Wang-Landau sampling with self-adaptive range

Andreas Tröster and Christoph Dellago
Faculty of Physics, University of Vienna, Boltzmanngasse 5, A-1090 Wien, Austria
(Received 31 January 2005; published 23 June 2005)

We report a self-adapting version of the Wang-Landau algorithm that is ideally suited for application to systems with a complicated structure of the density of states. Applications include determination of two-dimensional densities of states and high-precision numerical integration of sharply peaked functions on multidimensional integration domains.

DOI: 10.1103/PhysRevE.71.066705 PACS number(s): 05.10.−a, 64.60.Cn, 52.65.Pp

I. INTRODUCTION

The application of Monte Carlo methods for the simulation of condensed matter systems is often complicated by widely disparate time scales [1,2]. For instance, free energy barriers separating metastable from stable states at first-order phase transitions can prevent standard Metropolis Monte Carlo from sampling all important regions of configuration space. Similar problems arise due to rough energy landscapes or critical slowing down near second-order phase transitions. Several simulation algorithms, including umbrella sampling [3], multicanonical sampling [4], and parallel tempering [5], have been developed to alleviate such sampling problems. In these methods, bottlenecks in configuration space are overcome by sampling a modified Boltzmann weight. A different approach is taken in the recently proposed Wang-Landau method [6,7], in which the density of states $g(E)$ (essentially the number of states available to the system at energy E) is calculated in an iterative fashion. From the density of states one can then calculate the partition function and, by taking appropriate derivatives, the thermodynamic properties of the system. Wang-Landau sampling has been successfully applied to a variety of systems ranging from spin models [6] to fluids [8], polymers [9,10], and proteins [11]. Furthermore, the method has been generalized for the calculation of free energy profiles along selected reaction coordinates [12].

The Wang-Landau approach is based on the observation that if configurations (states) x with total energy $\mathcal{H}(x)$ are sampled with a probability proportional to $1/g(\mathcal{H}(x))$ the resulting energy histogram is flat. The density of states $g(E)$, however, is usually unknown. Indeed, it is the goal of the Wang-Landau method to calculate this function. This is achieved in the following way. First, the density of states is initialized with a guess, say, $g(E)=1$. A random walk through configuration space is then carried out by randomly changing configurations and accepting or rejecting them according to the weight $1/g(\mathcal{H}(x))$ using the Metropolis rule [1]. Each time a certain energy E is visited the corresponding density of states is multiplied with a factor $f>1$, such that it becomes less likely to visit states with the same energy again. Due to this iterative adjustment of the sampling weight all energies in a given range are then generated roughly with the same probability. If the factor f is slowly decreased, the energy distribution will eventually become flat and the function $g(E)$ will converge towards the density of states.

One of the most appealing features of the Wang-Landau algorithm is that even for determining sharply peaked densities of states, virtually no knowledge of the behavior of the function is required. Instead of facing the problem of having to determine a bias function that closely resembles the desired density of state, one starts with a flat trial density, which automatically adapts and shapes itself with higher and higher accuracy during each Wang-Landau step. The Wang-Landau algorithm can thus be regarded as a non-Markovian iterative self-adjusting relative of umbrella sampling.

However, successful application of the Wang-Landau method *does* require one vital piece of information: In order to produce a flat histogram, we not only need to specify the sampling range in energy space, but to also make sure that for all energies in this range accessible configurations exist. Indeed, if the system is prevented from visiting certain energy values within the specified range, the corresponding energy histogram will fail to become flat and the algorithm does not converge.

At first thought, this may regarded as a trivial matter. One might, for instance, fix the problem of inaccessible energies by dividing the entire energy range into several overlapping windows and by separately carrying out a Wang-Landau simulation in each of these windows. Possible inaccessible energies are most likely to occur at the upper and lower limits of the energy range. Windows in which such energies exist are then simply discarded and the density of states is calculated only from the windows where the Wang-Landau calculation converges. In some cases, however, such an approach is not adequate. Problems can become particularly severe if densities are calculated as a function of more than one variable. In the next section, we will discuss how these difficulties arise in the calculation of the density of states $g(E,M)$ as a function of energy E and magnetization M for the two-dimensional (2d) Ising model. In Sec. III we will then present an algorithm for determining the energy range adaptively. We discuss two applications of this algorithm in Sec. V and draw some conclusions in Sec. VI.

II. ISING MODEL

As an example, consider the 2d nearest neighbor Ising model with Hamiltonian

$$\mathcal{H}(\boldsymbol{s},H) = 2N - \sum_{\langle ij\rangle} s_i s_j - H\sum_i s_i, \tag{1}$$

with spins $\boldsymbol{s}=(s_1,\ldots,s_N)$ on $N=L^2$ sites on a square lattice in an external field H, and with periodic boundary conditions. The normalization constant $2N$ is chosen only for convenience. Here each spin s_i is a discrete variable and can take only one of two values: +1 (up) and −1 (down). The notation $\langle ij\rangle$ in the first sum on the right-hand side of Eq. (1) indicates that this sum runs over all pairs s_i and s_j of spins that are nearest neighbors on the lattice. The second sum on the right-hand side of Eq. (1) describes the interaction of the spins with a homogeneous external field H.

It is convenient to rewrite the Hamiltonian (1) in terms of the following numbers. For each given spin configuration $\boldsymbol{s}$, let N_+ denote the number of up spins, and N_- the number of down spins. In addition, we introduce N_{++} as the number of nearest neighbor pairs, where both spins are up, N_{--} as the number of nearest neighbor pairs where both spins are down, and N_{+-} as the number of unequal nearest neighbor spin pairs. With these definitions, the Ising Hamiltonian $\mathcal{H}_0(\boldsymbol{s}) \equiv \mathcal{H}(\boldsymbol{s},0)$ for vanishing field can be rewritten as

$$\mathcal{H}_0(\boldsymbol{s}) = 2N - N_{++} - N_{--} + N_{+-}. \tag{2}$$

However, since the total number of nearest neighbor pairs on a 2d square lattice with N sites and periodic boundary conditions is $2N$, the identity

$$N_{++} + N_{--} + N_{+-} = 2N \tag{3}$$

holds, and we can simplify Eq. (2) to obtain

$$\mathcal{H}_0(\boldsymbol{s}) = 2N_{+-}. \tag{4}$$

Counting nearest neighbor pairs on the lattice in which at least one spin is up, one finds the relation [13] $4N_+=2N_{++}+N_{+-}$, and by symmetry also $4N_-=2N_{--}+N_{+-}$, such that finally

$$\mathcal{H}_0(\boldsymbol{s}) = -4N_{++} + 8N_+ = -4N_{--} + 8N_-. \tag{5}$$

It follows from this equation that for even N the possible energy values at vanishing field are

$$E = 0,4,8,\ldots,4N-4,4N. \tag{6}$$

The corresponding density of states $g(E)$, i.e., the number of configurations with energy E, can be calculated with the Wang-Landau algorithm with high precision [6].

The problem of how to generalize the Wang-Landau approach to determine the combined density of states $g(E,M)$ for the energy E and the total magnetization

$$M = \sum_i s_i = N_+ - N_- = 2N_+ - N \tag{7}$$

is considerably more complicated. Let $\delta(x)$ denotes the Kronecker delta δ_{x0} for an integer argument x; i.e., $\delta(x)=1$ if $x=0$ and $\delta(x)=0$ if $x\neq 0$. Using this discrete version of Dirac's delta function, the canonical partition function at magnetic field H and temperature T can be written as

$$Z(\beta,H) = \sum_{M,E} e^{-\beta(E-HM)} g(E,M), \tag{8}$$

where

$$g(E,M) = \sum_s \delta(E-\mathcal{H}_0(\boldsymbol{s}))\,\delta\Big(M - \sum_i s_i\Big) \tag{9}$$

counts the number g of states with energy E and magnetization M and $1/\beta=k_BT$ is the Boltzmann constant. Since according to Eq. (8) the partition function can be calculated from $g(E,M)$, all thermal and magnetic properties of the system are determined by this density of states.

In the following, it will be more convenient to work with the equivalent expression $g(E,N_+)$ [the quantities N_+ and M are simply related by Eq. (7)]. The corresponding set of allowed parameter values (E,N_+) is a subset of $4\mathbb{N}_0\times\mathbb{N}_0$, and its exact shape must be determined before the Wang-Landau algorithm can be implemented. To determine this region we have to determine the maximum and minimum energy for each given N_+.

From Eq. (5) one can calculate the maximum energy $E_{\max}(N_+)$ for any given value $0\leqslant N_+\leqslant N$. For $N_+<N/2$ there is always at least one configuration for which $N_{++}=0$, which leaves us with $E_{\max}(N_+<N/2)=8N_+$. From symmetry, it follows that also $E_{\max}(N_+>N/2)=8(N-N_+)$, while for $N_{++}=N/2$ the fully "antiferromagnetic" state is the state of highest energy with $E_{\max}(N/2)=4N$. On the other hand, the minimum energy $E_{\min}(N_+)$ is identical with the zero-temperature ground state of the system with an imposed value of N_+ and is therefore expected to decrease monotonically from a maximum value at $N_+=N/2$ to 0 at the perfectly ordered states corresponding to $N_+=0$ and $N_+=N$. At $N_+=N/2$, the system's energy is minimized by configurations displaying perfect phase separation of up and down spins separated by a single, perfectly straight domain wall. This results in the pure surface energy contribution $4\sqrt{N}$. As the linear interface moves through the system at constant energy for values of N_+ around $N/2$, in this region we also expect the function $E_{\min}(N_+)$ to be *flat*, with steps resulting from a geometric "lock in" at certain values commensurate with the underlying lattice structure. The detailed ground state energies found in these configurations will be discussed in more detail below. In any case, it is not straightforward to calculate $E_{\min}(N_+)$ for general N_+. In principle, we could try to determine $E_{\min}(N_+)$ for every single value N_+ using a variety of methods; for instance, with straightforward Monte Carlo minimization. In practice, this is both computationally expensive and sometimes of insufficient accuracy. For decreasing values of $N_+<N/2$ in a certain intermediate range, it becomes energetically more favorable for the system to switch from linear domain wall configurations to circular clusters, as they have a lower surface energy. However, to perform the transition from configurations with a planar to those with a circular interface *along paths of constant* N_+, the system would have to cross a large energy barrier. Such transitions are quite unlikely and certainly diminish speed and accuracy of the calculation. Obviously, a more sophisticated approach to determine the energy minima is needed.

However, even after determining the boundary of the allowed region in (E,N_+) space, we may be left with the possibility of the existence of *holes*, i.e., (E,N_+) values that are not realized, in the interior of this region. Hence, at these particular values, the density of states $g(E,N_+)$ vanishes. For instance, consider a "lock in" configuration as mentioned above. By this we mean a phase separated configuration consisting of two domains of up and down spins, which are separated by two (due to the periodic boundary conditions) perfectly linear domain walls. Obviously this is only possible if $N_+ \equiv n\sqrt{N}$ is an integer multiple of $\sqrt{N}$. For a fixed given value n around $\sqrt{N}/2$, this configuration will have the smallest "surface" N_{+-} of unequal spin pairs of all other configurations with the same magnetization. According to Eq. (4) its energy $4\sqrt{N}$ will thus be lower than that of any other configuration with the same total number of up spins, such that it constitutes a state of lowest energy for $N_+=n\sqrt{N}$. Flipping $|m|<\sqrt{N}$ spins now produces a value $N_+=n\sqrt{N}+m$, which is "incommensurate" with the underlying lattice. Among such "neighboring" configurations, those with a piecewise linear interface with exactly two "steps," will have the smallest "surface." As the corners of the steps produce two more uneven spin pairs, the corresponding energy of $4\sqrt{N}+4$ resides at +4 above the lowest energy found for the "commensurate" linear interface. On the other hand, to calculate the first "excited" energy, i.e., the first energy level above $4\sqrt{N}$ at the commensurate value $N_+=n\sqrt{N}$, we are only allowed to *exchange* spins among each other. However, starting from a linear interface, it is easy to see that any exchange of unequal spins produces an energy located not +4 but even +8 above the lowest energy $4\sqrt{N}$, leaving a "hole" at $4\sqrt{N}+4$. By a similar reasoning, it is easy to see that since the global energy maximum $E_{\max}(N/2)$ corresponding to the "antiferromagnetic" state where all nearest neighbor spin pairs are unequal and the magnetization is zero, the first possible lower energy level at magnetization zero is even separated from the top level by a gap of -12. Are there even more holes? This question is crucial. If just one of these holes remains undetected, the Wang-Landau histograms will never become flat and the algorithm fails to converge. For pure nearest neighbor Ising models the answer may be found analytically, but for more general couplings the task may be highly nontrivial.

In the case of continuous models the above problem of possible holes in the spectrum seems to be rather exotic. However, for discrete systems it is expected to be the rule rather than the exception. Summarizing our analysis so far, a modified Wang-Landau algorithm that takes care of both the boundary and possible holes of a multidimensional parameter region for the density of states would be highly useful. This can be achieved in a way explained below.

III. ALGORITHM

In the following, we will discuss the calculation of the density of states $g(E,M)$ as a function of energy E and magnetization M for a spin system, but we stress that the method we propose is very general and can easily be applied to a wide variety of systems. To overcome the problems outlined above, we have developed an algorithm in which the ranges of E and M are determined adaptively and on the fly. In order to set up multidimensional histograms, we first have to obtain upper and lower bounds on E and M. Determining a range of magnetizations usually poses no serious problem, but even the crude determination of useful upper and lower bounds on $E(M)$ for given magnetization M may be a nontrivial question. In the above example, these were fixed by analyzing the system configurations. In the case of continuous models these ranges may also be chosen deliberately from estimating the maximum energy or magnetization relevant up to a certain temperature T to which the result will be applied. In addition, an approach of dividing the parameter space into several smaller regions ("windows"), whose densities of states are then matched, may be chosen for efficiency. In any case, we confine the parameters to a rectangular region with the lower and upper bounds of energy and magnetization denoted by $(\underline{E},\underline{M})$ and $(\bar{E},\bar{M})$, respectively.

Next, we have to choose histogram widths for both E and M. Of course, to get accurate results, one would like to pick the finest resolution possible. For discrete systems, this offers another pitfall, since choosing a grid sizes too small in the direction of a discrete parameter will result in failure of the algorithm. Apart from such trivial considerations, the choice of grid widths has a major influence on the performance of the algorithm, as a multidimensional histogram grows rapidly with decreasing grid widths and may even force us to resort to an umbrella approach as mentioned above. Let n_E and n_M denote the numbers of histogram bins of width $(\bar{E}-\underline{E})/n_E$ and $(\bar{M}-\underline{M})/n_M$, respectively. We also denote the central values of bin (i,j) by (E_i,M_j). On this grid in the E-M space, two-dimensional arrays for the density of states, $g(E,M)$, and for the frequency of E-M pairs, $h(E,M)$, are set up.

The idea underlying our modified Wang-Landau algorithm is to successively record the absolute minimum and maximum values $E_{\min}(M_j)$ and $E_{\max}(M_j)$ for each magnetization index M_j in each step of the random walk. Suppose we now initialize our Wang-Landau random walk by choosing a random spin configuration with energy in the bin centered at E_k and a magnetization in the bin centered at M_l. These values then serve as initial values $E_{\max}(M_l)=E_{\min}(M_l)=E_k$. Whenever during the simulation a new magnetization occurs, this initialization procedure is carried out for that particular magnetization. The energy bounds $E_{\max}(M_j)$ and $E_{\min}(M_j)$ are updated every time an energy E outside the current energy range belonging to M_j is found. For all energy values between the "old" and the "new" energy bounds, the corresponding histogram and density of states entries $h(i,j)$ and $g(i,j)$ are initialized with 0 and 1, respectively. By iterating this procedure, the domain of the Wang-Landau simulation quickly spreads out in parameter space. Of course, flatness of the histogram should not be checked before a large number of, say, 10^6 random moves has been performed to avoid an untimely stop of this first "domain sampling run." In the course of the simulation, the histogram $h(i,j)$, should finally satisfy a certain flatness criterion *except* for points outside the bounds or certain isolated areas ("holes") *inside* this region, where the histogram en-

tries are strictly zero. As a second requirement, we now insist that each histogram bin be visited at least a minimum of, say, 10^6 times. Accordingly, it is clear how to identify the boundary and holes of the parameter domain: We will call a "hole" a bin (i,j) inside the parameter region found so far that has strictly *zero histogram entries*, while the remaining histogram is *flat* and remains so for a chosen large additional number of random moves. The same argument is also used to identify all other "forbidden" parameter regions outside of the domain of visited parameters found so far. Once the holes and the bins outside of the determined domain of parameters are determined, the standard Wang-Landau algorithm is carried out by simply ignoring these bins in checking for flatness of the histogram, which amounts to approximating $g(E,M)$ by $g(E,M)\approx 0$ for the corresponding (E,M) values. In the succeeding Wang-Landau runs, the parameter region found in this domain sampling run is frozen.

Of course, by choosing, e.g., poor moves, it is always possible that a Monte Carlo type of simulation fails to cover an important part of phase space. Therefore, we emphasize that efficiently designed Monte Carlo moves are absolutely indispensable for the above method to work. In principle, however, due to the increasing precision of the result acquired in each successive run, one can never exclude the possibility of discovering, e.g., "new" allowed pairs (E,M) in a later stage of the simulation. Nevertheless, by choosing rather strict parameters (flatness criterion, a large number of minimum hits for each bin, long constancy of flatness) for the initial run of the simulation, this possibility can be greatly reduced.

Still—how do we deal with such possible subsequent extensions of the valid parameter range? Obviously, the answer depends on the intended use of the result. For instance, suppose that we are interested in studying the low-temperature behavior of a certain system, and that a new lowest energy is found for a certain magnetization M at a later Wang-Landau run. Of course, it is always possible to complete the current Wang-Landau step, update the parameter range, and then restart the simulation. However, let us, for instance, suppose that we are interested in the calculation of the free energy of a system near its phase transition temperature. In studying this problem, one can expect that the dominant contributions to the free energy will result from higher energy ranges, and one can safely ignore these marginal points. In addition, to speed up the calculation in continuous systems in which holes are not expected to appear, it may be admissible to exclude, e.g., the very boundary bins of the determined parameter region from the flatness check. These points may correspond to parameter cells of which only a small volume fraction is actually accessible to the system, thus slowing down the algorithm without significantly increasing the accuracy of the result. Finally, when in doubt, it is always possible to further reduce the (E,M) region in order to estimate the error introduced by excluding boundary points.

IV. WANG-LANDAU INTEGRATION

The self-adapting Wang-Landau algorithm outlined above can also be applied to the problem of integrating strongly peaked functions in $d\times l$ dimensions. Such integrals typically arise in perturbation theory; e.g., in the context of lattice models in statistical mechanics [14] or lattice quantum field theory [15]. For instance, consider an Euclidean ϕ^4 model defined on a d-dimensional cubic lattice of lattice constant 1. Perturbation theory to loop order l involves ld-dimensional convolution integrals of a propagator of type $G(\boldsymbol{k},m)\sim 1/(4\Sigma_{i=1}^{d}\sin^2 k_i/2+m^2)$, where $m^2>0$ and $|k_i|<\pi$. A typical integral will be of the form

$$I(m^2)=\int_{[-\pi,\pi]^d} d^dp \int_{[-\pi,\pi]^d} d^dq G(\boldsymbol{p},m)G(\boldsymbol{q},m)G(\boldsymbol{p}+\boldsymbol{q},m), \tag{10}$$

which corresponds to the well-known $l=2$ "setting sun" Feynman diagram. More complicated integrals in higher dimensions occur for increasing orders of perturbation theory. Depending on the dimension d and the diagram under investigation, one has to deal with infrared singularities for $m^2\to 0$. For small values of m^2, the integrals are strongly peaked around the center as well as along certain diagonal directions of $\mathbb{R}^{ld}$. In this situation, numerical evaluation for smaller and smaller m^2 becomes increasingly difficult. To successfully apply Monte Carlo integration, we would have to construct a suitable umbrella function that resembles the integrand, within certain limits, which is *normalized*, or equivalently, whose integral on the domain of integration is known. Unfortunately, except for trivial cases, such a function is usually prohibitively difficult to find. As a matter of fact, the integrand itself would be the perfect umbrella function. However, normalizing it is just equivalent to actually computing the original integral. A slight variation of this idea would be the following. For values of m^2 exceeding a certain "large" value m_0^2 the integrals are no longer sharply peaked and are therefore are accessible to standard numerical integration. We then use this normalized integrand, which we will denote by $g(\boldsymbol{x},m_0^2)$, $x\in\mathbb{R}^{dl}$, as an umbrella function for computing our integral for a nearby parameter m_1^2 and so forth. However, in the resulting iterative procedure, care must be taken to control the unavoidable successive integration errors.

We now show how to compute integrals of the above type using the self-adaptive Wang-Landau algorithm sketched above. Let $f(\boldsymbol{x})>0$ denote a continuous and positive function on any compact subset $\mathbb{V}\subset\mathbb{R}^d$, such that the minimum $f_{\min}:=\min_{\boldsymbol{x}\in\mathbb{V}} f(\boldsymbol{x})$ and maximum $f_{\max}:=\max_{\boldsymbol{x}\in\mathbb{V}} f(\boldsymbol{x})$ are finite. We would like to compute the integral

$$Z[f]=\int_{\mathbb{V}} d^dx f(\boldsymbol{x}). \tag{11}$$

Let

$$\varphi(\boldsymbol{x}):=-\ln f(\boldsymbol{x})\Rightarrow f(\boldsymbol{x})=e^{-\varphi(\boldsymbol{x})} \tag{12}$$

denote the corresponding "energy" at temperature $k_BT=1$. We also set $\varphi_1:=-\ln f_{\min}$, $\varphi_0:=-\ln f_{\max}$ and $\Delta E:=\varphi_1-\varphi_0$. After a trivial manipulation, we obtain

$$Z[f] = \int_{-\infty}^{\infty} dE e^{-E} g_f(E), \tag{13}$$

where

$$g_f(E) := \int_{\mathbb{V}} d^d x \, \delta(E - \varphi(\boldsymbol{x})) \tag{14}$$

denotes the corresponding density of states. Dividing the energy interval $[\varphi_0, \varphi_1]$ into N subintervals of length $\epsilon := \Delta E/N$ and approximating the delta function by $\delta(E-\varphi(\boldsymbol{x})) \approx (1/\epsilon)\chi_\epsilon(E-\varphi(\boldsymbol{x}))$, where

$$\chi_\epsilon(e) := \begin{cases} 1, & |e| < \epsilon/2 \\ 0, & |e| \geqslant \epsilon/2 \end{cases} \tag{15}$$

denotes the "characteristic function" of energy $e \pm \epsilon/2$ gives

$$g_f(E) \approx \frac{1}{\epsilon} \int_{\mathbb{V}} d^d x \chi_\epsilon(E - \varphi(\boldsymbol{x})). \tag{16}$$

Defining the N energy values

$$E_n := \varphi_0 + (n + 1/2)\epsilon, \quad n = 0, \ldots, N-1, \tag{17}$$

we arrive at

$$Z[f] \approx \epsilon \sum_{n=0}^{N-1} e^{-E_n} g_f(E_n). \tag{18}$$

For arbitrary n, let $\mathbb{V}_n$ denote the subset of all $\boldsymbol{x} \in \mathbb{V}$ with energy $|\varphi(\boldsymbol{x}) - E_n| < \epsilon/2$. Then

$$Z[f] \approx V \sum_{n=0}^{N-1} e^{-E_n} w_\epsilon(E_n), \tag{19}$$

where

$$w_\epsilon(E_n) := \left(\frac{V_\epsilon^n}{V} \right) \tag{20}$$

is the volume fraction of all points $\boldsymbol{x}$ of $\mathbb{V}$ with energies within $\epsilon/2$ around E_n. Since trivially

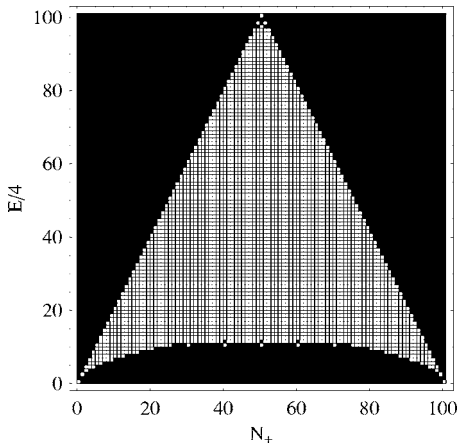

FIG. 1. (N_+, E)-domain of parameters for the 2d Ising model on a 10×10 lattice.

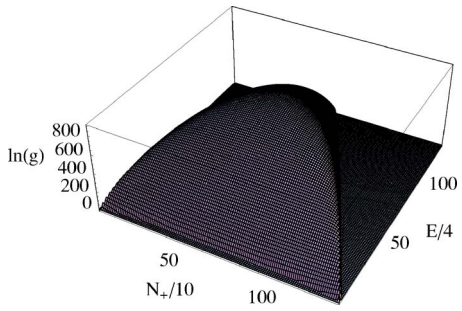

FIG. 2. $\ln g(N_+, E)$ as computed for the 2d Ising model on a 36×36 lattice.

$$\sum_{n=0}^{N-1} w_\epsilon(E_n) = \left(\frac{1}{V} \right) \sum_{n=0}^{N-1} V_\epsilon^n = \frac{V}{V} = 1, \tag{21}$$

the numbers $w_\epsilon(E_n)$ define a *normalized* distribution in *energy space*. However, this means that the $w_\epsilon(E_n)$ must be identical to

$$w_\epsilon(E_n) \equiv \hat{g}_f(E_n) := \frac{g_f(E_n)}{\sum_n g_f(E_n)}, \tag{22}$$

which can be determined from the Wang-Landau method by random walks in the volume $\mathbb{V}$. Note that the final formula

$$Z[f] \approx V \sum_{n=0}^{N-1} e^{-E_n} \hat{g}_f(E_n) \tag{23}$$

actually computes the integral; i.e., not just the integral up to a constant factor. This is because, although we were unable to normalize an umbrella function in direct space, due to the boundedness of f it is possible to normalize the density of states $g_f(E)$ in energy space. To carry out the integration procedure sketched above requires just two pieces of information. First we have to determine the volume V of the integration domain; i.e., the integral Z [1]. As a second ingredient, we would have to determine the energy bounds φ_0, φ_1. In the case of a complicated function on some complicated domain, even the determination of exact minima and maxima may be a difficult task. However, using our self-adaptive algorithm, all that is required is to find crude but safe estimates of these bounds, which is usually a trivial matter. Although the integrand may strongly peak in direct space with a peak height growing, e.g., like m^{-2n} for $m \to 0$, the corre-

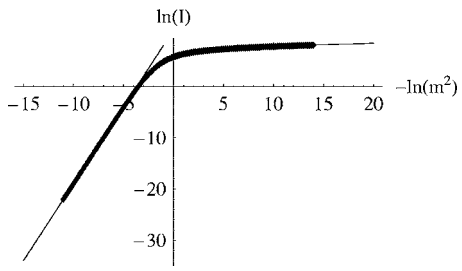

FIG. 3. Results for integral (10) completed by analytic approximations in the asymptotic small and large m^2 regions.

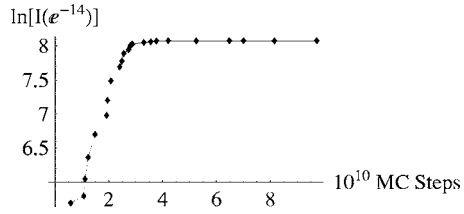

FIG. 4. Convergence of the numerical integration procedure for integral (10) at $-\ln(m^2)=14.0$ as a function of Monte Carlo steps.

sponding range in energy space only grows like $2n \ln m$. Therefore, the above method is ideally suited to tackle integrals of the type discussed.

V. NUMERICAL RESULTS

A. Ising model

As the first illustrative example of our algorithm, we calculate the density of states $g(E,M)$ of the 2d Ising model. The density of states calculated with the Wang-Landau method for the equivalent lattice gas model has been used by Jain and de Pablo to determine the surface free energy of the vapor-liquid interface [9]. Figure 1 shows the (E,N_+) parameter region obtained from our algorithm on a 10×10 Ising lattice. Notice the location of holes and the traces of the underlying lattice structure. The corresponding density of states $g(E,N_+)$ for a 36×36 lattice is shown in Fig. 2.

B. Numerical Integration

To illustrate the power of our numerical integration algorithm, we present the results of a calculation of integral (10) in the parameter range $0.4\leqslant-\ln(m^2)\leqslant14.0$. The resulting data were completed by conventional Monte Carlo integration data and analytic approximations of the integral in the asymptotic regions $-\ln(m^2)\gg14$ and $-\ln(m^2)\ll0$. We performed up to 22 successive Wang-Landau runs, using 15 000 bins in energy space and a flatness parameter of 0.7. The results are shown in Fig. 3. The computational effort is largest for small parameter values; i.e., $-\ln(m^2)$ near 14.0. For these values, although convergence sets in a lot faster, we used a total of approximately 10^{11} Monte Carlo moves of maximum width 1.0 in direct space. Figure 4 displays the numerical convergence of the integral as a function of Monte Carlo steps for this "worst case" scenario. The corresponding density of states is shown in Fig. 5. One notices nearly singular behavior at the lower and upper energy boundaries. These singularities, which are, of course, due to the "flatness" of the integrand in direct space, effectively put a limit to the use of the method at extreme parameter values as it is. However, useful results could still be obtained by sampling different "umbrella" regions near these boundaries in additional runs.

Let us return to Fig. 5. By close investigation, using the present flatness parameter of 0.7, the resulting density of states does not yield strong noise disturbance down to scales even much smaller than depicted here. However, we should like to mention that, as long as one is not interested in calculating the density of states but just the integral, the performance of our algorithm can be significantly increased by reducing the flatness parameter to smaller values. In fact, this may finally lead to noticeable noise in the density of states. However, the calculated value of the integral is not very sensitive to this noise, as the final formula (23) effectively performs a smoothening average.

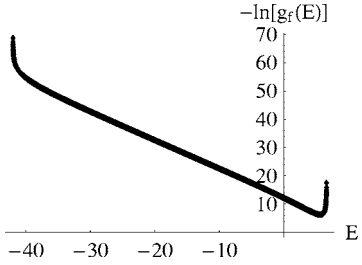

FIG. 5. Density of states $g_f(E)$ for integral (10) calculated at $-\ln(m^2)=14.0$.

VI. CONCLUSIONS

In the context of statistical mechanics, the self-adjusting Wang-Landau method presented above is ideally suited for computing one, or even multidimensional densities of states for systems whose energetic or configurational bounds are not known in advance. In fact, it can also be employed to calculate such bounds, such as e.g., energy minima or maxima as functions of an order parameter value, with high accuracy or detect forbidden areas in the space of admissible parameter values. The algorithm should thus be useful, for instance, for finding spin-glass ground states [16].

The self-adapting character of the algorithm also turns the Wang-Landau method into a powerful numerical integration tool. In passing, we note that such a numerical integration could also serve as a benchmark to study the efficiency of the Wang-Landau algorithm. First of all, the performance of the algorithm is certainly a function of tuning parameters such as histogram width and flatness percentage. In Ref. [6] the algorithm was applied to a 2d Ising model, where the results can be compared to analytical solutions. Quite recently, an analysis of the efficiency of the Landau-Wang method has been presented for Lennard-Jones and Dzugutov fluids [17], focusing on the optimal choice of energy windows in a parallel implementation. Compared to these examples, the comparison of the performance of the numerical Wang-Landau integration algorithm with different parameters, applied to a case wherein the value of the integral is actually known analytically, is easy.

ACKNOWLEDGMENTS

We would like to thank H. Oberhofer for useful discussions. This work was supported by the Austrian Science Fund (FWF) under Grant No. P17178-N02.

[1] D. P. Landau and K. Binder, *Monte Carlo Simulation in Statistical Physics* (Cambridge University Press, 2000).
[2] D. Frenkel and B. Smit, *Understanding Molecular Simulation* (Academic, San Diego, 2002).
[3] G. M. Torrie and J. P. Valleau, J. Comput. Phys. **23**, 187 (1977).
[4] B. A. Berg and T. Neuhaus, Phys. Rev. Lett. **68**, 9 (1992).
[5] E. Marinari and G. Parisi, Europhys. Lett. **19**, 451 (1992).
[6] F. Wang and D. P. Landau, Phys. Rev. Lett. **86**, 2050 (2001).
[7] F. Wang and D. P. Landau, Phys. Rev. E **64**, 056101 (2001).
[8] Q. L. Yan, R. Faller, and J. J. de Pablo, J. Chem. Phys. **116**, 8745 (2002).
[9] T. S. Jain and J. J. de Pablo, J. Chem. Phys. **118**, 4226 (2003).
[10] T. J. H. Vlugt, Mol. Phys. **100**, 2763 (2002).
[11] N. Rathore, T. A. Knotts, and J. J. de Pablo, J. Chem. Phys. **118**, 4285 (2003).
[12] F. Calvo, Mol. Phys. **100**, 3421 (2002).
[13] See, e.g., K. Huang, *Statistical Mechanics*, Second edition (Wiley, New York, 1987).
[14] H. Kleinert, Phys. Rev. D **57**, 2264 (1998); H. Kleinert and V. Schulte-Frohlinde, *Critical Properties of ϕ^4—Theories* (World Scientific, Singapore, 2001).
[15] Cf., e.g., M. Lüscher and P. Weisz, Nucl. Phys. B **445**, 429 (1995); S. Capitani *et al.*, Nucl. Phys. B (Proc. Suppl.) **63**, 802 (1998); R. Lewis and P. A. Ouimet, Phys. Rev. D **64**, 034005 (2001); T. Becher and K. Melnikov, *ibid.* **66**, 074508 (2002).
[16] J.-S. Wang and Y. Okabe, J. Phys. Soc. Jpn. **72**, 1380 (2003).
[17] M. S. Shell, P. G. Debenedetti, and A. Z. Panagiotopoulos, J. Comput. Phys. **23**, 187 (1977).