

# Geometric Properties of the Ising model on Interacting Self-Avoiding Walks

## Models

We consider several models: the first one is Ising model on interacting self-avoiding walk (further called Ising-ISAW). Considering the case of lack of outer magnetic field in this work, the Hamiltonian of the model of fixed conformation  $u$  with length  $N$  and strength of nearest-neighbors interaction  $J$  reads:

$$H_{u,N,\{\sigma\}} = - \sum_{\langle i,j \rangle} J \sigma_i \sigma_j, \quad i, j \in u, |u| = N$$

The summation runs through spins involved in conformation and only with the nearest neighbors. We also consider the parental model of interacting self-avoiding walk (further called ISAW), where all spins are equal 1.

Rules of being “the nearest neighbor” for monomers are defined by the used lattice. For example, a monomer on the square lattice has 4 potential nearest neighbors: on the left, right, front and back from the monomer, while on the triangle lattice two additional diagonal monomers are defined as nearest too.

## Methods

We define mean proportion of monomers with fixed number  $i$  of nearest neighbors  $\langle n_i \rangle$ , which is counted directly for every monomer in every simulated conformation of walk. As we are interested in comparing fraction in a range of spin-to-spin coupling strength  $J$ , we consider already learned critical values of  $J$  for both Ising-ISAW (left table) and ISAW (right table) models for several lattices. We suggest that  $kT = 1$ .

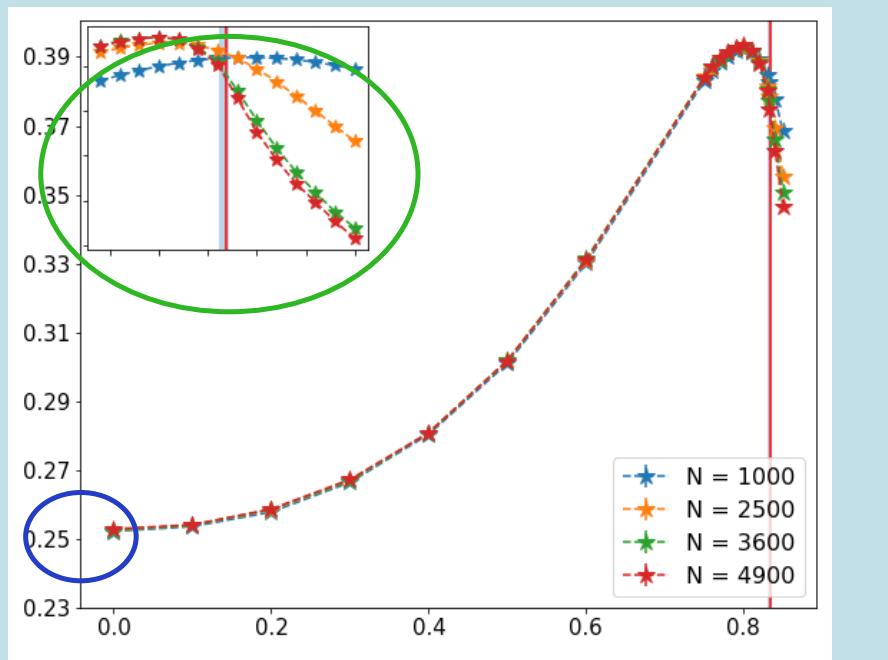
lattice	$J_c$
Square	0.8340(5) [1]
Cubic	$0.5263 \pm 0.055$ [2]

lattice	$J_c$
Square	0.6673(5) [3]
Cubic	$0.2779 \pm 0.0041$ [4]
Triangle	$0.405 \pm 0.07$ [5]

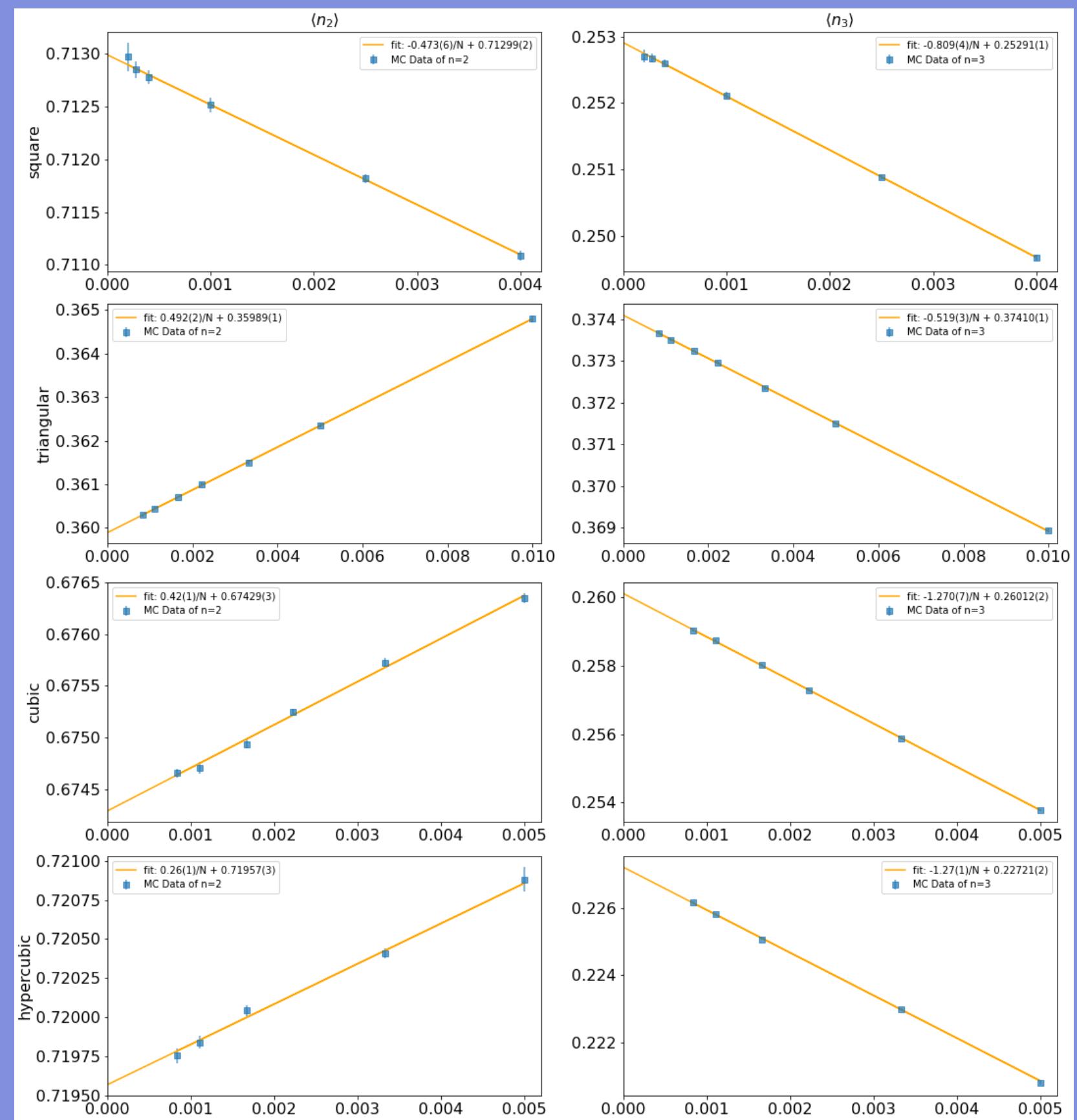
We performed Monte-Carlo simulations for studying the task of **annealed disorder**, where both shape of fixed length conformation (sequence of nodes on a lattice) and spin subsystem (values of spin on each node) changes on each step by Worm and Wolff algorithm respectively.

## Previous results - surface monomers

From work [1] it was established that in  $J=0$  mean fraction of “surface-like” monomers on Ising-ISAW conformation is **close to but numerically distinct from 0.25**. We performed same simulations of ISAW and Ising-ISAW models for triangular and cubic lattices with coordination number 6 to enumerate the distribution of monomers in a range of spin-spin coupling strength  $J$  with fixed number of neighbors 2-6. We also simulated the model on  $J=0$  for 2D-square, triangular, cubic and 4D-hypercubic lattices.



## Non-interacting limit of a simple SAW



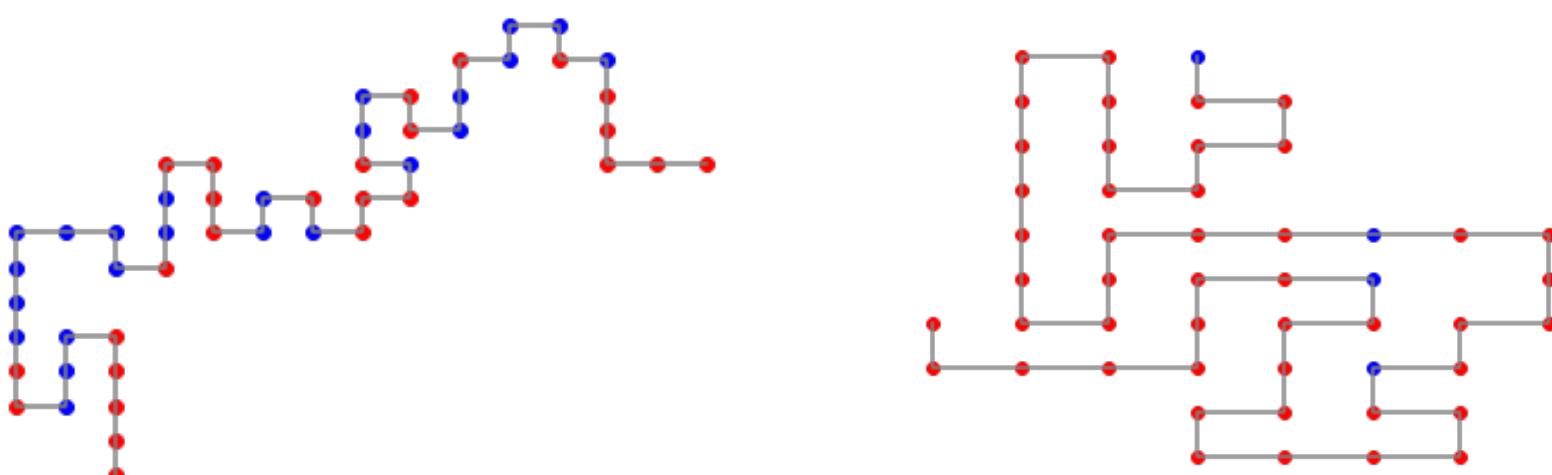
Lattice	$\langle n_2 \rangle$		$\langle n_3 \rangle$		k	$p^{(k)}$	i	$b(\langle n_i \rangle)$
Square	-0.473(6)	0.71299(2)	-0.809(4)	0.25291(1)	3	0.71114(3)	2	0.71299(2)
Triangular	0.492(2)	0.35989(1)	-0.519(3)	0.37410(1)	2	0.22500(2)	3	0.25291(1)
Cubic	0.42(1)	0.67429(3)	-1.270(7)	0.26012(3)	1	0.05476(1)	4	0.03410(1)
Hypocubic	0.26(1)	0.71957(3)	-1.27(1)	0.22721(2)	0	0.009096(4)	-	-

Figure shows results of Monte-Carlo simulations for mean fractions of monomers with 2 and 3 neighbors on a conformation of non-interacting SAW with length of  $N$  (monomers) as a function of  $1/N$ . As it seen, results, especially on triangular lattice, have strong linear approximation near 0, where length of the SAW-chain is close to infinite.

However, linear coefficients of approximation of the results for each lattice, which are presented on a left table, do not have any numerical similarities, except conformations of the triangular, cubic and hypercubic lattices have same signs of approximation coefficients. So, despite the unequal number of dimensions, the geometrical behaviour of conformations on a triangular lattice is more similar to ones on a lattice with same coordination number or higher.

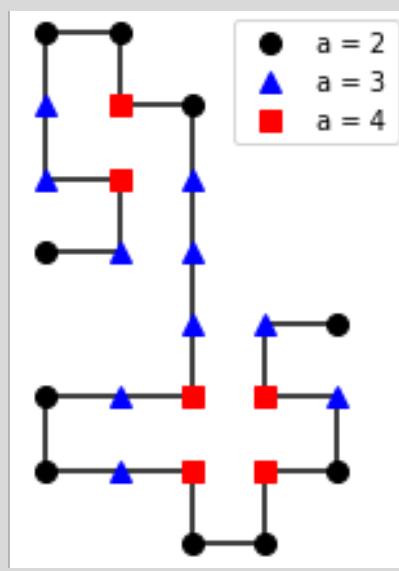
We also compared the constant terms of linear regression of Monte-Carlo results for square lattice with values of probability of a SAW with infinite length to have an atmosphere  $k$  (see right table [6]). Despite the fact that  $p^{(8)}$  and  $b(\langle n_2 \rangle)$  are quite close, all three pairs of constant are not equal within the scope of statistical errors, which means that these two concepts express different aspects of behaviour of model in case of infinite length.

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By adding interaction between nearest neighbors of monomers of the walk, we are allowed to study phase transition fixed between solvent conditions, so the given polymer in the thermal equilibrium become extended (the left example) in good-solvent conditions and collapsed (the right example) in poor-solvent one.

## Local coordination number and atmosphere of the walk



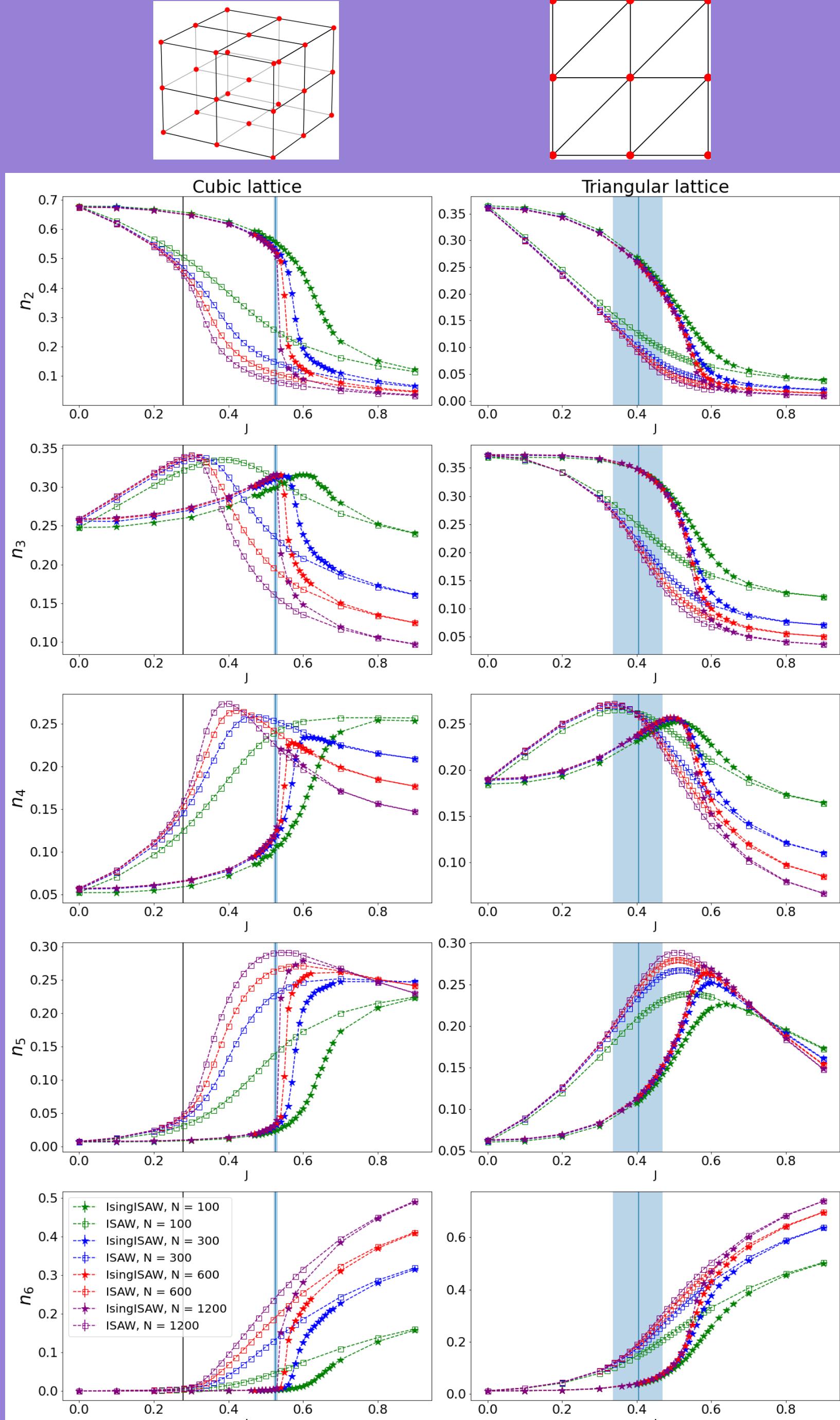
Example of SAW conformation with counted neighbors of each node.

- **one-dimensional chains** with monomers having only 2 neighbors (previous and the next ones in order of the walk)
- monomers with 3 neighbors which called **surface-like monomers**
- **bulk-like monomers** are located deep inside clusters and surrounded by all 4 possible neighbors

For lattices of higher dimensionality (3D-cubic and 4D-hypercubic) or higher coordination number of the lattice with fixed dimension (with new connections between nodes, as 2D-triangular) this classification become more complex, as in this case surface of dense clusters can be defined as a set of monomers with several numbers of neighbors.

In the work [6] about non-interacting SAW on a square lattice there was considered a concept of “atmosphere” of the walk  $k$ . It is a number of possible ways for a walk  $u$  with length  $N$  to add new  $N+1$ -th monomer. We suggested the connection between local coordination number, universal among every monomer of the chain including its ends and walk’s atmosphere.

## Cubic and triangular lattice comparison



As it is seen from left part of figure, increasing the strength of nearest-neighbors interaction  $J$  leads to conformation becoming more dense as proportions of monomers with higher numbers of close-range connections significantly increases after theta-transition located in a blue zone. We also repeated MC simulations for two-dimensional triangular lattice. Unlike the 3D-square lattice, the 5-th and 6-th possible neighbors located on the same plane as the first four, so conformations are expected to be more dense on this lattice.

Critical region of the model on a triangular lattice was not enumerated yet. But as it was suggested, density of conformations becomes higher as nearest-neighbors interaction  $J$  strengthen. Moreover, proportion of monomers with six neighbors on a triangular lattice is far higher than on a cubic one. It is also significant that “triangular” conformations with no inner interaction have almost twice shorter one-dimensional chains than conformations on a cubic lattice in the same conditions.

## References

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