Comment on "Efficient, multiple-range random walk algorithm to calculate the
density of states"

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In their recent Letter Wang and Landau \cite{1} have proposed a very effective MC method of producing evenly distributed histograms for the degeneracy $g(E_i)$ of the energy levels of different discrete spin models. The method suffers, however, from a drawback. In the course of their calculations Wang and Landau have to reduce their multiplication factor $f$ to a value $f_{\text{final}}$ which differs from 1 only by $10^{-8}$. At this stage the algorithm comes very close to entropic sampling. Indeed when $g(E_i)$ has the value $10^8$ then the modified density of states (DOS) $g(E_i) \to g(E_i) \ast f_{\text{final}}$ in the new algorithm and the modified DOS: $g(E_i) \to g(E_i) + 1$ in entropic sampling are identical. Thus the new method has the definite advantage of rapidly building a rough estimator for the DOS but in the end the work of refining it to useful accuracy is as time consuming as entropic sampling.

We have ourselves used a similar method as Ref. \cite{1} to calculate histograms of the degeneracy of $g(E_i)$ of three dimensional Ising models and of the degeneracy $g(E_0, M_i)$ of 2d-Ising models for a fixed value $E_0$ of the energy as a function of the magnetization $M_i$. We have also produced histograms for the three dimensional ANNNI-model. All these data are unpublished.

In our approach the acceptance probability of a spin flip is also governed by the density of states $g(E_i)$ which has been accumulated so far. In this respect our approach is identical to that of Wang and Landau, but it differs from Ref. \cite{1} in two important aspects: (i) the histogram $g(E_i)$ of the DOS is updated (multiplied by $f$) only every tenth step, (ii) the transition observables $T(E_i, \Delta)$ are also evaluated by recording all attempts to move from an energy $E_i$ to $E_i + \Delta$ with $\Delta = 0, \pm 4, \pm 8$ for the 2d-Ising model. On taking the logarithm one obtains the entropy $S(E_i) = \ln g(E_i)$ from the DOS and the inverse temperature $\beta = \ln [T(E_i + \Delta, -\Delta)/T(E_i, \Delta)]/\Delta$ from the transition observables. It turns out that the latter data suffer much less from statistical errors than the former. In contrast to Ref. \cite{1} we do not vary $f$ – it is kept constant during the simulation. In the examples which follow we have added $\eta = 0.004$ viz. $\eta' = 0.002$ to the entropy $S(E_i)$ after every 10 attempted spin flips. This leads to multiplication factors $f = e^\eta$ of 1.004 viz. 1.002.

It turns out that the error one makes is roughly proportional to $\eta$, i.e., $\ln g_{\ast}(E_i) \approx S(E_i) + \eta f(E_i) + K_{\eta}$ where $\eta f(E_i)$ is this error and $K_{\eta}$ is an unimportant constant. A very good approximation for $S(E_i)$ can therefore be determined from two MC runs with different values of $\eta$ and $\eta'$: $S(E_i) \approx [\eta \ln g_{\ast}(E_i) - \eta' \ln g_{\ast}(E_i)] / (\eta - \eta') + K$.

Fig. 1 has been produced for the $32 \times 32$ 2d-Ising model. It shows the second derivative $d^2 s(\varepsilon)/d\varepsilon^2$ of our simulated data. Here $s = S/N$ and $\varepsilon = E/N$ are the entropy and the energy per spin. These data scatter around the exact data of Beale \cite{2}. The difference to these data is shown in the inset. Gaussian smoothing over 20 channels reduces the maximum deviation to 0.005.

As the entropy is determined up to an unimportant constant, the derivatives of the entropy are more assertive. Therefore one should not compare the entropy itself, but its derivatives with the exact results \cite{2}. We have chosen the second derivative for this comparison because it enters into the microcanonically defined specific heat $c(\varepsilon) = -s'^{\prime\prime}(\varepsilon)/s'^{\prime}(\varepsilon)$ and it is thus very important that high quality data are obtained for it.

In summary: Because of our substraction scheme we can keep the entropy increment and concomitantly the effectivity of the simulation procedure five orders of magnitude above Ref. \cite{1}.

We thank Michael Promberger for his advice.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig1}
\caption{The second derivative $d^2 s(\varepsilon)/d\varepsilon^2$ and the difference to the exact data (inset).}
\end{figure}

\begin{itemize}
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\item \[1\] F. Wang and D. P. Landau, Phys. Rev. Lett. \textbf{86}, 2050 (2001).
\item \[2\] P. D. Beale, Phys. Rev. Lett. \textbf{76}, 78 (1996).
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