Performance of Wang-Landau algorithm in lattice model of liquid crystals

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We present a study on the performance of Wang-Landau algorithm in a lattice model of liquid crystals which is a continuous lattice spin model. We propose a novel method of the spin update scheme in a continuous lattice spin model. The proposed scheme reduces the autocorrelation time of the simulation and results in faster convergence.

I. INTRODUCTION

The Wang-Landau (WL) algorithm [1], introduced in 2001, has received much attention and has been applied to a wide range of problems [2–12]. In most of these investigations, the authors have applied the WL algorithm to systems with discrete energy levels. However, relatively fewer papers have so far appeared on lattice models with continuous energy spectrum [7, 13–17]. Techniques, in general, to improve the algorithm for different problems have also been proposed [18–33]. The review [34] illustrates the versatile applications of the WL algorithm in protein folding, fluid simulations, systems with first order phase transitions and other systems with rough energy terrain. Some authors find its applications in performing numerical integration [10, 28].

The WL algorithm allows us to calculate the density of states (DOS) as a function of energy or the joint density of states (JDOS) as a function of energy and a second variable [14]. For a macroscopic system, the DOS $\Omega(E_i)$ (where $i = 1, 2, \cdots, n$, n being the bin index) is a large number and it is convenient to work with its logarithm $g(E_i) = \ln \Omega(E_i)$. Since the DOS is independent of temperature and contains complete information about the system, the task is to determine it as accurately as possible. The next step involves the determination of partition function $Z(T) = \sum_E \Omega(E) e^{-\beta E}$ ($\beta = 1/T$, Boltzmann constant has been set to unity) at any temperature (T) by the standard Boltzmann reweighting procedure. Once the partition function is known, the model is essentially "solved" since most thermodynamic quantities at any temperature can be calculated from it. The algorithm is implemented by performing an one-dimensional random walk that produces a "flat" histogram in the energy space. For a continuous model, one needs to use a discretization scheme to divide the energy range of interest into a number of bins which label the macrostates of the system. In the WL algorithm, these macrostates are sampled with a probability which is proportional to the reciprocal of the current DOS. The estimate for the DOS

is improved at each step of the random walk using a carefully controlled modification factor f to produce a result that converges to the true DOS quickly. A histogram record $H(E_i)$ of all states visited is maintained throughout the simulation. When $g(E_i)$ corresponding to a certain macrostate is modified as $g(E_i) \rightarrow g(E_i) + \ln f$, the corresponding $H(E_i)$ is modified as $H(E_i) \rightarrow H(E_i) + 1$. In the original proposal of WL algorithm, an iteration is said to be complete when the histogram satisfies a certain "flatness" condition. This means that $H(E_i)$, for all values of i, has attained 90% (or some other preset value) of the average histogram. In the following iteration, f is reduced in some fashion, the $H(E_i)$'s are reset to zero and the process is continued till $\ln f$ is as small as 10^{-8} or 10^{-9}. Since the history of the entire sampling process determines the DOS, the WL algorithm is non-Markovian besides being multicanonical in nature.

In course of the random walk in a WL simulation, the fluctuations of energy histogram, for a given modification factor f, initially grows with time and then saturates to a certain value. Zhou and Bhatt [27] carried out a mathematical analysis of the WL algorithm. They provided a proof of the convergence of the iterative procedure and have shown that the fluctuations in histogram, proportional to $1/\sqrt{\ln f}$ for a given f, cause statistical errors which can be reduced by averaging over multiple simulations. They have also shown that the correlation between adjacent records in the histogram introduces a systematic error which is reduced at smaller f. The prediction in Ref. [27] has been numerically verified by different authors independently [17, 29]. Although to obtain a flat histogram is the initial motivation behind the WL algorithm, Ref. [27] concluded that flatness is not a necessary criterion to achieve convergence and suggested that one should instead focus on the fluctuations of the histogram rather than the "flatness". They had shown that $1/\sqrt{\ln f}$ visits on each macroscopic state is enough to guarantee the convergence. In fact, fluctuations in the histogram is intrinsic to WL algorithm. These fluctuations lead to a statistical error in the DOS which scales as $\sqrt{\ln f}$, for a given f. The iterative WL algorithm partially reduces this statistical fluctuations by decreasing f monotonically. However Ref. [32] clearly illustrates that even if f is reduced to a very small value according to

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the original prescription, the statistical error stops to decrease at a certain point. In practice there always exists a systematic error in the simulation which is a function of f and the correlation between adjacent records in the histogram. Ref. [27] observed that this systematic error decreases when either f or the correlation decreases. In this context, we refer to the work of Morozov and Lin [31] who presented a study on the estimations of accuracy and convergence of the Wang-Landau algorithm on a two level system with a significant efficiency improvement in [35]. The WL algorithm compares $\Omega(E_i)$ and $\Omega(E_f)$, i.e, DOS before and after an attempted move, but it does not require E_i to be close to E_f. This is why Ref. [27] suggested the use of cluster algorithms that allow "nonlocal" moves in the parameter space. The Ref. [33] rightly pointed out that the update schemes for the underlying model certainly have an effect on the outcome. In the present paper we suggest a method for the spin update scheme of a lattice model with continuous energy spectrum, which reduces the autocorrelation time by an appreciable amount compared to the conventional spin update scheme. The suggested spin update method to obtain a less correlated configuration has also the advantage that this method is free from tuning any adjustable parameter. The method is described in Section III. We also investigate the growth of the histogram fluctuations in the one-dimensional Lebwohl-Lasher (LL) model, described in Section II, to check if the nature of the dependence of the maximum of the histogram fluctuations on the modification factor f is model independent or not. We mention in passing that Ref. [29] suggested the model-independent nature of the maximum of the histogram fluctuations by performing simulations on two discrete Ising models and concluded that many more simulations on different models are needed to confirm this universality nature. Ref. [17] confirmed this universality behavior for two continuous lattice spin models with spin dimensionality two. We have found that for the present model (spin dimensionality three), the fluctuations in the energy histogram, after an initial increase, saturates to a value which is inversely proportional to $\sqrt{\ln f}$ and confirm that this feature is generic to the WL algorithm. In the second part of the work, we have carried out the WL simulation with the proposed spin update scheme to estimate the canonical averages of various thermodynamic quantities for lattices of reasonably large size where minimum number of visits to each macrostate are $1/\sqrt{\ln f}$. Results obtained from our simulation are compared with the exact results available for the model.

The rest of the paper is arranged as follows. In Section II, we have described the model. The computational techniques are discussed in Section III. Section IV presents our results and discussions. Section V draws the conclusions.

II. MODEL

For the purpose of investigation, we have chosen an one-dimensional array of three-dimensional spins ($d = 1, l = 3$, where d is the space dimensionality and l is the spin dimensionality) interacting with nearest neighbors (nn) via a potential

$$V_{ij} = -P_2(\cos\,\theta_{ij}) \tag{1}$$

where P_2 is the second Legendre polynomial and θ_{ij} is the angle between the nearest neighbor spins i and j (the coupling constant in the interaction has been set to unity). 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. The model, known as the Lebwohl-Lasher (LL) model [36], is the lattice version of the Maier-Saupe (MS) model [37] which describes a nematic liquid crystal in the mean field approximation. Being a low-dimensional model with nn interaction, the $1d$ LL model does not exhibit any finite temperature phase transition. This model has been solved exactly by Vuillermot and Romerio [38] in 1973, using a group theoretical method. The results obtained in [38] are quoted below. The partition function $Z_N(\widetilde{K})$ for the N-particle system is given by

$$Z_N(\widetilde{K}) = \widetilde{K}^{N/2}\exp\left[\frac{2}{3}N\widetilde{K}\right]D^N(\widetilde{K}^{1/2}) \tag{2}$$

where $\widetilde{K} = 3/2T$ is a dimensionless quantity. D is the Dawson function [39] given by

$$D(x) = \exp(-x^2)\int_0^x e^{u^2}\,du \tag{3}$$

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

$$\frac{2U_N(\widetilde{K})}{N} = 1 + \frac{3\widetilde{K}^{-1}}{2} - \frac{3}{2}\widetilde{K}^{-1/2}D^{-1}\left(\widetilde{K}^{1/2}\right) \tag{4}$$

$$\frac{S_N(\widetilde{K})}{N} = \frac{1}{2} + \widetilde{K} - \frac{1}{2}\widetilde{K}^{1/2}D^{-1}\left(\widetilde{K}^{1/2}\right) \\ + \ln\left[\widetilde{K}^{-1/2}D\left(\widetilde{K}^{1/2}\right)\right] \tag{5}$$

$$\frac{2C_N(\widetilde{K})}{N} = 1 - \widetilde{K}^{3/2}\left[\frac{\widetilde{K}^{-1}}{2} - 1\right]D^{-1}\left(\widetilde{K}^{1/2}\right) \\ - \frac{1}{2}\widetilde{K}D^{-2}\left(\widetilde{K}^{1/2}\right) \tag{6}$$

We decided to choose this model to test the performance of WL algorithm using the suggested spin update scheme so that a comparison can be made with the exact results available for the model.

III.   COMPUTATIONAL TECHNIQUES

In the first part of this Section, we will describe the computational techniques used to determine the fluctuations in the energy histogram. In the later part of this Section, we will discuss the method for the new spin update scheme.

Let us first explain the notations and symbols relevant to the present work. The saturation value of the energy histogram fluctuation in the kth iteration is represented by β_k. Let f_k be the modification factor for the kth iteration. One usually starts with a modification factor $f = f_1 \geq 1$ and uses a sequence of decreasing f_k's ($k = 1, 2, 3, \cdots$) defined in some manner. One Monte Carlo (MC) sweep is taken to be completed when the number of attempted single spin moves equals the number of spins in the system. The error in the DOS after the nth iteration is directly related to β_i for $i > n$, the saturation values of the fluctuations. In the WL algorithm the logarithm of the DOS after n iterations is given by

$$g_n(E_i) = \sum_{k=1}^{n} H_k(E_i) \ln(f_k) \tag{7}$$

where $H_k(E_i)$ is the accumulated histogram count for the ith energy bin during the kth iteration. In order to get an idea of the fluctuations in the histogram and its growth with the number of MC sweeps, we subtract the minimum of the histogram count h_k^j which occurs in the histogram after the jth MC sweep has been completed during the kth iteration, i.e., we consider the quantity

$$\widetilde{H}_k^j(E_i) = H_k^j(E_i) - h_k^j \tag{8}$$

It may be noted that h_k^j does not refer to any particular bin and may occur in any of the visited bins. The quantity $\widetilde{H}_k^j(E_i)$ is now summed over all bins to give ΔH_k^j.

$$\Delta H_k^j = \sum_i \widetilde{H}_k^j(E_i) \tag{9}$$

ΔH_k^j is thus a measure of the fluctuations which occurs in the jth MC sweep during k^{th} iteration and is a sort of average over all macrostates or bins. ΔH_k^j fluctuates with j because of statistical errors and its mean value taken over j is nothing but β_k. The error of the logarithm of the DOS, summed over all energy levels or bins, after the completion of n iterations is therefore given by [29]

$$\eta_n = \sum_{k=n+1}^{\infty} \beta_k \ln(f_k) \tag{10}$$

Eq. (10) means that the error depends only on the fluctuations in histogram and the sequence of modification factors. When the values of f_k are predetermined, the fluctuations in histogram, i.e., ΔH_k^j, becomes the only determining factor for the error. For this reason the observable ΔH_k^j, defined by Eq. (9), is considered to be

a good measure of the fluctutations in histogram. However, we point out that because of the summation over the index i in Eq. (9), the nature of the distribution of the errors over the energy bins is not reflected in the summed quantity ΔH_k^j. What we get instead is an error which has been summed over all the energy bins. Since the predicted value of the error η_n is of the order of $\sqrt{\ln f_n}$ [27], one expects that the histogram saturation value β_n, for the nth iteration, should be proportional to $1/\sqrt{\ln f_n}$.

A.   Proposal for a novel spin update method

Now we discuss the method to generate a subsequent less-correlated spin configuration. In the conventional spin update method for a continuous lattice spin model, the orientation of each spin $\vec{s}$ is stored in terms of the direction cosines (l_1, l_2, l_3). To generate a new configuration (microstate), a spin is selected at random and each direction cosine of it is updated as $l_i \to l_i + p * x_i$ for $(i = 1, 2, 3)$ where the parameter "p" denotes the amplitude of the random angular displacements, chosen such that approximately half of the configurations are accepted and half rejected [40] and x_i is a random number between -1 to 1. We have seen for a number of continuous lattice spin models that the results for the thermodynamic quantities become very sensitive to the value of the parameter "p". "p" is generally taken such that $p < 1$ and the choice of "p" also depends on the systems we are working on. The reason for taking $p < 1$ is that small values of "p" correspond to small changes in the direction of the spin, i.e., the energy cost of an attempted move will be small. However, this is not the only form of update, nor is it known whether this is the most efficient form. The thing is, there is quite a lot of flexibility about the choice of the new state for the spins. A good discussion of it may be found in Ref. [41].

In the present work, we propose a novel protocol to generate a less-correlated spin configuration in the following manner. We take a random unit vector $\vec{r}$ and a spin update $\vec{s} \to \vec{s}\,'$ is defined as $\vec{s}\,' = \vec{s} - 2\,(\vec{s} \cdot \vec{r})\,\vec{r}$ where $(\vec{s} \cdot \vec{r})$ is the dot product of $\vec{s}$ and $\vec{r}$. This represents a reflection with respect to the hyperplane orthogonal to $\vec{r}$ and this is an idempotent operation. The idea came from Wolff [42]. One may think of a linear transformation $R(\vec{r})$ such that $\vec{s}\,' = R(\vec{r})\vec{s}$. This linear transformation has the property

$$R(\vec{r})^2 = 1 \tag{11}$$

i.e., idempotent and

$$[R(\vec{r})\vec{s}_1] \cdot [R(\vec{r})\vec{s}_2] = \vec{s}_1 \cdot \vec{s}_2 \tag{12}$$

i.e., the Hamiltonian (1) is invariant under global R transformations. This spin update method reduces the autocorrelation time to a considerable amount and consequently systematic error decreases. Moreover, defining a spin update in that way, the algorithm becomes free

from tuning any adjustable parameter even while simulating a lattice spin model with continuous energy spectrum. This spin update method has resulted in efficient simulation of continuous lattice spin models with XY symmetry [43, 44].

The energy of the $1d$ LL model is a continuous variable and it can have any value between $-L$ to $L/2$ where L is the system size. To discretize the system, we have chosen an energy range $(-L, 0)$ and divided this energy range into a number of bins (macrostates) each having a width, say w. In the present work, the bin width is taken to be 0.2.

IV. RESULTS AND DISCUSSIONS

We have determined for the lattice model we have defined, the dependence of the quantity ΔH_k^j, given by Eq. (9), on j, the number of MC sweeps for a given iteration denoted by k. For the purpose of testing the fluctuations in histogram, we have taken linear spin chains of length $L = 80$ and 160. Nearest neighbor interactions along with periodic boundary conditions were always used. The starting value of the modification factor $\ln f_1$ was taken to be 0.1 and the sequence $\ln f_{n+1} = (\ln f_n)/10^{1/4}$ was chosen and for the purpose of determination of fluctuations, the minimum $\ln f$ used was 10^{-5}. Clearly, the chosen sequence of f is to ensure that it gets reduced by a factor of 10 after four iterations. We have determined the quantity ΔH_k^j defined by Eq. (9) at intervals of 10^3 MC sweeps and the maximum number of sweeps chosen for a given value of f is such that the saturation of the histogram is clearly evident. The system energy is always considered up to $E = 0$. The lower limit of the energy for $L = 80$ is taken to be -78 and for $L = 160$, it is -158, while 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, though the small cut near the ground state is necessary, as configurations near the minimum energy take a very long time to be sampled during the random walk.

In Fig. 1, we have plotted the fluctuations in the histogram ΔH_k^j against the number of MC sweeps j for four values of the modification factor f. The plots shown are for $L = 160$ lattice and for $\ln f$ equal to 10^{-2}, 10^{-3}, 10^{-4} and 10^{-5}. We did not go to values of $\ln f$ less than 10^{-5} as it takes a very large CPU time. Averages were taken over hundred independent simulations to improve the statistics and accuracy. Similar plots are also taken for the $L = 80$ lattice. It is evident from Fig. 1 that ΔH_k^j increases initially and then saturates and as f gets smaller, the saturation value as well as the number of MC sweeps necessary to reach the saturation ($\mathtt{MCS_{sat}}$) increases. Fig. 2 explicitly reveals this fact. The standard error calculated from the hundred independent simulations are also shown in Fig. 1. In Fig. 3, we have plotted the logarithm of saturation value β_k, i.e., $\ln(\beta_k)$ vs $\ln(\ln f)$ for system sizes $L = 80$ and $L = 160$. From this

figure, it is clear that

$$\beta_k \propto (\ln f)^\alpha \qquad (13)$$

where the index $\alpha = -0.50133 \pm 0.007$ for $L = 80$ and $\alpha = -0.50844 \pm 0.005$ for $L = 160$ respectively. This is in agreement with the prediction of Zhou and Bhatt [27]. Certainly, this result is not new. It confirms the previous results that the values of the slope is generic to the WL algorithm, in this case, it is a continuous lattice spin model with spin dimensionality three.

Now we present the results of various thermodynamic quantities obtained from the simulation. In Fig. 4, we have plotted the average energy per spin against temperature (T) for $L = 220$. The results have been compared with the exact values of this observable obtained from Ref. [38]. The specific heat, calculated as fluctuations of the energy, has been plotted against T in Fig. 5 for $L = 220$ and compared with the exact results. In the inset of Fig. 5, the percentage error (ϵ) in the C_v near the peak in comparison with the exact results is shown. Percentage error is a measure of how inaccurate (or accurate) a measurement is and is defined by the formula $\frac{\mathtt{measured\ value} - \mathtt{actual\ value}}{\mathtt{actual\ value}} \times 100\%$. Exact results show that the specific heat peak is maximum at a temperature $T_{max}^{ex} = 0.24$ and from our simulation we obtain the temperature at which the peak of the specific heat is maximum is $T_{max}^{sim} = 0.2351$ for $L = 220$. This implies that the percentage error in temperature at which the peak of the specific heat is maximum is 2.04%. Fig. 6 shows the variation of entropy per particle for $L = 220$ and the exact results are also shown in the same plot.

The attention is now focused on the autocorrelation time of the simulation. The autocorrelation function for an observable $O(t)$ is given by

$$\chi(t) = \int dt'(O(t') - \langle O \rangle)(O(t' + t) - \langle O \rangle) \qquad (14)$$

where $O(t)$ is the instantaneous value of the observable at time t and $\langle O \rangle$ is the average value. The integrand in the above equation actually measures the correlation between the fluctuation of the observables at two different times, one an interval t later than the other. So $\chi(t)$ will take a nonzero value if on the average the fluctuations are correlated, otherwise it is zero. Thus when t is just a single MC step apart, we will have a large positive autocorrelation. For large t, $\chi(t)$ will be zero and the measurements are totally uncorrelated. The autocorrelation is expected to fall off exponentially at long times thus:

$$\chi(t) \sim \mathtt{e}^{-t/\tau} \qquad (15)$$

where τ is a measure of autocorrelation time of our simulation. At time $t = \tau$, the autocorrelation function, which is a measure of the similarity of the two states, is only a factor of $1/\mathtt{e}$ down from its maximum value at $t = 0$. We have estimated the autocorrelation time both for the simulations with the conventional spin update method
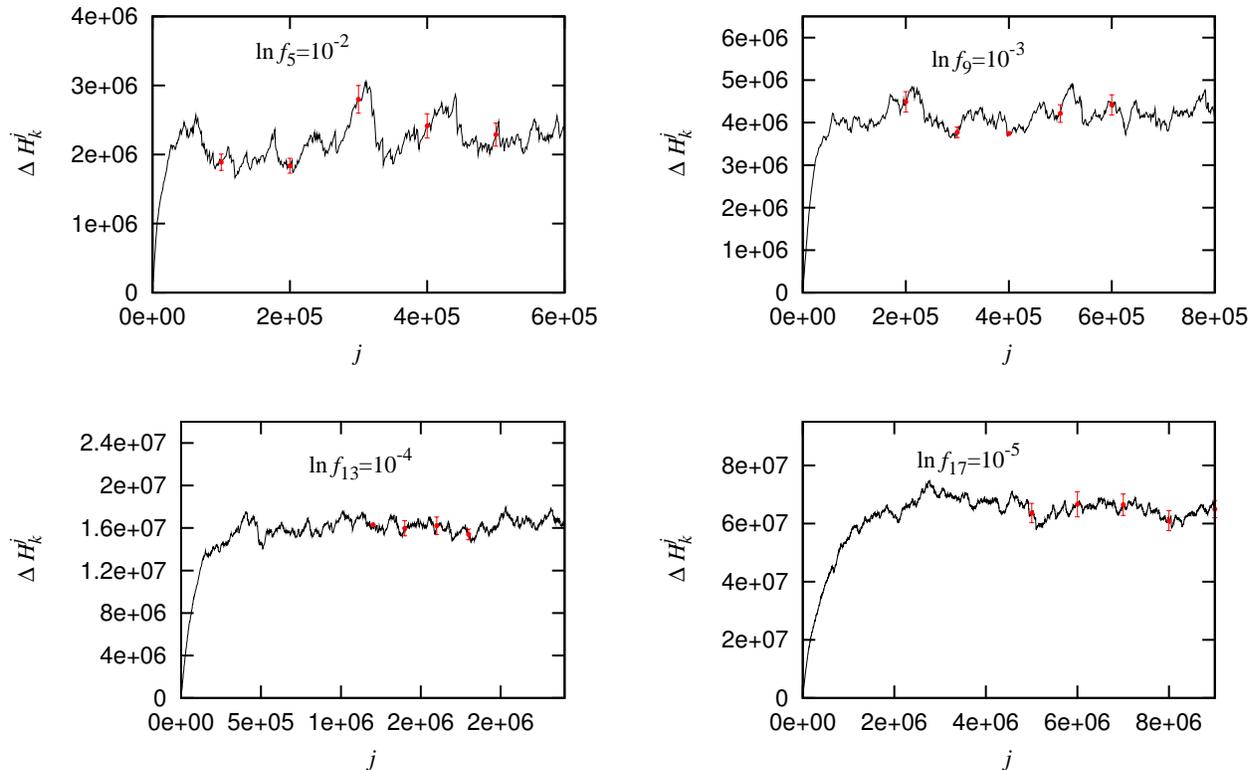
FIG. 1. (Color online) The histogram fluctuations ΔH_k^j for the kth iteration are plotted against the MC sweeps j for the $L = 160$ lattice. The values of $\ln f_k$ are indicated in the figures. The histograms are averaged over 100 independent simulations.
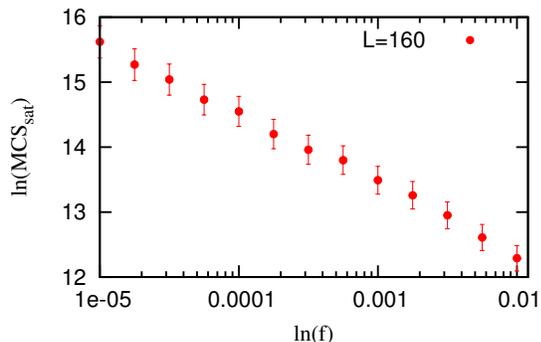

FIG. 2. (Color online) Logarithm of the MC sweeps required to reach the saturation is plotted against $\ln f$ for $L = 160$ system size. The errorbars are shown in the figure.
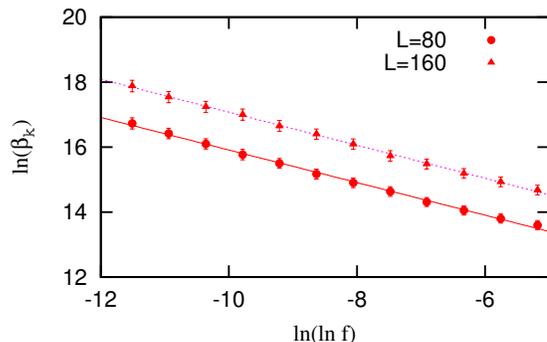

FIG. 3. (Color online) Logarithm of the saturation values of the histogram fluctuations $\ln(\beta_k)$ is plotted against $\ln(\ln f)$ for $L = 80$ and $L = 160$ systems with the error bars. The slopes of the two linear fits are given in the text.

and the proposed spin update method. The autocorrelation time is calculated following the method proposed by Madras and Sokal [45]. In the conventional spin update scheme, when we flip a single spin in each update, the total energy can only change by a small amount every time. In the proposed spin update scheme, the change in total energy is greater compared to that in the conven-

tional scheme. As the WL algorithm does not require E_i to be close to E_f, but compares only $\Omega(E_i)$ and $\Omega(E_f)$, the convergence becomes faster with the proposed scheme than with the conventional scheme.
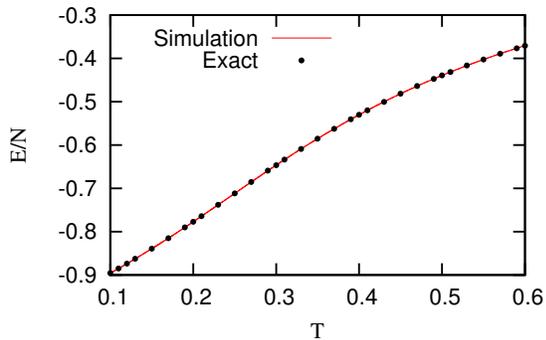
We have found that the autocorrelation time (τ) ex-

FIG. 4. (Color online) The variation of the average energy per particle is plotted against T (solid line) for $L = 220$. Exact results, indicated by the filled circle, are also plotted in the same graph. The error bars are of the dimensions smaller than the symbols used for plotting.
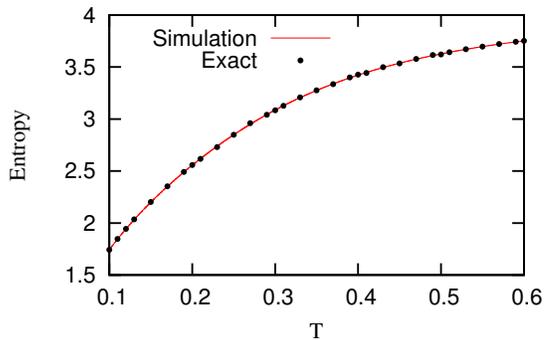

FIG. 6. (Color online) The variation of the entropy per particle is plotted against T (solid line) for $L = 220$. The filled circle indicates the exact results. The error bars are of the dimensions smaller than the symbols used for plotting.
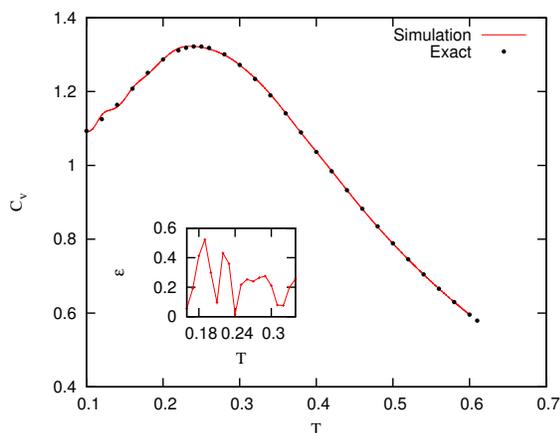
FIG. 5. (Color online) The specific heat is plotted against T (solid line) for $L = 220$. Exact results are indicated by the filled circle. The error bars are of the dimensions smaller than the symbols used for plotting. The percentage error in the C_v in comparison with the exact results is shown in the inset.
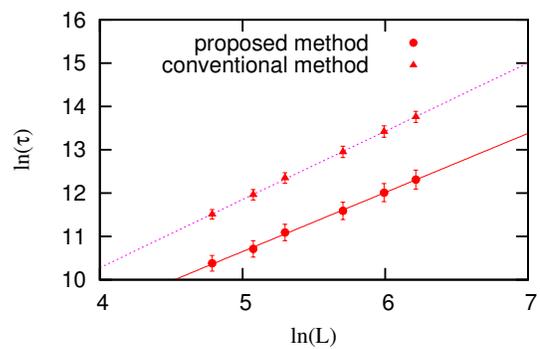

FIG. 7. (Color online) Scaling of the autocorrelation time as a function of system size L for $\ln f = 0.01$ with the error bars shown. The scaling exponents are mentioned in the text.

hibits a power law scaling with system size, i.e.,

$$\tau \propto L^z \qquad (16)$$

The scaling exponent (z) is determined from a linear fit of the plot $\ln \tau$ versus $\ln L$. The logarithm of the autocorrelation time for both the conventional and the proposed spin update scheme has been plotted against $\ln L$ for $\ln f = 0.01$ in Fig. 7. The scaling exponent for the proposed spin update scheme (z_{new}) is found to be $z_{\text{new}} = 1.36351 \pm 0.024$ while that for the conventional spin update scheme (z_{old}) is found to be $z_{\text{old}} = 1.57591 \pm 0.013$. The proposed spin update scheme significantly decreases the scaling exponent. We would like to point out that the autocorrelation time (τ) increases rapidly as the modification factor (f) becomes smaller and for a larger system

size, the calculation of τ, specially for smaller f, becomes very much costly in terms of CPU time. The autocorrelation time for a number of modification factors f for $L = 200$ for both the proposed and the conventional spin update schemes is listed in Table I and plotted in Fig. 8.

TABLE I. Autocorrelation time (in units of MC sweep) for different $\ln f$ for $L = 200$.

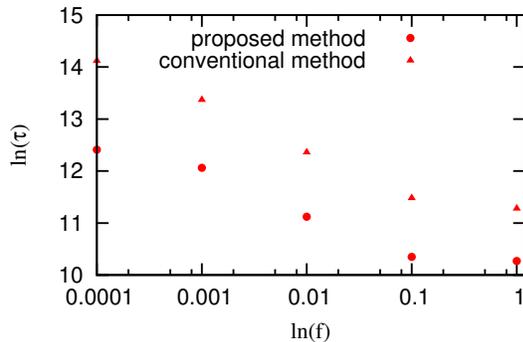| $\ln f$	τ_{new}	τ_{old}
1.0	28954	78966
0.1	31226	96902
0.01	67642	234502
0.001	173250	638082
0.0001	246118	1359694

FIG. 8. (Color online) Logarithm of the autocorrelation time plotted against $\ln f$ for system size $L = 200$ for both the proposed and the conventional spin update method.

V. CONCLUSIONS

To summarize, we have tested the performance of the WL algorithm in a continuous lattice spin model, namely, the $1d$ LL model which describes a nematic liquid crystal in the mean field approximation. The results obtained from our simulation are compared with the exact results available for this model. It has been observed that the results obtained tally accurately with the exact results. We focus on the fluctuations of histogram and replace the "flatness" criterion with that of minimum histogram. We have found that in this continuous lattice model, the fluctuations in the energy histogram, after an initial accumulation stage, saturates to a value that is proportional to $1/\sqrt{\ln f}$ where f is the modification factor in the WL algorithm and confirm that this behavior is generic to the WL algorithm. We also present a novel method for spin update scheme to obtain a subsequent configuration which is less-correlated than the previous method. The proposed spin update scheme makes the WL "driver"

to move from one sampling point to the next faster. As a result, the autocorrelation time between successive moves decreases and the convergence becomes faster. It may be noted that the WL algorithm only asks for the next sampling point (say X) with probability distribution $P(X) \propto \Omega(X)/\Omega(\bar{X})$ where $\Omega(X)$ and $\Omega(\bar{X})$ are the exact and the estimated DOS respectively. A previous study [20] suggested that N-fold way updates yields better performance in flat-histogram sampling. However, Dayal $et.al$ [25] argued that the performance is limited by the added expense of the CPU time needed to implement the N-fold way updates. The proposed method is simple to implement and has also the merit that it makes us free from tuning any adjustable parameter while simulating a continuous lattice spin model. Although the method has been applied to a liquid crystalline system in the present work, the method can, in general, be applied to any lattice spin model with continuous energy spectrum. This method has resulted in efficient simulation of continuous models with XY symmetry [43, 44]. Finally, we stress that the focus in this paper is to test the performance of the WL algorithm in continuous lattice spin models with the proposed spin update scheme. We hope that this spin update method will be of general interest in the area of research in Monte Carlo simulations of continuous lattice spin models.

VI. ACKNOWLEDGEMENTS

[1] F. Wang and D. P. Landau, Phys. Rev. Lett. **86**, 2050 (2001); Phys. Rev. E **64**, 056101 (2001).
[2] C. Yamaguchi and Y. Okabe, J. Phys. A **34**, 8781 (2001).
[3] Y. Okabe, Y. Tomita and C. Yamaguchi, Comput. Phys. Commun. **146**, 63 (2002).
[4] M. S. Shell, P. G. Debenedetti and A. Z. Panagiotopoulos, J. Chem. Phys **119**, 9406 (2003).
[5] N. Rathore and J. J. de Pablo, J. Chem. Phys **116**, 7225 (2002); N. Rathore, T. A. Knotts and J. J. de Pablo, *ibid.* **118**, 4285 (2001).
[6] T. S. Jain and J. J. de Pablo, J. Chem. Phys **116**, 7238 (2002).
[7] Q. Yan, R. Faller and J. J. de Pablo, J. Chem. Phys **116**, 8745 (2002); E. B. Kim, R. Faller, Q. Yan, N. L. Abbott and J. J. de Pablo, *ibid.* **117**, 7781 (2002).
[8] D. Jayasri, V. S. S. Sastry and K. P. N. Murthy, Phys. Rev. E **72**, 036702 (2005).

[9] M. Chopra and J. J. de Pablo, J. Chem. Phys **124**, 114102 (2006); E. A. Mastny and J. J. de Pablo, *ibid.* **122**, (2005).
[10] Y. W. Li, T. Wust, D. P. Landau and H. Q. Lin, Comput. Phys. Commun. **177**, 524 (2007).
[11] T. Wust and D. P. Landau, Phys. Rev. Lett. **102**, 178101 (2009).
[12] D. T. Seaton, T. Wust and D. P. Landau, Phys. Rev. E **81**, 011802 (2010).
[13] P. Poulain, F. Calvo, R. Antoine, M. Broyer and P. Dugourd, Phys. Rev. E **73**, 056704 (2006).
[14] C. Zhou, T. C. Schulthess, S. Torbrugge and D. P. Landau, Phys. Rev. Lett. **96**, 120201 (2006).
[15] K. Mukhopadhyay, N. Ghoshal and S. K. Roy, Phys. Lett. A **372**, 3369 (2008).
[16] S. Bhar and S. K. Roy, Comput. Phys. Commun. **180**, 699 (2009).

[17] S. Sinha and S. K. Roy, Phys. Lett. A **373**, 308 (2009).
[18] C. Yamaguchi and N. Kawashima, Phys. Rev. E **65**, 056710 (2002).
[19] B. J. Schulz, K. Binder and M. Muller, Int. J. Mod. Phys. C, **13**, 477 (2002).
[20] B. J. Schulz, K. Binder, M. Muller and D. P. Landau, Phys. Rev. E, **67**, 067102 (2003).
[21] B. A. Berg, Comput. Phys. Commun. **153**, 397 (2003).
[22] Q. Yan and J. J. de Pablo, Phys. Rev. Lett. **90**, 035701 (2003);
[23] M. S. Shell, P. G. Debenedetti and A. Z. Panagiotopoulos, J. Phys. Chem. B **108**, 19748 (2004).
[24] S. Trebst, D. A. Huse and M. Troyer, Phys. Rev. E **70**, 056701 (2004).
[25] P. Dayal, S. Trebst, S. Wessel, D. Wurtz, M. Troyer, S. Sabhapandit and S. N. Coppersmith, Phys. Rev. Lett. **92**, 097201 (2004).
[26] P. Virnau, M. Muller, L. G. Macdowell, K. Binder, J. Chem. Phys **121**, 2169 (2004).
[27] C. Zhou and R. N. Bhatt, Phys. Rev. E **72**, 025701(R) (2005).
[28] A. Troster and C. Dellago, Phys. Rev. E **71**, 066705 (2005).
[29] H. K. Lee, Y. Okabe and D. P. Landau, Comput. Phys. Commun. **175**, 36 (2006).
[30] D. Earl and M. Deem, J. Phys. Chem. B **109**, 6701 (2005).
[31] A. N. Morozov and S. H. Lin, Phys. Rev. E **76**, 026701 (2007).
[32] R. E. Belardinelli and V. D. Pereyra, Phys. Rev. E **75**, 046701 (2007); J. Chem. Phys. **127**, 184105 (2007).
[33] C. Zhou and J. Su, Phys. Rev. E **78**, 046705 (2008).
[34] D. P. Landau, S. H. Tsai and M. Exler, Am. J. Phys. **72**, 1294 (2004).
[35] A. N. Morozov and S. H. Lin, J. Chem. Phys **130**, 074903 (2009).
[36] P. A. Lebwohl and G. Lasher, Phys. Rev. A **6**, 426 (1972).
[37] W. Maier and A. Saupe, Z. Naturforsch. A **13**, 564 (1958); *ibid.* **14**, 882 (1959); *ibid.* **15**, 287 (1960).
[38] P. A. Vuillermot and M. V. Romerio, J. Phys. C **6**, 2922 (1973); Commun. Math. Phys. **41**, 281 (1975).
[39] M. Abramowitz and I. Stegun, A Handbook of Mathematical Functions, Dover, New York, 1970.
[40] C. Zannoni (Chapter 9) in The Molecular Physics of Liquid Crystals edited by G. R. Luckhurst and G. W. Gray, Academic Press, 1979.
[41] Monte Carlo methods in Statistical Physics, edited by M. E. J. Newman and G. T. Barkema, (Clarendon, Oxford, 1999).
[42] U. Wolff, Phys. Rev. Lett. **62**, 361 (1989); Nucl. Phys. B **322**, 759 (1989).
[43] S. Sinha and S. K. Roy, phys. Rev. E **81**, 041120 (2010).
[44] S. Sinha, phys. Rev. E **84**, 010102(R) (2011).
[45] N. Madras and A. D. Sokal, J. Stat. Phys. **50**, 109 (1988).