Magnetic and Geometric Properties of the Ising Model on Lattice Random Walks

Ilya Pchelintsev
Scientific Advisor: Burovsky Evgeny Andreevich

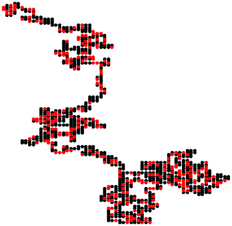
The Department of Applied Mathmatics
National Research University "Higher School of Economics"
The Moscow Institute of Electronics and Mathematics
Moscow, Russia

Outline

- Introduction and the main directions of the work:
  1. Ising model on a SAW conformation
  2. Rectangular Ising model
  3. Lattice modifications of the Ising-ISAW
  4. Methods and observables
- Results
  1. Critical asphericity research
  2. Local coordination number reseacrh

Ising-ISAW model

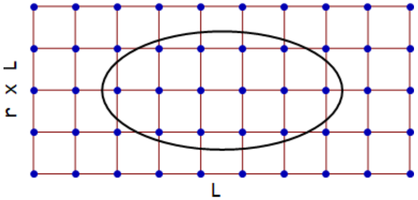
- Linear self-avoiding conformation (**SAW**-models)
- Spin subsistem inside of the monomers (regular **Ising model**)
- Close-range interaction (1)
- Tricriticality of the phase transition point [1]



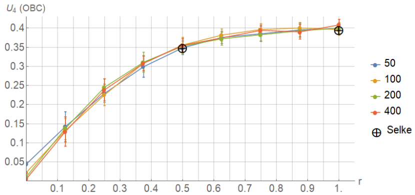
$$H_{u,N,\{\sigma\}} = -\sum_{\langle i,j\rangle} J\sigma_i\sigma_j, \quad i,j \in u, \ |u| = N \tag{1}$$

Universality of critical properties of the regular Ising model

$$H_{L,r,\{\sigma\}} = -\sum_{\langle i,j \rangle} J\sigma_i\sigma_j \qquad (2)$$



(a) Example of the regular Ising model and its gyration ellipse

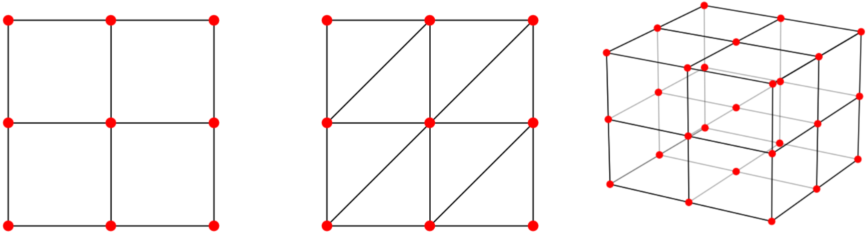


(b) Critical cumulant as a function of the lattice ratio [2]

Question №1

Equal critical geometrical properties ⇒ equal critical magnetic ones?

Lattice nearest-neighbors modifications



Question №2

Universality of lattices with equal numbers of dimensions OR equal coordination numbers?

SAW-confromations: Worm algorithm

- Gyration tensor of the SAW-system [3]:

$$Q_{N,\alpha\beta} = \frac{1}{N}\sum_{i=1}^{N}(w_{i,\alpha} - w_{c,\alpha})(w_{i,\beta} - w_{c,\beta}) \tag{3}$$

- Aspect ratio [3]:

$$r = \sqrt{\frac{\langle q_1 \rangle_N}{\langle q_2 \rangle_N}} \tag{4}$$

- Asphericity [3]:

$$\mathcal{A} = \left\langle \frac{(q_1 - q_2)^2}{(q_1 + q_2)^2} \right\rangle_N \tag{5}$$

Methods and Observables II

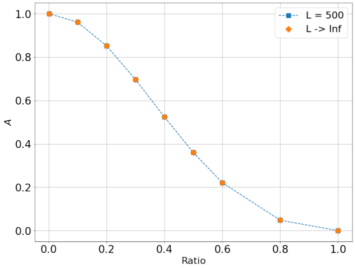
Spin-subsystem / Regular Ising: cluster update of Wolff algorithm

- Critical cumulant:

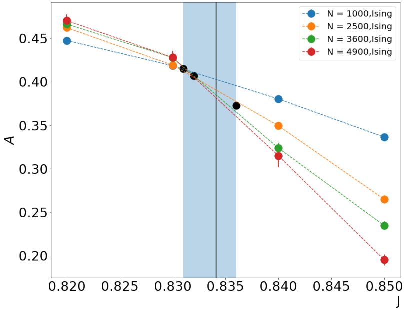
$$U_4 = 1 - \frac{\langle m^4 \rangle}{3\langle m^2 \rangle^2} \tag{6}$$

$\langle m^4 \rangle$ and $\langle m^2 \rangle$ - mean fourth/second order of spin magnetisation

Critical Asphericity



(a) Asphericity of the regular Ising as a function of the lattice ratio



(b) Asphericity of the Ising-ISAW as a function of J in the crit. region

Structure	lattice	J_c
SAW	Square	0.8340(5) [4]
lattice	Rectangular	$\ln(1+\sqrt{2})/2$ [5]

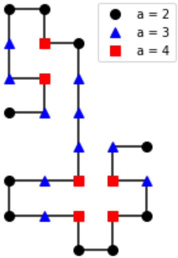
Ising-ISAW			
J	$\mathcal{A}$	r	U_4 *Rectangular*
0.831	0.415	0.465	0.338 ± 0.006
0.832	0.4072	0.47	0.343 ± 0.006
0.836	0.373	0.492	0.349 ± 0.006

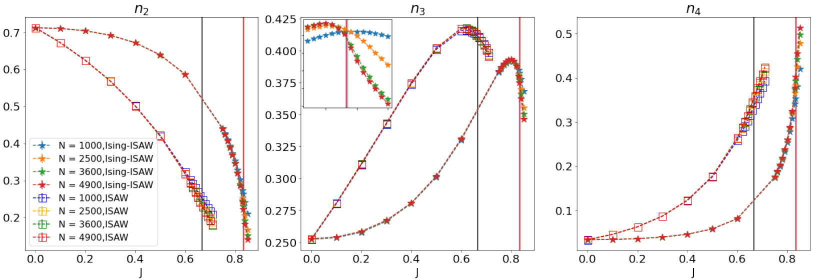
Result

As for Ising-ISAW $U_4 = 0.308(8)$ [4], critical cumulant showed complete mismatch.

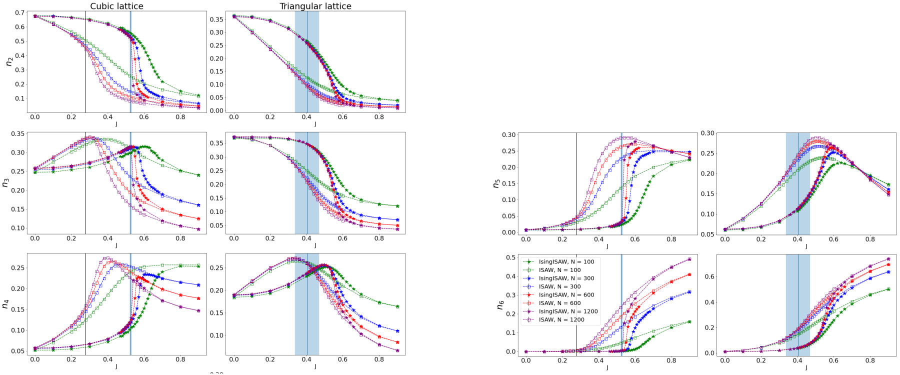
Monomer classes according to the number of interactions:

- 2 neighbors - 1D-chains
- 3 neighbors - boundaries of the cluster
- 4 neighbors - core of the cluster



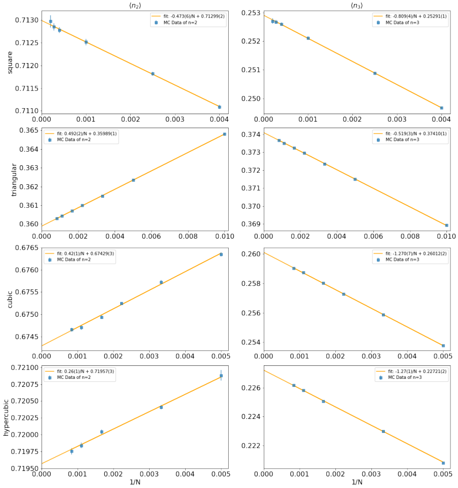


Bulk results



- First order transition was determined in cubic Ising-ISAW
- Continious transition in triangular Ising-ISAW
- Clear depiction of the chain consolidation

Anticipated results



J=0 case research

- fractions scaling nature as functions of the chain length?
- comparability of the lattice modifications

References I

- P.-G. de Gennes, *Scaling concepts in polymer physics*. Cornell University Press, 1979.
- W. Selke, "Critical Binder cumulant of two-dimensional Ising models," *Eur. Phys. J. B*, vol. 51, no. 2, pp. 223–228, 2006.
- S. Caracciolo, M. Gherardi, M. Papinutto, and A. Pelissetto, "Geometrical properties of two-dimensional interacting self-avoiding walks at the θ-point," *J. Phys. A: Math. Theor.*, vol. 44, no. 11, pp. 1–24, 2011.
- K. Faizullina, I. Pchelintsev, and E. Burovski, "Critical and geometric properties of magnetic polymers across the globule-coil transition," 2021.
- L. Onsager, "Crystal statistics. i. a two-dimensional model with an order-disorder transition," *Phys. Rev.*, vol. 65, pp. 117–149, Feb 1944. [Online]. Available: https://link.aps.org/doi/10.1103/PhysRev.65.117

References II

K. Binder, "Finite size scaling analysis of Ising model block distribution functions," *Z. Phys. B*, vol. 43, p. 119, 1981.

D. Foster and D. Majumdar, "Critical behavior of magnetic polymers in two and three dimensions," *Phys. Rev. E*, vol. 104, p. 024122, Aug 2021. [Online]. Available: https://link.aps.org/doi/10.1103/PhysRevE.104.024122

T. Garel, H. Orland, and E. Orlandini, "Phase diagram of magnetic polymers," *Eur. Phys. J. B*, vol. 12, pp. 261–268, 1999.

H. Arkın and W. Janke, "Gyration tensor based analysis of the shapes of polymer chains in an attractive spherical cage," *J. Chem. Phys.*, vol. 138, no. 5, p. 054904, 2013. [Online]. Available: https://doi.org/10.1063/1.4788616

References III

V. Privman, "Study of the point by enumeration of self-avoiding walks on the triangular lattice," vol. 19, no. 16, pp. 3287–3297, nov 1986. [Online]. Available: https://doi.org/10.1088/0305-4470/19/16/027

M. C. Tesi, E. J. J. van Rensburg, E. Orlandini, and S. G. Whittington, "Interacting self-avoiding walks and polygons in three dimensions," vol. 29, no. 10, pp. 2451–2463, may 1996. [Online]. Available: https://doi.org/10.1088/0305-4470/29/10/023

S. Livne and H. Meirovitch, "Computer simulation of long polymers adsorbed on a surface. i. corrections to scaling in an ideal chain," *The Journal of Chemical Physics*, vol. 88, no. 7, pp. 4498–4506, 1988. [Online]. Available: https://doi.org/10.1063/1.45389

N. Madras and A. D. Sokal, "The pivot algorithm: a highly efficient monte carlo method for the self-avoiding walk," *Journal of Statistical Physics*, vol. 50, no. 1, pp. 109–186, 1988.

References IV

A. Owczarek and T. Prellberg, "Scaling of the atmosphere of self-avoiding walks," *Journal of Physics A: Mathematical and Theoretical*, vol. 41, no. 37, p. 375004, 2008.

——, "First-order scaling near a second-order phase transition: Tricritical polymer collapse," *Europhysics Letters*, vol. 51, no. 6, p. 602, 2000.

H. Arkın and W. Janke, "Gyration tensor based analysis of the shapes of polymer chains in an attractive spherical cage," *The Journal of chemical physics*, vol. 138, no. 5, p. 054904, 2013.

Thank you for your attention!