Statistical thermodynamics of lattice-gas model with directional interactions: tensor-networks approach

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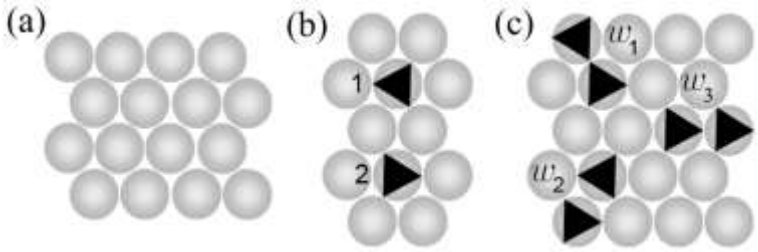
Lately, methods based on the language of tensor networks (TRG, TNR, MPS, PEPS, MERA etc.) have been increasingly used [1–4]. They have a huge potential for application in the study of many-body systems and are currently used mainly for the study of quantum models [5]. On the other hand, now there is only a small amount of work on the application of this approach to the study of classical systems [2, 6, 7]. In this work we propose to use the tensor networks approach for studying the thermodynamic characteristics of the lattice-gas model of functional organic molecules adsorption in terms of pair directional interactions. In fact, here we consider a lattice model for the adsorption of trimesic acid on a surface with triangular symmetry. We investigated this model earlier in [8,9] using the Monte Carlo and transfer-matrix methods. The use of tensor networks avoids the limitations imposed by these methods (small size of the system, long equilibration, difficulties in estimating the equilibrium etc.) and allows conducting a more complete study of this system. Next, briefly describe the studied model. The surface is a set of adsorption centers located at the nodes of a triangle lattice (Fig. a).



The adsorbed molecule has three functional groups and two possible orientations at the surface (Fig. b). Depending on the mutual orientation of the molecules on the surface, various directional interactions can form between them w1<0 (attraction), w2 and w3. Varying these energies significantly changes the behavior of the model. As a result, adsorption isotherms, graphs of the entropy and heat capacity dependence on the chemical potential were obtained, and the temperature stability of the resulting ordered structures was investigated. In addition, the computational characteristics of using approach were compared with Monte Carlo and transfer-matrix methods. All computations were conducted with in-house code SUSMOST [10].

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References:
[1] R. Orús, Annals of Physics **349**, 117 (2014).
[2] M. Levin, C. P. Nave, Physical Review Letters **99**, 120601 (2007).
[3] G. Evenbly, G. Vidal, Physical Review Letters **115**, 180405 (2015).
[4] L. Kohn et al., Physical Review E **97**, 013301 (2018).
[5] A. Kshetrimayum, H. Weimer, R. Orús, Nature communications **8**, 1291 (2017).
[6] K. Roychowdhury, C. Y. Huang, Physical Review B **91**, 205418 (2015).
[7] J. F. Yu et al., Physical Review E **89**, 013308 (2014).
[8] V. A. Gorbunov, V. A et al., Adsorption **19**, 571 (2013).
[9] S. S. Akimenko et al., Physical Review E **93**, 062804 (2016).
[10] Susmost: Surface science modeling and simulation toolkit, http://susmost.com.