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Extremality of Gibbs measures for the DNA-Ising molecule model on the Cayley tree

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Abstract We examine a model of a DNA-Ising molecule on a Cayley tree of order $k \geq 2$. For this model, we derive a system of functional equations, where each positive solution corresponds to a Gibbs measure. On the general order Cayley tree, we can solve the model exactly. Specifically, we can find the exact value of the critical temperature T_c for any $k \geq 2$ so that, if $T \geq T_c$, there is a unique translation-invariant Gibbs measure (TIGM), and if $T < T_c$, there are three TIGMs. We determine the model's typical configurations and stationary distributions for high enough and low enough temperatures. The primary attention is focused on the systematic study of the structure of the set of the Gibbs measures. In this paper, we present a non-trivial adaptation of famous techniques, such as the Martinelli-Sinclair-Weitz criterion for determining the extremality of TIGMs and the Kesten-Stigum criterion for determining the non-extremality of TIGMs. One of the important contributions of this paper is the resolution of the extremality versus non-extremality regions for one of the TIGMs on a Cayley tree of the general order. For the other TIGMs, the extremality and non-extremality regions are determined on Cayley trees of orders up to 5.

Keywords DNA, temperature, Cayley tree, Gibbs measure, translation-invariant measures, extreme of measure

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1. Introduction and Definitions

The Ising model is the most basic and widely used phase transition model in statistical physics, and it has a long and significant history. The significance of the statistical theory of the Ising model is described through the fact that it is used to investigate a wide variety of both magnetic and non-magnetic systems.

Translation-invariant, periodic and weakly periodic Gibbs measures for the Ising model on the Cayley tree were researched by U.A. Rozikov, M.M. Rakhmatullaev [1, 2]. In the studies by P.M. Blekher and N.N. Ganikhodzhaev [3], the existence of a continuum number of Gibbs measures was proved.

In the research performed by U.A. Rozikov, D. Gandolfo, J. Ruiz, H. Akin, S. Temur, and F.Kh. Khaydarov, the limit Gibbs measures for the Ising model were investigated using a method based on the theory of Markov random fields and the recurrent equations (see [4–6]).

In recent years, the thermodynamics of certain DNA models has been investigated in the field of statistical physics. For instance, in [7–12], the Holliday junctions of the DNA molecule of the Ising, Potts, and Blume-Capel models on the Cayley tree were studied. In [13], statistical mechanics methods, specifically the theory of Gibbs measures, are employed to analyze the thermodynamic properties of a new model. Using these measures, the phases (states) of the DNA-RNA system are characterized, and the conditions (in temperature) for DNA-RNA renaturation are outlined. The book [14] discusses the latest mathematical results regarding Gibbs measures for the Potts model with q states, focusing on both the integer lattice and Cayley trees. It also demonstrates various applications of the Potts model to real situations such as biology, physics, financial engineering, medicine, sociology, neural networks, and other scientific fields.

It is widely acknowledged that the nucleotide sequence of DNA encodes genetic information [15]. Each DNA molecule consists of a double helix made up of two complementary nucleotide chains connected by base pairs through $G + C$ and $A + T$ bonds. In this context, C stands for cytosine, G for guanine, A for adenine, and T for thymine. Genetic information is replicated by utilizing one DNA strand as a template to synthesize a complementary strand. The genetic information encoded in an organism's DNA provides the instructions for the synthesis of all the proteins that the organism will produce throughout its life.

The structure of DNA can be analyzed using statistical physics approaches (see [16, 17]), representing a single DNA strand as a stochastic system of interacting bases that exhibit long-range correlations. This analysis reveals a significant link between the structure of the DNA sequence and temperature; for instance, phase transitions in this system can be understood as conformational changes.

It is recognized [2, 18–23] that the set of Gibbs measures constitutes a non-empty, convex, and compact subset within the space of probability measures. Additionally, every Gibbs measure can be represented as an integral of extreme Gibbs measures, a concept referred to as extreme decomposition [18]. As a result, the extreme points play a crucial role in characterizing the entire convex set of Gibbs measures. The extreme disordered phases of lattice models are especially important in the context of information flow theory [2, 24–26]. In this paper, we present a non-trivial adaptation of established methods, such as the Kesten-Stigum criterion [32] for determining the non-extremality of translation-invariant Gibbs measures, and the Martinelli-Sinclair-Weitz method [33] for assessing the extremality of these measures.

The organization of the paper is as follows: Chapter 2 introduces the fundamental definitions from biology and mathematics. In Chapter 3, we formulate a system of functional equations, where each solution characterizes a family of finite-dimensional Gibbs distributions and ensures the existence of a thermodynamic limit for these distributions. Moreover, we investigate the nature of DNA interactions by exploring the properties of Markov chains (with the corresponding Gibbs measures). At extremely high and low temperatures, we derive stationary distributions and typical configurations of the model. In Chapters 4 and 5, we analyze the (non)extremity problem related to the obtained TIGMs.

2. Description of DNA as a Cayley tree

Following [2, 7, 9], we review some definitions.

A Cayley tree Γ^k of order $k \geq 1$ is an infinite tree, which is defined as a graph without cycles, where exactly $k+1$ edges converge at each vertex. Let $\Gamma^k = (V, L, i)$, where V denotes the set of vertices of Γ^k, L is the set of edges and i is the incidence function that assigns each edge $l \in L$ to its endpoints $x, y \in V$. If $i(l) = \{x, y\}$, x and y are called nearest neighbors, represented as $l = \langle x, y\rangle$. The distance $d(x, y)$, $x, y \in V$ on a Cayley tree is defined as the number of edges in the shortest path connecting x to y:

$$d(x,y) = \min\{d|\exists x = x_0, x_1, ..., x_{d-1}, x_d = y \in V \text{ such that } \langle x_0, x_1\rangle, ..., \langle x_{d-1}, x_d\rangle\}.$$

For a fixed $x^0 \in V$, we define $W_n = \{x \in V \mid d(x, x^0) = n\}$,

$$V_n = \{x \in V \mid d(x, x^0) \leq n\}, \quad L_n = \{l = \langle x, y\rangle \in L \mid x, y \in V_n\}. \tag{1}$$

Let $\mathbb{Z} = \{..., -2, -1, 0, 1, 2, ...\}$. In [27], it was established that the vertices of the Cayley tree can be partitioned into equivalence classes that are indexed by integers, and for each vertex in the $m-$ equivalence class, there is a unique path such that the equivalence class numbers of the successive vertices along this path create an infinite sequence in both directions: $..., m-2, m-1, m, m+1, m+2, ...$. It is called the $\mathbb{Z}-$path.

Because each vertex x has its own $\mathbb{Z}-$path, it is evident that the Cayley tree encompasses an infinite number of (countable) sets of $\mathbb{Z}-$paths. We define the hierarchy of the Cayley tree of a set of DNA molecules as follows.

Given a configuration σ on the Cayley tree, the presence of countably many $\mathbb{Z}-$ paths implies that there are also countably many distinct DNAs. We define two DNAs as *neighbors* if there is an edge in the Cayley tree such that one endpoint is part of the first DNA and the other endpoint is part of the second DNA. By construction, it is evident that there is a unique edge for every pair of neighboring DNAs. This edge has equivalent endpoints, meaning that both ends belong to the same equivalence class for some $m \in \mathbb{Z}$.

A hierarchy is created by a countable, infinite set of DNA molecules where

(i) No two DNAs ever intersect,

(ii) every DNA possesses its own countable set of neighboring DNAs,

(iii) for any two neighboring DNAs, denoted as D_1 and D_2, there exists a unique edge $l = l(D_1; D_2) = \langle x, y\rangle$ where $x \sim y$ that connects these DNAs, and

(iv) The ball V_n intersects only finitely many DNAs for any finite $n \geq 1$.

Model. A configuration $\sigma = \sigma(x), x \in V$ on the vertex set of a Cayley tree is defined as the function σ that assigns a value $\sigma(x) \in \{-1, 1\}$, to each vertex $x \in V$, here -1 and 1 accordingly represents the base pairs $A+T$ and $C+G$. The sets of all configurations on V and V_n are accordingly denoted by Ω and Ω_n. The restriction of a configuration to a $\mathbb{Z}-$path is termed DNA. This type of problem is discussed in the work [9]. Here, two potentials define the energies of the DNA molecule set's configuration σ: one on the $\mathbb{Z}-$path and the other off the $\mathbb{Z}-$path. The DNA molecule's configuration energies σ on the path $\mathbb{Z}$ and outside of it are determined by the same potentials in this work, namely, the Ising model of the configuration energies σ of the DNA molecule set is considered

$$H(\sigma) = J \sum_{\langle x,y\rangle \in L} \sigma(x)\sigma(y), \tag{2}$$

here the vertices of the closest neighbors are indicated by $\langle x, y\rangle$, $J > 0$ is the coupling constant between neighboring DNAs, and $\sigma(x) \in \{-1, 1\}$.

3. Thermodynamics of the DNA molecule system.

We establish a finite-dimensional distribution for the probability measure μ on the set Ω_n of all conceivable configurations on V_n

$$\mu_n(\sigma_n) = Z_n^{-1} \exp\{\beta H_n(\sigma_n) + \sum_{y\in W_n} h_{\sigma(y),y}\}, \tag{3}$$

where Z_n^{-1} is the normalizing coefficient, $\beta = \frac{1}{T}$, $T > 0$ is the temperature,

$$H_n(\sigma_n) = \sum_{\langle x,y\rangle\in L_n} \sigma_n(x)\sigma_n(y)$$

and $\{h_{i,x} \in \mathbb{R}, i = -1, 1, x \in V_n\}$

Remark 1. The quantities $e^{h_{i,x}}$ define the boundary law in the sense of definition 12.10 in [18] (see also [28–30]). In our case, these quantities define the boundary law of the biological DNA system.

We will refer to the probability distributions (3) as consistent if, for all $n \geq 1$ and $\sigma_{n-1} \in \Omega_{n-1}$:

$$\sum_{\omega_n\in\Omega_{W_n}} \mu_n(\sigma_n \vee \omega_n) = \mu_{n-1}(\sigma_{n-1}), \tag{4}$$

where $\sigma_n \vee \omega_n$ is the union of configurations.

For $x \in V_{n-1}$, we define the set $S(x) = \{t \in V_n : \langle x, t\rangle\}$. For $x \in V$, we define $x_\downarrow$ as the unique point in the set $\{y \in V : \langle x, y\rangle\} \setminus S(x)$. It is evident that

$$S(x) \cap \mathbb{Z}\text{-path} = \begin{cases} \{x_0, x_1\} \subset V, \text{ if } & \langle x_\downarrow, x\rangle \notin \mathbb{Z} - \text{path}, \\ \{x_1\} \subset V, \text{ if } & \langle x_\downarrow, x\rangle \in \mathbb{Z} - \text{path}. \end{cases}$$

We introduce the notation

$$S_0(x) = S(x) \setminus \{x_0, x_1\}, \langle x_\downarrow, x\rangle \notin \mathbb{Z}\text{-path},$$
$$S_1(x) = S(x) \setminus \{x_1\}, \langle x_\downarrow, x\rangle \in \mathbb{Z}\text{-path}.$$

A specific instance of Theorem 1 from [9] is the following theorem.

Theorem 1. *The probability distributions μ_n in (3) are consistent if and only if the equations*

$$\begin{aligned} z_x &= \frac{\theta^2 \hat{z}_{x_0} + 1}{\hat{z}_{x_0} + \theta^2} \cdot \frac{\theta^2 \hat{z}_{x_1} + 1}{\hat{z}_{x_1} + \theta^2} \prod_{t\in S_0(x)} \frac{\theta^2 z_t + 1}{z_t + \theta^2}, \langle x_\downarrow, x\rangle \notin \mathbb{Z}\text{-}path, \\ \hat{z}_x &= \frac{\theta^2 \hat{z}_{x_1} + 1}{\hat{z}_{x_1} + \theta^2} \prod_{t\in S_1(x)} \frac{\theta^2 z_t + 1}{z_t + \theta^2}, \langle x_\downarrow, x\rangle \in \mathbb{Z}\text{-}path, \end{aligned} \tag{5}$$

holds for any $x \in V \setminus \{x^0\}$. Here

$$\theta = e^{-J\beta},$$
$$z_x = e^{h_{1,x}-h_{-1,x}}, \langle x_\downarrow, x\rangle \notin \mathbb{Z}\text{-}path,$$
$$\hat{z}_x = e^{h_{1,x}-h_{-1,x}}, \langle x_\downarrow, x\rangle \in \mathbb{Z}\text{-}path.$$

Remark 2. The difference between the present paper and [9] is that here the number of parameters is reduced, but the tree order is increased to $k = 2, 3, 4, 5$ and the results are obtained for these cases. At the same time, in these cases, we consider the problem of extremity of Gibbs measures which is a new problem in the set of DNA molecules.

It follows from Theorem 1 that for any set of vectors $\mathbf{z}$=$\{(z_x, \hat{z}_t)\}$ satisfying the system of functional equations (5), there exists a unique Gibbs measure μ and vice versa. But the analysis of this system of nonlinear functional equations is not easy. In the next subsection, we will find several of its solutions.

Remark 3. The number of solutions of the system (5) depends on the temperature and the interaction parameters θ. If this system has more than one solution, then there is more than one Gibbs measure (i.e., a phase transition occurs in the DNA model).

We find solutions of the system of equations (5) of the form

$$z_x = u, \text{ for all } \langle x_\downarrow, x\rangle \notin \mathbb{Z}\text{-path},$$
$$\hat{z}_x = v, \text{ for all } \langle x_\downarrow, x\rangle \in \mathbb{Z}\text{-path}.$$

The Gibbs measures corresponding to such solutions are called *translation-invariant.*

From (5), we obtain

$$\begin{aligned} u &= \left(\frac{\theta^2 v+1}{v+\theta^2}\right)^2 \left(\frac{\theta^2 u+1}{u+\theta^2}\right)^{k-2}, \\ v &= \left(\frac{\theta^2 v+1}{v+\theta^2}\right) \left(\frac{\theta^2 u+1}{u+\theta^2}\right)^{k-1}, \end{aligned} \tag{6}$$

where $u, v > 0$. Clearly, $u = v = 1$ satisfies system (6) for any $k \geq 2$ and $\theta > 0$.

Now, in the general case, we solve the system of equations (6). To do this, we divide the first equation by the second of this system. Then we get

$$\frac{u}{v} = \frac{\theta^2 v+1}{v+\theta^2} \cdot \frac{u+\theta^2}{\theta^2 u+1},$$

or

$$(u-v)(\theta^2 uv + \theta^4(u+v) + \theta^2) = 0.$$

The last equation is true if and only if $u = v$. Since $u, v, \theta > 0$, then $\theta^2 uv + \theta^4(u+v) + \theta^2 > 0$.

Therefore, it is sufficient to find a solution to the system of equations (6) in the case $u = v$, i.e.

$$u = \left(\frac{\theta^2 u+1}{u+\theta^2}\right)^k. \tag{7}$$

Denoting $x = \sqrt[k]{u}$ from (7), we obtain

$$x^{k+1} - \theta^2 x^k + \theta^2 x - 1 = 0. \tag{8}$$

Equation (7) has a solution $x = 1$ regardless of the parameters (θ, k). Dividing the both parts of (7) by $x - 1$, we obtain

$$x^k - (\theta^2 - 1)(x^{k-1} + x^{k-2} + \cdots + x) + 1 = 0. \tag{9}$$

The following lemma gives one the number of solutions of the equation (9):

Lemma 1. [31] *For each $k \geq 2$, there exists exactly one critical value of θ, i.e. $\theta_{\mathrm{c}} = \theta_{\mathrm{c}}(k) := \sqrt{\frac{k+1}{k-1}}$, such that*

(1) *if $\theta < \theta_{\mathrm{c}}$, then equation (9) does not have a positive solution;*
(2) *if $\theta = \theta_{\mathrm{c}}$, then equation (9) has a unique solution $x_1^{(k)} = 1$;*
(3) *if $\theta > \theta_{\mathrm{c}}$, then equation (9) has exactly two solutions (both different from 1), denoted as $x_2^{(k)}$, $x_3^{(k)}$.*

Thus, the corresponding solutions (7) are equal to

$$\begin{aligned} &1)\ 1 \text{ for } \theta \leq \theta_c, \\ &2)\ 1,\ \left(x_2^{(k)}\right)^k,\ \left(x_3^{(k)}\right)^k \ \text{ for } \theta > \theta_c. \end{aligned} \tag{10}$$

For $k \geq 2$, we can prove the following lemma.

Lemma 2. *Let $k \geq 2$ and $\theta_{cr} = \sqrt{\frac{k+1}{k-1}}$. Then the following statements hold*:

- *if $\theta = exp(-J\beta) \leq \theta_c$, then system (6) has a unique solution*

$$\mathbf{z}_1^{(k)} = (u_1^{(k)}, u_1^{(k)}) = (1, 1);$$

- *if $\theta > \theta_c$, then system (6) has three solutions*

$$\mathbf{z}_1^{(k)} = (u_1^{(k)}, u_1^{(k)}) = (1, 1), \mathbf{z}_2^{(k)} = (u_2^{(k)}, u_2^{(k)}), \mathbf{z}_3^{(k)} = (u_3^{(k)}, u_3^{(k)}),$$

where

$$u_i^{(k)} = \left(x_i^{(k)}\right)^k, i = 2, 3, \ \ u_2^{(k)} u_3^{(k)} = 1.$$

Let us denote by $\mu_i^{(k)}$ the Gibbs measures corresponding to the solutions $\mathbf{z}_i^{(k)}$, $i = 1, 2, 3$. Let us define the critical temperature

$$T_c := T_c(k) = \frac{J}{\ln \sqrt{\frac{k-1}{k+1}}}.$$

Thus, summarising, we obtain the following result

Theorem 3. *For the DNA-Ising molecule model on the Cayley tree of order $k \geq 2$, the following statements are true*:
1) *if $T \geq T_c$, then there exists a unique translation-invariant Gibbs measure $\mu_1^{(k)}$;*

2) *if* $T < T_c$, *then there exist three translation-invariant Gibbs measures* $\mu_1^{(k)}, \mu_2^{(k)}, \mu_3^{(k)}$, *i.e. a phase transition occurs.*

Remark 4. Note that, in comparison with work [9], the exact value of the critical temperature is found here for any $k \geq 2$, and the analysis of the equations in these works is different.

For further discussion, we will need an explicit solution of the system of equations (6), i.e. equation (7).

Equation (7) has the following explicit solutions:

- for $k = 2$ there is a unique solution $u_1^{(2)} = 1$ for $0 < \theta \leq \sqrt{3}$ and there are three positive solutions for $\theta > \sqrt{3}$:

$$u_1^{(2)} = 1, u_{2,3}^{(2)} = \frac{\theta^4 - 2\theta^2 - 1 \pm \sqrt{(\theta^4 - 2\theta^2 - 1)^2 - 4}}{2}. \tag{11}$$

- for $k = 3$ there is a unique solution $u_1^{(3)} = 1$ in the interval $0 < \theta \leq \sqrt{2}$ and there are three positive solutions in the interval $\theta > \sqrt{2}$:

$$u_1^{(3)} = 1, u_{2,3}^{(3)} = \frac{\theta^6 - 3\theta^2 \pm \sqrt{(\theta^6 - 3\theta^2)^2 - 4}}{2}. \tag{12}$$

- for $k = 4$ there is a unique solution $u_1^{(4)} = 1$ in the interval $0 < \theta \leq \sqrt{\frac{5}{3}}$ and for $\theta > \sqrt{\frac{5}{3}}$ there are three positive solutions:

$$u_1^{(4)} = 1, u_{2,3}^{(4)} = \left(\frac{z_1 \pm \sqrt{z_1^2 - 4}}{2}\right)^4, \tag{13}$$

  where

$$z_1 = \frac{\theta^2 - 1 + \sqrt{(\theta^2 - 1)^2 + 4(1 + \theta^2)}}{2}.$$

- for $k = 5$ there is a unique solution $u_1^{(5)} = 1$ in the interval $0 < \theta \leq \sqrt{\frac{3}{2}}$ and for $\theta > \sqrt{\frac{3}{2}}$ there are three positive solutions:

$$u_1^{(5)} = 1, u_{2,3}^{(5)} = \left(\frac{z_2 \pm \sqrt{z_2^2 - 4}}{2}\right)^5. \tag{14}$$

  where

$$z_2 = \frac{\theta^2 + \sqrt{\theta^4 + 4}}{2}.$$

Markov chains. The transition matrix of a Markov chain (with a given Gibbs measure) is defined as (see [9])

$$\mathbb{P}^{\langle x,y\rangle} = (P_{i,j}^{\langle x,y\rangle})_{i,j=1,2} = \begin{cases} \begin{pmatrix} \frac{\theta^2 u}{\theta^2 u + 1} & \frac{1}{\theta^2 u + 1} \\ \frac{u}{u + \theta^2} & \frac{\theta^2}{u + \theta^2} \end{pmatrix}, & \langle x,y\rangle \in \mathbb{Z}\text{-}path, \\ \begin{pmatrix} \frac{\theta^2 v}{\theta^2 v + 1} & \frac{1}{\theta^2 v + 1} \\ \frac{v}{v + \theta^2} & \frac{\theta^2}{v + \theta^2} \end{pmatrix}, & \langle x,y\rangle \notin \mathbb{Z}\text{-}path, \end{cases}$$

where (u, v) is the solution of system (6) (mentioned in Lemma 2). Note that each matrix $\mathbb{P}^{\langle x,y\rangle}$ does not depend on $\langle x, y\rangle$ itself, but depends on the $\mathbb{Z}-$path to which it belongs.

Stationary distributions are easy to find:

$$\pi^{\langle x,y\rangle} = \begin{cases} \left(\frac{\theta^2 u^2 + u}{\theta^2 u^2 + 2u + \theta^2}, \frac{u + \theta^2}{\theta^2 u^2 + 2u + \theta^2}\right), & \langle x,y\rangle \in \mathbb{Z}\text{-}path, \\ \left(\frac{\theta^2 v^2 + v}{\theta^2 v^2 + 2v + \theta^2}, \frac{v + \theta^2}{\theta^2 v^2 + 2v + \theta^2}\right), & \langle x,y\rangle \notin \mathbb{Z}\text{-}path. \end{cases}$$

The following statement is known as the ergodic theorem for positive stochastic matrices (see [18]).

Theorem 4. *Let* $\mathbb{P}$ *be a positive stochastic matrix and* π *be the unique probability vector with* $\pi\mathbb{P} = \pi$ *(i.e.* π*is a stationary distribution). Then*

$$\lim_{n\to\infty} x\mathbb{P}^n = \pi$$

for all initial vectors x.

In the case where the Gibbs measure (and the corresponding Markov chains) are not unique, we have different stationary states for different measures. These states depend on the temperature and the fixed measure.

Recall that a DNA molecule is a configuration $\sigma \in \{-1,1\}^{\mathbb{Z}}$ on a $\mathbb{Z}-$path. According to the definition of our model, only neighboring DNAs can interact. Interaction occurs through an edge $l = \langle x,y \rangle \notin \mathbb{Z}-$path connecting two DNA molecules when the configuration at the ends of this edge satisfies $\sigma(x) = \sigma(y)$. Neighboring DNAs do not interact if $\sigma(x) \neq \sigma(y)$.

The following theorem can be proved similarly to Theorem 4 in [9].

Theorem 5. *In the stationary state of the DNA set we have the following statements:*

1. Two neighboring DNAs do not interact with probability (here and below, index i *corresponds to measure* $\mu_i^{(k)}$, $i = 1,2,3$*)*

$$\mathbb{P}_{i,k} = \frac{2v_i^{(k)}}{\theta^2 \left(v_i^{(k)}\right)^2 + 2v_i^{(k)} + \theta^2},$$

where $(u_i^{(k)}, v_i^{(k)})$ *are defined in Lemma 2 and, therefore, interact with probability* $1 - \mathbb{P}_{i,k}$.

2. Two neighboring base pairs (on the vertices of an edge $l = \langle x,y \rangle \in \mathbb{Z}-$*path) in a DNA molecule have distinct values (i.e.,* $\sigma(x) \neq \sigma(y)$*) with the probability*

$$\mathbb{Q}_{i,k} = \frac{2u_i^{(k)}}{\theta^2 \left(u_i^{(k)}\right)^2 + 2u_i^{(k)} + \theta^2},$$

and they consequently have the same value with the probability $1 - \mathbb{Q}_{i,k}$.

Remark 5. Since each DNA molecule has a countable set of neighboring DNA molecules, at the same temperature it can interact with several of its neighbors. In the case where DNA does not interact with its neighbors, it is isolated. We can consider the interacting DNA molecules as a branched DNA molecule. In the case of coexistence of more than one Gibbs measure, the branches of the DNA molecule can consist of different phases and different stationary states.

We are interested in the stationary distributions of $\pi^{\langle x,y \rangle, i,k}$ for $k = 2,3,4,5$ (which correspond to the Markov chain generated by the Gibbs measure μ_i) in the cases when the temperature $T \to 0$ and $T \to +\infty$. To calculate the limit, note that $u_i^{(k)}$ and $v_i^{(k)}$, $i = 1,2,3$, vary with $T = 1/\beta$.

Proposition 1. *Regardless of the edge* $\langle x,y \rangle$ *for* $k = 2,3,4,5$, *we have the following limit relations*

$$\lim_{T\to 0} \pi^{\langle x,y \rangle,1,k} = \left(\frac{1}{2}, \frac{1}{2}\right), \quad \lim_{T\to 0} \pi^{\langle x,y \rangle,2,k} = (0,1), \quad \lim_{T\to 0} \pi^{\langle x,y \rangle,3,k} = (1,0)$$

in case of low temperatures and

$$\lim_{T\to +\infty} \pi^{\langle x,y \rangle,1,k} = \lim_{T\to T_c} \pi^{\langle x,y \rangle,i,k} = \left(\frac{1}{2}, \frac{1}{2}\right), \quad i = 1,2,3$$

in case of high temperatures.

Proof. The proof is obtained from the explicit formulas for $k = 2,3,4,5$ for $u_i^{(k)}$ and $v_i^{(k)}$, $i = 1,2,3$, respectively, by direct calculations.

Remark 6. Using this proposition, we obtain the structure of DNA at $k = 2,3,4,5$ for low and high temperatures.

In the case of $T \to 0$, the DNA set has the following stationary states (configurations).

For a measure of $\mu_1^{(k)}$, the base pairs $-1 = A + T$ and $1 = C + G$ at each point of the DNA molecule are found with equal probability $1/2$ for states -1 and 1.

For measure $\mu_2^{(k)}$ all DNAs are rigid and interact, and $\sigma(x) = 1$ for all $x \in \mathbb{Z}-$paths.

For measure $\mu_3^{(k)}$, all DNAs are rigid and interact, and $\sigma(x) = -1$ for all $x \in \mathbb{Z}-$paths.

In the case $T \to +\infty$, the sequence of states -1 and 1 in the DNA molecule on the $\mathbb{Z}-$path is free, the states are independent and identically distributed. There is a state -1 with probability $1/2$ and a state 1 with probability $1/2$.

4. Conditions (not) extremes of measures $\mu_1^{(k)}$, $\mu_2^{(k)}$, $\mu_3^{(k)}$

It is known that the set of all limit Gibbs measures (corresponding to a given Hamiltonian) forms a non-empty convex compact subset in the set of all probability measures. In this connection, the description of all extreme points of this convex set, i.e. extreme Gibbs measures, is of particular interest.

To check the (non)extremality of the measure, we use the methods from [32,33]. For this, we consider Markov chains with states $\{-1,1\}$ and the matrix P_μ of probability transitions $P_{\sigma(x)\sigma(y)}$ defined by the given translation-invariant Gibbs measure μ, i.e. $P_{\sigma(x)\sigma(y)}$ is the probability of a shift from the state $\sigma(x)$ to the state $\sigma(y)$.

A sufficient condition for the Gibbs measure corresponding to the matrix P_μ to be non-extreme is that $k\lambda_2^2 > 1$, where λ_2 is the second largest eigenvalue of the matrix P_μ (the Kesten-Stigum condition).

To check this condition, we need to know the explicit form of the solution of the system (6). Exact solutions are currently known to us only for $k \leq 5$.

It is clear that for $k \geq 2$, the system of equations (6) for $\theta \leq \theta_{cr} = \sqrt{\dfrac{k+1}{k-1}}$ has a unique solution $(u_1^{(k)}, u_1^{(k)}) = (1,1)$ and for $\theta > \theta_{cr} = \sqrt{\dfrac{k+1}{k-1}}$ has three solutions $(u_1^{(k)}, u_1^{(k)}) = (1,1), (u_2^{(k)}, u_2^{(k)}), (u_3^{(k)}, u_3^{(k)})$.

Let us find the conditions for non-extremality of the measures corresponding to these solutions. Since $u = v$ for any $\langle x, y\rangle \in L$. Then we obtain

$$\mathbb{P}_k^{\langle x,y\rangle} = \mathbb{P}_k = \begin{pmatrix} \dfrac{\theta^2 u^{(k)}}{\theta^2 u^{(k)}+1} & \dfrac{1}{\theta^2 u^{(k)}+1} \\ \dfrac{u^{(k)}}{u^{(k)}+\theta^2} & \dfrac{\theta^2}{u^{(k)}+\theta^2} \end{pmatrix}. \tag{15}$$

It is clear that eigenvalues of this matrix

$$s_1^{(k)} = 1, s_2^{(k)} = \frac{u^{(k)}(\theta^4-1)}{(\theta^2 u^{(k)}+1)(\theta^2+u^{(k)})}.$$

First, we check the condition of non-extremity of the measure $\mu_1^{(k)}$ corresponding to the solution $(u_1^{(k)}, u_1^{(k)}) = (1,1)$.

Now let us check the condition of non-extreme measures: $k \cdot \left(s_2^{(k)}\right)^2 > 1$. For the solution under consideration, this inequality will take the form:

$$k \cdot \left(\frac{\theta^2-1}{\theta^2+1}\right)^2 > 1. \tag{16}$$

By solving inequality (16), one comes to the following theorem.

Theorem 6. *Let $k \geq 2$. Then for the DNA-Ising model of the molecule the measure $\mu_1^{(k)}$ at*

$$\theta \in \left(0; \sqrt{\frac{\sqrt{k}-1}{\sqrt{k}+1}}\right) \bigcup \left(\sqrt{\frac{\sqrt{k}+1}{\sqrt{k}-1}}; +\infty\right)$$

is not extreme.

We check the condition of non-extremity of the measures $\mu_2^{(k)}$, $\mu_3^{(k)}$ for $k = 2$, corresponding to the solutions $(u_2^{(2)}, u_2^{(2)}), (u_3^{(2)}, u_3^{(2)})$. Now let us check the condition of non-extreme measure: $2 \cdot \left(s_2^{(2)}\right)^2 > 1$. For solutions $(u_2^{(2)}, u_2^{(2)})$ and $(u_3^{(2)}, u_3^{(2)})$ this inequality will take the form:

$$2 \cdot \left(\frac{u_{2,3}^{(2)}(\theta^4-1)}{(\theta^2 u_{2,3}^{(2)}+1)(\theta^2+u_{2,3}^{(2)})}\right)^2 > 1. \tag{17}$$

In (17), substituting our expressions $u_{2,3}^{(2)}$ and reducing them, we obtain

$$2 \cdot \left(\frac{1}{\theta^2-1}\right)^2 > 1. \tag{18}$$

Since $\theta > \sqrt{3}$, inequality (18) does not have a solution. Thus, for $k = 2$, the non-extreme condition does not exist for the solution $(u_2^{(2)}, u_2^{(2)}), (u_3^{(2)}, u_3^{(2)})$. This means that the measures corresponding to these solutions might be extreme. We will check this in further studies.

We check the condition of non-extremity of the measures $\mu_2^{(k)}$, $\mu_3^{(k)}$ for $k = 3$, corresponding to the solutions $(u_2^{(3)}, u_2^{(3)}), (u_3^{(3)}, u_3^{(3)})$. Let us check the condition of non-extreme measure: $3 \cdot \left(s_2^{(3)}\right)^2 > 1$. For solutions $(u_2^{(3)}, u_2^{(3)})$ and $(u_3^{(3)}, u_3^{(3)})$, this inequality will take the form:

$$3 \cdot \left(\frac{u_{2,3}^{(3)}(\theta^4-1)}{(\theta^2 u_{2,3}^{(3)}+1)(\theta^2+u_{2,3}^{(3)})}\right)^2 > 1. \tag{19}$$

In (19), substituting our expressions $u_{2,3}^{(3)}$ and reducing them, we obtain

$$3 \cdot \left(\frac{1}{\theta^4-1}\right)^2 > 1. \tag{20}$$

Since $\theta > \sqrt{2}$, inequality (20) does not have a solution. Thus, for $k = 3$, the non-extreme condition does not exist for the solution $(u_2^{(3)}, u_2^{(3)})$, $(u_3^{(3)}, u_3^{(3)})$. This means that the measures corresponding to these solutions might be extreme. We will check this in further studies.

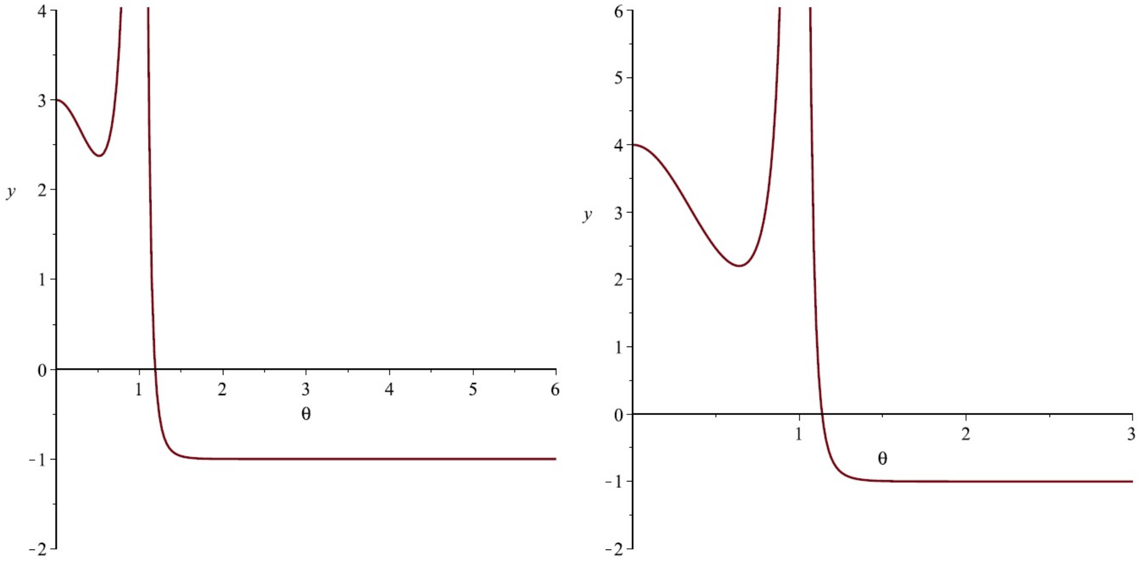

FIG. 1. Plots of the functions $4\cdot\left(s_2^{(4)}\right)^2-1$ (left) and $5\cdot\left(s_2^{(5)}\right)^2-1$ (right)

We check the condition of non-extremity of the measures $\mu_2^{(k)}$, $\mu_3^{(k)}$ for $k=4$, corresponding to the solutions $(u_2^{(4)},u_2^{(4)})$, $(u_3^{(4)},u_3^{(4)})$, i.e. we check the condition: $4\cdot\left(s_2^{(4)}\right)^2>1$. For solutions $(u_2^{(4)},u_2^{(4)})$ and $(u_3^{(4)},u_3^{(4)})$ this inequality will take the form:

$$4\cdot\left(\frac{u_{2,3}^{(4)}(\theta^4-1)}{(\theta^2u_{2,3}^{(4)}+1)(\theta^2+u_{2,3}^{(4)})}\right)^2>1. \tag{21}$$

Finding an analytical solution to inequality (21) is difficult. Using the Maple program, one can see that the last inequality is not satisfied for any $\theta>\sqrt{\frac{5}{3}}$ (see Fig. 1). Thus, for $k=4$, the non-extreme condition does not exist for the solution $(u_2^{(4)},u_2^{(4)})$, $(u_3^{(4)},u_3^{(4)})$. This means that the measures corresponding to these solutions might be extreme. We will check this in further studies.

We check the condition of non-extremity of the measures $\mu_2^{(k)}$, $\mu_3^{(k)}$ for $k=5$, corresponding to the solutions $(u_2^{(5)},u_2^{(5)})$, $(u_3^{(5)},u_3^{(5)})$. Now let us check the condition of non-extreme measure: $5\cdot\left(s_2^{(5)}\right)^2>1$. For solutions $(u_2^{(5)},u_2^{(5)})$ and $(u_3^{(5)},u_3^{(5)})$ this inequality will take the form:

$$5\cdot\left(\frac{u_{2,3}^{(5)}(\theta^4-1)}{(\theta^2u_{2,3}^{(5)}+1)(\theta^2+u_{2,3}^{(5)})}\right)^2>1. \tag{22}$$

Using the Maple program, one can see that the last inequality is satisfied for any $\theta>\sqrt{\frac{3}{2}}$ (see Fig. 1). Thus, for $k=5$, the non-extreme condition does not exist for the solution $(u_2^{(5)},u_2^{(5)})$, $(u_3^{(5)},u_3^{(5)})$. This means that the measures corresponding to these solutions might be extreme. We will check this in further studies.

5. Conditions of extremity of measures $\mu_1^{(k)}$, $\mu_2^{(k)}$, $\mu_3^{(k)}$

Methods from [33] are known for studying the extremum. Let us carry out the necessary definitions from [33]. If we remove an arbitrary edge $\langle x^0,x^1\rangle=l\in L$ from the Cayley tree Γ^k, then it is separated into two components $\Gamma^k_{x^0}$ and $\Gamma^k_{x^1}$, each of which is called a semi-infinite tree or a semi-Cayley tree.

Consider a finite complete subtree $\Im$ that contains all initial points of the half-tree $\Gamma^k_{x^0}$. The boundary $\partial\Im$ of the subtree $\Im$ consists of the nearest neighbors of its vertices that lie in $\Gamma^k_{x^0}\setminus\Im$. We identify the subtree $\Im$ with the set of its vertices. By $E(A)$ we denote the set of all edges of A and ∂A.

In [33], two key quantities were introduced: κ and γ, which play an important role in studying the extremity of the TI of Gibbs measures. These quantities are properties of the set of Gibbs measures $\{\mu^\tau_\Im\}$, where the boundary condition τ is fixed and $\Im$ is an arbitrary, initial, complete, final subtree of $\Gamma^k_{x^0}$. Given an initial subtree $\Gamma^k_{x^0}$ and a vertex $x\in\Im$, we write $\Im_x$ for the (maximal) subtree of $\Im$ with initial point at x. When x is not the initial point of $\Im$, we denote by

$\{\mu^s_{\Im}\}$ the Gibbs measure in which the "ancestor" of x has spin s and the configuration on the lower bound of $\Im_x$ (i.e. on $\partial\Im\backslash\{$"ancestor" of $x\}$) is given by Γ.

For two measures on Ω, let μ_1 and μ_2, let us denote the distance in the norm

$$\parallel \mu_1 - \mu_2 \parallel_x = \frac{1}{2}\sum_{i\in\{-1,1\}} \mid \mu_1(\sigma(x)=i) - \mu_2(\sigma(x)=i) \mid .$$

Let $\eta^{x,s}$ be a configuration η with spin at x set at s.

Following [33], we define

$$\kappa \equiv \kappa(\mu) = \sup_{x\in\Gamma^k} \max_{x,s,s'} \parallel \mu^s_{\Im_x} - \mu^{s'}_{\Im_x} \parallel_x,$$

$$\gamma \equiv \gamma(\mu) = \sup_{A\subset\Gamma^k} \max \parallel \mu_A^{\eta^{y,s}} - \mu_A^{\eta^{y,s'}} \parallel_x,$$

where the maximum is taken over all boundary conditions η, all $y \in \partial A$, all neighbors $x \in A$ of vertex y and all spins $s, s' \in \{-1,1\}$.

First, we find the condition for the extremity of the measure μ_0.

Note that κ has a particularly simple formula

$$\kappa = \frac{1}{2}\max \sum_{l\in\{-1,1\}} \mid P_{il} - P_{jl} \mid .$$

Then for κ we get

$$\kappa^{(k)} = \frac{u^{(k)} \mid \theta^4 - 1 \mid}{(\theta^2 u^{(k)} + 1)(\theta^2 + u^{(k)})}.$$

Now, similar to the work ([33], p. 15), we will look for an estimate for γ, in the following form:

$$\gamma = \max\{\parallel \mu_A^{\eta^{y,1}} - \mu_A^{\eta^{y,-1}} \parallel_x\},$$

where

$$\parallel \mu_A^{\eta^{y,1}} - \mu_A^{\eta^{y,-1}} \parallel_x = \frac{1}{2}\sum_{s\in\{-1,1\}} \mid \mu_A^{\eta^{y,1}}(\sigma(x)=s) - \mu_A^{\eta^{y,0}}(\sigma(x)=s) \mid .$$

Then for γ, we also have

$$\gamma^{(k)} = \frac{u^{(k)} \mid \theta^4 - 1 \mid}{(\theta^2 u^{(k)} + 1)(\theta^2 + u^{(k)})}.$$

First, we check the condition of extremity of the measure $\mu_1^{(k)}$ corresponding to the solution $(u_1^{(k)}, u_1^{(k)}) = (1,1)$.

Now let's check the condition of extreme measures: $k\kappa^{(k)}\gamma^{(k)} < 1$, i.e.

$$k \cdot \left(\frac{u^{(k)} \mid \theta^4 - 1 \mid}{(\theta^2 u^{(k)} + 1)(\theta^2 + u^{(k)})}\right)^2 < 1.$$

Remark 7. Note that $\kappa^{(k)}\gamma^{(k)} = \left(s_2^{(k)}\right)^2$.

For the solution under consideration, this inequality will take the form:

$$k \cdot \left(\frac{\theta^2 - 1}{\theta^2 + 1}\right)^2 < 1. \tag{23}$$

By solving inequality (23), one comes to the following theorem.

Theorem 7. *Let $k \geq 2$. Then for the DNA-Ising molecule model the measure μ_1 at*

$$\theta \in \left(\sqrt{\frac{\sqrt{k}-1}{\sqrt{k}+1}}; \sqrt{\frac{\sqrt{k}+1}{\sqrt{k}-1}}\right)$$

is extreme.

Remark 8. Note that, in comparison with the work [9], in the present work we also study extremality problems for these measures.

Now let us check the condition of extremity of the measures $\mu_2^{(k)}$, $\mu_3^{(k)}$ for $k = 2$, corresponding to the solutions $(u_2^{(2)}, u_2^{(2)})$, $(u_3^{(2)}, u_3^{(2)})$. Now let us check the condition of the extreme measure: $2\kappa^{(2)}\gamma^{(2)} < 1$. For solutions $(u_2^{(2)}, u_2^{(2)})$ and $(u_3^{(2)}, u_3^{(2)})$ this inequality will take the form:

$$2 \cdot \left(\frac{u_{2,3}^{(2)}(\theta^4 - 1)}{(\theta^2 u_{2,3}^{(2)} + 1)(\theta^2 + u_{2,3}^{(2)})}\right)^2 < 1. \tag{24}$$

In (24), substituting our expressions $u_{2,3}^{(2)}$ and reducing them, we get

$$2 \cdot \left(\frac{1}{\theta^2 - 1} \right)^2 < 1. \tag{25}$$

For $\theta > \sqrt{3}$ the above inequality is satisfied. It follows that in the case $k = 2$ the condition of extremity of the measures $\mu_2^{(k)}$ and $\mu_3^{(k)}$ is satisfied, where they exist.

Now let us check the condition of extremity of the measures $\mu_2^{(k)}$, $\mu_3^{(k)}$ for $k = 3$, corresponding to the solutions $(u_2^{(3)}, u_2^{(3)})$, $(u_3^{(3)}, u_3^{(3)})$.

Now let us check the condition of the extreme measure: $3\kappa^{(3)}\gamma^{(3)} < 1$. For solutions $(u_2^{(3)}, u_2^{(3)})$ and $(u_3^{(3)}, u_3^{(3)})$ this inequality will take the form:

$$3 \cdot \left(\frac{u_{2,3}^{(3)}(\theta^4 - 1)}{(\theta^2 u_{2,3}^{(3)} + 1)(\theta^2 + u_{2,3}^{(3)})} \right)^2 < 1. \tag{26}$$

In (26), substituting our expressions $u_{2,3}^{(3)}$ and reducing them, we get

$$3 \cdot \left(\frac{1}{\theta^4 - 1} \right)^2 < 1. \tag{27}$$

For $\theta > \sqrt{2}$ the above inequality is satisfied. It follows that in the case $k = 3$, the condition of extremity of the measures $\mu_2^{(k)}$ and $\mu_3^{(k)}$ is satisfied, where they exist.

We check the condition of extremity of the measures $\mu_2^{(k)}$, $\mu_3^{(k)}$ for $k = 4$, corresponding to the solutions $(u_2^{(4)}, u_2^{(4)})$, $(u_3^{(4)}, u_3^{(4)})$. Now let us check the condition of the extreme measure: $4\kappa^{(4)}\gamma^{(4)} < 1$. For solutions $(u_2^{(4)}, u_2^{(4)})$ and $(u_3^{(4)}, u_3^{(4)})$ this inequality will take the form:

$$4 \cdot \left(\frac{u_{2,3}^{(4)}(\theta^4 - 1)}{(\theta^2 u_{2,3}^{(4)} + 1)(\theta^2 + u_{2,3}^{(4)})} \right)^2 < 1. \tag{28}$$

This inequality is valid for all values of $\theta > 1.187$ (see Fig. 1). Consequently, in the case $k = 4$ the condition of extremity of the measures $\mu_2^{(k)}$ and $\mu_3^{(k)}$ is satisfied for any values of $\theta > \sqrt{\frac{5}{3}}$, i.e. in the domain of existence of these measures.

Now let us check the condition of extremity of the measures $\mu_2^{(k)}$, $\mu_3^{(k)}$ for $k = 5$, corresponding to the solutions $(u_2^{(5)}, u_2^{(5)})$, $(u_3^{(5)}, u_3^{(5)})$. We check the condition of the extreme measure: $5\kappa^{(5)}\gamma^{(5)} < 1$. For solutions $(u_2^{(5)}, u_2^{(5)})$ and $(u_3^{(5)}, u_3^{(5)})$ this inequality will take the form:

$$5 \cdot \left(\frac{u_{2,3}^{(5)}(\theta^4 - 1)}{(\theta^2 u_{2,3}^{(5)} + 1)(\theta^2 + u_{2,3}^{(5)})} \right)^2 < 1. \tag{29}$$

This inequality is valid for all values of $\theta > 1.136$ (see Fig. 1). Consequently, in the case $k = 5$ the condition of extremity of the measures $\mu_2^{(k)}$ and $\mu_3^{(k)}$ is satisfied for any values of $\theta > \sqrt{\frac{3}{2}}$, i.e. in the domain of existence of these measures. Thus, we have proven the following theorem.

Theorem 8. *Let* $k \in \{2, 3, 4, 5\}$. *Then for the DNA-Ising molecule model with* $\theta > \theta_{cr} = \sqrt{\frac{k+1}{k-1}}$ *the measures* $\mu_2^{(k)}$ *and* $\mu_3^{(k)}$ *are extreme.*

From this theorem, using the methods of work [3], it is easy to prove the following theorem.

Theorem 9. *Let* $k \in \{2, 3, 4, 5\}$. *Then for the DNA-Ising molecule model with* $\theta > \theta_{cr} = \sqrt{\frac{k+1}{k-1}}$ *there exists a continuum of Gibbs measures that are not translation-invariant.*

6. Conclusion

In this study, we have investigated the thermodynamic properties of the DNA-like system using the Ising model applied to a nano-scale system. The results presented in this paper have direct implications for biophysics, particularly in DNA studies. The Ising-like representation allows us to model the stability of DNA under thermal fluctuations, which is crucial for applications in molecular biology, nanotechnology, and genetic sequencing. Specifically, the phase diagrams obtained (Fig. 1) demonstrate how external parameters influence DNA stability, offering insights into experimental DNA denaturation curves.

Future work could extend this study by incorporating sequence heterogeneity and external factors such as ionic strength and molecular crowding, which are known to influence DNA stability. Furthermore, experimental validation of these theoretical predictions would help bridge the gap between computational models and real biological systems.

In summary, our study contributes to the theoretical understanding of DNA stability and denaturation by utilizing an adapted Ising model approach. This work not only refines theoretical predictions but also offers a foundation for future experimental and computational studies in DNA biophysics.

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