Worm algorithm for the 6-vertex model

João F. Bravo

Computational Many-Body Physics

Prof. Michael Knap

Prof. Frank Pollmann

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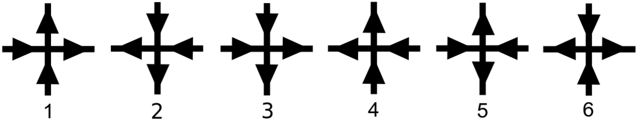
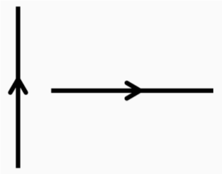
6-vertex model

- Model for crystal lattices with coordination number 4 & hydrogen bonds.
- Square lattice with periodic boundary conditions
  $\Longrightarrow$ **translational & rotational invariance**.
- **Ice rule**: satisfy two-in/two-out constraint at each vertex
  $\Longrightarrow$ vertices have zero charge $q = 1/2 \sum_i s_i$.
- **Ice model**: all allowed configurations are equally likely ($T = \infty$).

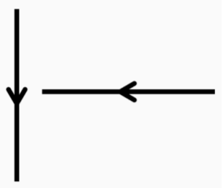


- Important to model real crystals with hydrogen bonds, such as:
  - **water ice** (oxygen: vertices, hydrogen bonds: edges);
  - **ferroelectric** & **antiferroelectric** crystals.

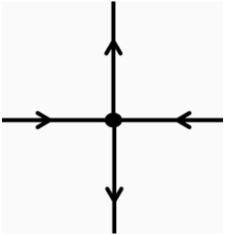
Bond-value choices



$s_{up} = s_{right} = 1$



$s_{down} = s_{left} = -1$



Relative to each vertex:

- $s_{in} = 1$
- $s_{out} = -1$

Worm algorithm

Single-spin flip updates break the 6-vertex model constraints!

Worm algorithm:

1. Start from stable configuration;
2. Flip 1 bond arrow $\implies$ create 2 defects;
3. Propagate 1 defect randomly until the two meet & annihilate:
   3.1 Randomly flip one of the vertex's other arrows, subject to **ice rule**;
   3.2 Repeat for vertex connected by chosen bond;
   3.3 Stop when next vertex is the other initial defect
   $\implies$ new stable configuration.
4. Measure (back to *1.*).

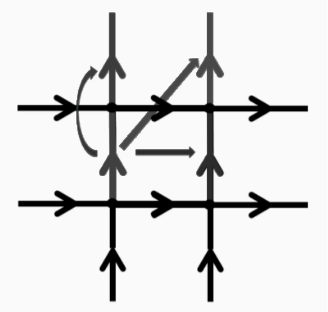
Simulation steps

1. Start from stable configuration;
2. Thermalize system;
3. Run worm N times & measure all spin correlations $\langle s_0 s_r \rangle$ after each time;
4. Average correlations with *binning analysis*, considering translational & rotational invariance to reduce errors;
5. Fit & plot results.

Remarks:

- Partial loop *(worm)* performs random walk on lattice $\implies$ **global updates** $\implies$ **short autocorrelation times** expected $\implies$ measuring after each update should only decrease variances slightly.
- **Binning analysis**: N measures $\rightarrow$ C_i bins with average of N_i measures $\rightarrow$ compute std. dev. of those averages $\implies$ errors: $\sigma_{C_i} / \sqrt{\# C_i}$.
- **Autocorrelation time** τ factor in error can be neglected since $N_i >> \tau$ $\implies$ bins become uncorrelated.

Spin correlations with distance



8 types:

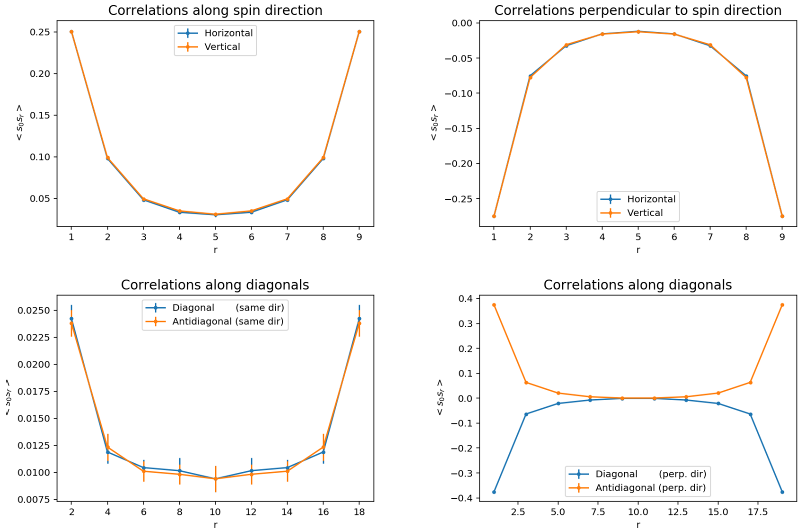
- For horizontal spins:
  - $\boldsymbol{H_1}$: Along spin direction;
  - $\boldsymbol{H_2}$: Perpendicular to spin direction.
- For vertical spins: same $\boldsymbol{V_1}$ & $\boldsymbol{V_2}$;
- Diagonal correlations:
  - $\boldsymbol{D_1}$: Same-direction spins;
  - $\boldsymbol{D_2}$: Perpendicular-direction spins.
- Antidiagonal correlations: same $\boldsymbol{A_1}$ & $\boldsymbol{A_2}$.

Considerations:

- **Rotational invariance**: can average $\boldsymbol{H_i} + \boldsymbol{V_i}$ & $\boldsymbol{D_i} + \boldsymbol{A_i}$.
- **Translational invariance**: for each type, can translate origin along lattice & average all those measures.
- Power-law behaviour expected: $\boxed{\langle s_0 s_r \rangle \propto 1/r^a}$
- Should decrease until $L//2$ & increase until L.

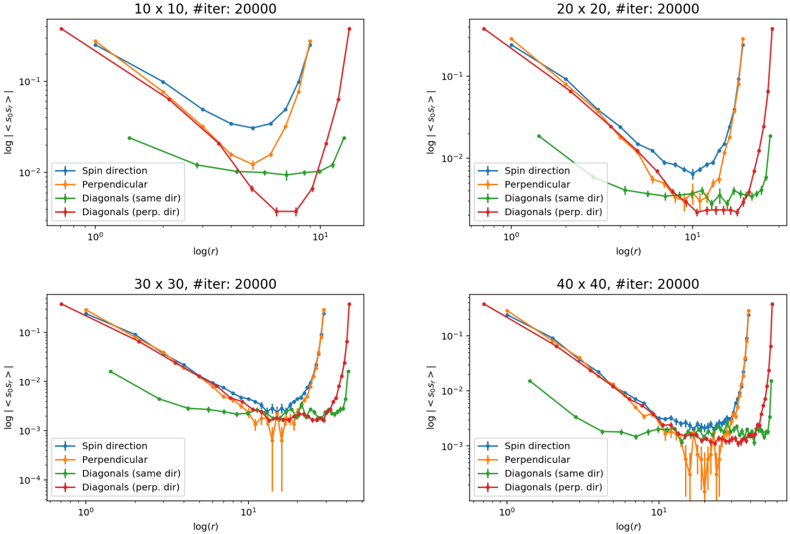
Testing rotational invariance

Lattice size: 10x10, #iter: 20000



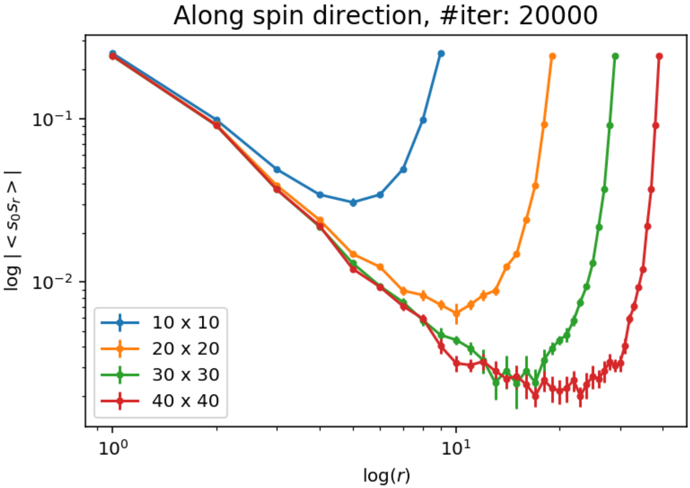
- Turning point at $L//2$ as expected.

Increasing system size L



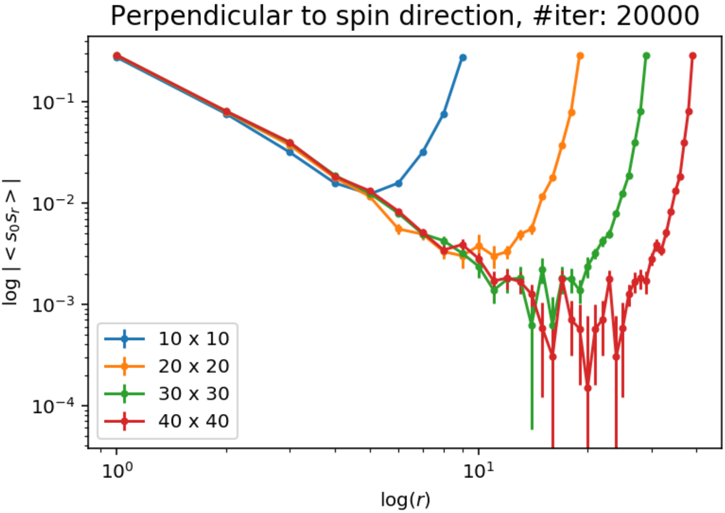
- Along spin direction: decay the slowest relative to L.
- Along diagonals with same-direction spins: 1 order of magnitude weaker.
- Behaviour of other 3 more similar with increasing L.

Correlations along the spin direction



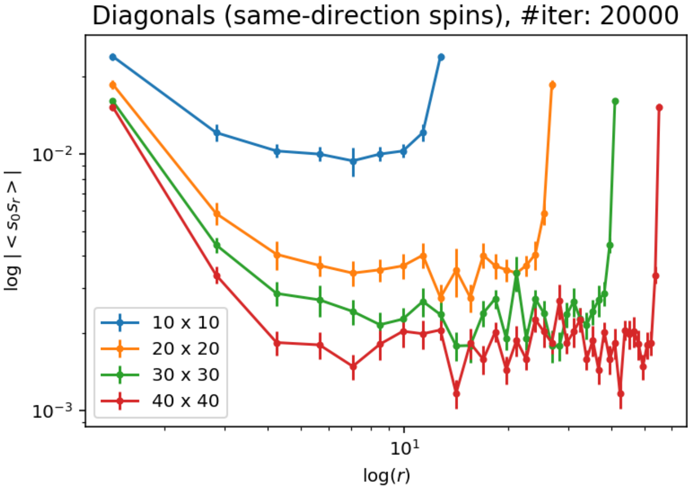
- Turning point: scales linearly with L.
- Short-range correlations: independent of L.
- Decay: increases slightly with small L. Independent of L for large L.

Correlations perpendicular to the spin direction



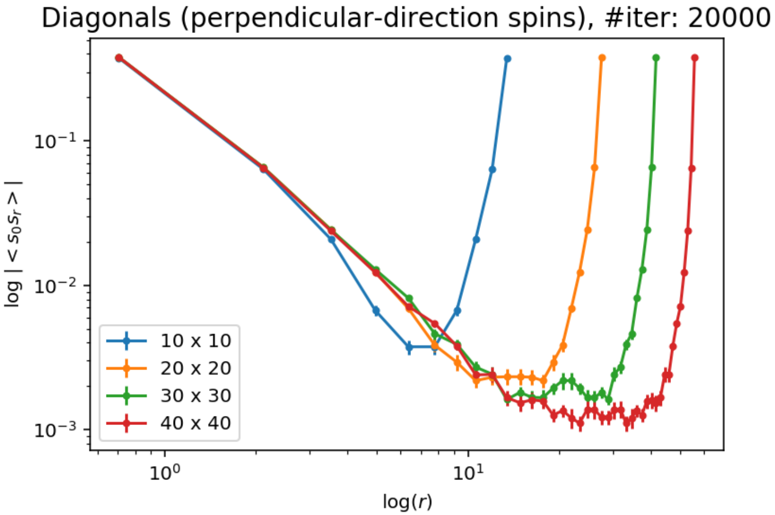
- Short-range correlations: independent of L.
- Decay: seems independent of L.

Correlations along diagonals



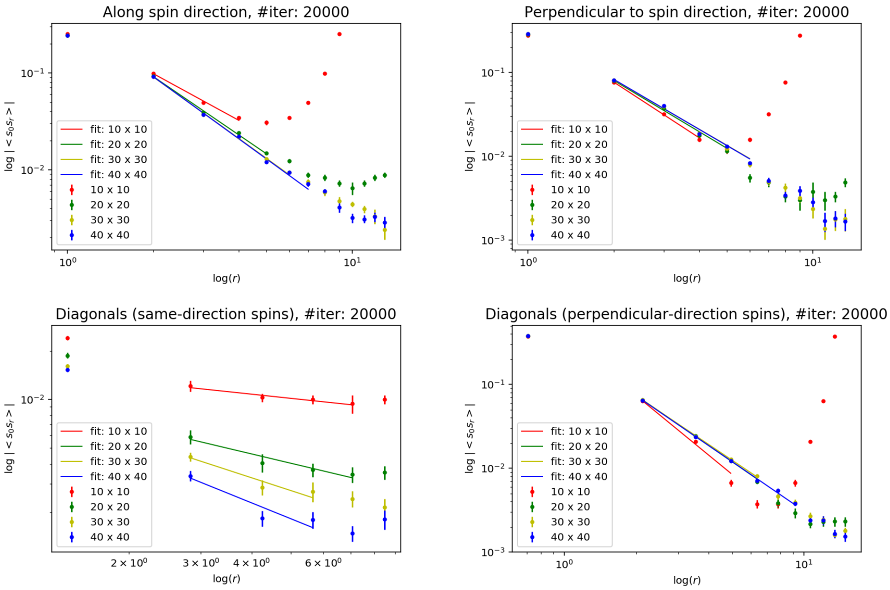
- Short-range correlations: smaller with increasing small L. Seem independent of L for large L.
- Decay: increases with small L. Probably independent of L for large L.

Correlations along diagonals



- Short-range correlations: independent of L.
- Decay: increases with small L. Independent of L for large L.

Fitting in log *vs.* log



Fitting in log *vs.* log

$$\boxed{\langle s_0 s_r \rangle \propto \frac{1}{r^a}} \quad \Longrightarrow \quad \log \left| \langle s_0 s_r \rangle \right| = -a \cdot \log r + b$$

	Along spin dir		Perp. to spin dir	
L	a	b	a	b
10	1.60 $\pm$ 0.12	-1.21 $\pm$ 0.11	2.21 $\pm$ 0.06	-1.04 $\pm$ 0.05
20	2.00 $\pm$ 0.07	-1.01 $\pm$ 0.07	2.04 $\pm$ 0.11	-1.11 $\pm$ 0.09
30	2.11 $\pm$ 0.05	-0.94 $\pm$ 0.04	1.97 $\pm$ 0.10	-1.14 $\pm$ 0.10
40	2.13 $\pm$ 0.05	-0.92 $\pm$ 0.04	1.99 $\pm$ 0.11	-1.12 $\pm$ 0.11

	Diagonals (same dir)		Diagonals (perp. dir)	
L	a	b	a	b
10	0.27 $\pm$ 0.06	-4.16 $\pm$ 0.09	2.34 $\pm$ 0.24	-0.99 $\pm$ 0.20
20	0.60 $\pm$ 0.10	-4.55 $\pm$ 0.15	1.97 $\pm$ 0.04	-1.24 $\pm$ 0.03
30	0.82 $\pm$ 0.21	-4.58 $\pm$ 0.27	1.92 $\pm$ 0.02	-1.29 $\pm$ 0.02
40	1.02 $\pm$ 0.35	-4.67 $\pm$ 0.46	1.96 $\pm$ 0.02	-1.26 $\pm$ 0.02

- Correlations other than along diagonals with same-direction spins: approx. inverse-square-law decay for $L \neq 10$. Values closer for larger L as expected.
- Along diagonals with same-direction spins: Increasing decay with L. Cannot tell if decay converges for large L.

Conclusions

- **Translational invariance** holds for *PBC*.
- **Rotational invariance** holds for *PBC*, except along diagonals for spins with same direction.
- Nearby spins tend to be **aligned** along the direction they point in & **antialigned** perpendicular to it. Alignment of spins along a diagonal is less likely.
- Correlations along diagonals with same-direction spins decay faster with increasing system size.
- Correlations other than those:
  - follow **inverse-square-law** decay;
  - **short-range** independent of system size;
  - behaviour becomes more similar with increasing system size.

References

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L. Pauling, *The Structure and Entropy of Ice and of Other Crystals with Some Randomness of Atomic Arrangement*, Journal of the American Chemical Society 1935, vol.57, p.2680-2684

https://en.wikipedia.org/wiki/Vertex_model, July 2019

https://en.wikipedia.org/wiki/Ice-type_model, July 2019