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Improving Wang-Landau sampling with adaptive windows

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Wang-Landau sampling (WLS) of large systems requires dividing the energy range into "windows" and joining the results of simulations in each window. The resulting density of states (and associated thermodynamic functions) is shown to suffer from boundary effects in simulations of lattice polymers and the five-state Potts model. Here, we implement WLS using *adaptive* windows. Instead of defining fixed energy windows (or windows in the energy-magnetization plane for the Potts model), the boundary positions depend on the set of energy values on which the histogram is flat at a given stage of the simulation. Shifting the windows each time the modification factor f is reduced, we eliminate border effects that arise in simulations using fixed windows. Adaptive windows extend significantly the range of system sizes that may be studied reliably using WLS.

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In recent years Wang-Landau sampling (WLS) [1–4] has become an important algorithm for Monte Carlo (MC) simulations and is being applied to a vast array of models in statistical physics and beyond [4]. WLS uses a random walk in energy (E) space to estimate the density of states, $g(E)$; to sample well the full range of energies, the walk is adjusted to spend approximately equal time intervals at each energy value. The estimate for $g(E)$ is refined successively in a series of random walks. WLS has been used, for example, to simulate polymers [5–8] and proteins [9,10] and to calculate the joint density of states (JDOS) of two or more variables [11]: e.g., $g(E,M)$ of magnetic systems (M is the magnetization).

For models with a complex energy landscape, WLS permits simulation of larger systems than can be studied using conventional MC approaches. Because sampling the full range of energies of a large system is not viable using a single walk, one divides the energy range into slightly overlapping subintervals ("windows") and samples each separately. The density of states, $g(E)$, for the full energy range is then obtained via a matching procedure that consists of multiplying $g(E)$ in each window by a factor to force continuity of this function at the borders. This yields $g(E)$ to within an overall multiplicative factor, permitting evaluation of canonical averages.

Does sampling restricted to windows yield reliable estimates for $g(E)$ near the boundary energy values? Wang and Landau suggested that boundary effects would be negligible if adjacent windows were defined with a suitably large overlap [2]. On the other hand, Schulz *et al.* [12] suggest that whenever a configuration is rejected because its energy is greater than the maximum value $E_>$ of a given window, one should update $g(E)$ for the current energy value. These prescriptions are effective for Ising models, but do not eliminate boundary effects in all instances: e.g., in simulations of polymers [13] and systems where the JDOS is required [14].

Here we present an implementation of WLS that eliminates border effects and apply it to two examples with severe border problems: a lattice polymer with attractive interactions between nonbonded nearest-neighbor monomers [5,15,16], simulated via reptation [17], and the calculation of $g(E,M)$ in the five-state Potts model [18]. (Although reptation is not suitable for sampling the most compact configurations, this does not affect the conclusions presented here.) We note that the present method is distinct from "self-adaptive" WLS [19], used for determining the JDOS when the range over which $g(E,M)$ is nonzero is not known *a priori*.

To begin, we document border effects in fixed-window simulations of polymers, focusing on the specific heat $c(T)$ (calculated from the variance of the energy). The polymer is modeled as a self-avoiding walk on the square lattice. The energy is $E=-N_{nb}$, with N_{nb} the number of nearest-neighbor contacts between nonconsecutive monomers; our simulations sample the entire energy range. We encounter strong border effects, even if, following the suggestion of Ref. [12], we use three overlapping levels at the border(s). Varying the border energy E_b, we find that the temperature T_m at which $c(T)$ is maximum varies (a smaller E_b corresponds to a smaller T_m), signaling a systematic error (see Fig. 1). We stress that such a distortion does not arise in WLS of the two-dimensional Ising model [2], for which simulations using fixed windows have been performed on lattices of up to 256×256 sites.)

We now show how to eliminate the boundary effects described above. Recall that WLS begins with an arbitrary configuration and with $g(E)=1$ for all energies E. A random walk in energy space is realized by generating trial configurations and accepting them with probability $p(E_1\rightarrow E_2)=\min(g(E_1)/g(E_2),1)$, where E_1 is the current energy value and E_2 that of the trial configuration $\mathcal{C}_2$. If $\mathcal{C}_2$ is accepted, we update $g(E_2)\rightarrow f\times g(E_2)$ and $H(E_2)\rightarrow H(E_2)+1$; otherwise, $g(E_1)\rightarrow f\times g(E_1)$ and $H(E_1)\rightarrow H(E_1)+1$. The histogram $H(E)$ records the number of visits to energy E, and f is the modification factor, initially set to $e=2.718\,28\ldots$. When $H(E)$ is sufficiently *flat*, it is reset to zero and a new random walk is initiated, with a smaller f: e.g., $f\rightarrow\sqrt{f}$, used to update

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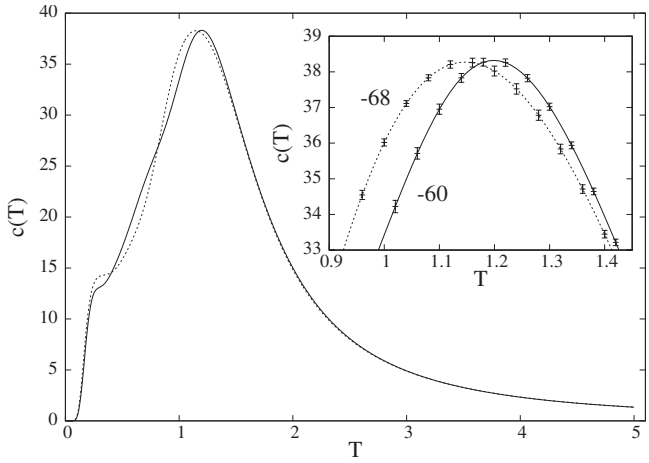

FIG. 1. Specific heat of a polymer of $N=100$ monomers on the square lattice using two windows and border energies $E_b=-68$ and -60. Inset: neighborhood of the maximum. Average values and uncertainties are calculated using ten independent runs.

$g(E)$. The simulation ends when f is sufficiently close to 1: e.g., $f \approx 1+10^{-7}$.

The histogram is said to be flat if, for all energies in the window of interest, $H(E) > \kappa \bar{H}$, where the overbar denotes an average over energies. (Typically, $\kappa=0.8$, as used here.) In WLS with fixed windows, this criterion is applied in each window. Here, by contrast, we determine the range over which the histogram is flat at various stages of the simulation.

Initially, we allow the WLS random walk to visit all energies $E_{min} \leqslant E \leqslant E_{max}$, accumulating the histogram in the usual manner. After a certain number N_1 of Monte Carlo steps (we use $N_1=10^4$), we check if the histogram is flat on the interval $E_w \leqslant E \leqslant E_{max}$. (Here $E_w=E_{max}-W$, with W defining the minimum acceptable window size.) If it is not flat, we perform an additional N_1 Monte Carlo steps and check again, repeating until the histogram is flat on the minimal window. Once this condition is satisfied, we check whether the histogram is in fact flat on a larger window. We include the energy level just below E_w in $\bar{H}$ and check if the flatness criterion holds in the enlarged window. Adding levels one by one, we identify the largest window over which flatness is satisfied. Let $E^* \leqslant E_w$ be the smallest energy such that the histogram, restricted to the interval $[E^*, E_{max}]$, is flat, and let $E_1=E^*+\Delta E$, where ΔE determines the overlap between adjacent windows. At the next stage, we restrict the random walk to energies $E_{min} \leqslant E \leqslant E_1+\Delta E$. After N_1 steps we check if the histogram is flat on the interval $[E_1+\Delta E-W, E_1+\Delta E]$ and proceed as above, until all energies have been included in a window with a flat histogram (see Fig. 2). To avoid problems that might arise with very small windows, the final window (with lower limit E_{min}) always has a width $\geqslant W$. In the studies shown below we use $W=(E_{max}-E_{min})/10$ and $\Delta E=3$ for lattice polymers ($\Delta E=1$ or $\Delta M=1$ for the Potts model). Once all energies have been sampled, we connect the functions $g(E)$ associated with the various windows by imposing continuity at $E_1, E_2, \ldots, E_n$. Then the entire procedure is repeated using

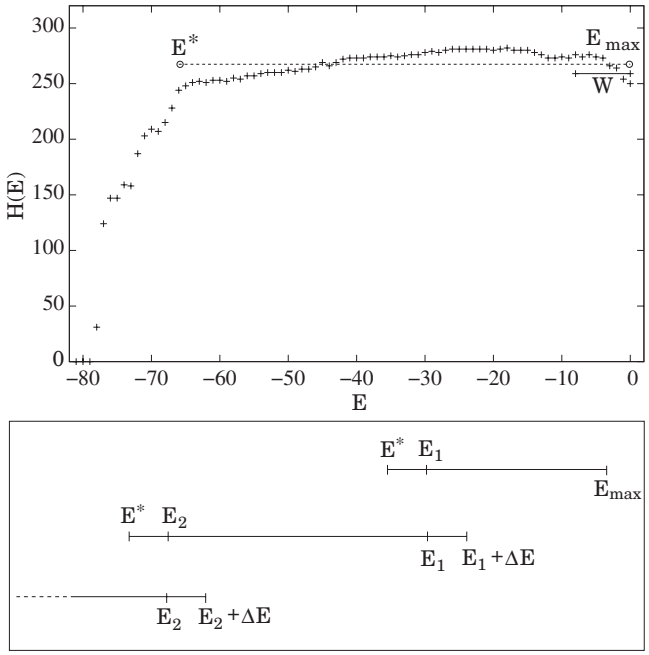

FIG. 2. Lower panel: schematic of adaptive windows; the value of E_{max} depends on the model, while ΔE is chosen to ensure sufficient overlap. E^* and E_1, E_2, etc., are determined during the simulation not fixed beforehand. Upper panel: example of a histogram and associated window in the lattice polymer simulation.

the next value of the modification factor f—that is, $f \to \sqrt{f}$; the simulation ends once $f-1<10^{-7}$.

Note that at each iteration (using a different value of f), the borders E_j are chosen differently: repetition of a border value in successive iterations is prohibited. This point is crucial to the functioning of our method; if the borders were fixed, errors incurred at a given iteration (similar to those seen in Fig. 1) would accumulate, rather than being corrected in subsequent iterations.

Energy windows are necessary in studies of large systems; without them, WLS does not converge. Thus, the largest polymer we are able to study without windows is $N=70$; using adaptive windows, the entire energy range is accessible for $N=300$ or more. To test our method, we compare $g(E)$ (for $N=200$), given by our scheme, with that obtained using high-resolution Metropolis Monte Carlo (MMC) simulations [17]; excellent agreement is found (see Fig. 3). MMC simulations are performed at temperatures $T=1.0$, 1.5, 3.0, and 10.0, using 10^8 MC steps per study, with the RAN2 random number generator [20]. In MMC simulations, the expected number $m(E)$ of visits to energy E satisfies $m(E)/m(E_{ref})=e^{-(E-E_{ref})/k_BT} g(E)/g(E_{ref})$. Equating $m(E)$ to the number of visits to energy E, we determine the ratios $g(E)/g(E_{ref})$. At a given T, a certain range of energies is well sampled; we take the reference energy E_{ref} as the most visited value at that temperature. The resulting values for $g(E)$ are normalized by equating $g(E_{ref})$ to the corresponding value obtained via WLS. We also find that the specific heat obtained using adaptive windows agrees to within uncertainty (i.e., one standard deviation) with that found using MMC simulations, while that obtained using fixed windows does not.

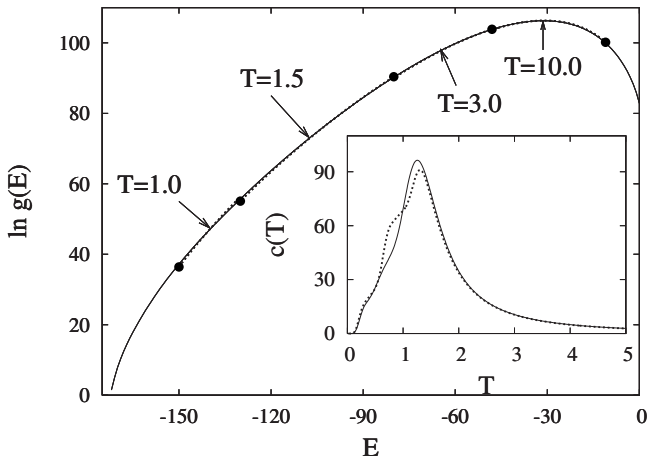

FIG. 3. Density of states $g(E)$ of two-dimensional polymers, $N=200$. Solid line: adaptive-window sampling. Dashed line: Metropolis sampling, using the ratios $g(E)/g(E_{ref})$. Circles denote the limits of the energy ranges associated with each temperature in Metropolis sampling. Inset: specific heat vs temperature for $N=200$. Solid line: adaptive windows: Dotted line: fixed windows.

We turn now to the Potts model [18], with Hamiltonian $\mathcal{H}=-J\Sigma_{\langle ij\rangle}\delta_{\sigma_i,\sigma_j}-h\Sigma_i\delta_{\sigma_i,1}$ where $\sigma_i=1,2,\ldots,Q$; $\langle ij\rangle$ denotes pairs of nearest-neighbor spins, $J>0$ is a ferromagnetic coupling, and h is an external field that couples to state 1. (Our units are such that $J/k_B=1$.) We study the $Q=5$ model on square lattices of 32×32 sites with periodic boundaries using the R1279 shift register random number generator [17].

Let $E=-\Sigma_{\langle ij\rangle}\delta_{\sigma_i,\sigma_j}$ and $M=\Sigma_i\delta_{\sigma_i,1}$. We determine the JDOS $g(E,M)$ via fixed-window WLS by dividing the parameter space into (i) strips of restricted values of E and unrestricted M or (ii) restricted M and unrestricted E and (iii) rectangles with both E and M restricted. Independent random walks are carried out in parallel and the densities of states from adjacent regions normalized at a single common (E,M) point or by minimizing the least-squares distance between an overlapping (E,M) region. The resulting JDOS exhibits small discontinuities which affect the probability distributions of energy and magnetization, as illustrated by the dashed line in Fig. 4 for $P(M,T,h)$ for case (ii) above. This curve was obtained with one simulation (hence no error bars are displayed); the temperature is taken such that $P(M,T,h)$ has two peaks of approximately equal height. When we average $P(M,T,h)$ from multiple independent simulations, the jumps are somewhat smoothed out; nevertheless, the thermodynamic quantities obtained with these implementations of parallel WLS suffer from a small systematic error, as illustrated in Fig. 5 for the specific heat.

The discontinuities in $P(M,T,h)$ arise because the slope of the JDOS is discontinuous at the borders between windows. This can be partly circumvented by using a larger overlap region, but there is no guarantee that these regions will be sampled properly. Using adaptive windows, by contrast, the slopes of the JDOS at the borders of neighboring windows are equal to within numerical uncertainty. In WLS with adaptive windows, we normalize the JDOS via a least-squares-difference criterion along the line of overlap between neighboring windows.

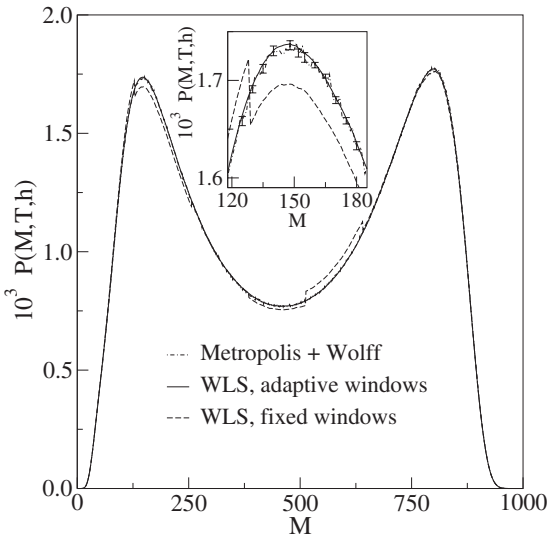

FIG. 4. Magnetization probability distribution $P(M,T,h)$ for the five-state Potts model with $T=0.86177$ and $h=0.005$, computed from $g(E,M)$ obtained via WLS with fixed windows using restricted M and unrestricted E (dashed line), adaptive windows (solid line), and from a hybrid MC method (dot-dashed line). In the inset only a few typical error bars are shown for the hybrid MC result (error bars for the WLS with adaptive windows are slightly smaller).

The magnetization probability distribution computed from $g(E,M)$ (obtained from an average over ten independent runs using WLS with adaptive windows), shown in Fig. 4 (solid line), is in good agreement with the distribution obtained using a hybrid MC method [17] with 10^8 MC steps. Here one MC step comprises $4L^2$ single spin-change trials (Metropolis algorithm) and 6 Wolff cluster updates. (In the main graph of Fig. 4 the result from adaptive-window WLS is almost indistinguishable from that using the hybrid MC method.) The specific heat obtained with WLS using adaptive windows is also in excellent agreement with that of the hybrid MC method, as shown in Fig. 5. Although we illustrate the effectiveness of WLS with adaptive windows for $L=32$, a relatively small lattice size, we note that we are performing *two-dimensional* random walks; the parameter space is much

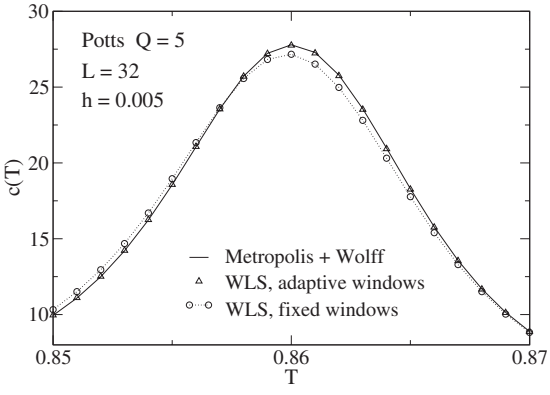

FIG. 5. Specific heat versus temperature for the five-state Potts model with $h=0.005$, obtained via sampling methods as indicated. Error bars are smaller than the symbol sizes.

larger than for a one-dimensional random walk using the same system size. Since the five-state Potts model has a very weak first-order phase transition, the hybrid MC method, employed here to test our new method, can sample equilibrium states; however, as Q increases, it becomes forbiddingly difficult for this method to equilibrate the system. In contrast, WLS works well even at strong first-order phase transitions and, when combined with the adaptive-window method, can be used for quite large systems.

Comparing the efficiency of adaptive versus fixed-window WLS is subtle because the convergence time in the latter case depends on how the window boundaries are defined. The adaptive window algorithm typically uses four windows for this size; fixed-window WLS with window boundaries similar to those of the adaptive case (i.e., smaller windows in the low-energy region) has a convergence time similar to that for adaptive windows. Recall, however, that fixed-window WLS does not yield reliable results in this case. In a pair of studies of the five-state Potts model ($L=32$), one using adaptive windows and the other dividing the range of the magnetization into eight equal windows (with no restrictions on energy), the adaptive-windows simulation ran in about 60% of the time required for fixed windows.

In summary, we show how WLS may be applied reliably to large systems without border effects. For the models considered here, such effects are strong and effectively prohibit the study of large systems using fixed windows. In our method, errors that may arise near the border of a given window are corrected in subsequent stages, in which the border positions are shifted.

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