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Ising spins on randomly multi-branched Husimi square lattice: Thermodynamics and phase transition in cross-dimensional range

Ran Huang [a,b,*]

[a] State Key Laboratory of Microbial Metabolism and School of Life Sciences and Biotechnology, Shanghai Jiao Tong University, Shanghai 200240, China
[b] Department of Materials Technology and Engineering, Research Institute of Zhejiang University-Taizhou, Taizhou, Zhejiang 318000, China

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ABSTRACT

An inhomogeneous random recursive lattice is constructed from the multi-branched Husimi square lattice. The number of repeating units connected on one vertex is randomly set to be 2 or 3 with a fixed ratio P_2 or P_3 with $P_2 + P_3 = 1$. The lattice is designed to describe complex thermodynamic systems with variable coordinating neighbors, e.g. the asymmetric range around the surface of a bulk system. Classical ferromagnetic spin-1 Ising model is solved on the lattice to achieve an annealed solution via the local exact calculation technique. The model exhibits distinct spontaneous magnetization similar to the deterministic system, with however rigorous thermal fluctuations and significant singularities on the entropy behavior around the critical temperature, indicating a complex superheating frustration in the cross-dimensional range induced by the stochasticity. The critical temperature was found to be exponentially correlated to the structural ratio P with the coefficient fitted as 0.53187, while the ground state energy presents linear correlation to P, implying a well-defined average property according to the structural ratio.

1. Introduction

The Bethe or Bethe-like recursive lattices generally refer to the fractal arrangements of repeating units recursively connected to neighbors only on the sharing vertex, with no connection bond lies crossing layers. It has become a powerful methodology in various fields such as thermodynamics [1,2], graph theory [3], optimization problems [4,5] and so on. In statistical physics, one important application of the recursive lattice is to approximate the regular lattice with the identical coordination number to solve a thermodynamic system (e.g. Ising model) on it. As one of few exactly calculable models, it has been proven to be a reliable method [6], with the advantage of exact calculation and simple iterative approach [7], to be applied in numerous physical systems, e.g. alloy [8], spin glass [9], polymers [10], biomacromolecule [11] etc.

As a versatile extension of the Bethe lattice assembled by single dots and bonds, the Husimi lattice employing simple geographic shapes, such as square, triangle, tetrahedron, hexagon, or cube [12–14] has also been developed for decades to describe various systems with particular geographic properties [15–17]. Similar to the Bethe lattice, the independence feature of units enables the exact calculation on Husimi lattice regardless of the dimensions of the geographic unit, and mean field approximation is unnecessary since the interactions are confined within a unit and not shared by others. The calculation method usually relies on the recursive approach, which is featured as simple and less computation effort costing thanks to the homogeneous self-similar structure [13,18].

Nevertheless, the recursive feature is accompanied with several disadvantages of this lattice methodology. Firstly, the repeating structure implies a homogeneous system, it is only suitable to describe systems of uniform texture. Some particular however important cases, e.g. the confined geometry or structural transformation, are enormously difficult, if not impossible, to be simulated by the recursive lattices. Therefore, besides a few investigations on the thermodynamics on the surface/thin film employed moderately inhomogeneous structure to present the boundary of a bulk system [19,20], the reports on the application of recursive lattice onto inhomogeneous systems were very rare. Secondly, recursive lattice is considered to be a reliable approximation to regular lattice based on the identical coordination number q. Therefore, the manipulation of coordination number(s) is critical in constructing a recursive lattice for particular requirements. While it is easy to draw a regular lattice with an arbitrary q, achieving an odd q in recursive lattice usually requires awkward design of unit selection and branch number, and even worse a prime number of q

* Correspondence to: State Key Laboratory of Microbial Metabolism and School of Life Sciences and Biotechnology, Shanghai Jiao Tong University, Shanghai 200240, China.
E-mail address: ranhuang@sjtu.edu.cn.

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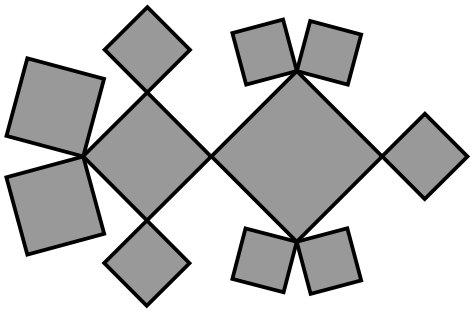

Fig. 1. A demonstration of Husimi lattice with randomly two or three branches joint on one vertex.

is impossible. Furthermore, when the randomness is necessary in a recursive lattice model, the common method is to add random terms in the Hamiltonian, e.g. a random external field as noise or random exchange couplings parameter J_{ij} [21,22], while the structural randomness is difficult to be presented due to the homogeneity of recursions.

Therefore, it is expected to be a considerable contribution to this field that if new designs of recursive lattice and calculation methods are developed to handle the above concerns, and make the recursive methodology more versatile in describing inhomogeneous systems. Recently we reported an Husimi lattice of random square-cube recursion, on which the simple Ising model can be solved by conventional exact calculation technique with moderate modification and exhibits well-defined thermal behaviors [23]. Following the same principle, in this work we have developed a randomly multi-branched Husimi square lattice and solved the simple ferromagnetic Ising model on it. The lattice is featured by randomly two or three square units connected on one vertex, then an inhomogeneous system of variable coordination numbers can be achieved with the identical unit cells. The spontaneous magnetization with critical temperature T_C, thermodynamics around the singularity, and the thermal fluctuation caused by stochastic structure, were investigated with the variation of structural ratio.

2. Modeling and calculation

2.1. Lattice construction

The original Husimi lattice was a tree-like graph assembled by squares with two units connecting on one vertex. Since its development, derivative structures of three and more squares connection have been also investigated. In this way, to achieve an inhomogeneous structure with variable q, it is a natural choice to have random number of branches connected in the lattice. To keep the investigation simple, in this work we will only study the randomly 2 or 3-branched Husimi square lattice with $q = 4$ or 6 as demonstrated in Fig. 1. A structural ratio P_2 or P_3 can be defined to indicate the probability to have 2 or 3 branches on one vertex, with obviously $P_2 + P_3 = 1$. However, as a probable reason why this type of lattice has not been reported before, the random structure destroys the recursive homogeneity and then makes the iterative approach unfeasible, therefore the lattice shown in Fig. 1 is not the actual model studied in this paper, and particular limitations on the structure must be applied to achieve an exact calculation, which will be detailed later.

While the branch number is randomly 2 or 3 in this lattice, with the structural ratio P we can define an "analog branch number" as

$$\text{analog } B = 2 \times P_2 + 3 \times P_3, \tag{1}$$

to present the average branch number of the lattice, and similarly an analog coordination number q can also be defined as analog $q = 2 \times$ analog B. By this means, the term "cross-dimensional" in this paper refers to the gradient of analog q: Taking a finite regular cubic lattice with a 2D surface as an example, we have $q = 5$ on the surface and $q = 6$ in the bulk, then in the near-surface region a randomly sampled site will has a probability to be of either q depending on the depth. Therefore, a gradually variation of analog q from 5 to 6 well represents the cross-dimensional range from the surface to bulk in this case. Similarly, the case of a 2D layer crossing to thin film can be described by the variation of analog q from 4 to 6. For an additional clarification, both 3-branched Husimi square lattice and Husimi cubic lattice have been proved to be a good approximation to the regular cubic lattice [13].

The simplest ferromagnetic spin ± 1 Ising model was applied on the lattice in this paper:

$$E = \sum_{<i,j>} -J_{ij} S_i S_j, \tag{2}$$

without external magnetic field H. The weights of one configuration γ of a square unit is given by

$$w(\gamma) = exp(-\beta \sum_{<i,j>}^{4} -J S_i S_j), \tag{3}$$

where β is the inverse temperature as $1/k_B T$, the Boltzmann constant k_B is set as one. We have the partition function of the entire system as

$$Z = \sum_{\Gamma} \prod_{\alpha} w(\gamma_\alpha), \tag{4}$$

where the $\Gamma = \bigotimes_\alpha \gamma_\alpha$ denotes the state of the lattice as an ensemble of unit α.

In this paper we setup a uniform ferromagnetic coupling $J_{ij} = 1$, then the state of system only depends on the structural properties. Without external magnetic field, we can expect a half–half probability of spin state on each site at high temperature, a uniform orientation pointing to either up or down of all spins at low temperature, and a spontaneous magnetization occurring in between. The only question being focused on in this paper is that, how this transition behaves in the cross-dimensional situation on an inhomogeneous lattice.

2.2. Partial partition function and cavity field

The lattice is designed of infinite size, nevertheless for an iterative approach it is necessary to imagine an original point where the entire lattice contribute to. Furthermore, the structure must be symmetrical to the original point, and subsequently the symmetry of sub-trees contributing onto one unit is required, otherwise the unique structure of an arbitrary sub-tree is impossible to be tracked and accounted in iterative calculation. Therefore, the unlimited random structure shown in Fig. 1 is not the actual lattice we are going to study, and two important principles have to be settled here: 1) the branch number on the vertices of one unit must be the same excluding the base vertex; 2) for any arbitrary square the three sub-trees contributing onto it towards to the original point should be identical. And the branch number on the vertices of different levels are random with the structural ratio P. A sample structure is presented in the Fig. 2a.

Although these two limitations confine a locally ordered configuration on the same levels and impair the randomness of the lattice, from a general view of the infinitely large structure, we still have two or three branched vertex randomly appears with a fixed probability. Therefore, we may say that this paper discussed a special case of the ideally random multi-branched lattice with identical sub-trees contributions.