Wang-Landau sampling: A criterion for halting the simulations

A. A. Caparica
Instituto de Física, Universidade Federal de Goiás. C.P. 131, CEP 74001-970, Goiânia, GO, Brazil
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In this work we propose a criterion to finish the simulations of the Wang-Landau sampling. Instead of determining a final modification factor for all simulations and every sample size, we investigate the behavior of the temperature of the peak of the specific heat during the simulations and finish them when this value varies below a given limit. As a result, different runs stop at different final modification factors. We show that in place of the temperature of the peak of the specific heat one can adopt alternatively the integrated heat transfer as a reference quantity. We apply this technique to the two-dimensional Ising model and a homopolymer. We verify that for the Ising model the mean order of the final modification factors is roughly the same for all lattice sizes, but for the homopolymer the order of the final modification factors increases with increasing polymer sizes. The results show that the simulations can be halted much earlier than is conventional in Wang-Landau sampling, but manifold finite-size simulations are required in order to obtain accurate results. A brief application to the three-dimensional Ising model is also available.

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I. INTRODUCTION

Wang-Landau sampling (WLS) [1,2] can be considered a well-established Monte Carlo method, since it has been applied efficiently to many systems. Nevertheless the method is still in development and new ideas have contributed to increase the degree of efficiency and accuracy of the algorithm.

The method is based on the fact that if one performs a random walk in energy space with a probability proportional to the reciprocal of the density of states, a flat histogram is generated for the energy distribution. Since the density of states produces huge numbers, instead of estimating $g(E)$, the simulation is performed for $S(E) \equiv \ln g(E)$. At the beginning we set $S(E) = 0$ for all energy levels. The random walk in the energy space runs through all energy levels from $E_{\min}$ to $E_{\max}$ with a probability $p(E \to E') = \min(\exp[S(E) - S(E')], 1)$, where E and E' are the energies of the current and the new possible configurations. Whenever a configuration is accepted we update $H(E') \to H(E') + 1$ and $S(E') \to S(E') + F_i$, where $F_i = \ln f_i$, $f_0 \equiv e = 2.71828\ldots$, and $f_{i+1} = \sqrt{f_i}$ (f_i is the so-called modification factor). The flatness of the histogram is checked after a number of Monte Carlo steps and usually the histogram is considered flat if $H(E) > 0.8\langle H\rangle$, for all energies, where $\langle H\rangle$ is an average over energies. If the flatness condition is fulfilled we update the modification factor to a finer one and reset the histogram $H(E) = 0$. The original version of WLS prescribes that simulations should be in general halted when $f \sim 1 + 10^{-8}$. Having in hand the density of states, one can calculate the canonical average of any thermodynamic variable X as

$$\langle X\rangle_T = \frac{\sum_E \langle X\rangle_E g(E) e^{-\beta E}}{\sum_E g(E) e^{-\beta E}}, \tag{1}$$

where $\langle X\rangle_E$ is the microcanonical average accumulated during the simulations and $\beta = 1/k_B T$, k_B is the Boltzmann constant, and T is the temperature.

Recent works [3–5] have demonstrated that (a) instead of updating the density of states after every move, one ought to update it after each Monte Carlo sweep (MCS) [6]; (b) WLS should be carried out only up to $\ln f = \ln f_{\text{final}}$ defined by the canonical averages during the simulations; and (c) the microcanonical averages should not be accumulated before $\ln f \leqslant \ln f_{\text{micro}}$ defined by the microcanonical averages during the simulation. The adoption of these easily implementable changes leads to more accurate results and saves computational time. They investigated the behavior of the maxima of the specific heat,

$$C(T) = \langle (E - \langle E\rangle)^2\rangle / T^2, \tag{2}$$

and the susceptibility,

$$\chi(T) = L^2 \langle (m - \langle m\rangle)^2\rangle / T, \tag{3}$$

where E is the energy of the configurations and m is the corresponding magnetization per spin, during the WLS for the Ising model on a square lattice. They observed (as in [7–11]) that a considerable part of the conventional Wang-Landau simulation is not very useful because the error saturates. They demonstrated in detail that in general no single simulation converges to the true value, but to a particular value of a Gaussian distribution of results around the correct value. The saturation of the error coincides with the convergence to this value. Continuing the simulations beyond this limit leads to irrelevant variations in the canonical averages of all thermodynamic variables. In order to define f_{final} to a given model one should take a representative size [$L = 32$ for the two-dimensional (2D) Ising model and $N = 50$ for the homopolymer] and find out when the corresponding canonical averages obtained from a few independent runs would come to steady values. In that study they concluded that f_{final} should be f_{13} and f_{18} for the 2D Ising model and the homopolymer, respectively.

In the present work we propose a criterion for finishing the simulations which turns the choice of f_{final} automatic for each independent run. As a result the simulated data become more accurate and one has no need to find out f_{final} before initiating the simulations. We found out also that two independent finite-size scaling procedures can lead to results that do not agree within the error bars and therefore the final results should be obtained from manifold independent procedures.

II. A CRITERION FOR FINISHING THE SIMULATIONS

From time to time during the WLS the random walker pauses the simulation in order to check the histogram for flatness.

Applying WLS to the two-dimensional Ising model, beginning from f_5, we calculate the temperature of the peak of the specific heat defined in Eq. (2) using the current $g(E)$ and from this time on this mean value is updated whenever the histogram is checked for flatness. When the histogram is considered flat, we save the value of the temperature of the peak of the specific heat $T_c(0)$. We then update the modification factor $f_{i+1} = \sqrt{f_i}$ and reset the histogram $H(E) = 0$. During the simulations with this new modification factor we continue calculating the temperature of the peak of the specific heat $T_c(t)$ whenever we check the histogram for flatness and we also calculate the checking parameter,

$$\varepsilon = |T_c(t) - T_c(0)|. \tag{4}$$

If the number of MCS before verifying the histogram for flatness is chosen not too large, say 10 000, then during the simulations with the same modification factor the checking parameter ε is calculated many times. The idea of the proposed criterion is that if ε remains less than a predefined threshold limiting value, which we will refer to as *limit*, until the histogram meets the flatness criterion for this WL level, then we save the density of states and the microcanonical averages and stop the simulations. The expedient of observing the behavior of the specific heat to end simulations has been used in a more informal way in Ref. [12].

The top of Fig. 1 shows the evolution of the temperature of the peak of the specific heat beginning from f_5 calculated

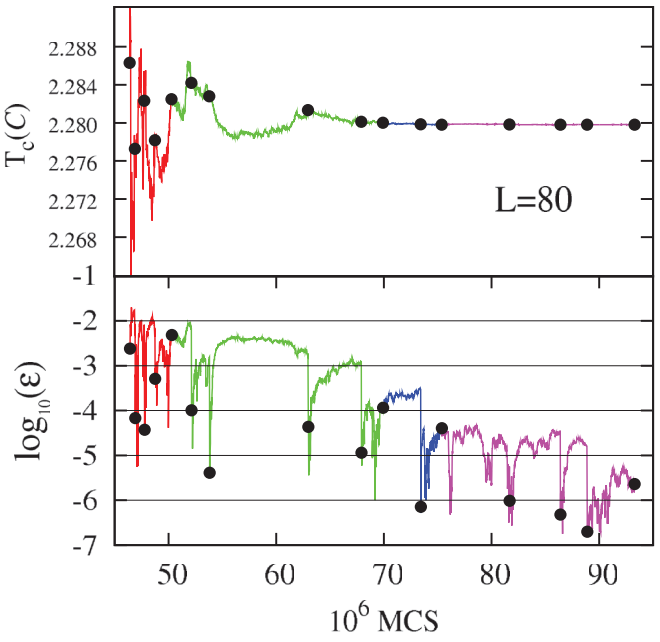

FIG. 1. (Color online) (Upper panel) Evolution of the temperature of the maximum of the specific heat during the WLS, beginning from f_5 for a single run. The dots show where the modification factor was updated. (Lower panel) Evolution of the logarithm of the checking parameter ε during the same simulation.

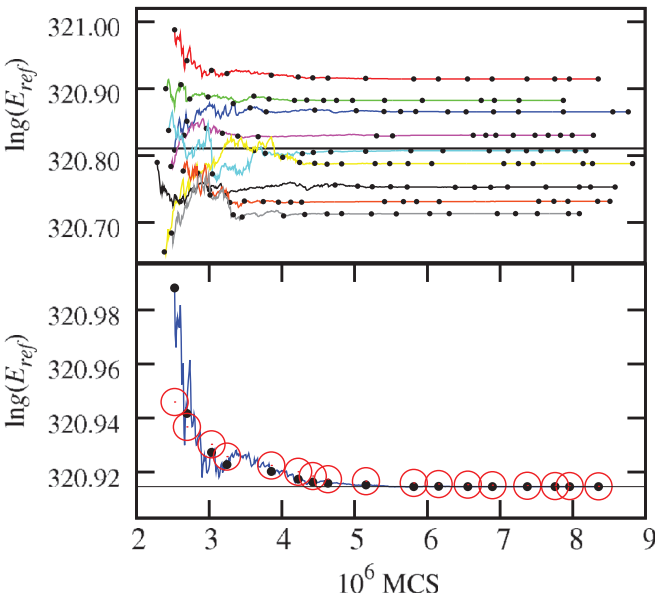

FIG. 2. (Color online) (Upper panel) Evolution of $\ln g(E_{\rm ref})$ during the WLS, beginning from f_{11} for nine independent runs. The dots show where the modification factor was updated and the straight line indicates the exact value $\ln g_{\rm exact}(E_{\rm ref})$ from Ref. [14]. (Lower panel) The uppermost curve alone. The straight line indicates the value $\ln g_{\rm final}$ to which this simulation converges and the open circles correspond to $\ln g_{\rm final} + \sqrt{\ln f}$.

for $L = 80$ as a function of the MCS using the 80% flatness criterion. The dots show where the modification factor was updated. The lower panel shows the evolution of the logarithm of the checking parameter ε during the same simulation. In this example one can see that for *limit* $= 10^{-2}$, 10^{-3}, 10^{-4}, and 10^{-5}, the simulation would be finished at f_8, f_{13}, f_{15}, and f_{19}, respectively.

The convergence of the temperature of the peak of the specific heat to a value of a Gaussian distribution around the true value is assured by the convergence of the density of states itself. Zhou and Bhatt [13] demonstrated that when f is close to 1 the relative error $\delta g/g = \delta \ln g$ scales as $\sqrt{\ln f}$.

In order to illustrate this convergence, using the exact density of states provided by Beale [14] we calculated the exact temperature of the maximum of the specific heat of a 32×32 lattice: $T_c = 2.29392897$. For this temperature the exponential e^{-E/k_BT} is maximum at $E_{\rm ref} = -1424$. We take this level as a reference. In the top of Fig. 2 we show the evolution of $\ln g(E_{\rm ref})$ during the simulations, beginning from f_{11} for nine independent runs. One can see that they all do converge to steady, but different values. In the lower panel we show only the uppermost one which converges to $\ln g_{\rm final} = 320.914628304468$, while the exact value is $\ln g_{\rm exact}(E_{\rm ref}) = 320.810960956218$ [14]. The open cycles display $\ln g_{\rm final} + \sqrt{\ln f}$. One can see that these results corroborate that the relative error scales with $\sqrt{\ln f}$, but not with respect to the true value. Based on the results of Ref. [3] we can presume that these values also fall into a Gaussian distribution around the exact value.

In order to define which would be the optimal value for the quantity *limit*, we performed finite-size scaling simulations

TABLE I. Ten finite-size results for the critical temperature for outputs at the end of f_{13} and for decreasing the threshold *limit*, using the 80% flatness criterion. The last line shows the average values over all the runs.

Exact	$T_c = 2.2691853\ldots$		
f_{13}	$\varepsilon < 10^{-3}$	$\varepsilon < 10^{-4}$	$\varepsilon < 10^{-5}$
2.26864(24)	2.26845(21)	2.26883(26)	2.26889(25)
2.26857(26)	2.26870(31)	2.26862(24)	2.26869(20)
2.26905(22)	2.26905(26)	2.26921(20)	2.26920(18)
2.26915(13)	2.26941(17)	2.26922(12)	2.26918(11)
2.26943(13)	2.26955(19)	2.26937(11)	2.26937(11)
2.26920(30)	2.26939(32)	2.26923(26)	2.26903(26)
2.26999(28)	2.27000(27)	2.26948(24)	2.26938(20)
2.26871(28)	2.26877(34)	2.26894(22)	2.26901(20)
2.26912(24)	2.26889(32)	2.26899(22)	2.26878(15)
2.26987(28)	2.27023(34)	2.26964(27)	2.26948(23)
2.26917(15)	2.26925(18)	2.26916(10)	2.26910(10)

TABLE II. Ten finite-size scaling results for the critical exponent γ for outputs at the end of f_{13} and for decreasing threshold *limit*, using the 80% flatness criterion. The last line shows the average values over all the runs.

Exact	$\gamma = 1.75$		
f_{13}	$\varepsilon < 10^{-3}$	$\varepsilon < 10^{-4}$	$\varepsilon < 10^{-5}$
1.7618(41)	1.7615(34)	1.7615(45)	1.7586(34)
1.7584(69)	1.7579(86)	1.7599(47)	1.7573(36)
1.7642(58)	1.7614(69)	1.7585(53)	1.7580(38)
1.7550(42)	1.7534(50)	1.7569(41)	1.7579(23)
1.7643(29)	1.7629(46)	1.7624(22)	1.7656(32)
1.7608(46)	1.7606(44)	1.7606(34)	1.7642(34)
1.7546(40)	1.7560(33)	1.7578(31)	1.7584(21)
1.7663(70)	1.7661(76)	1.7614(55)	1.7603(41)
1.7601(48)	1.7583(58)	1.7616(53)	1.7601(31)
1.7632(51)	1.7623(51)	1.7648(41)	1.7649(26)
1.7609(12)	1.7600(11)	1.7605(10)	1.7605(10)

taking outcomes when the criterion mentioned above was satisfied for *limit* $= 10^{-3}$, 10^{-4}, and 10^{-5}.

According to finite-size scaling theory [15–17] from the definition of the free energy one can obtain the zero field scaling expressions for the magnetization and the susceptibility, respectively, by

$$m \approx L^{-\beta/\nu}\mathcal{M}(tL^{1/\nu}), \tag{5}$$

$$\chi \approx L^{\gamma/\nu}\mathcal{X}(tL^{1/\nu}). \tag{6}$$

We see that the locations of the maxima of these functions scale asymptotically as

$$T_c(L) \approx T_c + a_q L^{-1/\nu}, \tag{7}$$

where a_q is a quantity-dependent constant, allowing then the determination of T_c.

Using these scaling functions and assuming $\nu = 1$, we estimated the critical temperature and the critical exponents β and γ.

In our initial attempts of using this checking parameter we produced also outcomes when the simulations reached the end of the modification factor f_{13}, as prescribed in Ref. [3] in order to reproduce those results. Surprisingly we found out that two independent similar finite-size scaling procedures can lead to very different results for the critical temperature, as $T_c = 2.26864(24)$ and $T_c = 2.26987(28)$, for example, which do not agree within the error bars. In order to circumvent this difficulty, we performed 10 independent Wang-Landau simulations for $L = 32$, 36, 40, 44, 48, 52, 56, 64, 72, and 80 with $N = 24, 24, 20, 20, 20, 16, 16, 16, 12$, and 12 independent runs for each size, respectively.

In Table I we show the results for the critical temperature obtained from these 10 independent finite-size scaling simulations and the mean values in the last line. Each temperature in this table is the mean value between the extrapolations of the temperatures of the peaks of the specific heat and the susceptibility. One can see that each single result can be particularly bad or good, but the average values for the temperature are excellent even for the less stringent *limit* $= 10^{-3}$.

This criterion for finishing the WLS has two main advantages. First of all it is not necessary to determine f_{final} for a representative size, as prescribed in Ref. [3] because it is defined automatically for each independent run. The second convenience is that different runs can proceed up to different final modification factors, depending on the evolution of the simulation.

In Table II we show the finite-size scaling results for the exponent γ. As in Ref. [3], they are a little bit above the exact value. For calculating the exponent β we used the averaged temperatures obtained in Table I for each case. In Table III we present the results for β. Again we can see that the results are in very close agreement with the exact value even for *limit* $= 10^{-3}$.

III. AN ALTERNATIVE QUANTITY FOR CALCULATING THE CHECKING PARAMETER

The use of the peak of the specific heat for calculating the checking parameter may in some cases be tricky because

TABLE III. Ten finite-size scaling results for the critical exponent β for outputs at the end of f_{13} and for decreasing threshold *limit*, using the 80% flatness criterion. The last line shows the average values over all the runs.

Exact	$\beta = 0.125$		
f_{13}	$\varepsilon < 10^{-3}$	$\varepsilon < 10^{-4}$	$\varepsilon < 10^{-5}$
0.1263(21)	0.1276(17)	0.1255(22)	0.1251(20)
0.1281(17)	0.1284(19)	0.1280(20)	0.1267(14)
0.1263(17)	0.1268(19)	0.1252(17)	0.1245(15)
0.1256(12)	0.1249(13)	0.1251(11)	0.1248(11)
0.1255(15)	0.1260(15)	0.1256(14)	0.1254(13)
0.1257(19)	0.1252(25)	0.1253(16)	0.1256(18)
0.1216(19)	0.1211(16)	0.1235(16)	0.1235(14)
0.1260(18)	0.1257(21)	0.1248(13)	0.1244(10)
0.1250(19)	0.1264(25)	0.1257(17)	0.1258(11)
0.1219(23)	0.1221(28)	0.1227(22)	0.1234(18)
0.12520(63)	0.12541(72)	0.12514(44)	0.12491(32)

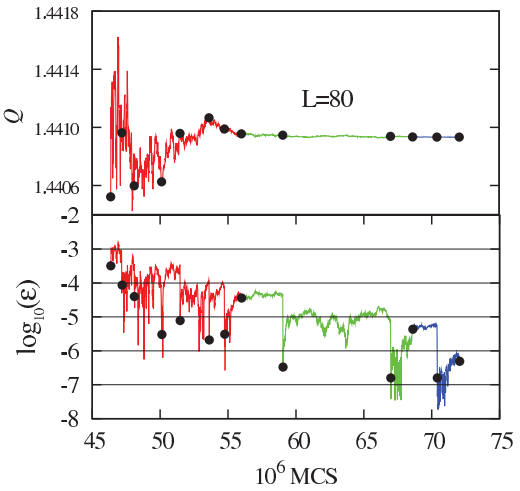

FIG. 3. (Color online) (Upper panel) Evolution of the temperature of the maximum of the specific heat during the WLS, beginning from f_5 for a single run. The dots show where the modification factor was updated. (Lower panel) Evolution of the logarithm of the checking parameter ε calculated using the quantity Q during the same simulation.

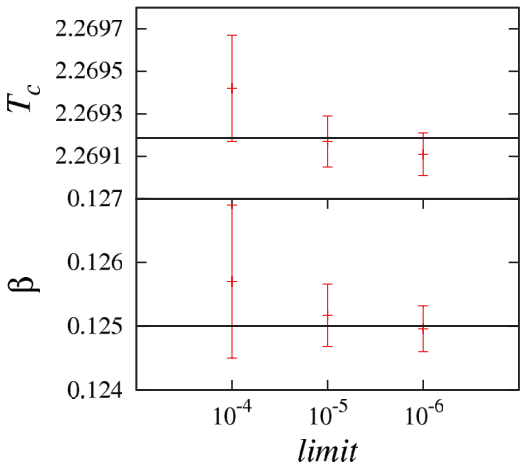

FIG. 4. (Color online) (Upper panel) Mean critical temperature from 10 independent finite-size scaling for three levels of demand for the checking parameter, using the quantity Q as a reference. (Lower panel) The exponent β from the same simulations. The straight lines in both panels refer to the exact values $T_c = 2.2691853\ldots$ and $\beta = 0.125$.

there are systems that exhibit more than one peak or that may behave unexpectedly. In such situations, another quantity may be used, namely, the heat transfer per unit calculated by the integrated specific heat in a broad temperature interval.

$$Q = \frac{1}{N}\int_{T_i}^{T_f} C(T)dT, \tag{8}$$

where $C(T)$ is the specific heat defined by Eq. (2) and N is the number of units in the system (number of spins, monomers, etc.).

The checking parameter ε can then be defined analogously as

$$\varepsilon = |Q(t) - Q(0)|, \tag{9}$$

where as before, $Q(0)$ is the last value calculated in the previous modification factor and $Q(t)$ are the values calculated during the current WL level. The integrals in Eq. (8) were calculated for $T_i = 1.0$ and $T_f = 4.0$, using a step $\Delta T = 0.01$.

In Fig. 3 we show the evolution of the heat transfer per spin during the WLS and the logarithm of the checking parameter. We see that the behavior of this integrated quantity is similar to the temperature of the peak of the heat capacity, but the stabilization happens for $limit = 10^{-4}$, 10^{-5}, and 10^{-6}.

Using this new variant for calculating the checking parameter we obtained results for T_c, γ, and β from 10 independent finite-size scaling simulations. In order to have a good ground for comparing both criteria, we repeated in this case exactly the same simulations that were performed in the previous section.

The top of Fig. 4 displays the overall mean results for the critical temperature for $limit = 10^{-4}$, 10^{-5}, and 10^{-6}. The bottom shows the results for the exponent β. The results for γ are 1.7631(12), 1.7610(10), and 1.7605(10), respectively, again above the exact value, while the outcomes for the critical temperature and the exponent β are in very good agreement with the exact data starting from $limit = 10^{-4}$. In Fig. 5 we show the mean final orders of the modification factor for each variant of the checking parameter for three levels of demand. One can see that using $T_c(t)$ the orders are roughly size independent, but if the quantity $Q(t)$ is adopted the orders of the final modification factor have a slight decrease with increasing lattice sizes.

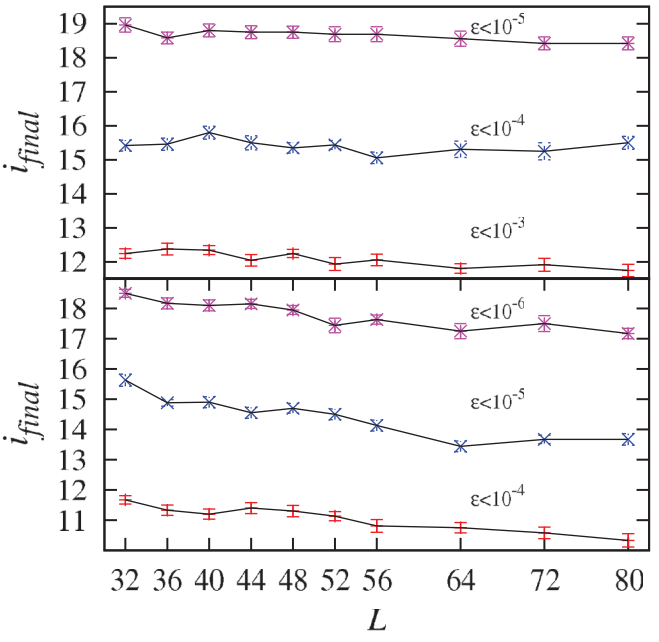

FIG. 5. (Color online) (Upper panel) Mean final order of the modification factor for three levels of demand for the checking parameter, using $T_c(C)$ as a reference. (Lower panel) The same using the quantity Q for calculating the checking parameter.

TABLE IV. Five independent runs using the checking parameter defined by the peak of the specific heat. Each procedure is the result of 10 finite-size scaling extrapolations for the critical temperature and the exponents γ and β for outputs at the end of f_{13} and for decreasing ε, using the 80% flatness criterion.

f_{13}	$\varepsilon < 10^{-3}$	$\varepsilon < 10^{-4}$	$\varepsilon < 10^{-5}$
	$T_c = 2.2691853\ldots$		
a. 2.26917(15)	2.26925(18)	2.26916(10)	2.26910(10)
b. 2.26914(18)	2.26929(19)	2.26915(14)	2.26911(14)
c. 2.26915(11)	2.26909(16)	2.26913(10)	2.26912(10)
d. 2.26930(14)	2.26921(17)	2.26928(12)	2.26927(10)
e. 2.26925(15)	2.26916(16)	2.26928(15)	2.26926(12)
	$\gamma = 1.75$		
a. 1.7609(12)	1.7600(11)	1.7605(10)	1.7605(10)
b. 1.7586(15)	1.7579(19)	1.7587(11)	1.7589(10)
c. 1.7597(15)	1.7601(18)	1.7584(11)	1.7580(10)
d. 1.7568(16)	1.7576(18)	1.7571(13)	1.7573(10)
e. 1.7590(11)	1.7590(15)	1.7577(10)	1.7576(10)
	$\beta = 0.125$		
a. 0.12520(63)	0.12541(72)	0.12514(44)	0.12491(32)
b. 0.12526(72)	0.12540(79)	0.12529(65)	0.12523(60)
c. 0.12560(56)	0.12561(56)	0.12548(48)	0.12516(45)
d. 0.12572(74)	0.12528(84)	0.12554(65)	0.12547(52)
e. 0.12559(52)	0.12559(56)	0.12554(46)	0.12554(34)

TABLE V. Five independent runs using the checking parameter defined by the heat transfer. Each procedure is the result of 10 finite-size scaling extrapolations for the critical temperature and the exponents γ and β for outputs at the end of f_{13} and for decreasing ε, using the 80% flatness criterion.

f_{13}	$\varepsilon < 10^{-4}$	$\varepsilon < 10^{-5}$	$\varepsilon < 10^{-6}$
	$T_c = 2.2691853\ldots$		
a. 2.26917(15)	2.26942(25)	2.26917(12)	2.26911(10)
b. 2.26914(18)	2.26944(27)	2.26913(17)	2.26911(14)
c. 2.26915(11)	2.26921(16)	2.26918(11)	2.26914(11)
d. 2.26930(14)	2.26936(21)	2.26928(13)	2.26927(11)
e. 2.26925(15)	2.26959(20)	2.26926(15)	2.26925(13)
	$\gamma = 1.75$		
a. 1.7609(12)	1.7631(12)	1.7610(10)	1.7605(10)
b. 1.7586(15)	1.7590(21)	1.7582(12)	1.7593(10)
c. 1.7597(15)	1.7615(14)	1.7590(11)	1.7587(11)
d. 1.7568(16)	1.7568(16)	1.7568(16)	1.7571(10)
e. 1.7590(11)	1.7588(11)	1.7589(11)	1.7577(10)
	$\beta = 0.125$		
a. 0.12520(63)	0.1257(12)	0.12517(49)	0.12496(36)
b. 0.12526(72)	0.12560(97)	0.12525(68)	0.12520(60)
c. 0.12559(56)	0.12588(79)	0.12550(52)	0.12522(45)
d. 0.12572(74)	0.12619(85)	0.12565(67)	0.12543(57)
e. 0.12559(52)	0.12655(71)	0.12557(50)	0.12549(40)

IV. RESULTS

A. 2D Ising model

Aware of the peculiarities of WLS, in order to test the reproductivity of the outcomes shown above we carried out four more independent simulations using the two versions of the checking parameter. In Table IV we show the results using the peak of the specific heat as a reference. The exponent γ remains stubbornly above the exact value in all cases, but regarding the critical temperature and the exponent β, we see that although the results for $limit = 10^{-3}$ are quite reasonable, the error bars are in general larger then those of the last two columns, which are roughly equivalent. The differences between the simulation values and the exact values are in most cases less then the standard deviations σ of the simulations. Only the exponent β in the fifth simulation is slightly beyond the error bars. These results give us confidence to define $limit = 10^{-4}$ as the ideal threshold for halting the simulations when the checking parameter is defined by the temperature of the peak of the specific heat.

Table V shows the results for the same independent finite-size scaling simulations using the heat transfer to define the checking parameter for halting the process. We see that the overall results for $limit = 10^{-4}$ are inaccurate. One can observe that the results using $limit = 10^{-5}$ and $limit = 10^{-6}$ are equivalent. We conclude therefore that if the second criterion is being used the ideal value to stop the simulations should be $limit = 10^{-5}$.

If adaptive windows [18] are being used in the simulations, both checking parameters can be applied. For calculating the peak of the specific heat or the heat transfer during the simulations one should just virtually joint the current windows. As demonstrated in Ref. [18] the use of fixed overlapping windows is not advisable in many models, but in the case that it is being adopted, the second checking parameter may still be applied. Instead of taking the canonical averages defined in Eq. (1) over all the energy spectrum, one should carry out the summations over the energy levels of each window. Naturally the resulting calculation loses the meaning of specific heat and the integral of Eq. (8) either can be interpreted as the heat transfer, but this integrated value can nonetheless be used to define the checking parameter. In order to demonstrate the validity of such a procedure, we divided the spectrum of the $L = 32$ Ising model lattice in four windows and carried out $N = 24$ independent simulations for each of them using $limit = 10^{-5}$ for halting the simulations. The resulting mean final orders of the modification factor were 14.32(21), 14.65(18), 14.43(20), and 14.71(19), respectively, which are compatible with the result of Fig. 5 using the full spectrum, although slightly below.

Such large repetitious handling of data for obtaining all these canonical averages and finite-size extrapolations were possible only by using shell scripting [19–23]. This is an exceptional tool for those who work with simulations.

B. 3D Ising model

In order to illustrate the applicability of this technique to a three-dimensional system, we performed WLS for the 3D Ising model on a $20 \times 20 \times 20$ lattice. The behavior of the canonical averages is similar to the 2D Ising model and shows that our method for halting the simulations can be applied to a three-dimensional system as well. The top of Fig. 6 shows the evolution of the temperature of the peak of the specific heat beginning from f_8, and the bottom displays the logarithm

of the checking parameter. In this case the simulations would stop at the end of f_{10}, f_{13}, and f_{18} for *limit* $= 10^{-3}$, 10^{-4}, and 10^{-5}, respectively.

C. Homopolymer

As a new application of the criterion, we consider a homopolymer consisting of N monomers which may assume any self-avoiding walk (SAW) configuration on a two-dimensional lattice [24,25]. Assuming that the polymer is in a bad solvent, there is an effective monomer-monomer attraction in addition to the self-avoidance constraint representing excluded volume. For every pair of nonbonded nearest-neighbor monomers the energy of the polymer is reduced by ϵ. The Hamiltonian for the model can be written as

$$\mathcal{H} = -\epsilon \sum_{\langle i,j \rangle} \sigma_i \sigma_j, \tag{10}$$

where $\sigma = 1(0)$ if the site i is occupied (vacant), and the sum is over nearest-neighbor pairs [26]. (The sum is understood to exclude pairs of bonded segments along the chain.) We used the so-called reptation or "*slithering snake*" move which consists of randomly adding a monomer to one end of the chain and removing a monomer from the other end, maintaining the size of the polymer constant. (Although reptation is not suitable for sampling the most compact configurations, this does not affect the conclusions presented here.) We define one Monte Carlo step as N attempted moves.

We performed simulations for polymers of sizes $N = 50,70,\ldots,150$ taking 10 independent runs for each size and finishing the process when the condition,

$$|T_c(t) - T_c(0)| < 10^{-4}, \tag{11}$$

was satisfied in the course of the whole simulation of a modification factor, where again, $T_c(0)$ is the last temperature of the peak of the specific heat in the previous modification factor.

In Fig. 7 we show the evolution of the temperature of the peak of the specific heat of a polymer of $N = 90$, beginning from f_{10}. In the lower panel the logarithm of the checking parameter ε of the same simulation is displayed. The simulations were started from constructed ground-state configurations [27].

In Fig. 8 we show the mean order of the final modification factor for each polymer size. One can see that unlike the two-dimensional Ising model, in this case the order of the final modification factor increases with increasing polymer sizes. Adopting the proposed criterion for halting the simulations ensures that each particular run proceeds up to the real stabilization of the results.

Often one faces difficulties in sampling conformations with lowest energies and reaching the flatness criterion. Many ingenious protocols of evolution of polymers have been proposed, e.g., Ref. [28]. The use of the criterion for halting the simulations developed in this work can enhance accuracy and save a lot of CPU time.

V. CONCLUSIONS

We proposed a criterion to finish the simulations of the Wang-Landau sampling. Instead of determining a final modification factor f_{final} for all simulations and every lattice size, the behavior of the temperature of the peak of the specific heat or the heat transfer per unit are checked during

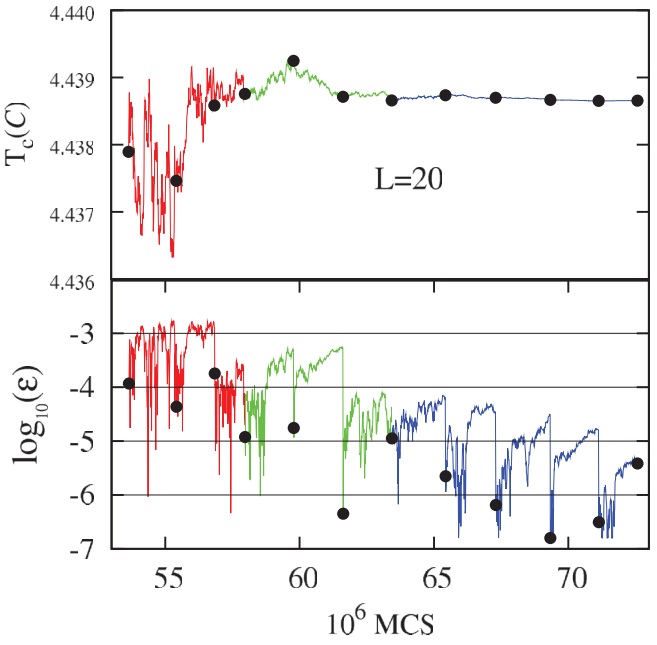

FIG. 6. (Color online) (Upper panel) Evolution of the temperature of the maximum of the specific heat during the WLS of the 3D Ising model, beginning from f_8 for a single run. The dots show where the modification factor was updated. (Lower panel) Evolution of the logarithm of the checking parameter ε during the same simulation.

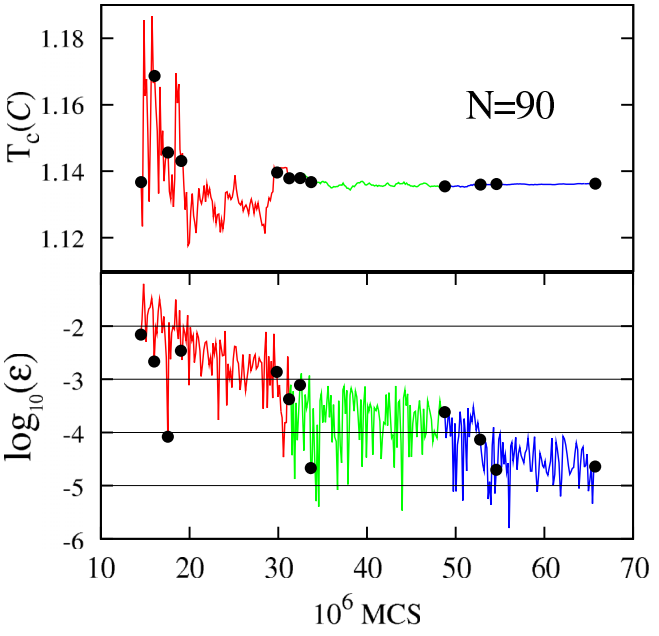

FIG. 7. (Color online) (Upper panel) Evolution of the temperature of the maximum of the specific heat of the self-avoiding homopolymer of $L = 90$ during the WLS, beginning from f_{10} for a single run. The dots show where the modification factor was updated. (Lower panel) Evolution of the logarithm of the checking parameter ε during the same simulation.

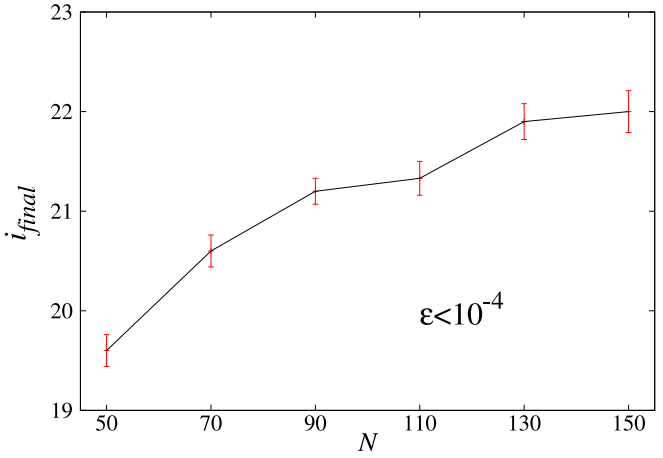

FIG. 8. (Color online) Mean order of the final modification factor for each simulated size of homopolymers using the 80% flatness criterion.

the simulations and the process is halted when these values vary below a given limit during the whole simulation of a modification factor. As a result, different runs stop at different final modification factors. Our results define that the ideal *limit* should be 10^{-4} if the peak of the specific heat is used and 10^{-5} if one adopts the heat transfer per unit. We demonstrated that reliable and accurate results are obtained only by taking averages over manifold simulations. We applied this technique to the two-dimensional Ising model and a homopolymer and found that for the Ising model the mean final order of the modification factors are roughly the same for all lattice sizes, but for the homopolymer the final order of the modification factor increases with increasing polymer sizes. We also presented a brief application of the criterion to the three-dimensional Ising model.

Finally it should be pointed out that Wang-Landau variants that do not require the use of the modification factor, e.g., Refs. [9,29] may benefit from the ideas proposed in this work by defining a suitable number of MCS, after which the checking parameter would be calculated. If ε remains below a predefined *limit* for, say, 10 consecutive checks the simulation could be halted.

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