 1$ and the updated $\Omega(E)$ is used for the next step of random walk. The modification factor f is controlled carefully in the following iterations and finally when $f \approx 1$ the density of states $\Omega(E)$ converges very close to its true value. The accuracy of the estimated density of states depends on many factors involved in the implementation part of the algorithm such as the final value of the modification factor, flatness criterion, system size etc. Since density of states $\Omega(E)$ is a large quantity, it is convenient to use $ln[\Omega(E)]$ in simulation and we denote it by $g(E)$.

The steps of the Wang Landau algorithm in a lattice-spin system having discrete energy values goes like this:

1. Set $g(E) = 0$ and $h(E) = 0$ for all E, here $h(E)$ is the histogram count. Also choose $\ln f = 1$ (the initial value of the modification factor may be $f = e^1$ which is suitable for a faster estimation of $\Omega(E)$).

2. Pick a single spin at random and flip it.

3. Whether the move is accepted or not is decided by the transition probability

$$p_{i \to j} = min \left[\frac{\Omega(E_i)}{\Omega(E_j)}, 1 \right]$$

or,

$$p_{i \to j} = min \left[exp[g(E_i) - g(E_j)], 1 \right],$$

where E_i and E_j are respectively the system energies before and after a spin is flipped. Generate a random number r such that its value lies between 0 and 1. If r is less than $p_{i \to j}$ flip the spin. Otherwise restore the previous configuration.

4. If the proposed state j is accepted, make

$$g(E_j) = g(E_j) + \ln f, \qquad h(E_j) = h(E_j) + 1$$

otherwise make

$$g(E_i) = g(E_i) + \ln f, \qquad h(E_i) = h(E_i) + 1$$

5. Repeat steps 2, 3, and 4 for about 10^4 MC sweeps and check the flatness of the histogram. One Monte Carlo sweep consists of a sequence of moves whose number is equal to the number of spins in the system. Since it is not possible to obtain a perfectly flat (100%) histogram, the flatness check is performed by calculating the average histogram $< h(E) >$ averaged over E and verifying the condition $\frac{h(E)}{<h(E)>} \geq x$ for all E where x can be chosen according to the size and complexity of the system (for example x may be chosen to be 0.9). When the flatness criterion is satisfied for all E we say that one iteration is completed.

6. In the next iteration reset the histogram counts to zero, reduce the modification factor as $f \to \sqrt{f}$ *i.e.* $\ln f \to \ln f / 2$. The steps (from 2 to 5) are repeated until $\ln f$ becomes smaller than a very small predefined value say $\sim 10^{-8}$ or 10^{-9}.

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In order to obtain a good estimate of the density of states $\Omega(E)$ multiple measurements with different sequences of random numbers should be performed and an average of these independent values of $\Omega(E)$ should be used for the calculation of partition function $Z(\beta)$ and other relevant thermodynamic quantities. Apart from multiple measurements one may try to minimize correlations between adjacent moves i.e. by increasing the separation between successive records in the histogram $h(E)$ to obtain a more accurate estimate of $\Omega(E)$. In the original Wang Landau algorithm one record is inserted into $h(E)$ for every trial spin-flip.

Any successful MC simulation algorithm must satisfy the conditions of ergodicity and detailed balance. By ergodicity we mean that starting from any microsate it should be possible to visit any other microstate if the run is long enough. Any algorithm based on single spin moves, like the Metropolis algorithm, satisfies the ergodicity condition. A single spin move may not take the spin system directly to any state starting from a given state but there always is a path connecting two states via a sequence of single step moves.

The condition of detailed balance means that the probabilities of moving into and moving out from a microstate are equal. The random walk process in the WL algorithm does not satisfy this condition initially as the density of states $\Omega(E)$ is rapidly being modified. In the late stage, when only fine adjustment are made to the density of states, *i.e.* the modification factor is close to 1, detailed balance is very close to being fulfilled. This can be seen very easily as the transition probability $p(E_1 \rightarrow E_2)$ is inversely proportional to $\Omega(E_2)$:

$$\frac{p(E_1 \rightarrow E_2)}{p(E_2 \rightarrow E_1)} = \frac{\Omega(E_1)}{\Omega(E_2)}, \tag{4}$$

$$i.e. \quad \frac{1}{\Omega(E_1)} p(E_1 \rightarrow E_2) = \frac{1}{\Omega(E_2)} p(E_2 \rightarrow E_1) \tag{5}$$

hence,

$$\sum_{E_1} \frac{1}{\Omega(E_1)} p(E_1 \rightarrow E_2) = \sum_{E_1} \frac{1}{\Omega(E_2)} p(E_2 \rightarrow E_1) \tag{6}$$

The quantity on the L.H.S. is the product of probability of occurrence of the state E_1 and the probability of the transition from $E_1 \rightarrow E_2$ and is summed over E_1. Hence it represents the probability of moving into the state E_2. Similarly the quantity on the R.H.S. represents the same for the reverse transition and the Equation 5 expresses the condition of detailed balance.

3. Wang-Landau algorithm for the one-dimensional Lebwohl-Lasher model

3.1 The one-dimensional Lebwohl-Lasher model and the exact results

The Lebwohl-Lasher model is the lattice version of the Maier-Saupe model (Priestly et al., 1976) which describes a nematic liquid crystal in the mean field approximation. This is a system of a one-dimensional array of three-dimensional spins ($d = 1$, $n = 3$, where d is the system dimensionality and n is the spin dimensionality) interacting with nearest neighbours via a potential $-P_2(cos\theta_{ij})$, where P_2 is the second Legendre polynomial and θ_{ij} is the angle between the nearest neighbour spins i and j (the coupling constant in the interaction has been set to unity).

The one-dimensional LL model ($d = 1$, $n = 3$), has an exact solution and we decided to choose this simple model to apply and test the performance of the WL algorithm for simulation of joint density of states so that a comparison can be made with the exact results available.

The Hamiltonian of the Lebwohl-Lasher model is given by

$$H = - \sum_{\langle i,j \rangle} P_2(\cos \theta_{ij}) \tag{7}$$

where P_2 is the second order Legendre polynomial and θ_{ij} is the angle between the nearest neighbour spins i and j. The spins are three dimensional and headless, *i.e.* the system has the O(3) as well as the local Z_2 symmetry characteristic of a nematic liquid crystal. A vector order parameter is inadequate for the system and a traceless second rank tensor Q, as defined below, is used to describe the orientational order of the system (Chaikin & Lubensky, 1995). One uses,

$$Q_{ij} = \frac{1}{N} \sum_{t=1}^{N} \left(n_i^t n_j^t - \frac{1}{3} \delta_{ij} \right) \tag{8}$$

where n_i^t is the i-th component of the unit vector $\hat{n}$, which points along the spin at the site t. N is the number of particles in the system. In the ordered state $\langle \underline{Q} \rangle$ is non-zero. In a coordinate system with the Z-axis pointing along the direction of molecular alignment (director) the matrix $\langle Q \rangle$ is diagonal and for a uniaxial system,

$$\langle \underline{\mathbf{Q}} \rangle = S \begin{pmatrix} -1/3 & 0 & 0 \\ 0 & -1/3 & 0 \\ 0 & 0 & 2/3 \end{pmatrix} \tag{9}$$

where,

$$S = \frac{1}{2} \langle (3 \cos^2 \theta^t - 1) \rangle = \langle P_2(\cos \theta^t) \rangle \tag{10}$$

where θ^t is the angle between a spin and the director. MC simulations demonstrate that a three dimensional Lebwohl-Lasher model (d=3, n=3) exhibits a weakly first order transition, characteristic of a nematic-isotropic transition which is available from the Maier-Saupe model of a nematic in the mean field approximation. On the other hand, for lattice dimensionality d=2 and 1, no true long range order is expected since Mermin-Wagner theorem (Mermin & Wagner, 1966) predicts a fluctuation destruction of long range order. The d=2 LL model has been investigated by a number of authors (Kunz & Zumbach, 1992; Mondal & Roy, 2003) and the system shows a behaviour qualitatively similar to the two dimensional XY model. A quasi-long range order has been observed in this system and this is believed to be related to the existence of topological defects in the system (Dutta & Roy, 2004).

The one-dimensional Lebwohl-Lasher model has been simulated by (Chiccoli et al., 1988) and has also been solved exactly (Vuillermot & Romerio, 1973; 1975). The system is known to be disordered at all finite temperatures and critical behaviour is expected only at T=0, which resembles an one-dimensional Ising model or the one dimensional Heisenberg model. The second rank spin-spin correlation function $\rho(r)$ is defined as

$$\rho(r) = \langle P_2(\cos \theta(r)) \rangle \tag{11}$$

where $\theta(r)$ is the angle between two spins, r lattice spacings apart. In the thermodynamic limit one would expect both S and $\rho(r)$ for $r \to \infty$ to vanish whereas in finite systems because of finite size effects both quantities may appear to have small but finite values.

Vuillermot and Romerio (Vuillermot & Romerio, 1973; 1975) presented an exact solution of the planar (n=2) and spatial (n=3) versions of the Lebwohl-Lasher model in one dimension

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(d=1) for a nematic liquid crystal, without periodic boundary conditions. They also calculated the two-molecule correlation functions and have shown that these models do not exhibit any finite temperature order-disorder phase transition.

The partition function $Z_N(\tilde{K})$ for the N-particle system is given by

$$Z_N(\tilde{K}) = \tilde{K}^{-N/2} \exp[\frac{2}{3}N\tilde{K}]D^N(\tilde{K}^{1/2}) \tag{12}$$

where $\tilde{K}$=3/2T and D is the Dawson function (Abramowitz & Stegun, 1970).

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

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

$$\frac{2U_N(\tilde{K})}{N} = 1 + \frac{3\tilde{K}^{-1}}{2} - \frac{3}{2}\tilde{K}^{-1/2}D^{-1}(\tilde{K}^{1/2}) \tag{13}$$

$$\frac{S_N(\tilde{K})}{N} = \frac{1}{2} + \tilde{K} - \frac{1}{2}\tilde{K}^{1/2}D^{-1}(\tilde{K}^{1/2}) + \ln\left[\tilde{K}^{-1/2}D(\tilde{K}^{1/2})\right] \tag{14}$$

and

$$\frac{2C_N(\tilde{K})}{N} = 1 - \tilde{K}^{3/2}\left[\frac{\tilde{K}^{-1}}{2} - 1\right]D^{-1}(\tilde{K}^{1/2}) - \frac{1}{2}\tilde{K}D^{-2}(\tilde{K}^{1/2}). \tag{15}$$

The correlation function is given by

$$\rho_N(r) = \left[\frac{3}{4}\tilde{K}^{-1/2}D^{-1}(\tilde{K}^{1/2}) - \frac{3}{4}\tilde{K}^{-1} - \frac{1}{2}\right]^r \tag{16}$$

3.2 Computational details – how to handle a continuous model

In the model we have investigated, spins can take up any orientation in the three dimensional space and the orientation of each spin is stored in terms of the direction cosines (l_1, l_2, l_3). The starting configuration has always been chosen as a random one and to generate a new microstate, a randomly selected spin is chosen and each direction cosine is updated as $l_i \rightarrow l_i + p * r_i$ (for i=1,2,3) where p is a parameter to be chosen according to some criterion and r_i is a random number between -1 to +1. To preserve the unit magnitude of the spins, (l_1, l_2, l_3) is always normalized.

The energy of the system in the LL model is a continuous variable and in one dimension (d =1) it can have any value between $-L$ to $L/2$. To have a discretization scheme for the implementation of the WL algorithm and for an one dimensional random walk in the energy space, we have chosen an energy range from (-L to 0) and have divided this energy range into M bins each having a width d_e.

As already mentioned in the previous section we use $g(E_i) = \ln\Omega(E_i)$, $\Omega(E_i)$ being the number of micro-states corresponding to the i-th bin for which the mid-point has the value E_i. Initially we set all $g(E_i)$ (i=1,M) to zero and the logarithm of the modification factor $\ln f$ is taken as 1. Whenever a new microstate is generated by rotating a spin, the new system-energy and hence, the macrostate j is determined. Whether the move is accepted or not is decided according to the WL prescription (Wang & Landau, 2001) for the probability

$$p_{i \to j} = min\left(\frac{\Omega(E_i)}{\Omega(E_j)}, 1\right). \tag{17}$$

If the state j is accepted, we make $g(E_j) = g(E_j) + \ln f$ and $h(E_j) = h(E_j) +1$, where $h(E_j)$ is the histogram count. Otherwise we make $g(E_i) = g(E_i) + \ln f$ and $h(E_i) = h(E_i)$ + 1. This procedure is repeated for 10^4 MC sweeps (where one MC sweeps consists of L attempted moves) and the flatness of the histogram is checked and the cycle is repeated till 90% flatness in the histogram is reached. This completes one iteration, following which we reduce the logarithm of the modification factor $\ln f \to \ln f/2$, reset the histogram, and the whole procedure is repeated. For each lattice size we have continued with the iterations till $\ln f$ gets reduced to 10^{-9}. We have also calculated the quantity S (Equation 10) which gives us the magnitude of the order parameter obtained from the largest eigenvalue of the ordering matrix defined in Equation 9 and a two-dimensional random walk was performed in the (E-S) space for this purpose. The flatness check of the two-dimensional histogram thus generated needs to be reconsidered. For a given value of the energy of the system, the order parameter, S has a distribution over a certain range of values. The whole range of S is 0 to 1 and in order to perform the two dimensional random walk in the energy-order parameter (E-S) space we divide the two dimensional space into $M \times N$ bins. We represent by d_ϕ the bin-widths involving the parameter other than energy in the two-dimensional walk. Each microstate will now correspond to a macrostate labeled by the indices i and j and the acceptance probability given by Equation 17 is now modified to

$$p_{ij \to kl} = min\left(\frac{\Omega(E_i, S_j)}{\Omega(E_k, S_l)}, 1\right) \tag{18}$$

along with an appropriate modification of the procedure described after Equation 17 for the two-dimensional random walk. Here, for instance, $\Omega(E_i, S_j)$ is the density of states for the i-th energy and j-th order parameter bin. A two-dimensional random walk in the (E-S) space is a lot more expensive in terms of the CPU time than an one-dimensional walk in the energy space alone. The problem is particularly severe in a system with continuous energy and becomes worse as the lattice size increases. However, this ensures a much more uniform sampling of the order parameter bins that correspond to a particular energy bin and this improves the overall statistics of the work. It may be pointed out that it is impossible to arrive at a flat histogram in the (E-S) space if one attempts to visit the entire energy and order parameter ranges accessible to the system. For an one-dimensional walk one normally faces a problem in that, it takes a relatively long time to visit the lowest energy levels and this increases with the increase in system size. For a two-dimensional walk the possibility of uniformly visiting the entire rectangular (E-S) space is unphysical and one must have a prior knowledge of the range of S-bins which are likely to be visited while the system energy has a given value E_i. Our method of simulating the two dimensional random walk has resemblance to the work of Troster and Dellago (Troster & Dellago, 2005), who have applied the WL algorithm to evaluate multidimensional integrals of sharply peaked functions. Our modified approach is elaborated in the following paragraph. We have first mapped the (E-S) space which costed us 35×10^6 sweeps (to be called the pre-production run). The idea is to determine the minimum (S_{min}^i) and maximum (S_{max}^i) values of the S-bins which are visited while the system energy is E_i for i=1,M. We observe that there are always some S-bins within the range (S_{min}^i,S_{max}^i) for each E_i, where either no sampling or very low sampling takes place during the pre-production

run. We therefore checked the histograms of the (E_i, S_j) bins in the mapped region of the two-dimensional space and those which attain a 90% flatness (i.e. $x = 0.9$) during the pre-production run are marked with '1' while other bins are marked '0'. This may be clarified as follows. We calculate the average histogram value for those bins which have been visited at least once, thus discarding the bins which are not visited at all. The flatness test (which needs each of the visited bins to have a histogram count at least equal to 90% of the average histogram) is then applied only to those bins and these are labeled with '1'. In the 'production run' part of the rest of the simulation we check the flatness of only those bins which were marked '1' ignoring what is happening to the others. There is however, always a possibility, since the 'production run' generates many more microstates than that in the 'pre-production run', that larger areas in the (E-S) space would get included in the initial 'visit-map' or those bins, once marked '0', would subsequently qualify for the label '1'. But it is impossible to improve upon the accuracy of the work indefinitely and we decided to stick to the map we obtained during a reasonable amount of the 'pre-production run', ignoring what is happening to the discarded bins. In addition to the two-dimensional random walk in the (E-S) space we have also performed a number of other two-dimensional random walks. These involve the (E-$\rho(r)$) space where $\rho(r)$ is the correlation function defined in Equation 11. Random walks in E-$\rho(r)$ space are performed only for the L=160 lattice, for r ranging from 2 to 40 and the ensemble averages of $\rho(r)$ were evaluated for different temperatures using Equation 3.
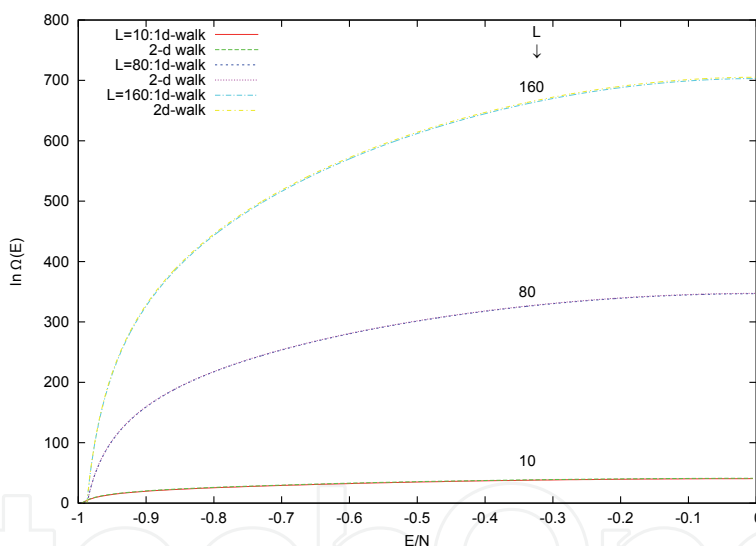
Fig. 1. Logarithm of the density of states, $\ln \Omega(E)$, for the 1-d Lebwohl-Lasher model for L=10, 80 and 160 obtained from 1-d and 2-d walks. In the resolution of the figure the data for 1-d and 2-d walks overlap.

3.3 How to choose different parameters for a continuous model

MC simulations using the WL algorithm in linear spin chains of length L where L=10, 20, 40, 80 and 160 have been performed. All the results we present are results of a single simulation for each lattice size and we did not perform averaging of results over multiple simulations although this surely is expected to reduce the errors. In a simulation involving a continuous model one is confronted with the proper choice of the values of two parameters, p and d_e. The former determines the amplitude of the random rotation of a spin and the latter is the energy bin width. In the case of a two dimensional random walk, another parameter d_ϕ,
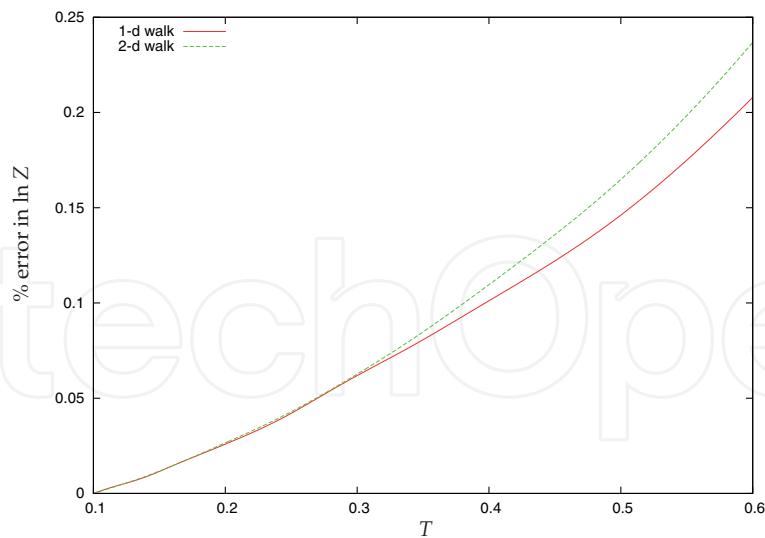
Fig. 2. Percentage error in the logarithm of partition function, $\ln Z$, for 1-d and 2-d walks, plotted against temperature T, for the 1-d Lebwohl-Lasher model for L=80. The errors are in comparison to the exact results.

which represents the width of the order parameter or the correlation function bin is also to be chosen. We have set d_e=0.1 for all the work reported in this paper. d_ϕ was taken to be 0.01 for both order parameter and correlation function. The parameter p was always 0.1, except for the two-dimensional walk involving the order parameter, where it was taken to be 0.2. For larger values of p, the CPU time is less, but the results of the simulation (like the position and height of the specific heat curve, for instance) tend to depend strongly on p. For the values of p in the neighbourhood of 0.1, the results depend very weakly on p. This is presumably due to the fact that, a small change in the orientation of a spin (one at a time) results in a systematic and uniform sampling in the phase space, but as a result of greater correlation of the successive configurations generated and the consequent slow movement of the representative point in phase space, the computer time involved is greater. For the two-dimensional walk involving the order parameter, since a lot of CPU time is necessary, we have chosen p=0.2, to reduce the time involved. The bin widths for energy or other variables were so chosen that for about 50% of the configurations generated by the spin rotation procedure, new bins are visited. This procedure was found to be optimum, as an attempt to visit new bins more frequently, would result in missing a vast majority of the microstates which correspond to each bin. A small value of p, the rotation amplitude, is justifiable from the same point of view. A relatively large value of p results in a poor sampling of the infinite number of closely spaced microstates contained in each bin and leads to poor results which tend to depend on the value of p, and consequently not in agreement with the exact results.

3.4 Results for the one-dimensional LL model: Comparison with exact results

In Fig. 1 we have plotted the quantity $g(E) = \ln \Omega(E)$ as a function of the energy per particle for L=10, 80 and 160 and the results obtained from one and two dimensional walks (in E-S space) have been compared. The system energy was always considered up to E=0. The lower limit of the energy for L=80 was -79 and for L=160, it was -158, where the corresponding ground state energies are -80 and -160. Thus, the visited energy range goes to a sufficiently low value to cover the entire range of interest but the small cut near the ground state was necessary, as it takes a huge time to sample these states for a relatively large lattice. The
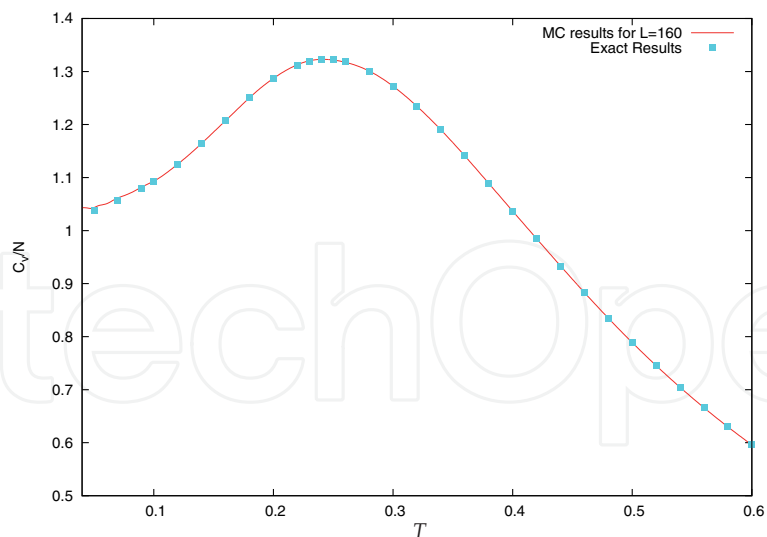
Fig. 3. The specific heat per particle, obtained as a fluctuation quantity, plotted against temperature, for L=160 and compared with the exact result.
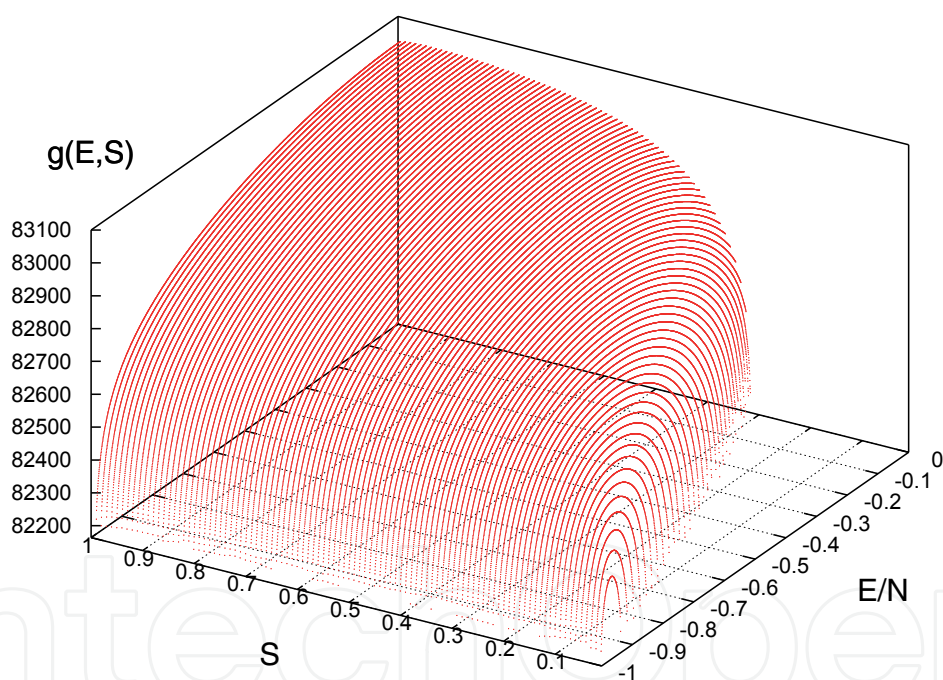

Fig. 4. Three dimensional $g(E, S)$ surface plotted against energy and the order parameter for L=160.

partition function, Z was calculated from a knowledge of the density of states, and the percentage error in $\ln Z$, in comparison with the exact results, has been shown in Fig. 2 for both 1-d and 2-d walk for the L=80 lattice. The error in $\ln Z$ slowly increases with temperature and, at the highest temperature we have investigated, (T=0.6), it is about 0.2%; the error in $\ln Z$ available from 2-d walk being marginally higher.

The specific heat per particle has been plotted against temperature in Fig. 3 for L=160 and compared with the exact results. The surface plot of joint density of states of energy and order parameter for one-dimensional LL model (L=160) is shown in Fig. 4. In Fig. 5 we have
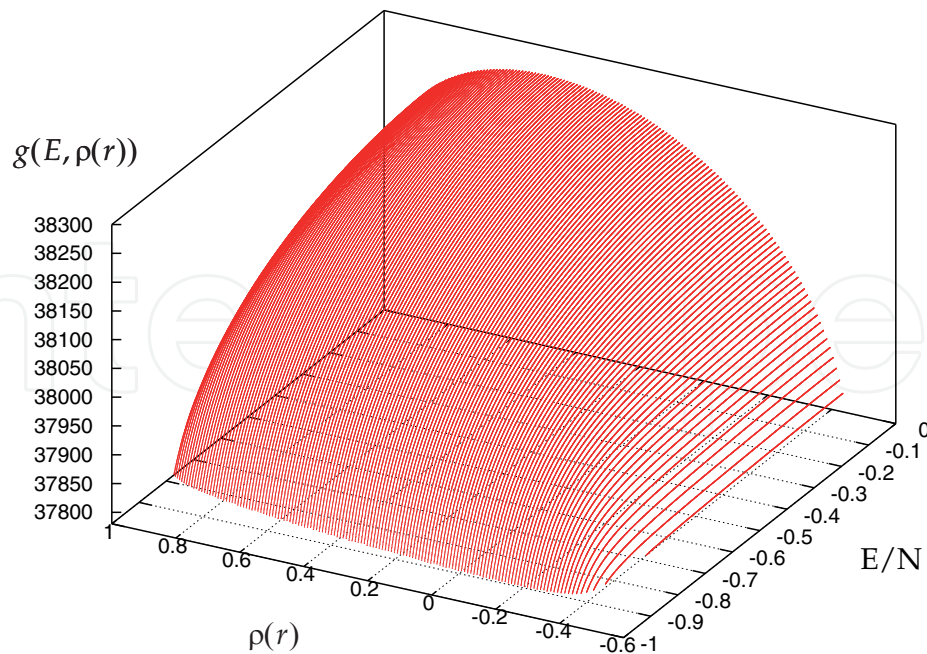
Fig. 5. Three dimensional $g(E, \rho(r))$ surface plotted against energy per particle and the correlation function for $r=5$ for the one-dimensional LL model of system size 160.
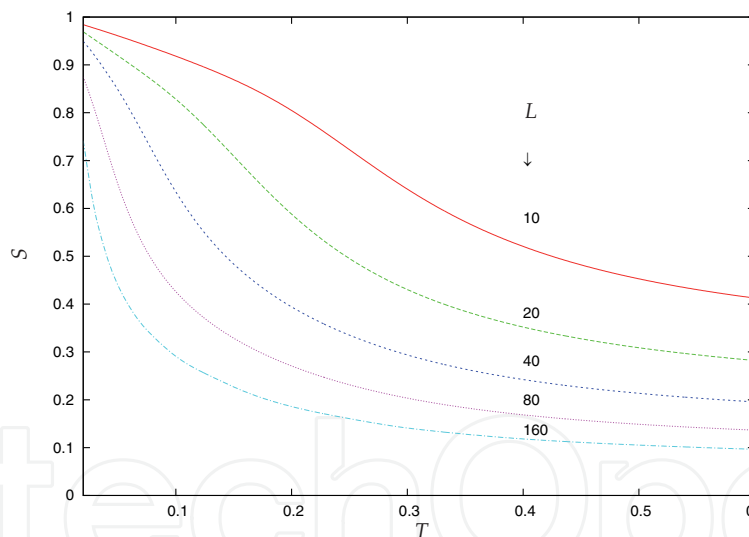
Fig. 6. The temperature variation of orientational order parameter for different lattice sizes for the LL model obtained from JDOS.

depicted the JDOS, $\ln \Omega[E, \rho(r)]$ for $r=5$. The scalar order parameter S, defined in Equation 10 has been plotted in Fig. 6 against temperature for all lattice sizes. It may be recalled that the system is disordered at all finite temperatures and one would expect $S=0$ for all values of T. For a given T (including $T=0$), S rapidly falls off with increase in system size, and in the thermodynamic limit will disappear altogether.

The correlation function $\rho(r)$ has been compared for the $L=160$ lattice using the two-dimensional random walk. We have performed simulations for 12 values of r, ranging from 1 to 40, and these have been plotted against temperature in Fig. 7 where comparison

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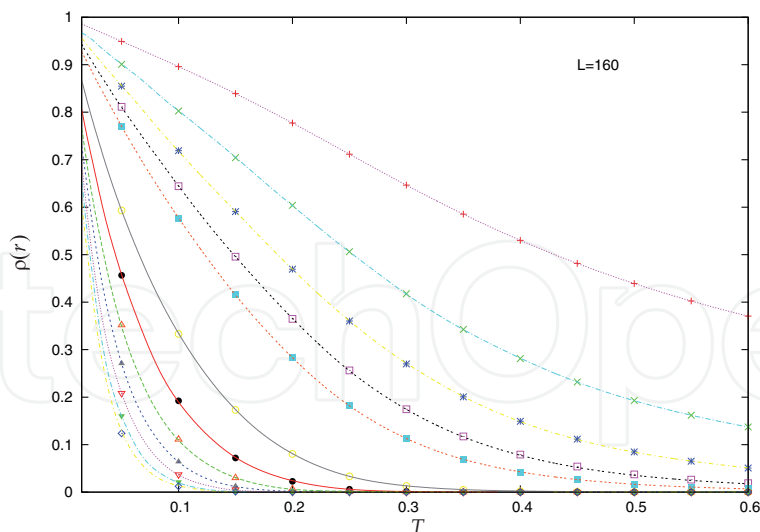
Fig. 7. Variation of correlation function $\rho(r)$ with temperature T for lattice size L=160. The points represented by different symbols are from the exact results. The curves are the results we obtained from the joint density of states. The values of r taken are 1, 2, 3, 4, 5, 10, 15, 20, 25, 30, 35 and 40. The topmost curve is for r=1 and the lower curves are for other values of r given in the sequence above and in ascending order of r.
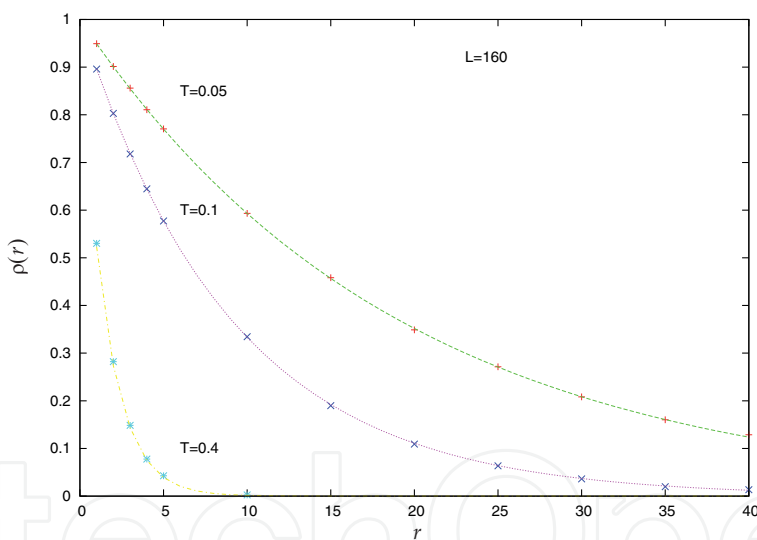
Fig. 8. Correlation function as a function of r at different temperatures for the LL model obtained using two-dimensional random walk.

has also been made with the exact results. It may be noted that, for each value of r, we had to run one simulation and the joint density of states were determined separately in each case. The same data has also been shown in Fig. 8 where for three temperatures $\rho(r)$ has been plotted against r. As one would expect in a disordered system, the correlation dies off quickly with increase in r. For $r \to \infty$, the spins are uncorrelated and $\rho(r)$ should approach S^2. However, verification of this result from our simulation data will not make much sense in a disordered system. The CPU time necessary for the L=160 lattice for one-dimensional walk is 10.6 hours and the two-dimensional walk involving correlation function is 70.5 hours. For the two-dimensional (E,S) walk the CPU time is 170 hours. The program was vectorized
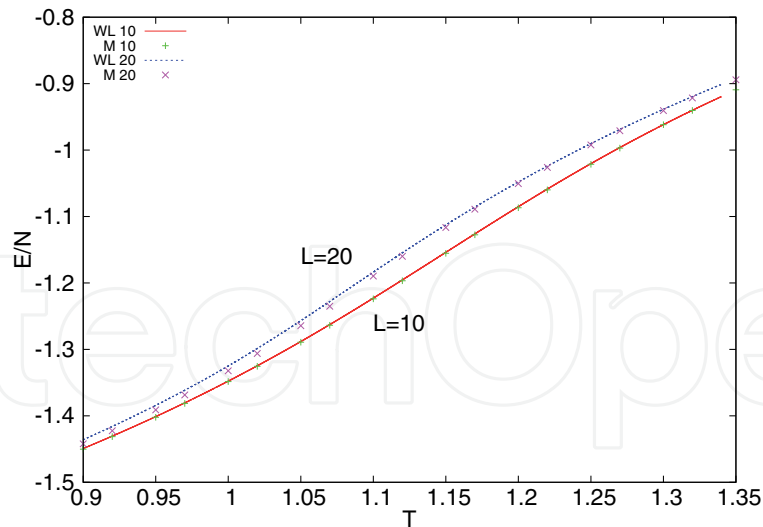
Fig. 9. The average energy per particle for the XY-model plotted against temperature for 10×10 and 20×20 lattice sizes, obtained using two MC methods namely, WL and M (Metropolis). All results are obtained by taking averages over 20 independent simulations. One-dimensional random walk has been used.
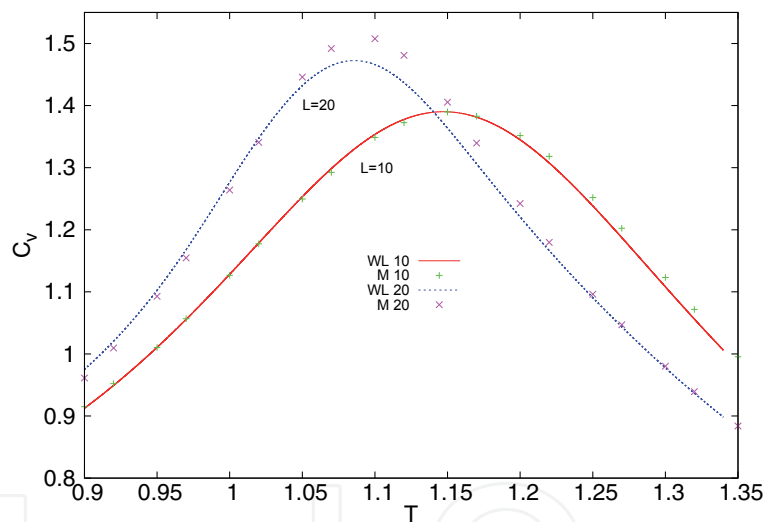

Fig. 10. The specific heat per particle for the XY-model plotted against temperature for 10×10 and 20×20 lattice sizes, obtained using two MC methods namely, WL and M (Metropolis). All results are obtained by taking averages over 20 independent simulations and one-dimensional random walk with 80% flatness of histogram was used.

(*i.e.* the 'do' loops parallelized) between two 3.0 GHz Xeon processors in a X226 IBM Server, automatically by the Intel Fortran Compiler, we used.

4. Wang Landau algorithm for two-dimensional XY-model

An XY model is a continuous spin model in which the spins on the lattice are confined to rotate in a plane. Unlike Ising and Potts models which have discrete energy values the XY model has a continuous range of energy values. In this section we consider a two-dimensional square lattice at every site of which is a spin confined to the XY-plane ($d = 2$, $n = 2$). Note that a
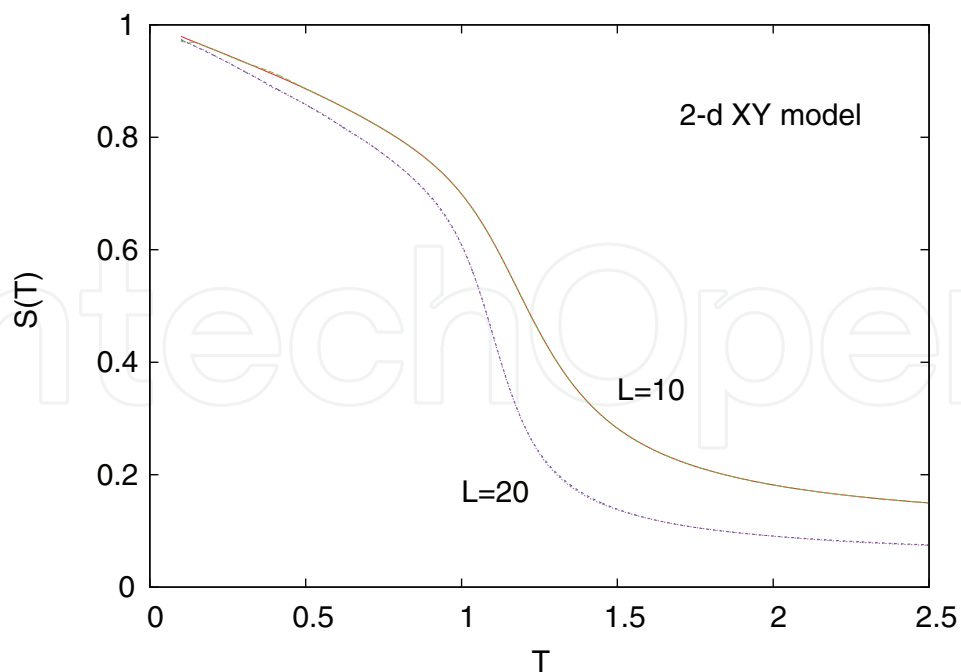
Fig. 11. The orientational order parameter for the XY-model is shown against temperature T for 10×10 and 20×20 lattice sizes. The results have been obtained from two-dimensional random walk.
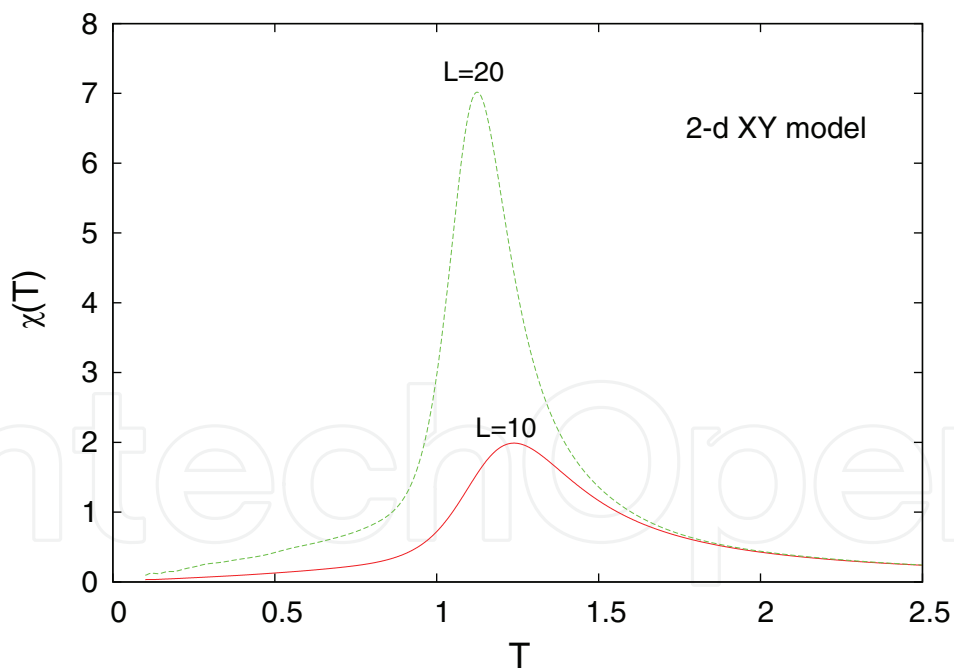

Fig. 12. The susceptibility for the XY-model is shown against temperature T for 10×10 and 20×20 lattice sizes.

lattice containing planar spins could have higher dimensions too, for example $d = 3$, $n = 2$ is also a possible choice.

4.1 The two-dimensional XY model

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

$$V(\theta_{ij}) = -\cos\theta_{ij} \tag{19}$$

where θ_{ij} is the angle between the nearest neighbour spins i and j. The XY-model is known to exhibit a quasi-long-range-order disorder transition which is mediated by unbinding of topological defects. It has also been the subject of extensive MC simulation over last few decades and some of the recent results may be found in (Bhar & Roy, 2009; Maucourt & Grempel, 1997; Olsson, 1995; Palma et al., 2002).

In this model, the orientational order parameter is defined as follows: let **n** be the unit vector (called the director) in the direction of maximum order prevailing in the system and **s** be the spin vector of unit magnitude, then the average order parameter S is given by

$$S(T) = \langle \mathbf{n} \cdot \mathbf{s} \rangle = \langle \cos\alpha \rangle \tag{20}$$

where α is the angle between the director and the spin. The order parameter susceptibility per spin is calculated from the fluctuations in the order parameter using the relation:

$$\chi(T) = \beta N \left(\langle \phi^2 \rangle - \langle \phi \rangle^2 \right) \tag{21}$$

where ϕ is the order parameter for a given configuration and N is the total number of spins of the system.

4.2 Computational details and results for the two-dimensional XY model

In this model simulations were carried out for lattice sizes 10×10 and 20×20 and the corresponding minimum of the energy range were chosen to be 3 for each. Histogram flatness was restricted to 80% (i.e. $x = 0.8$) in WL simulation. For the two-dimensional XY model of linear dimension L the system energy lies between $-2L^2$ and $2L^2$. In order to apply the WL algorithm we have restricted the random walk in the energy space from $-2L^2$ to 0 (actually a small energy band near the ground state was also excluded to avoid trapping of the random walker in these low energy states as these are scarcely visited during the simulation). The iterations are continued till logarithm of the modification factor $\ln f$ gets reduced to $ln f_{final} = 10^{-8}$ for the 10×10 lattice and to $ln f_{final} = 10^{-6}$ for the lattice size 20×20. 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 WL results with those obtained from simulation using the conventional Metropolis algorithm, which is known to work satisfactorily for this model (Palma et al., 2002). To increase the reliability of our results, we have performed 20 independent simulations for each of the Metropolis, and WL methods and have averaged over the respective results. In the Metropolis simulation the averaging was done directly over the observables while in the other case, 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 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 20×20 lattice.

In Figs. 9 and 10 the variations of the average energy, E and the specific heat, C_v with temperature are shown respectively for the 10×10 and 20×20 lattices. These are obtained

with the WL and Metropolis algorithms. This diagram and all the following diagrams, depicting the results of the XY-model, represent the results averaged over 20 independent simulations for the algorithm used. The order parameter S for two-dimensional XY model of linear lattice sizes 10 and 20 are plotted with temperature in Fig. 11. The system is known to possess no true long range order and a quasi-long range order-disorder transition takes place due to the unbinding of topological defects. Susceptibility of two-dimensional XY model is also plotted as a function of temperature for two lattice sizes in Fig. 12.

5. Conclusion

We end this chapter with discussions on the accuracy of the estimated density of states and alternative convergence methods. In course of the random walk in a Wang Landau simulation, the fluctuation of the energy histogram, for a given modification factor f, initially grows with the number of Monte Carlo sweeps and then saturates to a certain value. Because of the nature of this algorithm the value of the histogram fluctuation determines the error which is generated in the resulting density of states. Zhou and Bhatt carried out a mathematical analysis of the Wang Landau algorithm and proved the convergence of the iterative procedure. They have shown that the error in the density of states, for a given f, is of the order of $\sqrt{lnf}$. This finding has been tested by Lee *et al.* (Lee et al., 2006). who performed extensive numerical tests in two two-dimensional discrete models, namely, the ferromagnetic Ising model and the fully frustrated Ising model. They have shown that the fluctuation in the histogram increases during an initial accumulation stage and then saturates to a value which is inversely proportional to $\sqrt{lnf}$ and they were of the view that this feature is generic to the Wang Landau algorithm. The resulting error in the density of states was found to be of the order of $\sqrt{lnf}$, which is in agreement with the prediction of Zhou and Bhatt.

Convergence methods which are alternatives to the requirement of the histogram flatness, for deciding where to stop an iteration for a given modification factor, have been proposed in the work described in the references (Zhou & Bhatt, 2005), (Lee et al., 2006). According to Zhou and Bhatt an iteration may be stopped when the minimum number of visits to each macrostate is $1/\sqrt{lnf}$. On the other hand, Lee *et al.* proposed that an iteration can be stopped when the number of Monte Carlo sweeps, for a given value of f, is such that the saturation of the histogram fluctuation has been reached, since continuing the simulation for this particular modification factor is unlikely to reduce the error in the density of states any further. Sinha and Roy (Sinha & Roy, 2009) have investigated the growth of histogram fluctuations in two continuous lattice spin models. In these models where the spins reside at the sites of a two-dimensional square lattice, the interaction between nearest neighbours is given by

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

where q^2 is a positive number and θ_{ij} is the angle between the nearest neighbour spins i and j. For $q^2 = 1$, the model is simply the conventional XY model (except for an additive constant in the potential). This model has also been studied recently by Bhar and Roy (Bhar & Roy, 2009) using WL and Wang-Landau-Transition-Matrix Monte Carlo algorithm. For larger q^2 (say, $q^2 = 50$) the potential well has a sharp minimum and the system possesses a strongly first order phase transition. Sinha and Roy have observed that in these continuous models too, the fluctuations in the energy histogram after an initial increase saturates to a value proportional to $1\sqrt{(lnf)}$. Therefore, it may seem, in agreement with the proposal of Lee et al., that WL

sampling should be carried out only till the saturation value of the histogram sampling is reached. However it was found that this does not work even for systems of moderate size as an energy range near the ground state is not sampled at all. Even the idea of Zhou and Bhatt that $1\sqrt{(lnf)}$ visits to each bin does not seem to be a practical solution as it involves a huge CPU time even for continuous systems of moderate size. This remains a major problem with the feasibility of applying the WL method to continuous spin systems and problem is more tedious when one is determining the JDOS.

6. Acknowledgment

7. Appendix

In this appendix we show the technique for the evaluation of the partition function Z from the estimated density of states. The direct use of Equation 1 in evaluating partition function may cause overflow or underflow problem in the allowed range of real numbers on modern computers. In order to get around of this problem we may use the following trick. Suppose we have a system with four energy levels: E_1, E_2, E_3 and E_4 and the logarithms of the corresponding density of states are g_1, g_2, g_3 and g_4 the values of which are generated in simulations. Then the partition function of the system at temperature T is expressed as

$$Z = e^{v_1} + e^{v_2} + e^{v_3} + e^{v_4} \tag{22}$$

where $v_i = g_i - \beta E_i, \quad i = 1, 2, 3, 4.$

$$\begin{aligned}
Z &= e^{v_1} \left[e^{v_2 - v_1} + e^{v_3 - v_1} + e^{v_4 - v_1} \right] \\
&= e^{v_1} \left[1 + e^{v_2 - v_1} \left[1 + e^{v_3 - v_2} + e^{v_4 - v_2} \right] \right] \\
&= e^{v_1} \left[1 + e^{v_2 - v_1} \left[1 + e^{v_3 - v_2} \left[1 + e^{v_4 - v_3} \right] \right] \right]
\end{aligned} \tag{23}$$

This can further be written as

$$\begin{aligned}
Z &= e^{v_1} \left[1 + e^{v_2 - v_1} \left[1 + e^{\left[v_3 - v_2 + \ln\left[1 + e^{v_4 - v_3} \right] \right]} \right] \right] \\
&= e^{v_1} \left[1 + e^{\left[v_2 - v_1 + \ln\left[1 + e^{\left[v_3 - v_2 + \ln\left[1 + e^{v_4 - v_3} \right] \right]} \right] \right]} \right]
\end{aligned} \tag{24}$$

Therefore

$$\ln Z = v_1 + e^{v_1} \left[1 + e^{\left[v_2 - v_1 + \ln\left[1 + e^{\left[v_3 - v_2 + \ln\left[1 + e^{v_4 - v_3} \right] \right]} \right] \right]} \right] \tag{25}$$

Since the exponents of the exponential are now written as differences of two terms the problem of overflowing is avoided. Again, if each of the powers of the exponential in the above

equation are greater than a predefined large value say, 500, we can neglect 1. This also simplifies the evaluation of Z.

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