RUSSIAN ACADEMY OF SCIENCES
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Алгоритм Ванга-Ландау: случайное блуждание по спектру энергии и эффективная параллелизация

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Wang-Landau sampling method

Wang–Landau method is the random walk in the energy space with a flat histogram.

F. Wang and D.P. Landau, PRL **86** (2001) 2050 and PRE **64** (2001) 056101
D.P. Landau and K. Bunder, *A guide to Monte Carlo simulations in statistical physics*, Cambridge University Press, 2009

$$Z = \sum_{\text{configuration } i} e^{-E_i/k_B T} \equiv \sum_E g(E)\, e^{-E/k_B T}$$

where $g(E)$ is the density of state (DoS), the number of all possible states with the energy E of the system.

Wang-Landau algorithm

- set $g(E)=1$ *for all energy values* E;
- fix value of the modification factor $f = 2.718281828$;
- generate random state s_i ;
- calculate energy of the state E_k ;
- set auxiliary histogram $H(E)=0$ *for all* E;

- choose randomly spin s_i

  and calculate energy E_{k+1} *of* the state with the flipped spin $s_i \rightarrow -s_i$;

- If $g(E_{k+1}) < g(E_k)$, *then* ***accept*** *the new state.*

  If not, accept the new state with probability $g(E_k) / g(E_{k+1})$,

  Otherwise keep the current state unchanged (**not-accept**).

Wang-Landau algorithm /2

- Acceptance of the new state consists with the following steps:

  flip spin $S_i := - S_i$

  update DoS entry $g(E_{k+1}) := f\, g(E_k)$

  update histogram $H(E_{k+1}) := H(E_k) +1$,

- Non-acceptance of the new state consists with the following steps:

  update DoS entry $g(E_k) := f\, g(E_k)$

  update histogram $H(E_k) := H(E_k) +1$,

- Repeats steps between lines on the previous slide some MN *times, where* N is the number of spins and M is some large value (say 10^4) and check the “flatness” of the histogram (it is an empirical way to treat flatness and originally some 5% of flatness recommended).

Wang-Landau algorithm /3

If histogram is not “flat” enough, repeat additional MN *times, …*

If histogram is flat, decrease factor $f = f^{1/2}$,
normalize function $g(E)$ such that $g(E_0) = 1$, reset histogram H(E)=0
and with proceed the process …

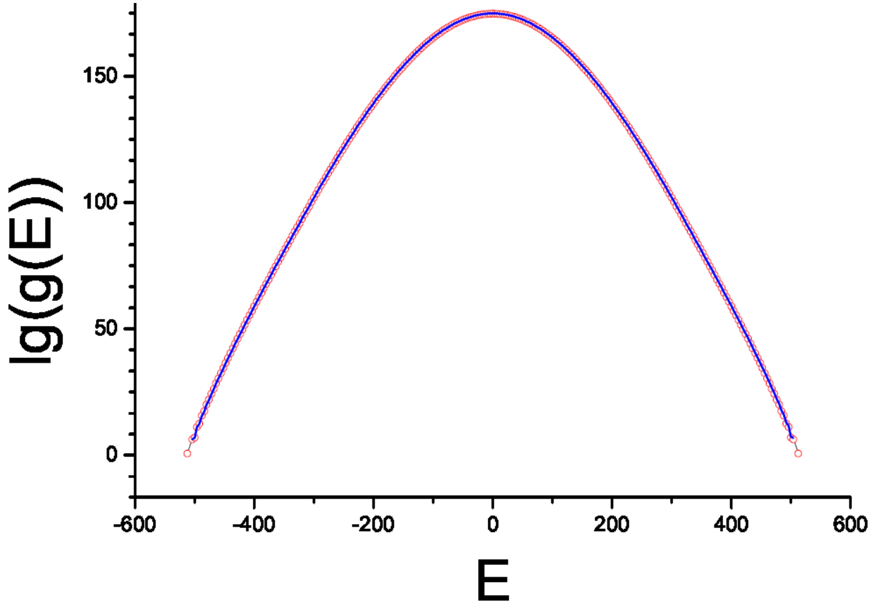
The algorithm may be stopped with some small value of f close enough to unity,
f.e. $\log f = 10^{-9}$

DoS of Ising model

$$Z = e^{2nmK} \sum_{k=0}^{nm} g_k x^{2k}$$

Exact - Beale, PRL 76 (1996) 78

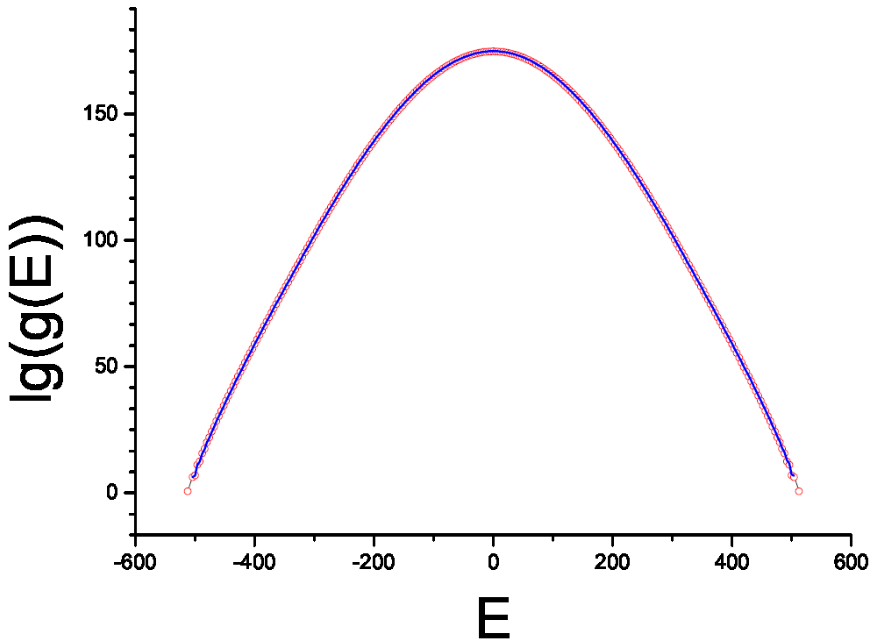
where $K = J/k_B T$, $x = e^{-2K}$, and g_k is the number of configurations with energy $4kJ$ above the ground state.



DoS *g(E) for Ising model 16x16. Circles - exact, line* - Wang-Landau sampling.

DoS of Ising model

$$Z = e^{2nmK} \sum_{k=0}^{nm} g_k x^{2k}$$



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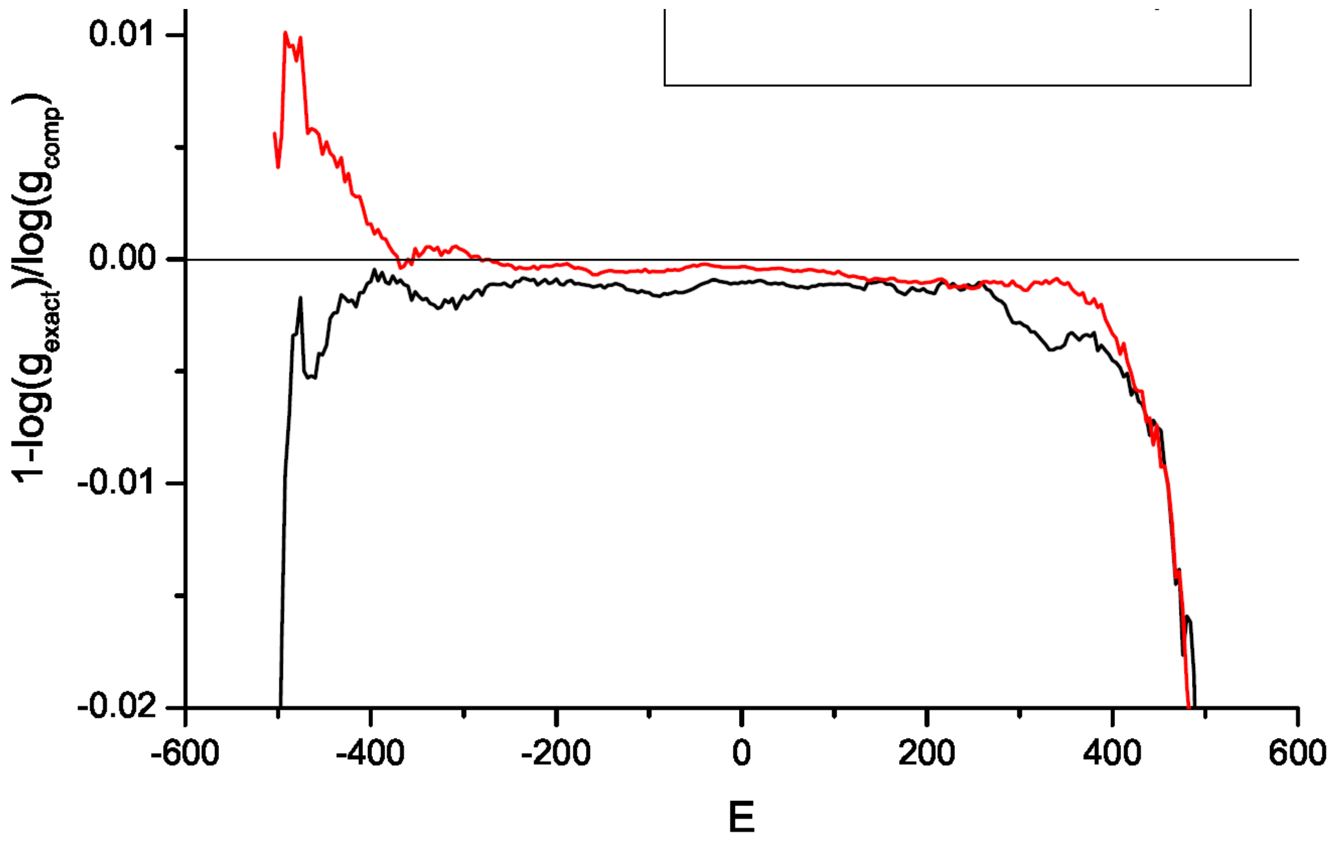
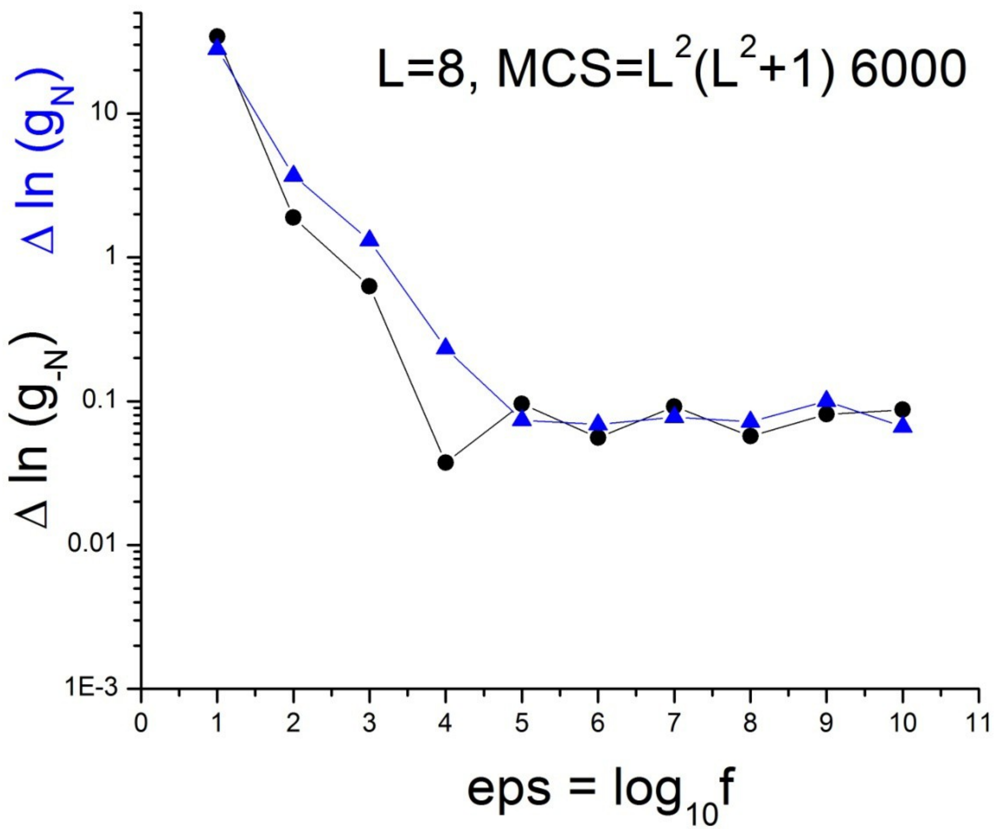
DoS of Ising model



DoS of Ising model



Transition matrix

Transition from level energy E_k to level energy $E_{k'}$

Count the number of transitions (k,k’). Build Matrix of that number M(k,k’).

The sum over the rows is the same in the large limit of events.
I.e. it is the Markov process in the energy space.

Result: instead of checking the flatness of the histogram, one has to check variation of the sum on the rows.

Stability of DoS

Exact DoS is not stable with respect of f-process

f-process drives DoS out of the exact solutions

f-process drives DoS to a little bit different limiting distribution

Parallelization

- Divide energy space on a number of intervals
- Perform F-process within each interval (accept only jumps within the interval) up to the flattness creterium
- Combine spectrum, decrease f
- - large errors at the edges
- solution – make intervals overlaps up to the middled and “combine” histogram, decrease f
- “Good” scalability
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Wang-Landau sampling method

Discussion and Conclusion:

- Wang-Landau method is less effective for large systems
  in comparison with MUCA
- Wang-Landau sampling method is a random walk in the configuration space and the Markov process in the energy space.
- What is the right algorithm with respect of the f-function? –
  ? the one which drives the system to the true DoS?
- Parallelization:
  + scalability is better for large systems
- - does not work properly for “complicated” systems
- + good for 1-st order phase transition