# Magnitude of the Wang-Landau error

**Gregory Brown[1], PA Rikvold[1], Kh Odbadrakh[2] and DM Nicholson[3]**

[1] Department of Physics, Florida State University, Tallahassee, FL 32306, USA
[2] Joint Institute for Computational Sciences at ORNL, University of Tennessee, Oak Ridge, TN 37831, USA
[3] Department of Physics, University of North Carolina Asheville, Asheville, NC 28804, USA

E-mail: `gbrown@fsu.edu`

**Abstract.** The Wang-Landau algorithm is an entropic sampling method that incoroporates an update factor $\ln f_i$, which introduces a self-avoidance tendency into the random walk. Continued sampling at constant $\ln f_i$ leads to a steady state estimate of the density of states $\ln g_i(E)$. We find numerically that the difference between $\ln g_i(E)$ and the true density of states $\ln g(E)$ is proportional to the update factor.

In general, the name "flat-histogram sampling" is applied to importance sampling Monte Carlo methods in which each proposed step in a Markov chain is accepted with probability $p(E \to E') = \min[1, g(E)/g(E')]$, with $g(E)$ the density of states (DOS). One result is that

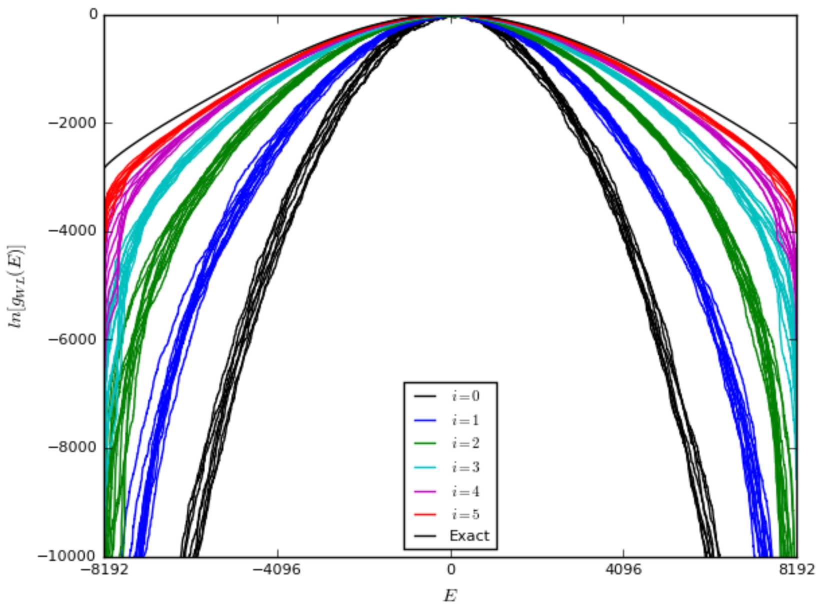


**Figure 1.** Snapshots of the estimated DOS $\ln[g_i(E)]$ for the $64 \times 64$ square-lattice Ising ferromagnet.

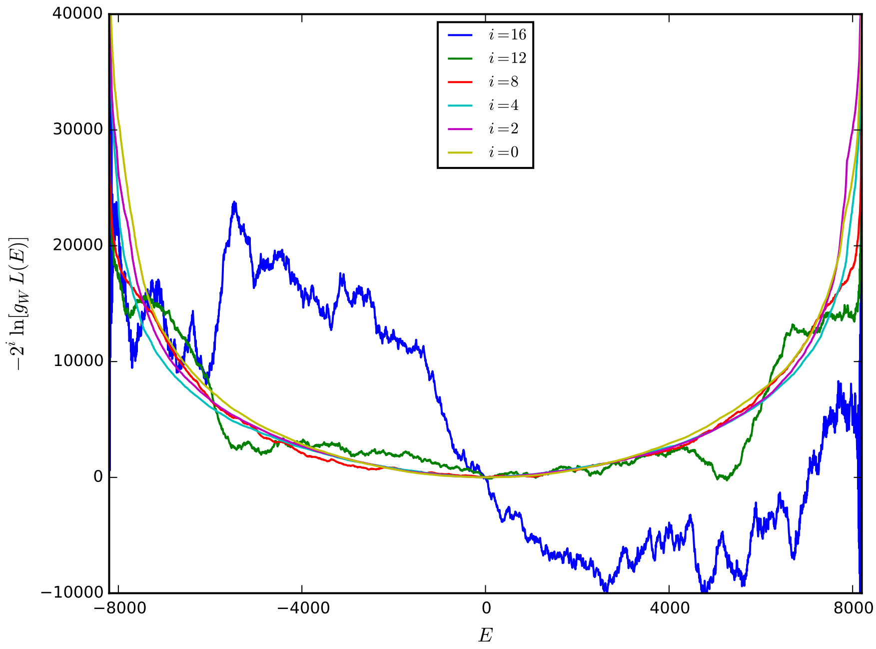


**Figure 2.** Wang-Landau error $g_{i,\mathrm{WL}}(E)$ scaled by the update factor $\ln f_i$ for several stages $i$ in the algorithm applied to the $64 \times 64$ square-lattice Ising ferromagnet. Here $\ln g_{\mathrm{FIX}}(E)$ is the exact result from Ref. [5].

the simulation-time-averaged histogram is a constant density with respect to energy, $h(E) = C$. When the DOS is not known, the Wang-Landau algorithm [1] can be used to generate an estimate of the DOS, $g_i(E)$. Each iterative stage $i$ of the algorithm is characterized by an update factor $\ln f_i$, which gets smaller as the stages progress. Typically $\ln f_i = 2^{-i}$ and the Wang-Landau estimated DOS becomes self-consistent as $\ln f_i \to 0$. Within each stage, the estimated DOS is dynamically updated after each step in the Markov chain by adding $\ln f_i$ to the logarithm of the estimated DOS at the current energy of the Monte Carlo walker, $\ln[g_i(E)] \leftarrow \ln[g_i(E)] + \ln f_i$. Within each stage $i$ of the Wang-Landau algorithm the dynamic estimate of the function $\ln[g(E)]$ will approach a steady-state value [2, 3]. In this way, the Wang-Landau algorithm can be said to produce a series of estimated DOS $g_i$ that converge to the true DOS $g$, particularly for the $1/t$ algorithm [3, 4].

The estimated DOS, $\ln[g_i(E)]$, for one run of the Wang-Landau algorithm is shown in Fig. 1 for the $64 \times 64$ square-lattice Ising ferromagnet. Several intermediate results are shown for each stage $i$ and the different stages are color coded (online), but can be easily distinguished visually. It is clear from these data that $\ln[g_i(E)]$ approaches a steady-state value for each $i$, and that this estimate relaxes to $\ln[g(E)]$ as $i$ increases. The exact DOS, as calculated using the result of Beale [5], is also shown.

In our implementation of the Wang-Landau algorithm, we have separated the estimated DOS at each stage into two factors

$$\ln[g_i(E)] = \ln[g_{\mathrm{FIX}}(E)] + \ln[g_{i,\mathrm{WL}}(E)] , \tag{1}$$

with $g_{\mathrm{FIX}}(E)$ fixed at the beginning of the Wang-Landau algorithm and unchanged throughout all stages. Then $g_{i,\mathrm{WL}}(E)$ isolates the dynamically changing part of the estimated DOS. In particular, if $g_{\mathrm{FIX}}$ is the true $g(E)$, then $\ln[g_{i,\mathrm{WL}}(E)] = \ln[g_i(E)] - \ln[g(E)]$ is the error in the

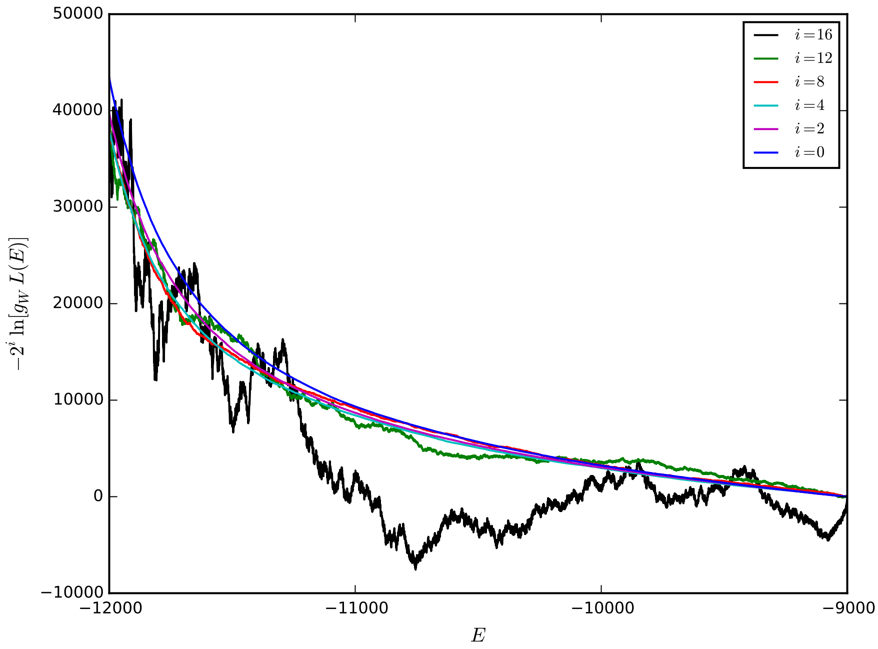


**Figure 3.** Wang-Landau error $g_{i,\mathrm{WL}}(E)$ scaled by the update factor $\ln f_i$ for several stages $i$ in the algorithm applied to the $16\times16\times16$ Heisenberg ferromagnet on a simple cubic lattice. Here $\ln g_{\mathrm{FIX}}(E)$ was estimated from a previous, identical calculation.

stage-$i$ Wang-Landau estimated DOS in the steady state limit. Using the exact result [5] as $g_{\mathrm{FIX}}(E)$, the error $g_{i,\mathrm{WL}}(E)$ is shown in Fig. 2. In this scheme the stages are run independently and the traditional flatness critierion is unimportant. Multiplying the DOS by the inverse update factor, $1/\ln f_i = 2^i$, results in good data collapse for a wide range of $\ln f_i$. As $\ln f_i$ get smaller, the noise in the error becomes more pronounced. For $i \geq 16$ the noise dominates. Similar behavior for the three-dimensional Heisenberg ferromagnet on a simple cubic lattice is shown in Fig. 3. For the Heisenberg ferromagnet, the energy has been restricted to the window $E \in [-12000, -9000]$ while the paramagnetic peak lies at $E=0$, in part because the DOS decreases rapidly near the ground state. We conjecture that it is a general feature of the Wang-Landau algorithm for the systematic error to include the update factor $\ln f_i$ as a multiplicative factor.

## Acknowledgments

GB and KO were supported by the Center for Defect Physics (CDP), an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences. PAR acknowledges support from NSF grant No. DMR-1104829. DMN was supported by the Materials Science an Engineering Division, Office of Basic Energy Sciences, US Department of Energy.

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