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Original article

The phase transition for the three-state SOS model with one-level competing interactions on the binary tree

Obid Sh. Karshiboev[1,a], Muzaffar M. Rahmatullaev[2,3,b]

[1]Namangan State University, Namangan, Uzbekistan

[2]V. I. Romanovskiy Institute of Mathematics, Uzbekistan Academy of Sciences, Tashkent, Uzbekistan

[3]New Uzbekistan University, Tashkent, Uzbekistan

[a]okarshiboevsher@mail.ru, [b]mrahmatullaev@rambler.ru,

Corresponding author: O. Sh. Karshiboev, okarshiboevsher@mail.ru

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Abstract In this paper, we consider a three-state solid-on-solid (SOS) model with two competing interactions (nearest-neighbor, one-level next-nearest-neighbor) on the Cayley tree of order two. We show that at some values of the parameters the model exhibits a phase transition. We also prove that for the model under some conditions there is no two-periodic Gibbs measures.

Keywords Cayley tree, Gibbs measure, SOS model, competing interactions

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1. Introduction

Recent advances in nanoscience and nanotechnology have led to significant interest in extending thermodynamics and statistical mechanics to small systems consisting of a finite number of particles, far below the thermodynamic limit [1, 2]. In nanoscale systems, structural characteristics exhibit dynamic behavior, in contrast to the static equilibrium observed in macroscopic phases. Phase coexistence in these systems is expected to occur over ranges of temperature and pressure rather than at sharp points, as seen in bulk materials. Consequently, the Gibbs phase rule is no longer strictly applicable, and various metastable phases may emerge that have no counterparts in macroscopic systems [3–5]. This introduces challenges in understanding property relations and phase transitions in small (nano) systems. Addressing these challenges requires the development of new working equations for thermodynamics and statistical mechanics tailored to small systems. Notably, the concept of molecular self-assembly-central to bottom-up nanotechnology-relies on phase transition principles, a concept highlighted by Feynman [6].

The solid-on-solid (SOS) model on a Cayley tree was introduced in [7] as a generalization of the Ising model. Since then, significant research has focused on investigating various properties of SOS models on Cayley trees (see, e.g., [8–14]; see also [15] for a comprehensive review).

In this paper, we investigate phase transitions in the three-state SOS model on a Cayley tree of order two with nearest-neighbor and one-level next-nearest-neighbor interactions. Phase transitions are a central topic in statistical mechanics [16]. The existence of the Gibbs measures for a given model defines the occurrence of a phase transition [15–21]. While previous studies [20, 21] have analyzed Gibbs measures for mixed-spin Ising models and continuous spin systems, our work focuses on a three-state SOS model with one-level competing interactions. Unlike [21], which examines translation-invariant measures under an external field, our study explores the impact of one-level next-nearest-neighbor interactions on phase transitions, revealing conditions under which multiple Gibbs measures emerge. For the classical models (Ising and Potts models) of statistical mechanics on Cayley trees within radius three interactions, this problem is well studied (for the Ising model see, e.g., [22–30], for the Potts model see, e.g., [31–34]).

We obtain a functional equation for the model using the self-similarity of the Cayley tree. Here we consider only the one-level next-nearest-neighbor interactions, since studying both one-level and prolonged next-nearest-neighbor interactions simultaneously usually lead to functional equations which are difficult to solve (this happens even for the Ising model, see, e.g., [35]). We prove that at some values of parameters the model possesses multiple Gibbs measures which implies the existence of phase transition. Moreover, imposing restrictions on interactions, we obtain some explicit conditions for which it is possible to establish the uniqueness or, conversely, the nonuniqueness of the Gibbs measures. We

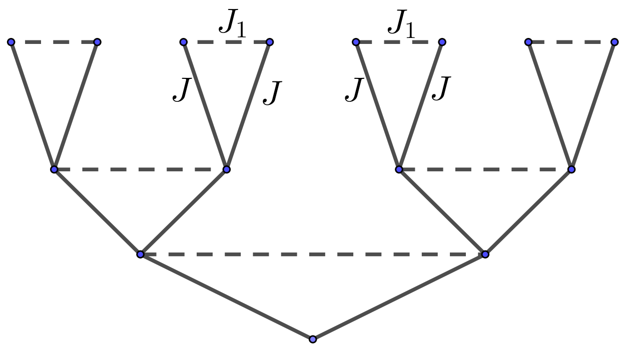

FIG. 1. The Cayley tree of order two with nearest-neighbor (———) and one-level next-nearest-neighbour (- - - - -) interactions

also show that under certain conditions, the model does not admit any two-periodic Gibbs measures. We also provide a conjecture on the absence of two-periodic Gibbs measure for the model on the invariant set.

The paper is organized as follows. Section 2 provides definitions of the model, the Cayley tree, and the Gibbs measures. In Section 3, we reformulate the problem of describing limiting Gibbs measures as a system of nonlinear functional equations. Section 4 establishes the existence of phase transitions in the model. Section 5 examines two-periodic Gibbs measures, while Section 6 summarizes the key findings and outlines potential directions for future research.

2. Preliminaries

Cayley tree. The Cayley tree Γ^k of order $k \geq 1$ is an infinite, cycle-free graph that exactly $k+1$ edges issue from each vertex. We denote by V the set of vertices and by L the set of edges. Two vertices x and y, where $x, y \in V$, are called nearest-neighbor if there exists an edge $l \in L$ connecting them, which is denoted by $l = \langle x, y \rangle$. The distance on this tree, denoted by $d(x, y)$, is defined as the number of nearest-neighbor pairs of the minimal path between the vertices x and y (where a path is a collection of nearest-neighbor pairs, two consecutive pairs sharing at least a given vertex).

For a fixed $x^0 \in V$, called the root, we set

$$W_n(x^0) = \{x \in V \mid d(x, x^0) = n\},\ V_n(x^0) = \bigcup_{m=0}^{n} W_m(x^0)$$

and denote by

$$S(x) = \{y \in W_{n+1}(x^0) : d(x, y) = 1\},\ x \in W_n(x^0)$$

the set of *direct successors* of x. We will omit x^0 in the notations W_n, and V_n because x^0 is fixed. For the sake of simplicity, we put $\mid x \mid = d(x, x^0),\ x \in V$. Two vertices $x, y \in V$ are called second nearest-neighbor if $d(x, y) = 2$. The second nearest-neighbor vertices x and y are called prolonged second nearest-neighbors if $\mid x \mid \neq \mid y \mid$ and is denoted by $> \widetilde{x, y} <$. The second nearest-neighbor vertices $x, y \in V$ that are not prolonged are called one-level next-nearest-neighbors since $\mid x \mid = \mid y \mid$ and are denoted by $> \overline{x, y} <$.

In this paper, we consider a semi-infinite Cayley Γ^k of order $k \geq 2$, i.e. a cycles-free graph with $(k+1)$ edges issuing from each vertex except for x^0 and with k edges issuing from the vertex x^0. According to well known theorems, this can be reconstituted as a Cayley tree [16, 31].

In the SOS model, the spin variables $\sigma(x)$ take values from the set $\Phi = \{0, 1, 2\}$, which is associated with each vertex of the tree Γ^k. The SOS model with nearest-neighbor and one-level next-nearest-neighbor interactions is defined by the following Hamiltonian:

$$H(\sigma) = -J \sum_{\langle x,y \rangle} \mid \sigma(x) - \sigma(y) \mid - J_1 \sum_{> \overline{x,y} <} \mid \sigma(x) - \sigma(y) \mid, \tag{1}$$

where the sum in the first term ranges all nearest-neighbors, the second sum ranges all one-level next-nearest-neighbors, and $J,\ J_1 \in \mathbb{R}$ are the coupling constants (see Fig. 1).

3. Recursive Equations

There are multiple approaches to derive the nonlinear functional equations governing the limiting Gibbs measures for lattice models on the Cayley tree. One approach utilizes properties of Markov random fields on Cayley trees (see, e.g., [7]). Another approach relies on recursive equations for partition functions (see, e.g., [31]). Both approaches ultimately yield the same equation (see, e.g., [15]). Since the second approach is more suitable for models with competing interactions, we adopt this approach.

Let Λ be a finite subset of V. We denote by $\sigma(\Lambda)$ the restriction of σ to Λ and let $\overline{\sigma}(V\backslash\Lambda)$ represent a fixed boundary configuration. The total energy of $\sigma(\Lambda)$, given the condition $\overline{\sigma}(V\backslash\Lambda)$, is defined as

$$\begin{gathered} H(\sigma(\Lambda) \mid \overline{\sigma}(V\backslash\Lambda)) = -J \sum_{\langle x,y\rangle : x,y\in\Lambda} \mid \sigma(x)-\sigma(y) \mid \\ -J_1 \sum_{>x,y<: x,y\in\Lambda} \mid \sigma(x)-\sigma(y) \mid -J \sum_{\langle x,y\rangle : x\in\Lambda, y\notin\Lambda} \mid \sigma(x)-\sigma(y) \mid, \end{gathered} \tag{2}$$

The partition function $Z_\Lambda(\overline{\sigma}(V\backslash\Lambda))$ over the finite volume Λ with boundary condition $\overline{\sigma}(V\backslash\Lambda)$ is defined as

$$Z_\Lambda(\overline{\sigma}(V\backslash\Lambda)) = \sum_{\sigma(\Lambda)\in\Omega(\Lambda)} \exp(-\beta H_\Lambda(\sigma(\Lambda) \mid \overline{\sigma}(V\backslash\Lambda))), \tag{3}$$

where $\Omega(\Lambda)$ is the set of all configurations in volume Λ and $\beta = \dfrac{1}{T}$ is the inverse temperature. Then the conditional Gibbs measure μ_Λ of a configuration $\sigma(\Lambda)$ is defined as

$$\mu_\Lambda(\sigma(\Lambda) \mid \overline{\sigma}(V\backslash\Lambda)) = \frac{\exp(-\beta\, H(\sigma(\Lambda) \mid \overline{\sigma}(V\backslash\Lambda)))}{Z_\Lambda(\overline{\sigma}(V\backslash\Lambda))}.$$

We consider the configuration $\sigma(V_n)$, the partition function Z_{V_n} and conditional Gibbs measure $\mu_\Lambda(\sigma(\Lambda) \mid \overline{\sigma}(V\backslash\Lambda))$ over the volume V_n. For simplicity, we denote them by σ_n, $Z^{(n)}$ and μ_n, respectively. The partition function $Z^{(n)}$ can be decomposed into the following summands:

$$Z^{(n)} = Z_0^{(n)} + Z_1^{(n)} + Z_2^{(n)}, \tag{4}$$

where

$$Z_i^{(n)} = \sum_{\sigma_n\in\Omega(V_n):\sigma(x^0)=i} \exp(-\beta H_{V_n}(\sigma \mid \overline{\sigma}(V\backslash V_n))),\ i=0,1,2. \tag{5}$$

Hereafter, we restrict our analysis to the case $k=2$.

Denote $\theta = \exp(\beta J),\ \theta_1 = \exp(\beta J_1)$. Let $S(x^0) = \{x^1,\ x^2\}$. If $\sigma(x^0) = i,\ \sigma(x^1) = j$ and $\sigma(x^2) = m$, then from (2) and (3), we we obtain the following relation

$$Z_i^{(n)} = \sum_{j,m=0}^{2} \exp(\beta J \mid i-j \mid +\beta J \mid i-m \mid +\beta J_1 \mid j-m \mid) Z_j^{n-1} Z_m^{(n-1)},$$

so that

$$\begin{aligned} Z_0^{(n)} &= \Big[\big(Z_0^{(n-1)}\big)^2 + 2\theta\theta_1 Z_0^{(n-1)} Z_1^{(n-1)} + 2\theta^2\theta_1^2 Z_0^{(n-1)} Z_2^{(n-1)} \\ &\quad +\theta^2\big(Z_1^{(n-1)}\big)^2 + 2\theta^3\theta_1 Z_1^{(n-1)} Z_2^{(n-1)} + \theta^4\big(Z_2^{(n-1)}\big)^2\Big], \\ Z_1^{(n)} &= \Big[\theta^2\big(Z_0^{n-1}\big)^2 + 2\theta\theta_1 Z_0^{(n-1)} Z_1^{(n-1)} + 2\theta^2\theta_1^2 Z_0^{(n-1)} Z_2^{(n-1)} \\ &\quad +\big(Z_1^{(n-1)}\big)^2 + 2\theta\theta_1 Z_1^{(n-1)} Z_2^{(n-1)} + \theta^2\big(Z_2^{(n-1)}\big)\Big], \\ Z_2^{(n)} &= \Big[\theta^4\big(Z_0^{(n-1)}\big)^2 + 2\theta^3\theta_1 Z_0^{(n-1)} Z_1^{(n-1)} + 2\theta^2\theta_1^2 Z_0^{(n-1)} Z_2^{(n-1)} \\ &\quad +\theta^2\big(Z_1^{(n-1)}\big)^2 + 2\theta\theta_1 Z_1^{(n-1)} Z_1^{(n-1)} + \big(Z_2^{n-1}\big)^2\Big]. \end{aligned}$$

Introducing the notations $u_n(x^0) = \dfrac{Z_1^{(n)}(x^0)}{Z_0^{(n)}(x^0)}$, $v_n(x^0) = \dfrac{Z_2^{(n)}(x^0)}{Z_0^{(n)}(x^0)}$, we obtain the following system of recurrent equations:

$$\begin{cases} u_n = \dfrac{\theta^2 + 2\theta\theta_1 u_{n-1} + 2\theta^2\theta_1^2 v_{n-1} + u_{n-1}^2 + 2\theta\theta_1 u_{n-1}v_{n-1} + \theta^2 v_{n-1}^2}{1 + 2\theta\theta_1 u_{n-1} + 2\theta^2\theta_1^2 v_{n-1} + \theta^2 u_{n-1}^2 + 2\theta^3\theta_1 u_{n-1}v_{n-1} + \theta^4 v_{n-1}^2} \\ \\ v_n = \dfrac{\theta^4 + 2\theta^3\theta_1 u_{n-1} + 2\theta^2\theta_1^2 v_{n-1} + \theta^2 u_{n-1}^2 + 2\theta\theta_1 u_{n-1}v_{n-1} + v_{n-1}^2}{1 + 2\theta\theta_1 u_{n-1} + 2\theta^2\theta_1^2 v_{n-1} + \theta^2 u_{n-1}^2 + 2\theta^3\theta_1 u_{n-1}v_{n-1} + \theta^4 v_{n-1}^2}. \end{cases} \tag{6}$$

Evidently,

$$u_n(x^0) = \frac{\mu_n(\sigma_n(x^0)=1)}{\mu_n(\sigma_n(x^0)=0)},\ v_n(x^0) = \frac{\mu_n(\sigma_n(x^0)=2)}{\mu_n(\sigma_n(x^0)=0)}.$$

If we can find the limit of $u_n(x^0)$ as n tends to infinity, we will find the ratio for the probability of value 1 to the probability of value 0 at the root for the limiting Gibbs measure. Similarly, if we can find the limit of $v_n(x^0)$ as n tends to infinity, we will find the ratio for the probability of value 2 to the probability of value 0 at the root for the limiting Gibbs measures. Thus, the fixed points of equation (6) describe the translation-invariant limiting Gibbs measure of the model (1).

If $u = \lim_{n\to\infty} u_n$ and $v = \lim_{n\to\infty} v_n$ then

$$\begin{cases} u = \dfrac{\theta^2 + 2\theta\theta_1 u + 2\theta^2\theta_1^2 v + u^2 + 2\theta\theta_1 uv + \theta^2 v^2}{1 + 2\theta\theta_1 u + 2\theta^2\theta_1^2 v + \theta^2 u^2 + 2\theta^3\theta_1 uv + \theta^4 v^2}, \\ \\ v = \dfrac{\theta^4 + 2\theta^3\theta_1 u + 2\theta^2\theta_1^2 v + \theta^2 u^2 + 2\theta\theta_1 uv + v^2}{1 + 2\theta\theta_1 u + 2\theta^2\theta_1^2 v + \theta^2 u^2 + 2\theta^3\theta_1 uv + \theta^4 v^2}. \end{cases} \tag{7}$$

Remark 1. The system (7) coincides with the classical result for the SOS model (see, e.g., [7,9]) when $\theta_1 = 1$ $(J_1 = 0)$, i.e.

$$\begin{cases} u = \left(\dfrac{u + \theta v + \theta}{\theta^2 v + \theta u + 1}\right)^2, \\ v = \left(\dfrac{\theta u + v + \theta^2}{\theta^2 v + \theta u + 1}\right)^2. \end{cases} \tag{8}$$

It is important to note that if there is more than one positive solution for system (7), then there is more than one translation-invariant limiting Gibbs measure corresponding to each solution. We say that a phase transition occurs for the model (1), if system (7) has more than one positive solution.

4. Translation-invariant Gibbs measures

In this section, we investigate phase transitions in the model. We consider dynamical system (6) and study its asymptotic behavior. Let $x = (u, v) \in \mathbb{R}^2_+$. The dynamical system $F : \mathbb{R}^2_+ \to \mathbb{R}^2_+$ is defined by

$$\begin{cases} u' = \dfrac{\theta^2 + 2\theta\theta_1 u + 2\theta^2\theta_1^2 v + u^2 + 2\theta\theta_1 uv + \theta^2 v^2}{1 + 2\theta\theta_1 u + 2\theta^2\theta_1^2 v + \theta^2 u^2 + 2\theta^3\theta_1 uv + \theta^4 v^2}, \\ \\ v' = \dfrac{\theta^4 + 2\theta^3\theta_1 u + 2\theta^2\theta_1^2 v + \theta^2 u^2 + 2\theta\theta_1 uv + v^2}{1 + 2\theta\theta_1 u + 2\theta^2\theta_1^2 v + \theta^2 u^2 + 2\theta^3\theta_1 uv + \theta^4 v^2}. \end{cases} \tag{9}$$

Then recurrent equations (6) can be rewritten as $x^{(n+1)} = F(x^{(n)}),\ n \geq 0$. Recall that the point x is a periodic point of period p if $F^p(x) = x$, where $F^p(x)$ stands for p-fold composition of F into itself, i.e., $F^p(x) = \underbrace{F(F(\dots F(x))\dots)}_{p}$. A point $x \in \mathbb{R}^2_+$ is called a fixed point for $F : \mathbb{R}^2_+ \to \mathbb{R}^2_+$ if $F(x) = x$ (see for more details [1, Chapter 1] or [36, Section 1]). To analyze phase transitions in the class of translation-invariant limiting Gibbs measures, it is necessary to characterize the fixed points of the mapping $F(x) = x$. We now describe the solutions of this equation. It follows that the set

$$I = \{x = (u, v) \in \mathbb{R}^2 : v = 1\}. \tag{10}$$

is invariant under the operator F. On the set I, system of equations (7) reduces to

$$u = f(u) \tag{11}$$

where

$$f(u) = f(u, \theta, \theta_1) := \frac{u^2 + 4\theta\,\theta_1\,u + 2\theta^2(\theta_1^2 + 1)}{\theta^2\,u^2 + 2\theta\,\theta_1(\theta^2 + 1)u + \theta^4 + 2\,\theta^2\theta_1^2 + 1}. \tag{12}$$

It is easy to see that the function $f(u)$ defined in (12) is continuous, bounded with $f(0) > 0$ and $\lim_{u\to+\infty} f(u) < +\infty$. Moreover, this function is decreasing for $\theta > 1$ and increasing for $\theta < 1$. Thus, it suffices to consider the case $\theta < 1$, since for $\theta > 1$ the equation (11) has a unique positive solution. From properties of the function f, it follows that the function f has at least one fixed point, say, u_*. We have

Theorem 1. Let $\theta < 1$. For the SOS model with one-level second nearest-neighbor interactions on the binary tree on the set I, if the condition $f'(u_*) > 1$, that is,

$$\frac{2(1-\theta^2)\Big(2\theta^3\theta_1^3 + 2\theta^2\theta_1^2 u_* + \theta\theta_1 u_*^2 + \theta^2 u_* + 2\theta\theta_1 + u_*\Big)}{\Big(2\theta^3\theta_1 u_* + \theta^4 + 2\theta^2\theta_1^2 + \theta^2 u_*^2 + 2\theta\theta_1 u_* + 1\Big)^2} > 1 \tag{13}$$

is satisfied, then there exist three distinct translation-invariant limiting Gibbs measures, i.e., the phase transition occurs.

Proof. When $f'(u_*) > 1$, u_* is unstable. Thus, a small neighborhood $(u_* - \varepsilon, u_* + \varepsilon)$ of u_* exists such that for $u \in (u_* - \varepsilon, u_*)$, $f(u) < u$, and for $(u_*, u_* + \varepsilon)$, $f(u) > u$. Since $f(0) > 0$, there exists a solution between 0 and u_*. Similarly, since $\lim_{u\to+\infty} f(u) < +\infty$ there is another solution between u_* and $+\infty$. Thus, there exist three solutions. Since there exist a bijection between the solutions of Eq. (11) and the translation-invariant limiting Gibbs measures, it follows that there exist three translation-invariant limiting Gibbs measures, which implies the existence of a phase transition. This completes the proof. □

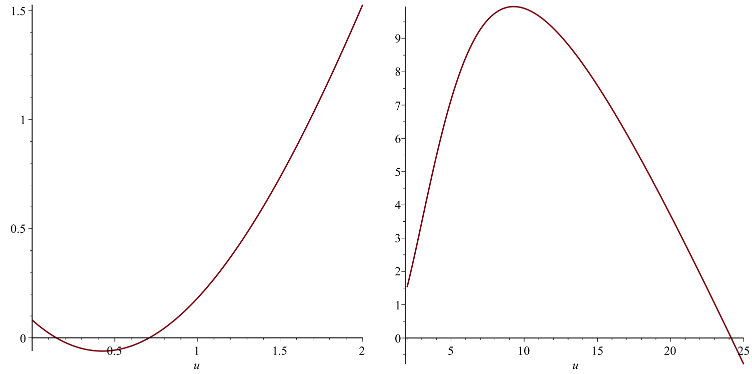

FIG. 2. The plot of $f(u) - u$ when $\theta = 0.2$, $\theta_1 = 0.5$. In this case, the function f has three positive fixed points: $\approx 0.1461;\ 0.7085;\ 24.1453$. The plot of the function is drawn for $u \in [0, 2]$, $u \in [2, 25]$ separately to show all three solutions

Remark 2. Note that the set of parameters which satisfy $f'(u_*) > 1$ is not empty, e.g., see Fig. 2.

Remark 3. In Theorem 1, we find sufficient conditions for Eq. (11) to possess multiple solutions, i.e., there might be multiple solutions for the equation even if $f'(u^*) \leq 1$.

Although solving the equation (11) for both parameters seems to be difficult, we could solve the equation in the case $\theta = \theta_1$. In this case, the equation (11) reads:

$$u^3 + A\,u^2 + B\,u + C = 0, \tag{14}$$

where

$$A = \frac{1}{\theta^2}\Big(\theta - \sqrt{\frac{\sqrt{3}-1}{2}}\Big)\Big(\theta + \sqrt{\frac{\sqrt{3}-1}{2}}\Big)\Big(\theta^2 + \frac{\sqrt{3}+1}{2}\Big),$$

$$B = (\theta - 1)(\theta + 1)(3\theta^2 - 1),\ C = -2\theta^2(\theta^2 + 1).$$

Note that $\sqrt{\frac{\sqrt{3}-1}{2}} \approx 0.605$ and $\frac{1}{\sqrt{3}} \approx 0.577$. According to the Descartes Rule of Signs (see, e.g., [37], Corollary 1), the equation (14) has at least one positive root and has at most three positive roots. We calculate the discriminant of (14) as in [38]:

$$\Delta'(\theta) := -\Delta(\theta) = 4A^3C - A^2B^2 - 18ABC + 4B^3 + 27C^2. \tag{15}$$

It is known (see [38], Theorem 4.3.8) that if $\Delta' > 0$ then the equation (14) has one real root and two imaginary roots. If $\Delta' = 0$ then the equation (14) has three real roots, at least two of which are equal. If $\Delta' < 0$ then the equation (14) has three distinct real roots. By the Descartes Rule of Signs, in order to have more than one distinct positive solutions, we should necessarily have

$$A < 0,\ B > 0,\ \Delta' \leq 0$$

which implies $\theta \leq \theta_c \approx 0.2729$, where θ_c solves the equation

$$100\,\theta^{14} + 8\,\theta^{12} + 372\,\theta^{10} - 56\,\theta^8 + 357\,\theta^6 - 155\,\theta^4 + 23\,\theta^2 - 1 = 0.$$

Summarizing, we have

Lemma 1. *There exists a unique* $\theta_c \approx 0.2729$ *such that*

- *If* $\theta > \theta_c$ *then Eq.* (14) *has one positive solution* $u_1 > 0$
- *If* $\theta = \theta_c$ *then Eq.* (14) *has two positive solutions* $u_2 < u_1$
- *If* $\theta < \theta_c$ *then Eq.* (14) *has three positive solutions* $u_3 < u_2 < u_1$.

See Fig. 3

We obtain

Theorem 2. For the SOS model with one-level next-nearest-neighbour interactions on the binary tree under condition $\theta = \theta_1$ on the set I there exists $\theta_c \approx 0.2729$ such that for $\theta \leq \theta_c$ there is a phase transition and for $\theta > \theta_c$ there is no phase transition.

Remark 4. In [9], the model is considered with only nearest neighbor interactions, and the critical value is found to be $\theta_{cr} \approx 0.1414$. We can see that the one-level next-nearest-interaction enlarges the phase transition interval.

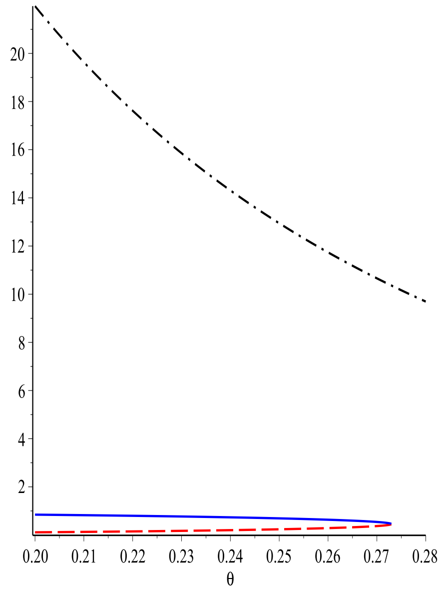

FIG. 3. The graph of functions $u_i = u_i(\theta)$, $i = 1, 2, 3$. Upper curve is u_1, middle curve is u_2 and lower curve is u_3

5. Two-periodic Gibbs measures

The notion of periodic Gibbs measures is discussed by Sinai [39] and Ganikhodjaev and Rozikov [40]. In this section, we examine periodic solutions of Eq. (6). To describe the 2-periodic Gibbs measures of the model within the set I given in (10), we will analyze the equation $f(f(u)) = u$, where the function f is defined by (12). In this case, the positive roots of the equation

$$\frac{f(f(u)) - u}{f(u) - u} = 0, \tag{16}$$

subject to the condition $f(u) \neq u$, describe the pure two-periodic Gibbs measures. By simplifying above equation, we obtain

$$A\,u^2 + B\,u + C = 0 \tag{17}$$

where

$$A := A(\theta;\theta_1) = \theta^6 + 2\theta^4\theta_1^2 + 2\theta^3\theta_1 + \theta^2 + 2\theta\theta_1 + 1,$$
$$B := B(\theta;\theta_1) = 2\theta^7\theta_1 + 4\theta^5\theta_1^3 + 2\theta^5\theta_1 + 6\theta^4\theta_1^2 + 4\theta^3\theta_1^3 - \theta^4 + 2\theta^3\theta_1 + 10\theta^2\theta_1^2 + 6\theta\theta_1 + 1,$$
$$C := C(\theta;\theta_1) = \theta^8 + 4\theta^6\theta_2 + 4\theta^4\theta_1^4 + 4\theta^5\theta_1 + 8\theta^3\theta_1^3 + 2\theta^4 + 6\theta^2\theta_1^2 + 2\theta^2 + 4\theta\theta_1 + 1.$$

Note that $A > 0$, $C > 0$ for any $\theta > 0$, $\theta_1 > 0$. According to Descartes' Rule of Signs (see, e.g., [37], Corollary 1) if $B \geq 0$ then the equation (17) does not have any positive solution (see Fig. 4). Thus, we have the following assertion:

Theorem 3. If

$$(\theta, \theta_1) \in \{(\theta, \theta_1) \in \mathbb{R}_+^2 : B \geq 0\}$$

then for the SOS model with one-level next-nearest-neighbour interactions on the binary tree there is no two-periodic (except for translation-invariant) Gibbs measures on the set I (10).

Based on Theorem 3, we now examine the case $B < 0$. If $B < 0$, then Eq. (17) may have two positive solutions. We compute the discriminant of Eq. (17):

$$D := D(\theta;\theta_1) = B^2 - 4\,A\,C.$$

It follows that if $B < 0$ and $D \geq 0$, then Eq. (17) has at least one positive solution. However, a computer analysis shows that the set

$$\mathcal{S} = \{(\theta, \theta_1) \in \mathbb{R}_+^2 :\ D \geq 0,\ B < 0\}$$

is empty. Summarising, we make

Conjecture 1. *The SOS model with one-level next-nearest-neighbor interactions on the binary tree admits no two-periodic Gibbs measures within the set* I (10).

Remark 5. a) Note that for the model (1) there might be two-periodic Gibbs measures outside of the set I (10).

b) In the case $\theta = \theta_1$ one can easily see that $B > 0$, thus, there is no two-periodic Gibbs measures.

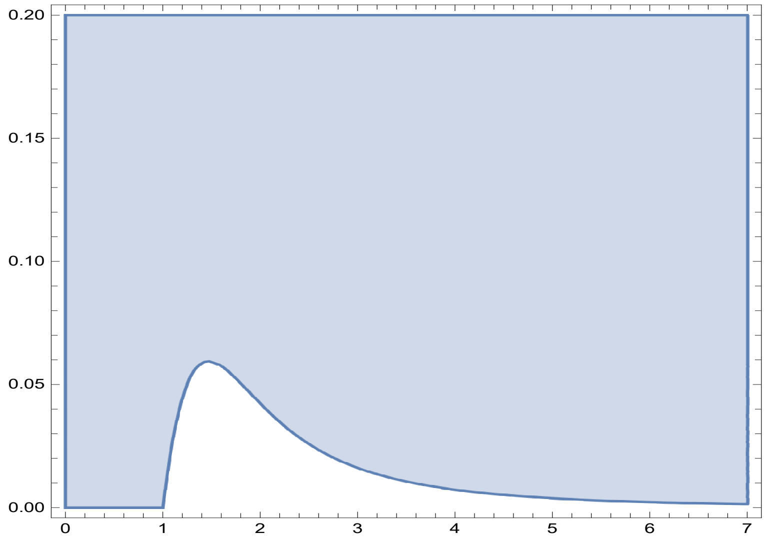

FIG. 4. The plot of $B(\theta, \theta_1)$ for $\theta \in (0, 7)$ and $\theta_1 \in (0, 0.2)$ The shaded area corresponds to $B(\theta, \theta_1) \geq 0$

6. Conclusion

In this paper, we have investigated phase transitions in the three-state solid-on-solid (SOS) model with one-level next-nearest-neighbor interactions on a Cayley tree of order two. Leveraging the self-similarity of the Cayley tree, we have derived a system of nonlinear recursive equations that describe the limiting Gibbs measures of the model. Our analysis revealed that for certain parameter values, the model exhibits multiple Gibbs measures, indicating the existence of a phase transition. Furthermore, we established explicit conditions under which the Gibbs measure is either unique or non-unique.

Additionally, we investigated the existence of two-periodic Gibbs measures and demonstrated that under certain conditions, no such measures exist in the model. We also proposed a conjecture stating the complete absence of two-periodic Gibbs measures on the invariant set. These results enhance our understanding of phase transitions in lattice models with competing interactions, which play a crucial role in statistical mechanics and mathematical physics.

From a broader perspective, our findings have implications for nanoscience, where phase transitions in nanoscale systems often exhibit unique characteristics due to finite-size effects. Studying Gibbs measures in these models provides insight into self-assembly processes and critical phenomena in nanomaterials. Future research may extend this approach to more complex lattice structures, higher-order interactions, or external fields to explore additional phase transition behaviors.

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Information about the authors:

Obid Sh. Karshiboev – Namangan State University, 161, Boburshox str, 160107, Namangan, Uzbekistan; ORCID 0000-0001-6204-4621; okarshiboevsher@mail.ru

Muzaffar M. Rahmatullaev – V. I. Romanovskiy Institute of Mathematics, Uzbekistan Academy of Sciences, 4-b, University str, 100174,Tashkent, Uzbekistan; New Uzbekistan University, 100000, Tashkent, Uzbekistan; ORCID 0000-0003-2987-7714; mrahmatullaev@rambler.ru

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