On the uniform sampling of ground states in the 2D $\pm J$ Ising spin glass model

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Outline

1. **Introduction**
   - Ising spin glass
   - Properties
2. **The Algorithm**
   - Basic idea
   - Determining the cluster configuration
   - Sampling ground states
3. **Results**
4. **Summary**

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ISG: EA model

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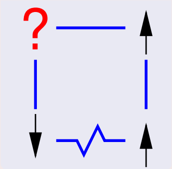
Edwards-Anderson model

The Hamiltonian in this model is given by:

$$\mathcal{H} = -\sum_{<i,j>} J_{ij} s_i s_j, \qquad \rightsquigarrow \text{frustration}$$



where $s_i = \uparrow\downarrow$, and the J_{ij} are randomly chosen from either a **Gaussian** or **bimodal ($\pm J$)** distribution (quenched disorder).

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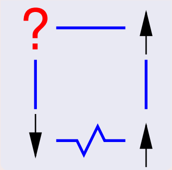

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Properties

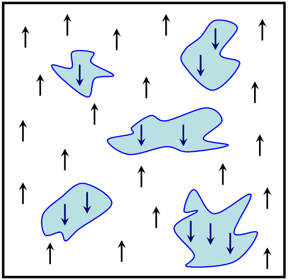
- Non-universality of coupling distribution.
- In $d = 2$, spin glass phase exists only at $T = 0$.

Ground state

In $d = 2$ exact ground state can be found in polynomial time by mapping to a minimum-weight perfect matching problem (MWPM).

The energy of the system can be written as:

$$\begin{aligned} E &= -\sum_{<i,j>} J_{ij} s_i s_j \\ &= -\sum_{s_i \parallel s_j} J_{ij} + \sum_{s_i \nparallel s_j} J_{ij} \\ &= -\sum_{s_i \parallel s_j} J_{ij} + \sum_{s_i \nparallel s_j} J_{ij} + \sum_{s_i \nparallel s_j} J_{ij} - \sum_{s_i \nparallel s_j} J_{ij} \\ &= -\sum_{<i,j>} J_{ij} + 2 \sum_{s_i \nparallel s_j} J_{ij} \end{aligned}$$



MWPM finds some loops such that the last term becomes minimum. Therefore it is able to calculate ground state ***energy*** as well as ground state ***spin configuration***.

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Defect energy

Ground state energy differences between systems with periodic and anti-periodic boundary conditions scale as

$$\Delta E(L) = |E_P - E_{AP}| \sim L^{\theta}.$$

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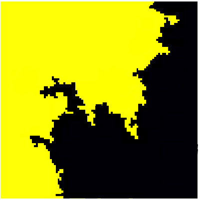
Domain wall

Comparing the ground state spin configuration of systems with periodic and anti-periodic boundary conditions leads to a domain wall. Domain wall lengths scale as $l_{\mathrm{DW}}(L) \sim L^{d_f}$, where d_f is known as *fractal dimension.*



Fractal dimension

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In order to have good statistics, we need to either

- consider **all** of the ground states (not possible except for very small system sizes)
- pick up some of the ground states, but **uniformly** (sufficient for practical purposes)

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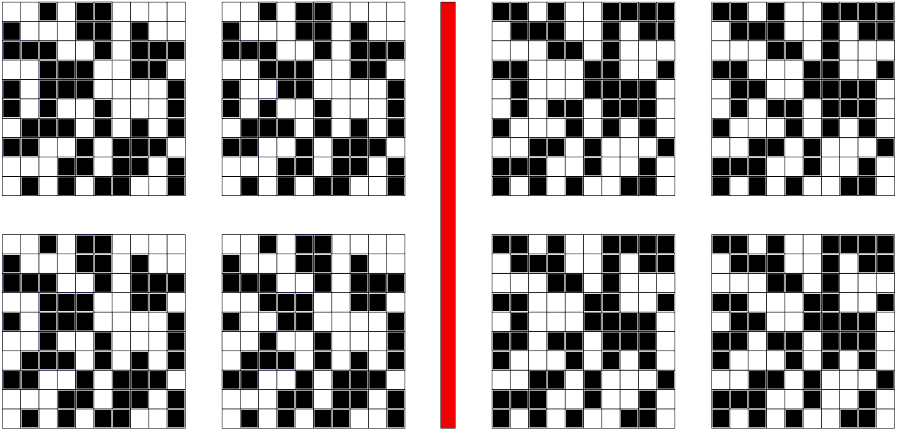
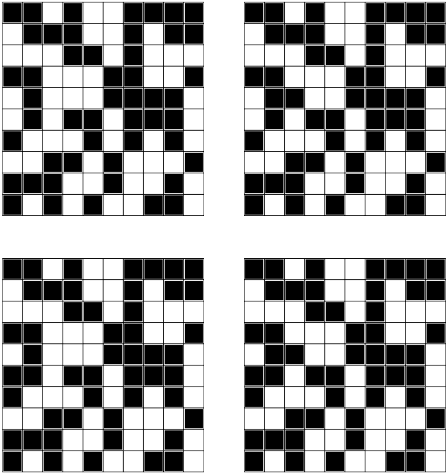
Example

Consider an example bond configuration with $N_{\mathrm{GS}} = 8$ ground states:



Example

We remove the global degeneracy and compare the remaining ground states:



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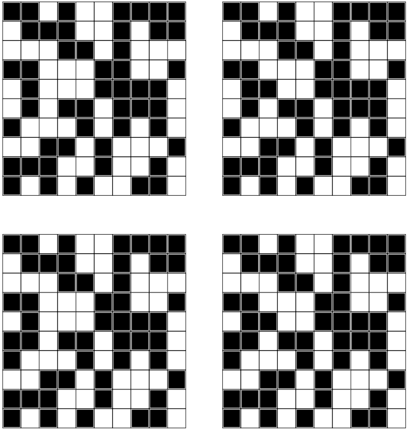

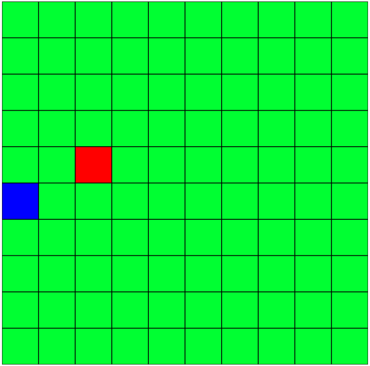

“cluster configuration”

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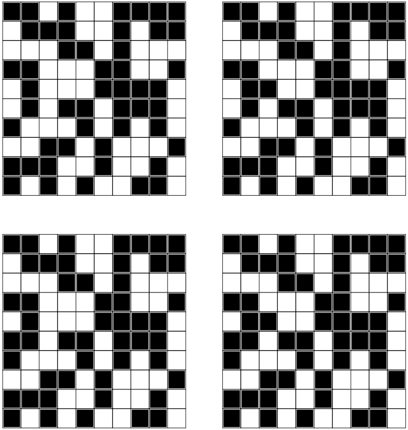
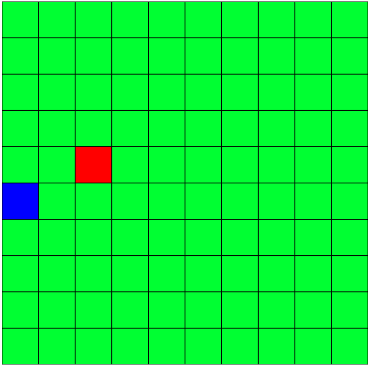




"cluster configuration"

If we know the **cluster configuration** and **one** of the spin configurations, we can generate **all** of the ground states!

Example

Question:

Do we need to know all of the ground states for determining the cluster configuration?

- answer:

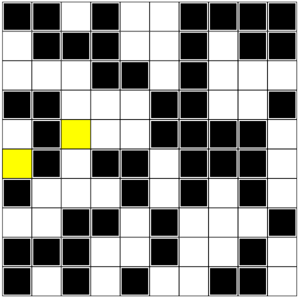
Example

Question:

Do we need to know all of the ground states for determining the cluster configuration?

- answer: NO!

if we consider only one ground state spin configuration and try to flip all of the spins one by one and check whether the energy changes or not, we are able to detect such clusters directly from even one ground state.



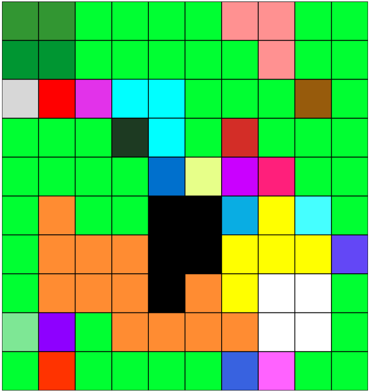
Free spins

Clusters of size one are usually called *free spins* because they are free to be either *up* (+1) or *down* (-1) in the ground state spin configuration.

Example

A general example

In the general case, we need N_{iGS} initial ground states, the system has both clusters of size one (free spins) and bigger than one. In addition, not all of the clusters are independent.



- $L = 10$
- $N_{\mathrm{GS}} = 2104568$
- $N_{\mathrm{iGS}} = 17$
- $N_{\mathrm{c}} = 28$

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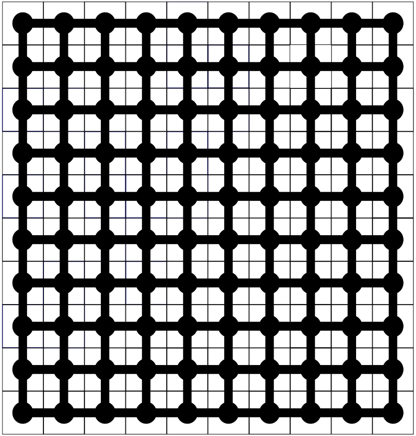
Replica

From now on, we consider a *replica* of the system. At the beginning all the nodes of the replica are connected to their nearest neighbours.



Steps

Our algorithm is based on 4 major steps:

- generating initial ground states
- determining free spins
- finding the flexible bonds
- cluster decomposition

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Generating initial ground states

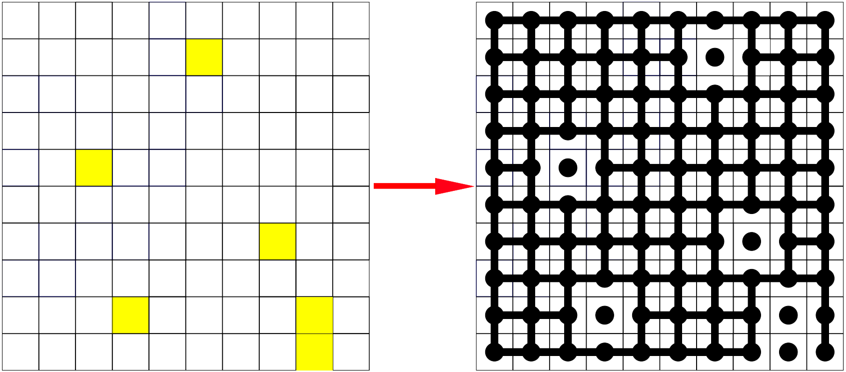
We use a technique based on MWPM and Gaussian noise:

- for a system with the set $\{J_{ij}\}$ of bonds, calculate $E_{\rm GS}$ and $\{S_{\rm GS}\}$
- add some infinitesimal Gaussian noise to each bond $J'_{ij} = J_{ij} + g_{ij}$
- calculate $\{S'_{GS}\}$ of the system with bonds $\{J'_{ij}\}$
- calculate the energy of the system with bonds $\{J_{ij}\}$ in respect to $\{S'\}$ i.e. E_{new}
- if $E_{\rm new} = E_{\rm GS}$, then $\{S'\}$ is a ground state spin configuration of the original system

Determining free spins

Finding free spins

For each initial ground state, we check all of the spins one by one to find *free spins*. As soon as we find a free spins, we disconnect it from its neighbour on the replica.

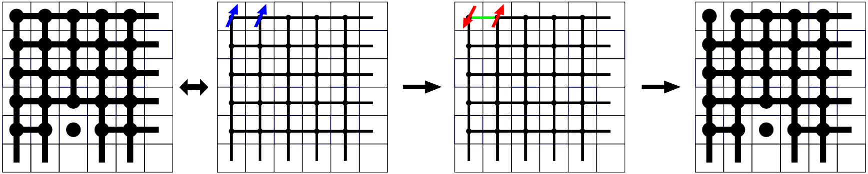


Finding the flexible bonds

Consider one ground state spin configuration and for each of the still existing bonds J_{ij} on the replica, we

- Flip s_i.
- Freeze the orientation of s_i and s_j.
- Calculate the new energy of the system using MWPM with the above constraint.
- If the new energy is the same as the ground state energy, J_{ij} is flexible. Therefore i and j on the replica will be disconnected.

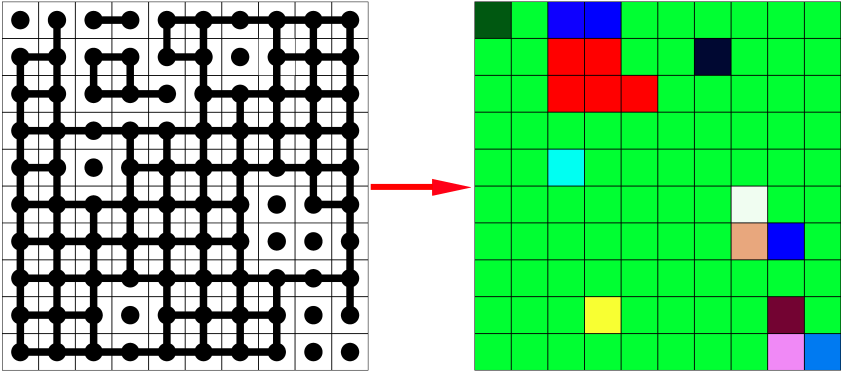
Note: This is an ***exact*** method to determine the flexible bonds.



Cluster decomposition

Calculate the cluster configuration

Now we can determine the cluster configuration from the replica by using one of the well known methods such as Hoshen-Kopelman's algorithm, breadth-first or depth-first search, etc.



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Advantage

- It is very fast.
- It generates the accessible ground states uniformly.

Disadvantage

- It is restricted to only one ground state valley.

second idea: Monte Carlo

- Consider a random cluster configuration.
- Consider a low enough temperature T.
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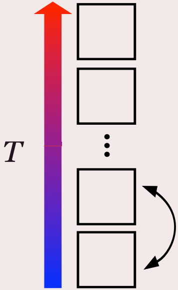
Disadvantage

- It is not able to over come the large energy barrier between different ground states valleys.
- It is not able to generate all of the ground states.

third idea: Parallel Tempering Monte Carlo

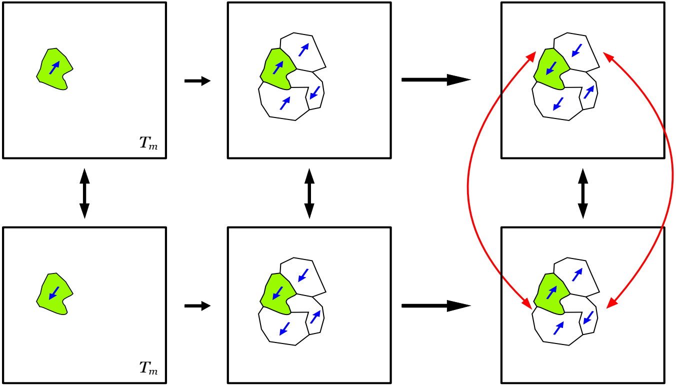
- Consider M copies of the system at different temperatures between $T_{\min}$ and $T_{\max}$ with random cluster configurations.
- For each copy, choose a cluster at random and flip it with probability $p = \min(1, e^{-\beta\Delta E})$ in which $\beta = 1/T$.
- For all pairs of the two neighbouring temperatures:
    - $\delta = (\beta_{m+1} - \beta_m)(E_m - E_{m+1})$.
    - If $\delta \leq 0$ we swap the temperatures $\beta_{m+1} \leftrightarrow \beta_m$.
    - If $\delta > 0$ we swap the temperatures by the probability $p = e^{-\delta}$.



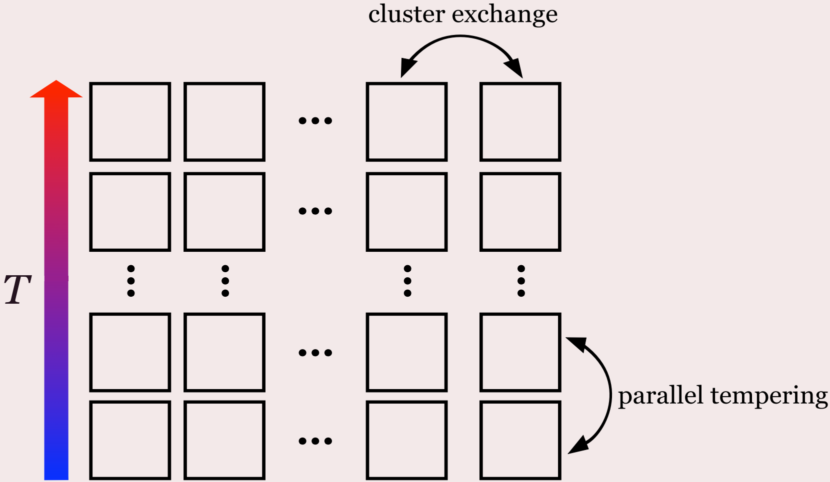
- Repeat everything until the system reaches the equilibrium.

An extra move: cluster exchange

- Consider N copies of the system at each temperature.
- Choose two configurations at the same T and one cluster randomly.
- If the cluster has different orientation in the configurations, exchange the domain of flipped clusters in both configurations.



Parallel tempering Monte Carlo with cluster exchange



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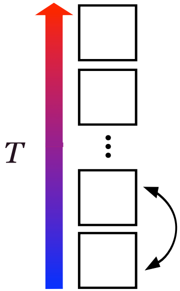
Number of copies per temperature N

- Increasing N will increase computational effort
- The minimum possible value $N_{min} = 2$ $\rightsquigarrow$ $N = 4$

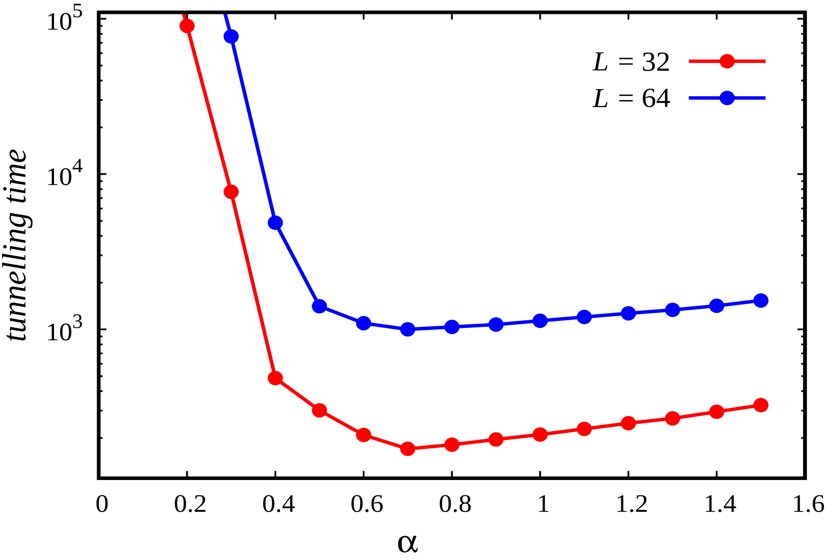
Parameters:

Number of temperatures M

- Increasing M will increase computational effort
- It should be large enough to have reasonable acceptance rate for low temperatures
- It should be small enough to have reasonable *tunnelling time*
  - The time (in MC steps) it takes for a copy of the system to go from T_{min} to T_{max} and comes back to T_{min} again.
- It depends on the system size $L \quad \rightsquigarrow \quad M = \alpha L$



Parameters: M



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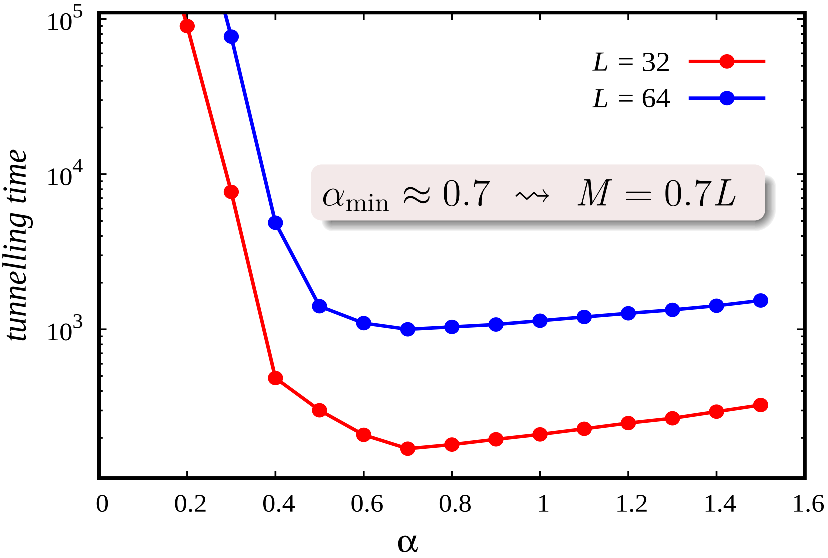
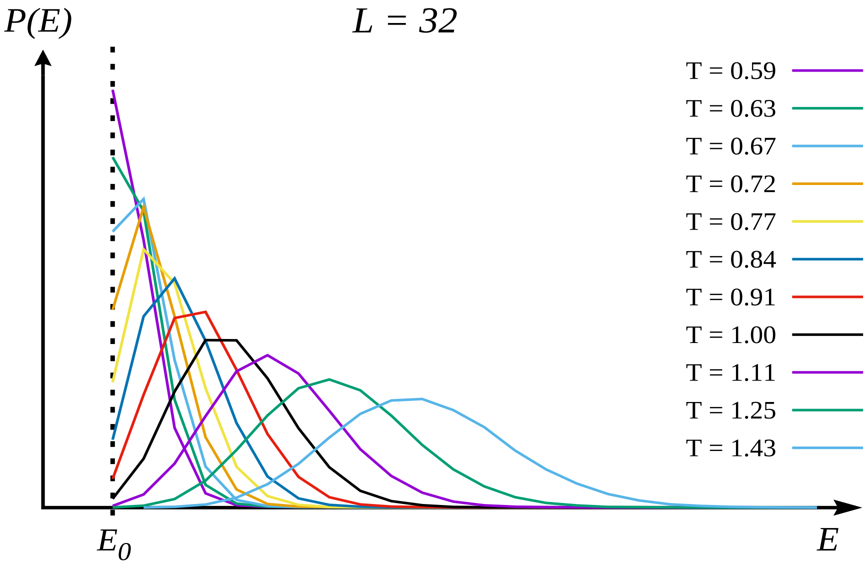


Parameters: T_{min}



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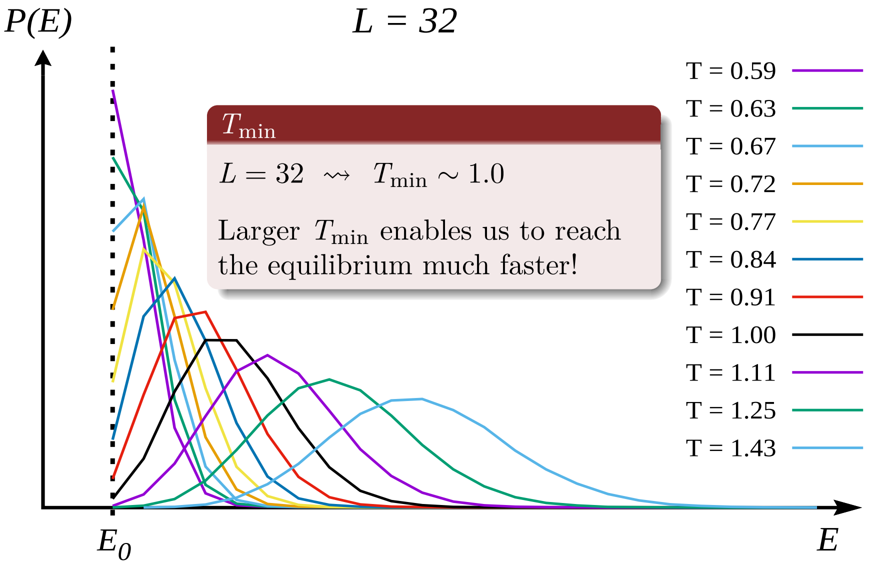
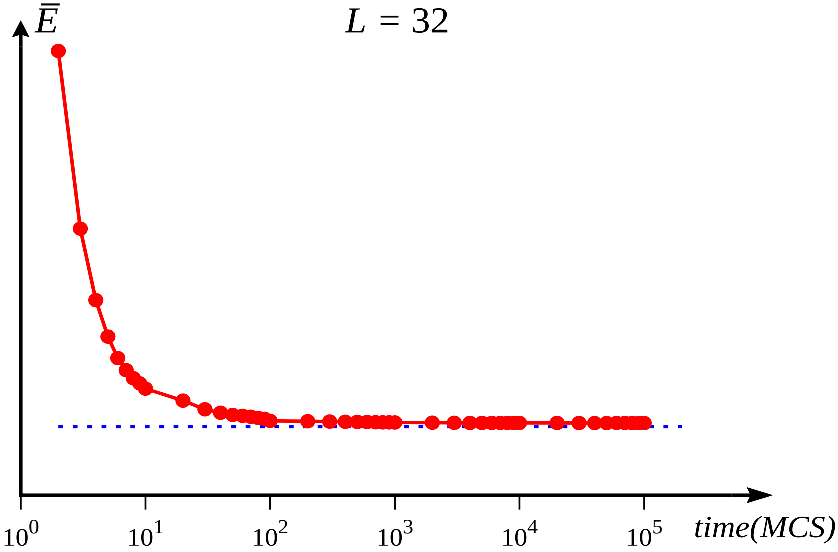
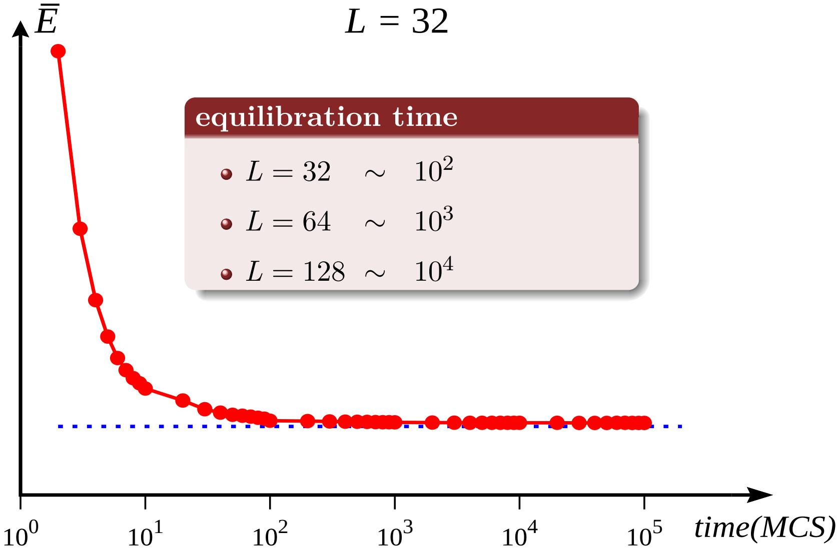


T_{min}

$L = 32 \quad \rightsquigarrow \quad T_{\text{min}} \sim 1.0$

Larger T_{min} enables us to reach the equilibrium much faster!


$\bar{E}$
$L = 32$
10^0
10^1
10^2
10^3
10^4
10^5
time(MCS)



equilibration time

- $L = 32 \quad \sim \quad 10^2$
- $L = 64 \quad \sim \quad 10^3$
- $L = 128 \quad \sim \quad 10^4$

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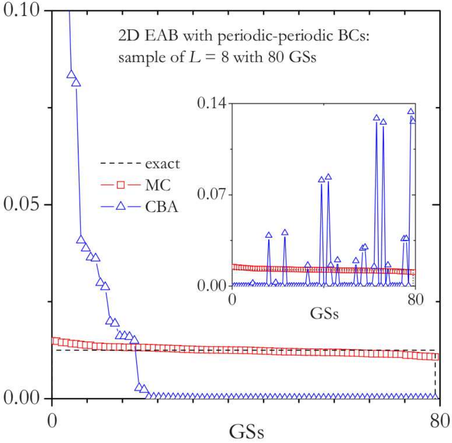
In the past...

Risau-Gusman *et al.* [Phys. Rev. B 77, 134435 (2008)]

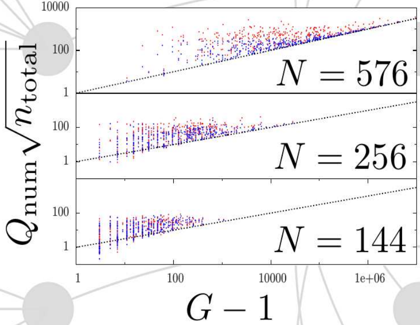


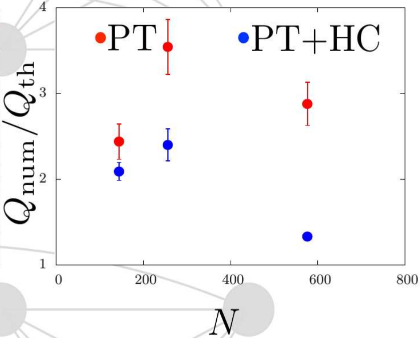
Results

Recently...

Zheng Zhu *et al.* [arXiv:1501.05630v2]

fluctuations: $Q_{\text{th}} = \sqrt{\frac{G-1}{n_{\text{total}}}}$ vs. $Q_{\text{num}} = \frac{\sigma(n)}{e(n)}$





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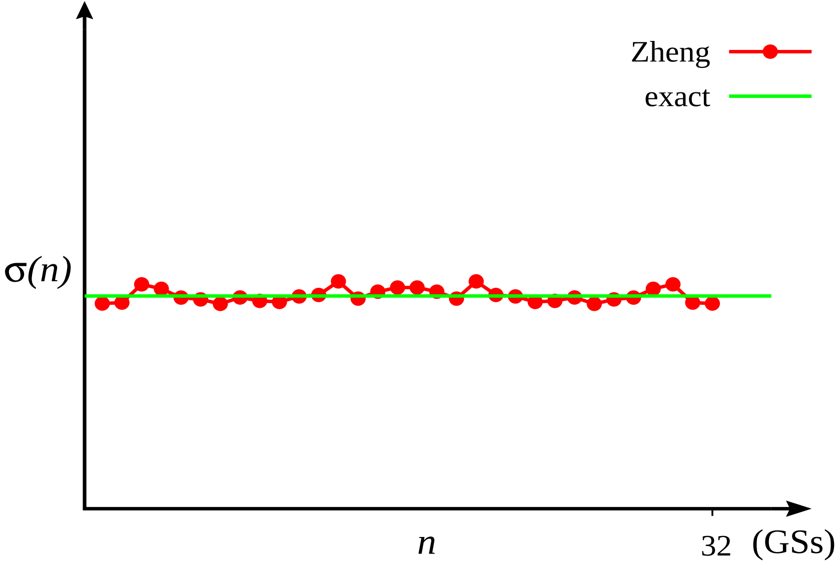

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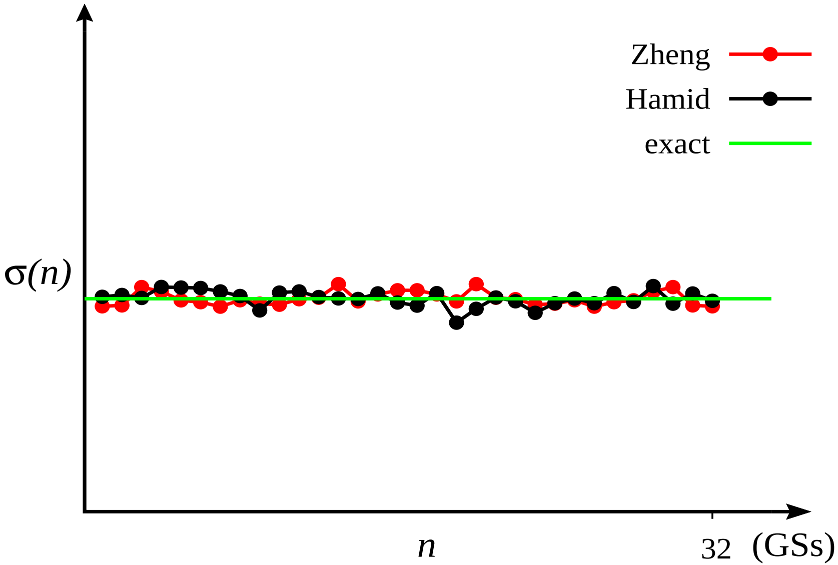

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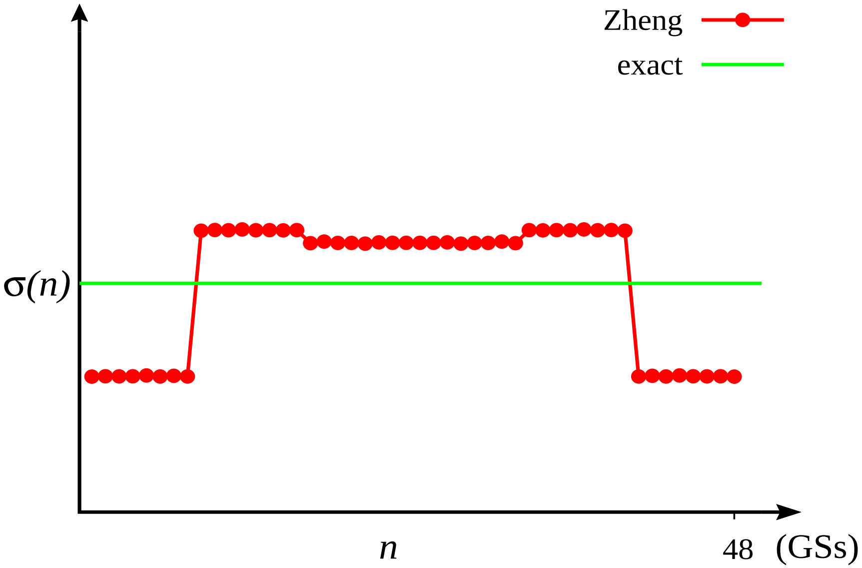

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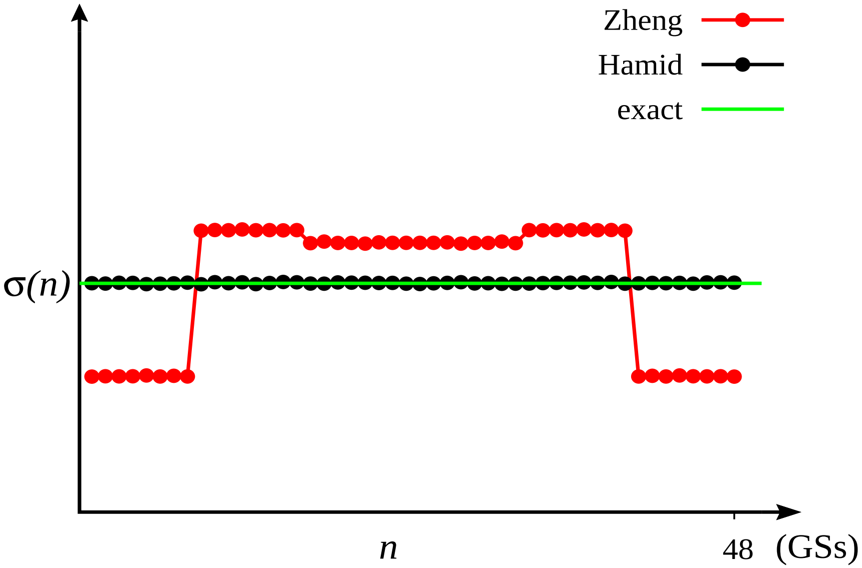

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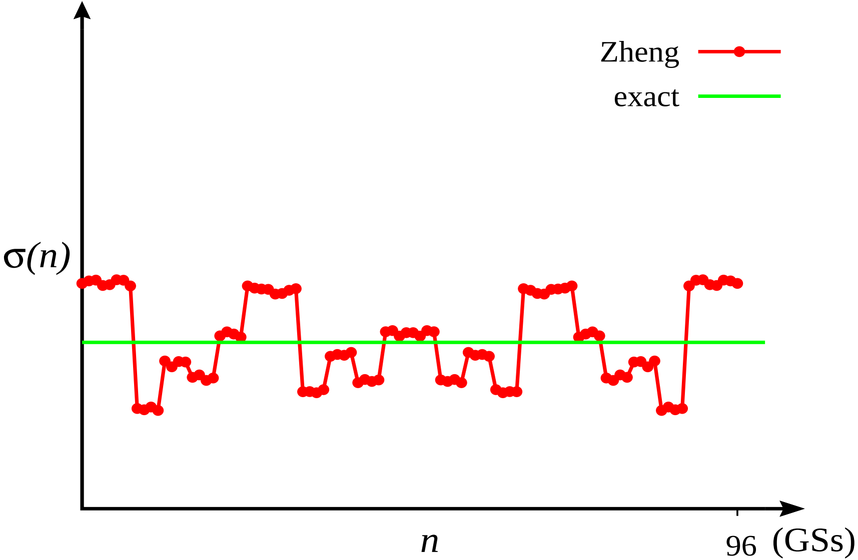

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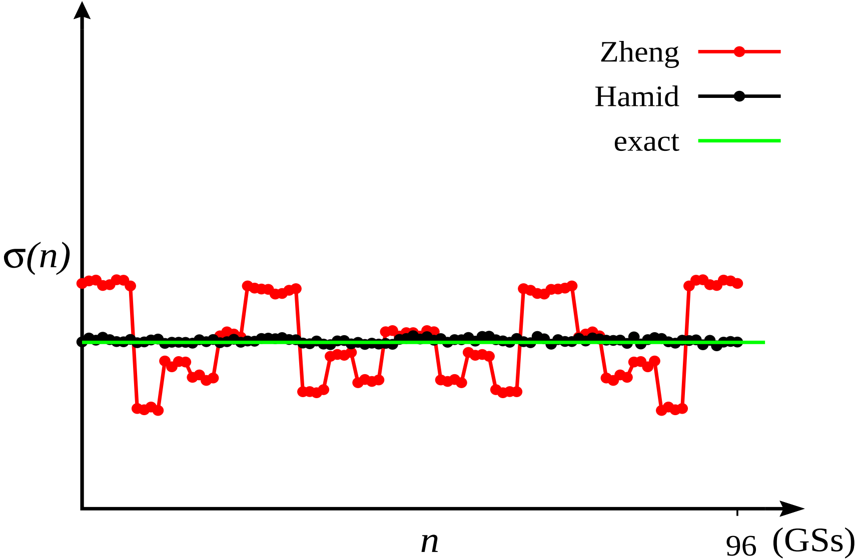
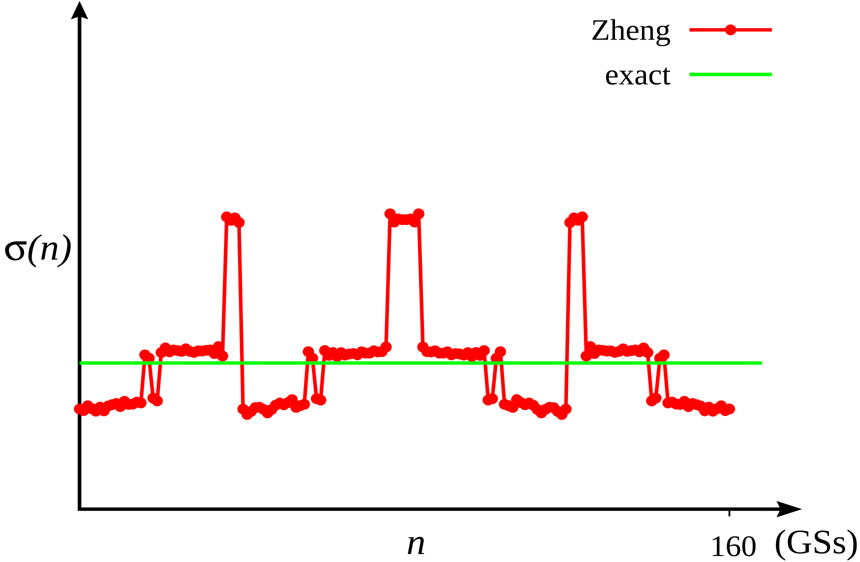
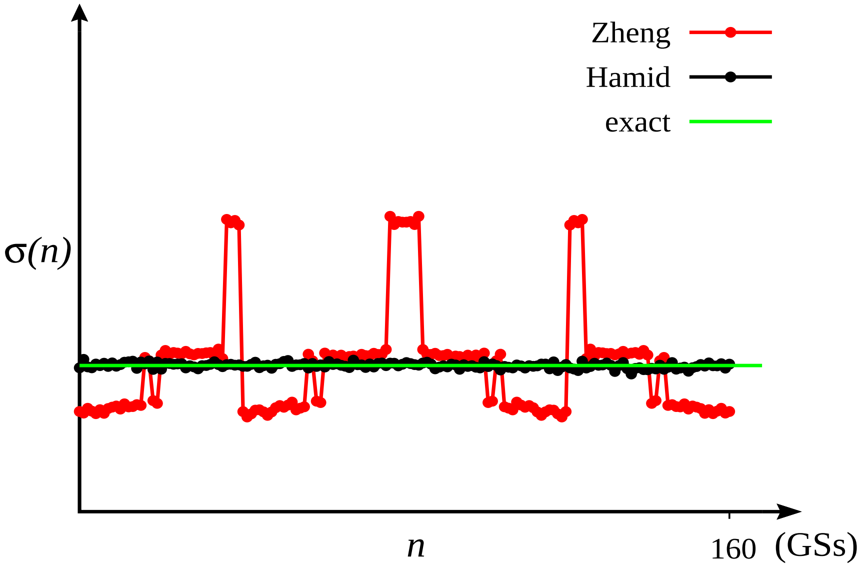


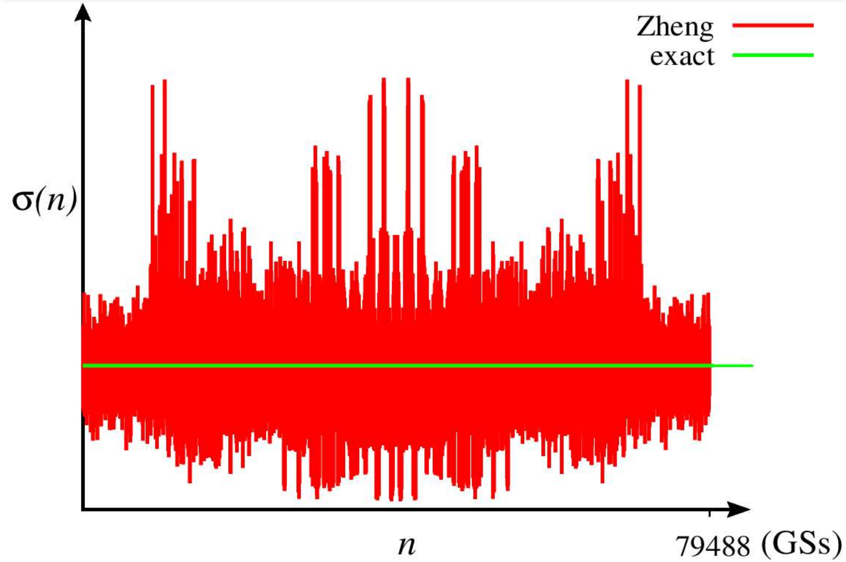
Results



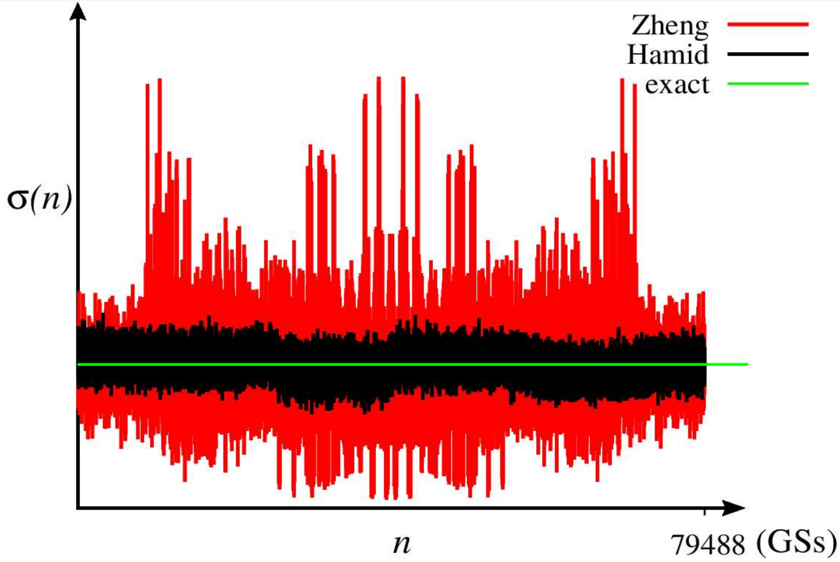
Results



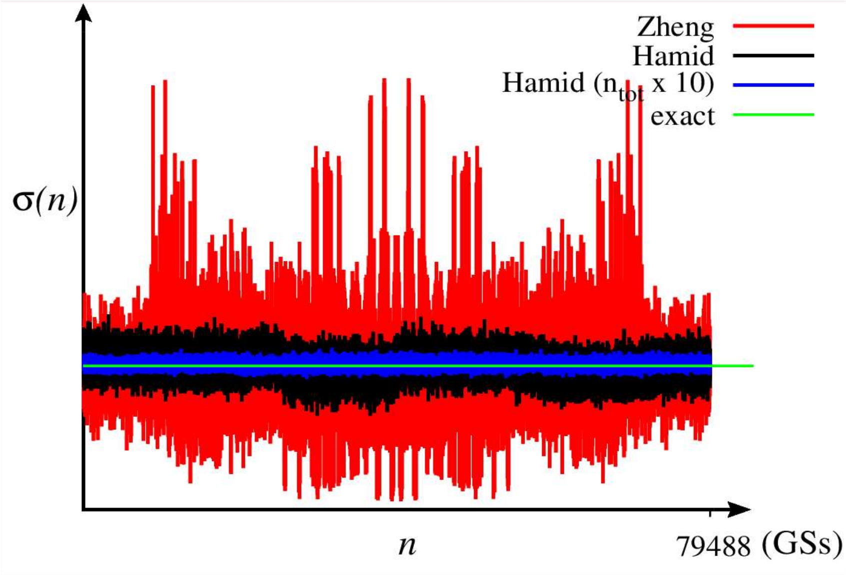
Results



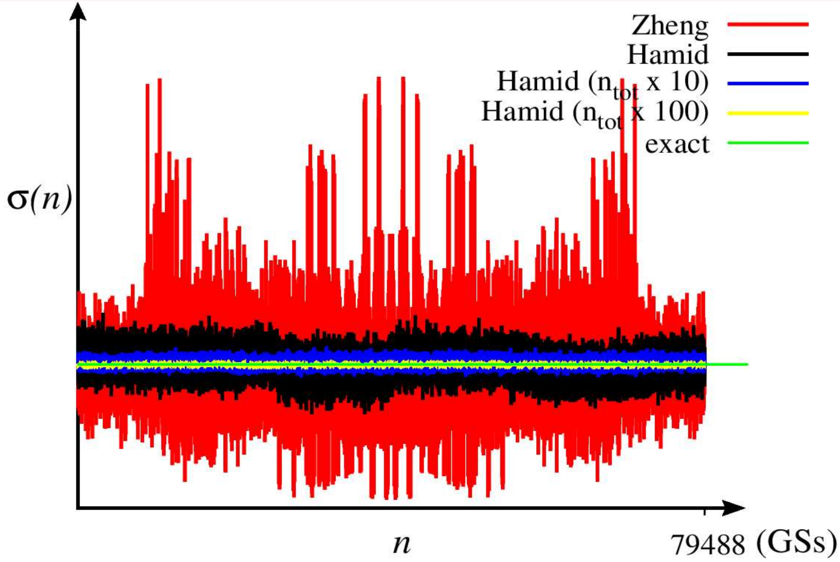
Results



Results



Results


Zheng
Hamid
Hamid (n_tot x 10)
Hamid (n_tot x 100)
exact
σ(n)
n
79488 (GSs)

Outline

1. **Introduction**
   - Ising spin glass
   - Properties
2. **The Algorithm**
   - Basic idea
   - Determining the cluster configuration
   - Sampling ground states
3. **Results**
4. **Summary**

Summary

- The $2D \pm J$ Ising spin glass system has been considered.
- Minimum perfect matching (MWPM) + Gaussian noise technique enables us to find degenerate ground state spin configurations.
- By comparing some of the ground state spin configurations, we can find the cluster configuration of the system.
- A combination of Parallel Monte Carlo algorithm and replica exchange cluster procedure results in an algorithm which generates ground states uniformly.
- Our algorithm enables us to have uniform sampling of the ground states up to system size $L = 156$.

Thank you for your attention

Distribution of the clusters