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THERMODYNAMICS AND HOLLIDAY JUNCTIONS OF THE DNA-POTTS MODEL FOR UNORDERED TRANSLATION-INVARIANT GIBBS MEASURES

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Abstract: *In this paper, DNA is modeled using a 4-state Potts model on a path of a Cayley tree. We introduce a Hamiltonian based on a 5-state Potts model with spin values and where 0 represents a vacant position. We investigate unordered translation-invariant Gibbs measures (UTIGMs) on a Cayley tree of order 5 and establish a unique critical temperature. For, there is one UTIGM; for, there are two; and for, there are three. These measures describe different phases of the DNA system. Finally, we study Holliday junction distributions and present their stationary distributions and typical configurations at very low temperatures.*$0, \pm 1, \pm 2, T_{cr} T < T_{cr} T = T_{cr} T > T_{cr}$

Keywords: *Cayley tree, Holliday junction, Potts model, Gibbs measure, phase transition.*

TARTIBLANMAGAN, SILJISHGA NISBATAN INVARIANT GIBBS O‘LCHOVLARI UCHUN DNK–POTTS MODELINING TERMODINAMIKASI VA HOLLIDAY BIRIKMALARI

Annotatsiya: *Ushbu maqolada DNK Cayley daraxtining bir yo‘li bo‘ylab 4 holatli Potts modeli yordamida modellashtiriladi. Biz spin qiymatlari* $0, \pm 1$ *va* ± 2 *bo‘lgan 5 holatli Potts modeliga asoslangan gamiltonian kiritamiz, bunda* 0 *bo‘sh pozitsiyani ifodalaydi. Biz tartiblanmagan, siljishga nisbatan invariant Gibbs o‘lchovlarini (UTIGM) tartibi 5 bo‘lgan Cayley daraxtida tadqiq qilamiz va yagona kritik harorat* T_{cr} *mavjudligini aniqlaymiz.* $T < T_{cr}$ *bo‘lganda bitta UTIGM mavjud;* $T = T_{cr}$ *bo‘lganda ikkita;* $T > T_{cr}$ *bo‘lganda esa uchta UTIGM mavjud bo‘ladi. Ushbu o‘lchovlar DNK tizimining turli fazalarini tavsiflaydi. Nihoyat, biz Holliday birikmalarining taqsimotlarini o‘rganamiz hamda juda past haroratlarda ularning statsionar taqsimotlari va tipik konfiguratsiyalarini taqdim etamiz.*

Kalit so‘zlar: *Keli daraxti, Holliday birikmasi, Potts modeli, Gibbs o‘lchovi, fazaviy o‘tish.*

ТЕРМОДИНАМИКА И СОЕДИНЕНИЯ ХОЛЛИДЕЯ В МОДЕЛИ ДНК-ПОТТСА ДЛЯ НЕУПОРЯДОЧЕННЫХ ТРАНСЛЯЦИОННО-ИНВАРИАНТНЫХ МЕР ГИББСА

Аннотация: *В данной работе ДНК моделируется с использованием модели Поттса с 4 состояниями на пути дерева Кэли. Мы вводим гамильтониан, основанный на модели Поттса с 5 состояниями, со значениями спина и, где обозначает вакантную позицию. Мы исследуем неупорядоченные трансляционно-инвариантные меры Гиббса (UTIGMs) на дереве Кэли порядка 5 и устанавливаем существование единственной критической температуры. При существует одна мера UTIGM; при — две; а при — три. Эти меры описывают различные фазы системы ДНК. Наконец, мы исследуем распределения соединений Холлидея и представляем их стационарные распределения и типичные конфигурации при очень низких температурах.*$0, \pm 1 \pm 20 T_{cr} T < T_{cr} T = T_{cr} T > T_{cr}$

Ключевые слова: *Дерево Кэли, соединение Холлидея, модель Поттса, мера Гиббса, фазовый переход.*

Introduction. It is known that each molecule of DNA is a double helix formed from two complementary strands of nucleotides held together by hydrogen bonds between and base pairs [1], where cytosine (C), guanine (G), adenine (A), and thymine (T).$G - CA - T$

A Holliday junction [2] is a branched nucleic acid structure consisting of four double-stranded arms joined together. It is formed during processes like DNA replication or repair, particularly during genetic recombination. The structure plays a crucial role in the crossing-over process, where two DNA strands exchange segments. The arms of the Holliday junction can adopt different conformations depending on external factors, such as the salt concentration in the buffer or the sequence of nucleotides near the junction.

At the microscopic level, DNA structure can be described using methods from statistical physics [3]. In this framework, a DNA strand is modeled as a stochastic system of interacting bases exhibiting long-range correlations. Such an approach establishes an important relationship between temperature and the structural organization of DNA. In particular, phase transitions in the corresponding statistical model can be interpreted as conformational or topological transformations of the molecule.

Among the models widely used in statistical physics [4], the Potts model with q states occupies a prominent place [5]. Introduced as a generalization of the Ising model to systems with more than two states, the Potts model possesses a rich mathematical structure, making it suitable for capturing complex interactions in multi-state systems.

Recent developments in statistical physics have significantly advanced the study of thermodynamic properties of DNA-based models. In particular, Holliday junctions between DNA molecules have been investigated within the frameworks of the Ising, Potts, and Blume–Capel models on the Cayley tree (see [6]–[7]). In [8], the Potts model was specifically adapted to describe a DNA molecule and to analyze its thermodynamic behavior. The UTIGMs for a system of DNA molecules on the Cayley tree were examined, and it was shown that their number may reach up to thirteen, depending on the temperature. Furthermore, the statistical properties of Holliday junctions and DNA branching structures were studied via the Markov chains associated with these UTIGMs. In particular, the stationary distributions and typical configurations of Holliday junctions were explicitly characterized in the low-temperature regime.

In this paper, we construct new UTIGMs for a system of DNA molecules modeled by the Potts model on a Cayley tree of order. In [9], this model was investigated for, where the uniqueness of the TIGM was established for. It was also shown that for, the number of UTIGMs does not exceed three. Using the obtained Gibbs measures, we analyze the thermodynamic behavior of the system. In particular, we describe the stationary distributions and typical configurations of Holliday junctions in both the high- and low-temperatures. This paper extends the results presented in [9], in which the collection of DNAs is analyzed as configurations of the Potts model defined on a Cayley tree.$k = 5k \geq 2k = 2,3,4k > 4$

In the article [10], the Holliday junctions and the extremality problem on the Cayley tree of order are studied for the DNA-Ising molecule model.$k \geq 2$

In this model, we consider a set of DNAs arranged along the edges of a Cayley tree. Let be an edge of the tree, and assign to it a function that assumes one of the five values, analogous to spin variables in statistical mechanics. The case means that the edge does not belong to any DNA strand (that is, it is empty). The remaining values correspond to the following pairings:$l\sigma(l)0, \pm 1, \pm 2\sigma(l) = 0l$

$$-1 = A - T,\ 1 = T - A,\ -2 = C - G,\ 2 = G - C.$$

If the edge lies between two DNA strands, then the condition indicates that these two DNAs are linked through a Holliday junction.$l\sigma(l) \neq 0$

1. Preliminaries.

We recall certain definitions following [6].

A Cayley tree of order is an infinite tree (that is, a graph without cycles) in which each vertex is incident to exactly edges. We denote, where is the set of vertices, is the set of edges, and is the incidence mapping that assigns to every edge its pair of endpoints. If, then the vertices and are said to be nearest neighbors, and the edge connecting them is written as.$\mathfrak{T}^k k \geq 1k + 1\mathfrak{T}^k = (V, L, i)VLil \in Lx, y \in Vi(l) = \{x, y\}xyl = \langle x, y\rangle$

For fixed we set,$x^0 \in VW_n = \{x \in V: d(x^0, x) = n\}$

$$V_n = \{x \in V: d(x^0, x) \leq n\}, L_n = \{l = \langle x, y\rangle \in L \mid x, y \in V_n\}\ (1.1).$$

where is the distance between vertices and on the Cayley tree, i.e. the number of edges of the shortest path connecting vertices and: $d(x, y)xyxyd(x, y) = \min\{d \mid \exists\, x = x_0, x_1, \ldots, x_{d-1}, x_d = y \in V \text{ such that } \langle x_0, x_1\rangle, \ldots, \langle x_{d-1}, x_d\rangle\}.$

Let. According to [11], the vertices of the Cayley tree admit a decomposition into equivalence classes indexed by integers. In addition, for every vertex belonging to the -th class, there exists exactly one infinite path passing through it such that the sequence of class indices encountered along this path is bi-infinite and has the form. Such a path is called a.$\mathbb{Z} = \{\ldots, -2, -1, 0, 1, 2, \ldots\}m \ldots, m-2, m-1, m, m+1, m+2, \ldots \mathbb{Z} - path$

Let be a set of edges of the Cayley tree. We define a function that assigns to each edge a value.$L\sigma l \in L\sigma(l) \in \{-2,-1,0,1,2\}$

A configuration on the edges of the Cayley tree is given by where the mapping assigns to each edge a value from the set. The collection of all such configurations on is denoted by. In the same way, configurations restricted to the subset are defined. The set of all configurations on is denoted by.$\sigma = \{\sigma(l), l \in L\} l \in L\{-2,-1,0,1,2\} L\Omega L_n \subset LL_n\Omega_n$

A configuration is called admissible if for every. Below, we consider DNAs that are restrictions of the admissible configuration on the.$\sigma = \{\sigma(l), l \in L\}\sigma(l) \neq 0 l \in \mathbb{Z} - path\mathbb{Z} - path$

We consider the Potts model describing the energy of a configuration for a system of DNA molecules [12]:σ

$$H(\sigma) = J \sum_{l,t \in L \times L} \delta_{\sigma(l),\sigma(t)}, \quad (1.2)$$

here, is the coupling constant, is the Kronecker delta,, and indicates that and are nearest-neighbor edges, meaning they share a common vertex.$J > 0 \delta\sigma(l) \in \{-2,-1,0,1,2\}\langle l,t\rangle lt$

We also define

$$E_n = \{\langle x,y\rangle \in L : x \in W_{n-1}, y \in W_n\}.$$

For, we introduce the notation$l \in E_{n-1}$

$$S(l) = \{t \in E_n : \langle l,t\rangle\}.$$

It is easy to observe that

$$S(l) \cap \mathbb{Z} - path = \begin{cases} \{l_0, l_1\} \subset L, & \text{if } l \notin \mathbb{Z} - path, \\ \{l_1\} \subset L, & \text{if } l \in \mathbb{Z} - path. \end{cases}$$

We define

$$S_0(l) = S(l) \setminus \{l_0, l_1\}, \quad \text{if } l \notin \mathbb{Z} - path,$$
$$S_1(l) = S(l) \setminus \{l_1\}, \quad \text{if } l \in \mathbb{Z} - path.$$

In [8], it was shown that analyzing Gibbs measures for the Potts model can be reduced to solving a system of the following functional equations:

if, then$l \notin \mathbb{Z} - path$

$$\begin{cases} u_{-1,l} = \prod_{i=0}^{1} \frac{1+\alpha v_{-1,l_i}+v_{1,l_i}+v_{2,l_i}}{\alpha+v_{-1,l_i}+v_{1,l_i}+v_{2,l_i}} \prod_{t \in S_0(l)} \frac{1+\alpha u_{-1,t}+u_{0,t}+u_{1,t}+u_{2,t}}{\alpha+u_{-1,t}+u_{0,t}+u_{1,t}+u_{2,t}}, \\ u_{0,l} = \prod_{i=0}^{1} \frac{1+v_{-1,l_i}+v_{1,l_i}+v_{2,l_i}}{\alpha+v_{-1,l_i}+v_{1,l_i}+v_{2,l_i}} \prod_{t \in S_0(l)} \frac{1+u_{-1,t}+\alpha u_{0,t}+u_{1,t}+u_{2,t}}{\alpha+u_{-1,t}+u_{0,t}+u_{1,t}+u_{2,t}}, \\ u_{1,l} = \prod_{i=0}^{1} \frac{1+v_{-1,l_i}+\alpha v_{1,l_i}+v_{2,l_i}}{\alpha+v_{-1,l_i}+v_{1,l_i}+v_{2,l_i}} \prod_{t \in S_0(l)} \frac{1+u_{-1,t}+u_{0,t}+\alpha u_{1,t}+u_{2,t}}{\alpha+u_{-1,t}+u_{0,t}+u_{1,t}+u_{2,t}}, \\ u_{2,l} = \prod_{i=0}^{1} \frac{1+v_{-1,l_i}+v_{1,l_i}+\alpha v_{2,l_i}}{\alpha+v_{-1,l_i}+v_{1,l_i}+v_{2,l_i}} \prod_{t \in S_0(l)} \frac{1+u_{-1,t}+u_{0,t}+u_{1,t}+\alpha u_{2,t}}{\alpha+u_{-1,t}+u_{0,t}+u_{1,t}+u_{2,t}}. \end{cases} \quad (1.3)$$

if, then$l \in \mathbb{Z} - path$

$$\begin{cases} v_{-1,l} = \frac{1+\alpha v_{-1,l_1}+v_{1,l_1}+v_{2,l_1}}{\alpha+v_{-1,l_1}+v_{1,l_1}+v_{2,l_1}} \prod_{t \in S_0(l)} \frac{1+\alpha u_{-1,t}+u_{0,t}+u_{1,t}+u_{2,t}}{\alpha+u_{-1,t}+u_{0,t}+u_{1,t}+u_{2,t}}, \\ v_{1,l} = \frac{1+v_{-1,l_1}+\alpha v_{1,l_1}+v_{2,l_1}}{\alpha+v_{-1,l_1}+v_{1,l_1}+v_{2,l_1}} \prod_{t \in S_0(l)} \frac{1+u_{-1,t}+u_{0,t}+\alpha u_{1,t}+u_{2,t}}{\alpha+u_{-1,t}+u_{0,t}+u_{1,t}+u_{2,t}}, \\ v_{2,l} = \frac{1+v_{-1,l_1}+v_{1,l_1}+\alpha v_{2,l_1}}{\alpha+v_{-1,l_1}+v_{1,l_1}+v_{2,l_1}} \prod_{t \in S_0(l)} \frac{1+u_{-1,t}+u_{0,t}+u_{1,t}+\alpha u_{2,t}}{\alpha+u_{-1,t}+u_{0,t}+u_{1,t}+u_{2,t}}. \end{cases} \quad (1.4)$$

Here,.$\alpha = exp(J\beta)$

For any set of vectors

$$z = \{(u_{i,l}, i = -1,0,1,2, l \notin \mathbb{Z} - path), (v_{j,t}, j = -1,0,1,2, t \in \mathbb{Z} - path)\},$$

If the variables satisfy the system of functional equations (1.3) and (1.4), then there exists a unique Gibbs measure, and conversely, each Gibbs measure corresponds to a solution of these equations. However, solving Equations (1.3) and (1.4) explicitly is generally difficult. Some particular solutions are presented in the next section.μ

1. UTIGM of the set of DNA molecules.

In this section, for the case, we find new solutions of the system of functional equations (1.3) and (1.4) that are independent of, i.e.,$J = 1z_l l$

$$u_{i,l} = u_i \quad \forall l \notin \mathbb{Z} - \text{path}, \quad v_{j,l} = v_j \quad \forall l \in \mathbb{Z} - \text{path}.$$

The Gibbs measure associated with a solution of this type is referred to as translation-invariant. From the system of equations (1.3) and (1.4), one can derive explicit expressions for the variables and.$u_i v_j$

$$\begin{cases} u_{-1} = \left(\frac{1+\alpha v_{-1}+v_1+v_2}{\alpha+v_{-1}+v_1+v_2}\right)^2 \left(\frac{1+\alpha u_{-1}+u_0+u_1+u_2}{\alpha+u_{-1}+u_0+u_1+u_2}\right)^{k-2}, \\ u_0 = \left(\frac{1+v_{-1}+v_1+v_2}{\alpha+v_{-1}+v_1+v_2}\right)^2 \left(\frac{1+u_{-1}+\alpha u_0+u_1+u_2}{\alpha+u_{-1}+u_0+u_1+u_2}\right)^{k-2}, \\ u_1 = \left(\frac{1+v_{-1}+\alpha v_1+v_2}{\alpha+v_{-1}+v_1+v_2}\right)^2 \left(\frac{1+u_{-1}+u_0+\alpha u_1+u_2}{\alpha+u_{-1}+u_0+u_1+u_2}\right)^{k-2}, \\ u_2 = \left(\frac{1+v_{-1}+v_1+\alpha v_2}{\alpha+v_{-1}+v_1+v_2}\right)^2 \left(\frac{1+u_{-1}+u_0+u_1+\alpha u_2}{\alpha+u_{-1}+u_0+u_1+u_2}\right)^{k-2}, \\ v_{-1} = \frac{1+\alpha v_{-1}+v_1+v_2}{\alpha+v_{-1}+v_1+v_2}\left(\frac{1+\alpha u_{-1}+u_0+u_1+u_2}{\alpha+u_{-1}+u_0+u_1+u_2}\right)^{k-1}, \\ v_1 = \frac{1+v_{-1}+\alpha v_1+v_2}{\alpha+v_{-1}+v_1+v_2}\left(\frac{1+u_{-1}+u_0+\alpha u_1+u_2}{\alpha+u_{-1}+u_0+u_1+u_2}\right)^{k-1}, \\ v_2 = \frac{1+v_{-1}+v_1+\alpha v_2}{\alpha+v_{-1}+v_1+v_2}\left(\frac{1+u_{-1}+u_0+u_1+\alpha u_2}{\alpha+u_{-1}+u_0+u_1+u_2}\right)^{k-1} \end{cases} \quad (2.1)$$

where. Under the assumption that, we have.$u_i, v_j > 0 J = 1 \alpha > 1$

The case and the following equation obtained from the second equation of system (2.1) were considered in [9]:$v_{-1} = v_1 = v_2 = u_{-1} = u_1 = u_2 = 1$

$$\left(\frac{4+\alpha u_0}{\alpha+3+u_0}\right)^{k-2} = \left(\frac{\alpha+3}{4}\right)^2 u_0 (2.2).$$

We note that at, the solutions of the equation (2.2) and the general statements for were found in [9].$k = 2,3,4 k \geq 5$

Let consider the case at. Then for Eq. (2.2), the following lemma holds.$k = 5$

Lemma 2.1. Let,, and. Then for the equation (2.2) the following assertions hold:$\alpha_{cr} \approx 8.252 u_0 > 0 k = 5 \alpha > 1$

The equation has one solution if.$\alpha < \alpha_{cr}$

The equation has two solutions if.$\alpha = \alpha_{cr}$

The equation has three solutions if.$\alpha > \alpha_{cr}$

Proof. If we give the notation, we then obtain the equation$x = \sqrt[3]{u_0}$

$$\left(\frac{\alpha+3}{4}\right)^{\frac{2}{3}} x^4 - \alpha x^3 + (\alpha+3)\left(\frac{\alpha+3}{4}\right)^{\frac{2}{3}} x - 4 = 0.$$

Let us get the function

$$f(x) = \left(\frac{\alpha+3}{4}\right)^{\frac{2}{3}} x^4 - \alpha x^3 + (\alpha+3)\left(\frac{\alpha+3}{4}\right)^{\frac{2}{3}} x - 4.$$

It is easy to see that and. Thus, the equation has at least one positive solution. Furthermore, it follows from the known Descartes theorem on the number of positive roots of a polynomial that this equation has at most three positive solutions.$f(0) < 0 f(1) > 0 f(x) = 0$

We now find the discriminant of the equation (2.3):

$$D(\alpha) = \frac{g(\alpha)}{(\alpha+3)^3},$$

where.$g(\alpha) = 37\alpha^8 + 312\alpha^7 - 660\alpha^6 - 18936\alpha^5 - 167874\alpha^4 + 131976\alpha^3 + 544940\alpha^2 - 718152\alpha - 2536443$

Using the Maple program, equation has one positive solution at (Fig. 1).$D(\alpha) = 0 \alpha = \alpha_{cr}$

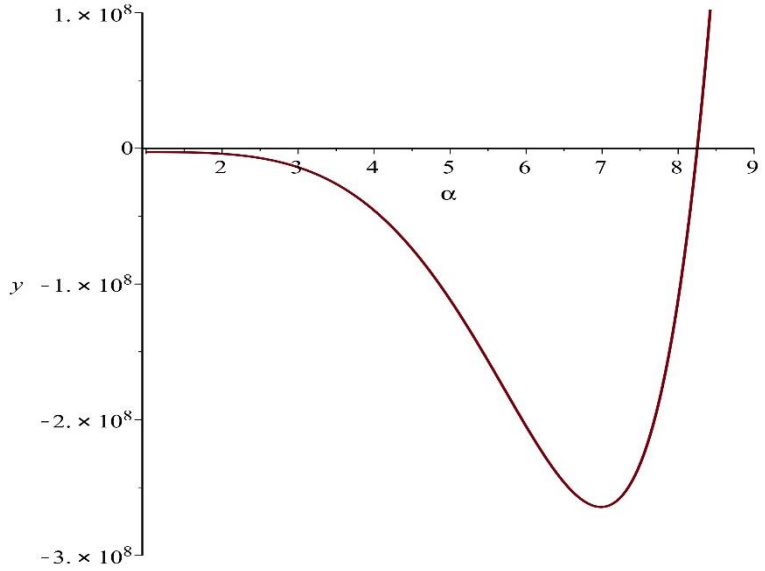


Figure 1. The graph of the function.$g(\alpha)$

The equation has one positive solution. According to the discriminant of the polynomial equation of degree four, the discriminant is zero if and only if at least two roots are equal at. If the coefficients are real numbers and the discriminant is negative, then there are two real roots and two complex conjugate roots at. Conversely, if the discriminant is positive, then the roots are all real at.$D(\alpha) = 0 \alpha = \alpha_{cr} \alpha < \alpha_{cr} \alpha > \alpha_{cr}$

We introduce the notations

$$p = -2^{\frac{4}{3}}\left(\frac{1}{\alpha+3}\right)^{\frac{2}{3}}(\alpha^2+3\alpha-16), \quad q = -\frac{(\alpha^2-2\alpha+9)(\alpha^2+14\alpha+9)}{(\alpha+3)^2},$$

$$y = \sqrt[3]{-\frac{q}{2} + \sqrt{\frac{q^2}{4} + \frac{p^3}{27}}} + \sqrt[3]{-\frac{q}{2} - \sqrt{\frac{q^2}{4} + \frac{p^3}{27}}},$$

$$A = \left(\frac{\alpha^2}{4}\left(\frac{4}{\alpha+3}\right)^{\frac{4}{3}} + y\right), \quad C = \left(\frac{y^2}{4} + 4\left(\frac{4}{\alpha+3}\right)^{\frac{2}{3}}\right).$$

In accordance with the Ferrari formula, we can find solutions of this equation through the following formulas:

$$x_1 = \frac{\frac{\alpha}{2}\left(\frac{4}{\alpha+3}\right)^{\frac{2}{3}} - \sqrt{A} + \sqrt{\left(\sqrt{A} - \frac{\alpha}{2}\left(\frac{4}{\alpha+3}\right)^{\frac{2}{3}}\right)^2 - 4\left(\frac{y}{2} - \sqrt{C}\right)}}{2},$$

$$x_2 = \frac{\frac{\alpha}{2}\left(\frac{4}{\alpha+3}\right)^{\frac{2}{3}} + \sqrt{A} - \sqrt{\left(\sqrt{A} + \frac{\alpha}{2}\left(\frac{4}{\alpha+3}\right)^{\frac{2}{3}}\right)^2 - 4\left(\frac{y}{2} + \sqrt{C}\right)}}{2},$$

$$x_3 = \frac{\frac{\alpha}{2}\left(\frac{4}{\alpha+3}\right)^{\frac{2}{3}} + \sqrt{A} + \sqrt{\left(\sqrt{A} + \frac{\alpha}{2}\left(\frac{4}{\alpha+3}\right)^{\frac{2}{3}}\right)^2 - 4\left(\frac{y}{2} + \sqrt{C}\right)}}{2}.$$

For, we then have the unique positive solution of equation (2.2):$\alpha < \alpha_{cr}$

$$u_0^{(1)} = x_1^3 \ (2.4)$$

At we get two positive solutions of equation (2.2):$\alpha = \alpha_{cr}$

$$u_0^{(1)} = x_1^3,$$
$$u_0^{(2)} = x_2^3.$$

where the values, are the positive solutions of equation (2.3).$x_1 \approx 0.18 x_2 \approx 2.728$

For we can obtain three positive solutions of equation (2.2):$\alpha > \alpha_{cr}$

$$\begin{cases} u_0^{(1)} = x_1^3, \\ u_0^{(2)} = x_2^3, \ (2.6) \\ u_0^{(3)} = x_3^3. \end{cases}$$

where the values $x_1, x_2, x_3$are the positive solutions of equation (2.3).

The statement of the lemma now follows. The lemma is proved.

We let denote the Gibbs measures corresponding to the solutions of system of equations (2.1) in the case. We call such measures unordered translation-invariant Gibbs measures (UTIGMs) because almost all coordinates of the solution of the corresponding measure are equal to unity.$\mu_i, i = 1,2,3 v_{-1} = v_1 = v_2 = u_{-1} = u_1 = u_2 = 1$

Define critical temperatures

$$T_{cr} = \frac{1}{\ln \alpha_{cr}^*}.$$

Summarizing the results discussed above, we can state the following theorem.

Theorem 2.1. For DNA model (1.2) on the Cayley tree of order, the following statements hold.$k = 5$

If the temperature, then there exists a unique UTIGM.$T < T_{cr} \mu_1$

If, then there are two UTIGMs.$T = T_{cr} \mu_1, \mu_2$

If, then there are three UTIGMs.$T > T_{cr} \mu_1, \mu_2, \mu_3$

Remark 2.1. We note that other TIGMs can exist in addition to the case. In contrast to [9], where the case was studied in a general framework, this paper focuses on. In this setting, we obtain an explicit description of translation-invariant Gibbs measures and determine the critical parameter (and), together with a refined characterization of the associated Markov chains describing Holliday junction distributions.$v_{-1} = v_1 = v_2 = u_{-1} = u_1 = u_2 = 1 k \geq 2 k = 5 \alpha^* T_c$

3. Markov chains corresponding to UTIGMs and the Holliday junction between DNA molecules.

To investigate the thermodynamics of Holliday junctions in the DNA molecule, it is enough to learn Markov chains on the subtree consisting of edges not lying on the $\mathbb{Z}$-path and the Markov chains on the $\mathbb{Z}$-path. In [10], these two Markov chains were defined as

$$\mathbb{P}_{(5\to5)}^{[l,t]} = \begin{pmatrix} \frac{\alpha}{Z_1} & \frac{u_{-1}}{\alpha u_{-1}} & \frac{u_0}{Z_1} & \frac{u_1}{Z_1} & \frac{u_2}{Z_1} \\ \frac{1}{Z_2} & \frac{Z_2}{u_{-1}} & \frac{Z_2}{u_0} & \frac{Z_2}{u_1} & \frac{Z_2}{u_2} \\ \frac{1}{Z_3} & \frac{u_{-1}}{Z_3} & \frac{u_0}{Z_3} & \frac{u_1}{Z_3} & \frac{u_2}{Z_3} \\ \frac{1}{Z_4} & \frac{u_{-1}}{Z_4} & \frac{u_0}{Z_4} & \frac{u_1}{Z_4} & \frac{u_2}{Z_4} \\ \frac{1}{Z_5} & \frac{u_{-1}}{Z_5} & \frac{u_0}{Z_5} & \frac{u_1}{Z_5} & \frac{u_2}{Z_5} \end{pmatrix}, \; l,t \notin \mathbb{Z}\text{-path},$$

where

$$Z_1 = \alpha + u_{-1} + u_0 + u_1 + u_2,\; Z_2 = 1 + \alpha u_{-1} + u_0 + u_1 + u_2,$$
$$Z_3 = 1 + u_{-1} + \alpha u_0 + u_1 + u_2,$$
$$Z_4 = 1 + u_{-1} + u_0 + \alpha u_1 + u_2,\; Z_5 = 1 + u_{-1} + u_0 + u_1 + \alpha u_2.$$

$$\mathbb{P}_{(4\to4)}^{[l,t]} = \begin{pmatrix} \frac{\alpha}{Y_1} & \frac{v_{-1}}{Y_1} & \frac{v_1}{Y_1} & \frac{v_2}{Y_1} \\ \frac{1}{Y_2} & \frac{\alpha v_{-1}}{Y_2} & \frac{v_1}{Y_2} & \frac{v_2}{Y_2} \\ \frac{1}{Y_3} & \frac{v_{-1}}{Y_3} & \frac{\alpha v_1}{Y_3} & \frac{v_2}{Y_3} \\ \frac{1}{Y_4} & \frac{v_{-1}}{Y_4} & \frac{v_1}{Y_4} & \frac{\alpha v_2}{Y_4} \end{pmatrix}, \; l,t \notin \mathbb{Z}\text{-path}.$$

Here

$$Y_1 = \alpha + v_{-1} + v_1 + v_2,\; Y_2 = 1 + \alpha v_{-1} + v_1 + v_2,$$
$$Y_3 = 1 + v_{-1} + \alpha v_1 + v_2,\; Y_4 = 1 + v_{-1} + v_1 + \alpha v_2.$$

The stationary distributions were also defined as

$$\pi_{(5\to5)} = \left(\pi_{(5\to5),-2}, \pi_{(5\to5),-1}, \pi_{(5\to5),0}, \pi_{(5\to5),1}, \pi_{(5\to5),2}\right)$$

for the matrix: $\mathbb{P}_{(5\to5)}^{[l,t]}$

$$\pi_{(5\to5)} = \frac{1}{N}\begin{pmatrix} \alpha + u_{-1} + u_0 + u_1 + u_2 \\ (1 + \alpha u_{-1} + u_0 + u_1 + u_2)u_{-1} \\ (1 + u_{-1} + \alpha u_0 + u_1 + u_2)u_0 \\ (1 + u_{-1} + u_0 + \alpha u_1 + u_2)u_1 \\ (1 + u_{-1} + u_0 + u_1 + \alpha u_2)u_2 \end{pmatrix}^t,$$

where is the normalization factor and N

$$\pi_{(4\to4)} = \frac{1}{M}\begin{pmatrix} \alpha + v_{-1} + v_1 + v_2 \\ (1 + \alpha v_{-1} + v_1 + v_2)v_{-1} \\ (1 + v_{-1} + \alpha v_1 + v_2)v_1 \\ (1 + v_{-1} + v_1 + \alpha v_2)v_2 \end{pmatrix}^t,$$

here is the normalization factor. M

By applying the ergodic theorem for stochastic matrices (see [20]) together with the formulas derived above, we arrive at the following result.

Theorem 3.1. In the stationary state of the set of DNA molecules, for any, there is no Holliday junction via the edge with the probability (with respect to the measures, corresponding to the solution of system (2.1)) $l \notin \mathbb{Z}\text{-path} l\mu_i,\ i = 1,2,3(u_{-1}, u_0, u_1, u_2)$

$$\pi_{(5\to5),0} = \frac{1}{N}(1 + u_{-1} + \alpha u_0 + u_1 + u_2)u_0.$$

Consequently, the probability that a Holliday junction forms is. We note that the probability can be expressed as a function of the solution of system (2.1) and the temperature. $1 - \pi_{(5\to5),0}\pi_{(5\to5),0}(u_{-1}, u_0, u_1, u_2)$

We now consider the limits of the vectors and of the stationary distributions as (corresponding to and) and as (corresponding to and). To compute these limits, it is necessary to know the explicit form of the solution to system (2.1). However, we have an explicit solution only for, given by formulas (2.4), (2.5), and (2.6). Using this solution, we can calculate the desired limits. $\pi_{(5\to5)}\pi_{(4\to4)} T \to 0 \beta \to \infty \alpha \to \infty T \to +\infty \beta \to 0 \alpha \to 1 k = 5$

Lemma 3.1. The following equalities hold

– The case of low temperature:

$$\lim_{T\to0} \pi^{(1)}_{(5\to5)} = \left(\frac{1}{4}, \frac{1}{4}, 0, \frac{1}{4}, \frac{1}{4}\right), \quad \lim_{T\to0} \pi^{(2)}_{(5\to5)} = (0,0,1,0,0),$$

$$\lim_{T\to0} \pi^{(3)}_{(5\to5)} = (0,0,1,0,0), \quad \lim_{T\to0} \pi^{(i)}_{(4\to4)} = \left(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right), i = 1,2,3.$$

– The case of high temperature:

$$\lim_{T\to+\infty} \pi^{(1)}_{(5\to5)} = \left(\frac{1}{5}, \frac{1}{5}, \frac{1}{5}, \frac{1}{5}, \frac{1}{5}\right),$$

$$\lim_{T\to T_c} \pi^{(1)}_{(5\to5)} = \left(\frac{1}{4}, \frac{1}{4}, 0, \frac{1}{4}, \frac{1}{4}\right),$$

$$\lim_{T\to T_c} \pi^{(i)}_{(5\to5)} = (0.00875, 0.00875, 0.965, 0.00875, 0.00875), i = 1,2,$$

$$\lim_{T\to+\infty} \pi^{(1)}_{(4\to4)} = \lim_{T\to T_{cr}} \pi^{(i)}_{(4\to4)} = \left(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right), i = 1,2,3.$$

Remark 3.1. Unlike in [9] where the measure was unique, extending the model to induces a phase transition, increasing the number of measures up to three. This is highlighted at, where the distribution splits and exhibits a sharply localized asymmetry with a dominant third component (0.965). $k = 5 T \to T_c$

4. Conclusion.

From Lemma 3.1, we deduce the following structural configurations for the set of DNA molecules.

As, the set of DNA molecules approaches the following stationary states (configurations): $T \to 0$

Case of the measure for: All neighboring DNA molecules are connected to each other via Holliday junctions. In this case, the connection occurs through one of the equally probable states for any edge. $\mu_1 k = 5 \sigma(l) \in \{-2, -1, 1, 2\} l \notin \mathbb{Z}\text{-path}$

Case of the measures for: All neighboring DNA molecules remain disconnected, meaning that no Holliday junctions are formed in this situation. $\mu_2, \mu_3 k = 5$

In these cases, the sequence of states along a DNA molecule on the is free; that is, it can be any sequence of independent, identically distributed random variables, each taking the values with equal probability. $\pm 1 \mathbb{Z}\text{-path} \pm 11/4$

As, the set of DNA molecules approaches the following stationary states: $T \to \infty$

Case of the measure for: All neighboring DNA molecules are connected via Holliday junctions with probability. In this case, the connection along an edge occurs through one of the states with probability. $\mu_1 k = 54/5 l \notin \mathbb{Z}\text{-path} \sigma(l) \in \{-2, -1, 1, 2\} 1/5$

In these cases, the sequence of states along a DNA molecule on the is free; that is, it can be any sequence of independent, identically distributed random variables, each occurring with equal probability. $\pm 1, \pm 2 \mathbb{Z}\text{-path} 1/4$

As, the set of DNA molecules attains the following stationary states: $T \to T_{cr}$

Case of the measure at: All neighboring DNA molecules are connected via Holliday junctions. In this situation, the connection occurs through one of the equally probable states for any edge. $\mu_1 k = 5\sigma(l) \in \{-2,-1,1,2\} l \notin \mathbb{Z}$-path

Case of the measures for: All neighboring DNA molecules are disconnected, with Holliday junctions forming with probability. In this case, a connection along an edge occurs through one of the states with probability. $\mu_2, \mu_3 k = 50.035 l \notin \mathbb{Z}$-path$\sigma(l) \in \{-1,1\} 0.00875$

In these cases, the sequence of states along a DNA molecule on the is free; that is, it may be any sequence of independent, identically distributed random variables, each occurring with equal probability. $\pm 1, \pm 2\mathbb{Z}$-path$1/4$

Remark 4.1. Compared to [9], the structural configurations of DNA molecules for exhibit a coexistence of distinct physical phases due to the non-uniqueness of Gibbs measures. Specifically, at low () and critical () temperatures, the system splits into a fully connected Holliday junction network under, and completely disconnected or weakly interacting (probability) molecular states under, which is a novel phenomenon missing in lower-order tree settings. $k = 5T \to 0T \to T_{cr} \mu_1 0.035 \mu_2, \mu_3$

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