NANOSYSTEMS: PHYSICS, CHEMISTRY, MATHEMATICS, 2021, 12 (5), P. 563–568

Holliday junctions in the HC Blume–Capel model in "one case" on DNA

N. M. Khatamov

Institute of mathematics, 4B, St. University, 100174, Tashkent, Uzbekistan

nxatamov@mail.ru

DOI 10.17586/2220-8054-2021-12-5-563-568

We consider a DNA as a configuration of HC Blume–Capel model and embed it on a path of Cayley tree. To study thermodynamic properties of the model of DNAs, we describe the corresponding translation-invariant Gibbs measures (TIGM) of the model on the Cayley tree. It is shown that, for $k \geq 2$, for any temperature $T > 0$ there is a unique TIGM. Using these results, we study the distributions of the Holliday junctions DNA. For very high and very low temperatures, we give stationary distributions and typical configurations of the Holliday junctions.

Keywords: DNA, Cayley tree, Blume–Capel model, Gibbs measure, Holliday junction.

Received: 23 June 2021

Revised: 30 June 2021

1. Introduction and definitions

It is known that each DNA molecule is a double helix formed by two complementary strands of nucleotides held together by hydrogen bonds between $C + G$ and $A + T$ base pairs, where cytosine (C), guanine (G), adenine (A) and thymine (T). The genetic information, stored in an organism's DNA, contains instructions for all proteins the organism will ever synthesize [1].

Holliday junctions [2] are cruciform structures that form during genetic recombination when two double-stranded DNA molecules split into four strands to exchange segments of genetic information.

In articles [3], [4–7] the Ising, Potts and Blume–Capel DNA models were considered in order to study their thermodynamics by Gibbs measures. Note that the non-uniqueness of the Gibbs measure corresponds to phase coexistence in the DNA system. By the properties of Markov chains (corresponding to TIGM) Holliday junctions and DNA branches are studied.

On the Cayley tree, the results for DNA were obtained only for cases $k = 2$. In this paper, the results are obtained for the case $k \geq 2$. For other results on the Blume–Capel model, see [8], [3, 9, 10].

In our model, we consider a set of DNA, as in [4], which "lives" on a tree graph. Suppose that on the edge l of this graph there is a function $\sigma(l)$ with three possible values $-1, 0, 1$ (an analog of the spin values in physical systems) in the case $\sigma(l) = 0$, we say that the edge l doesn't belong to DNA. If this l separates two DNAs, then the value $\sigma(l) = 1$ or $\sigma(l) = -1$ means that the two DNAs have a Holliday junction.

Now, following [4, 5, 12], we recall some definitions.

The Cayley tree Γ^k of order $k \geq 1$ is an infinite tree, i.e., a graph without cycles, such that exactly $k + 1$ edges originate from each vertex. Let $\Gamma^k = (V, L, i)$, where V is the set of vertices Γ^k, L the set of edges and i is the incidence function setting each edge $l \in L$ into correspondence with its endpoints $x, y \in V$. If $i(l) = \{x, y\}$, then, the vertices x and y are called the nearest neighbors, denoted by $l = \langle x, y\rangle$. The distance $d(x, y), x, y \in V$ on the Cayley tree is the number of edges of the shortest path from x to and 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 set $W_n = \{x \in V : d(x^0, x) = n\}$,

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

Let $\mathbb{Z} = \{..., -2, -1, 0, 1, 2, ...\}$. It was proved in [11] that all vertices of a Cayley tree can be partitioned into equivalence classes labeled by integers and that through each vertex belonging to the m-th equivalence class, there passes a unique path such that the labels of the equivalence classes to which successive vertices belong form an integer sequence $..., m-2, m-1, m, m+1, m+2, ...$, which is infinite in both directions. Each such path is called a $\mathbb{Z}$-path.

Let L be the set of edges of the Cayley tree. Consider the function σ, which assigns each edge $l \in L$ to the values $\sigma(l) \in \{-1, 0, 1\}$. The value $\sigma(l) = -1$ (respectively $+1$) means that the edge l is "occupied" $-1 = A + T$ (respectively $1 = C + G$) and $\sigma(l) = 0$ means that l is "vacant".

The configuration $\sigma = \{\sigma(l), l \in L\}$ on edges of the Cayley tree is given by a function from L to $\{-1, 0, 1\}$. The set of all configurations in L is denoted by Ω. Configurations in L_n are defined similarly and the set of all configurations in L_n are denoted by Ω_n.

In the case of a "one case", the configuration $\sigma = \{\sigma(l), l \in L\}$ is called *admissible*, if

1) $\sigma(l) \neq 0$ for any $l \in \mathbb{Z}$-path;
2) $\{\sigma(l), \sigma(t)\} \in \{\{0,0\}, \{0,-1\}, \{0,+1\}, \{-1,0\}, \{-1,+1\}\}$;

The restriction of an admissible configuration on a $\mathbb{Z}$-path is called *a DNA*.

We consider the following Blume–Capel model of energy configuration σ of a DNA set (see [4]):

$$H(\sigma) = J \sum_{\langle l,t\rangle \in L\times L;} (\sigma(l) - \sigma(t))^2, \tag{1}$$

where $J > 0$ is a coupling constant, $\sigma(l) \in \{-1, 0, 1\}$ and $\langle l, t\rangle$ denote the nearest neighboring edges, that is, the edges that have a common endpoint.

Let Ω_n^a (respectively Ω^a) be the set of all admissible configurations on L_n (respectively L).

Let us introduce designations as [4]:

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

$$\Omega_n^{ba} = \text{ the set of admissible configurations on } E_n.$$

For $l \in E_{n-1}$ denote:

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

It is easy to see that:

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

We denote:

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

Let $\widetilde{L}(G)$ be the set of "edge" of G. We define adjacency matrix of G by $A \equiv A^G = (\alpha_{ij})_{i,j=-1,0,+1}$, i.e.:

$$\alpha_{ij} \equiv \alpha_{ij}^G = \begin{cases} 1, & \text{if } \{i, j\} \in \widetilde{L}(G), \\ 0, & \text{if } \{i, j\} \notin \widetilde{L}(G). \end{cases}$$

In a standard way (see [4, 5, 12]), one can reduce the study of the Gibbs measures of the Blume–Capel model to the problem of finding solutions to the following system of functional equations:

$$z_{0,l} = \frac{\alpha_{0,+1}\lambda z_{l_0} + \alpha_{0,-1}\lambda}{a_{-1,+1}\lambda^4 z_{l_0} + \alpha_{-1,-1}} \cdot \frac{\alpha_{0,+1}\lambda z_{l_1} + \alpha_{0,-1}\lambda}{\alpha_{-1,+1}\lambda^4 z_{l_1} + \alpha_{-1,-1}} \cdot \prod_{t\in S_0(l)} \frac{\alpha_{0,+1}\lambda z_{+1,t} + \alpha_{0,-1}\lambda + \alpha_{0,0} z_{0,t}}{\alpha_{-1,+1}\lambda^4 z_{+1,t} + \alpha_{-1,-1} + \alpha_{-1,0}\lambda z_{0,t}},$$
$$l \notin \mathbb{Z}\text{-path},$$
$$z_{1,l} = \frac{\alpha_{+1,+1} z_{l_0} + \alpha_{+1,-1}\lambda^4}{\alpha_{-1,+1}\lambda^4 z_{l_0} + \alpha_{-1,-1}} \cdot \frac{\alpha_{+1,+1} z_{l_1} + \alpha_{+1,-1}\lambda^4}{\alpha_{-1,+1}\lambda^4 z_{l_1} + \alpha_{-1,-1}} \cdot \prod_{t\in S_0(l)} \frac{\alpha_{+1,+1} z_{+1,t} + \alpha_{+1,-1}\lambda^4 + \alpha_{+1,0}\lambda z_{0,t}}{\alpha_{-1,+1}\lambda^4 z_{+1,t} + \alpha_{-1,-1} + \alpha_{-1,0}\lambda z_{0,t}}, \tag{2}$$
$$l \notin \mathbb{Z}\text{-path},$$
$$z_l = \frac{\alpha_{+1,+1} z_l + \alpha_{+1,-1}\lambda^4}{\alpha_{-1,+1}\lambda^4 z_l + \alpha_{-1,-1}} \cdot \prod_{t\in S_1(l)} \frac{\alpha_{+1,+1} z_{+1,t} + \alpha_{+1,-1}\lambda^4 + \alpha_{+1,0}\lambda z_{0,t}}{\alpha_{-1,+1}\lambda^4 z_{+1,t} + \alpha_{-1,-1} + \alpha_{-1,0}\lambda z_{0,t}}, \quad l \in \mathbb{Z}\text{-path},$$

where:

$$\lambda = \exp(-J\beta). \tag{3}$$

Moreover, this means that for any set of vectors $\mathbf{z} = \{(z_{0,l}, z_{1,l}, z_t),\ l \notin \mathbb{Z}\text{-path},\ t \in \mathbb{Z}\text{-path}\}$ satisfying the system of functional equations (2), there exists the only Gibbs measure μ and vice versa. However, analyzing the (2) solutions is not easy. Here are some solutions (2).

2. TIGMs of the set of DNAs

Now, in this section, we find solutions $\mathbf{z}_l$ to the system of functional equations (2), which does not depend on l, i.e.:

$$z_{0,l} = u,\ z_{1,l} = v,\ \forall l \notin \mathbb{Z}\text{-path}; \quad z_l = w, \forall l \in \mathbb{Z}\text{-path}. \tag{4}$$

where $u, v, w > 0$ (by (2)) satisfy:

$$\begin{aligned}
u &= \left(\frac{\alpha_{0,+1}\lambda v + \alpha_{0,-1}\lambda + \alpha_{0,0}u}{\alpha_{-1,+1}\lambda^4 v + \alpha_{-1,-1} + \alpha_{-1,0}\lambda u}\right)^{k-2}\left(\frac{\alpha_{0,+1}\lambda w + \alpha_{0,-1}\lambda}{\alpha_{-1,+1}\lambda^4 w + \alpha_{-1,-1}}\right)^2,\\
v &= \left(\frac{\alpha_{+1,+1} v + \alpha_{+1,-1}\lambda^4 + \alpha_{+1,0}\lambda u}{\alpha_{-1,+1}\lambda^4 v + \alpha_{-1,-1} + \alpha_{-1,0}\lambda u}\right)^{k-2}\left(\frac{\alpha_{+1,+1} w + \alpha_{+1,-1}\lambda^4}{\alpha_{-1,+1}\lambda^4 w + \alpha_{-1,-1}}\right)^2,\\
w &= \left(\frac{\alpha_{+1,+1} v + \alpha_{+1,-1}\lambda^4 + \alpha_{+1,0}\lambda u}{\alpha_{-1,+1}\lambda^4 v + \alpha_{-1,-1} + \alpha_{-1,0}\lambda u}\right)^{k-1}\left(\frac{\alpha_{+1,+1} w + \alpha_{+1,-1}\lambda^4}{\alpha_{-1,+1}\lambda^4 w + \alpha_{-1,-1}}\right).
\end{aligned} \tag{5}$$

Consider in "one case":

$$\begin{aligned}
&\alpha_{-1,-1} = 0, \quad \alpha_{-1,0} = 1, \quad \alpha_{-1,1} = 1,\\
&\alpha_{0,-1} = 1, \quad \alpha_{0,0} = 1, \quad \alpha_{0,1} = 1,\\
&\alpha_{1,-1} = 1, \quad \alpha_{1,0} = 1, \quad \alpha_{1,1} = 0,
\end{aligned} \tag{6}$$

then system (5) we obtain:

$$\begin{aligned}
u &= \left(\frac{\lambda v + \lambda + u}{\lambda^4 v + \lambda u}\right)^{k-2} \cdot \left(\frac{\lambda w + \lambda}{\lambda^4 w}\right)^2\\
v &= \left(\frac{\lambda^4 + \lambda u}{\lambda^4 v + \lambda u}\right)^{k-2} \cdot \frac{1}{w^2}\\
w &= \left(\frac{\lambda^4 + \lambda u}{\lambda^4 v + \lambda u}\right)^{k-1} \cdot \frac{1}{w}.
\end{aligned} \tag{7}$$

We have the equation:

$$w^2 = \left(\frac{\lambda^4 + \lambda u}{\lambda^4 v + \lambda u}\right)^{k-1}, \tag{8}$$

from the last equation of the system (7). Then, from the second equation of the system (7), $v = 1$. From equation (8) we obtain $w = 1$. If we put them to the first equation of the system (7), then we have:

$$u = \frac{4}{\lambda^6}\left(\frac{u + 2\lambda}{\lambda^4 + \lambda u}\right)^{k-2}. \tag{9}$$

For $k \geq 2$ true the following.

Lemma 1. *If $k \geq 2$ and $0 < \lambda < 1$, then system* (7) *has unique solution:*

$$\mathbf{z} = (u, v, w) = (u_*, 1, 1),$$

where u_* is solution of equation (9).

Proof. We have seen above that at $k = 2$, equation (9) has a unique solution $u_* = \dfrac{4}{\lambda^6}$. Then in this case $\mathbf{z} = (u_*, 1, 1) = \left(\dfrac{4}{\lambda^6}, 1, 1\right)$. We write equation (9) in the form:

$$u = f(u), \tag{10}$$

where:

$$f(u) = \frac{4}{\lambda^6}\left(\frac{u + 2\lambda}{\lambda^4 + \lambda u}\right)^{k-2}.$$

Note that the derivative of the function $f(u)$:

$$f'(u) = (k-2)\frac{4}{\lambda^4}\left(\frac{u + 2\lambda}{\lambda^4 + \lambda u}\right)^{k-3}\frac{(\lambda - \sqrt{2})(\lambda + \sqrt{2})}{(\lambda^4 + \lambda u)^2} < 0$$

at the $0 < \lambda < 1$, i.e. the function $f(u)$ is decreasing for $u > 0$. Hence, equation (10) has a unique solution u_* for any $\lambda \in (0, 1)$. Then system (7) has unique solution $\mathbf{z} = (u, v, w) = (u_*, 1, 1)$. Lemma 1 is proved.

For some values of k one can give explicit form of the unique solution to (9). For example, if $k = 2$ then the unique solution of equation (7) is with:

$$u_*^{(2)} = \frac{4}{\lambda^6}, \tag{11}$$

i.e.,.:

$$\mathbf{z} = (u, v, w) = (u_*^{(2)}, 1, 1).$$

For $k = 3$ the system of equation (7) has unique solution for any $\lambda > 0$:

$$\mathbf{z} = (u, v, w) = (u_*^{(3)}, 1, 1),$$

where:

$$u_*^{(3)} = \frac{\sqrt{(\lambda^{10} - 4)^2 + 32\lambda^8} - (\lambda^{10} - 4)}{2\lambda^7}. \tag{12}$$

For $k = 4$ the system of equation (7) has unique solution:

$$\mathbf{z} = (u, v, w) = (u_*^{(4)}, 1, 1),$$

where:

$$u_*^{(4)}(\lambda) = \frac{1}{3\lambda^8}\left(\sqrt[3]{A + 6\sqrt{3B}} + \frac{C}{\sqrt[3]{A + 6\sqrt{3B}}} - 2\lambda^{11} + 4\right), \tag{13}$$

here:

$$A = \lambda^{33} + 30\lambda^{22} - 144\lambda^{20} + 216\lambda^{18} - 96\lambda^{11} + 288\lambda^9 + 64,$$

$$B = \frac{(\lambda^{24} - \lambda^{13} - 36\lambda^{11} + 108\lambda^9 + 32)(\lambda^2 - 2)^2}{\lambda},$$

$$C = \lambda^{22} - 16\lambda^{11} + 48\lambda^9 + 16.$$

On the cases $k > 4$, it is not possible to find an explicit form of the solution to equation (9).

Denote by μ the Gibbs measure which, by (2), correspond to the solution $\mathbf{z}$.

Thus we obtain the following.

Theorem 1. *For the HC Blume–Capel model in "one case" of DNAs on the Cayley tree of order $k \geq 2$ at the $T = \dfrac{J}{\ln \frac{1}{\lambda}} > 0$ there is unique translation-invariant Gibbs measure μ.*

3. Markov chains of TIGMs and Holliday junction of DNA

For marginals on the two-edge sets consisting of two neighboring edges l, t, taking into account the boundary law $\{(z_{0,l}, z_{1,l}, z_t),\ l \notin \mathbb{Z}\text{-path},\ t \in \mathbb{Z}\text{-path}\}$, i.e. solutions to the (2) system. This boundary law is normalized to -1, i.e., $z_{-1,l} = 1$. We have:

$$\mu(\sigma(l) = a, \quad \sigma(t) = b) = \frac{1}{Z} z_{a,l} \exp(J\beta(a - b)^2) z_{b,t}, \quad a, b = -1, 0, +1,$$

where Z is normalizing factor.

From this, using formulas (3) and (4) for solutions (u, v, w) to (7) we write the matrices of the tree-indexed Markov chains (related to Gibbs measures, see [4]) $\mathbb{P}^{[l,t]} = \left(P_{ij}^{[l,t]}\right)$:

$$\mathbb{P}^{[l,t]} = \mathbb{P}^{[l,t]}_{(3\to 3)} = \begin{pmatrix} 0 & \dfrac{\lambda u}{\lambda u + \lambda^4 v} & \dfrac{\lambda^4 v}{\lambda u + \lambda^4 v} \\ \dfrac{\lambda}{\lambda + u + \lambda v} & \dfrac{u}{\lambda + u + \lambda v} & \dfrac{\lambda v}{\lambda + u + \lambda v} \\ \dfrac{\lambda^4}{\lambda^4 + \lambda u} & \dfrac{\lambda u}{\lambda^4 + \lambda u} & 0 \end{pmatrix}, \quad \text{if } l, t \notin \mathbb{Z}\text{-path}.$$

$$\mathbb{P}^{[l,t]} = \mathbb{P}^{[l,t]}_{(3\to 2)} = \begin{pmatrix} 0 & 0 & 1 \\ \dfrac{1}{1 + w} & 0 & \dfrac{w}{1 + w} \\ 1 & 0 & 0 \end{pmatrix}, \quad \text{if } l \notin \mathbb{Z}\text{-path}, t \in \mathbb{Z}\text{-path}.$$

$$\mathbb{P}^{[l,t]} = \mathbb{P}^{[l,t]}_{(2\to 3)} = \begin{pmatrix} 0 & \dfrac{\lambda u}{\lambda u+\lambda^4 v} & \dfrac{\lambda^4 v}{\lambda u+\lambda^4 v} \\ * & * & * \\ \dfrac{\lambda^4}{\lambda^4+\lambda u} & \dfrac{\lambda u}{\lambda^4+\lambda u} & 0 \end{pmatrix}, \quad \text{if } l \in \mathbb{Z}\text{-path}, t \notin \mathbb{Z}\text{-path},$$

where $*$ means that $P^{[l,t]}_{0j}$ is not defined, because $\sigma(l) \neq 0$ for any $l \in \mathbb{Z}$-path.

$$\mathbb{P}^{[l,t]} = \mathbb{P}^{[l,t]}_{(2\to 2)} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \text{if } l \in \mathbb{Z}\text{-path}, t \in \mathbb{Z}\text{-path}.$$

Here, the matrix element $P^{[l,t]}_{ij}$ is the probablity of the transition from the state i on the edge l to the state j on the neighboring edge t.

Matrices $\mathbb{P}^{[l,t]}_{(2\to 3)}$, $\mathbb{P}^{[l,t]}_{(3\to 2)}$ do not define standard Markov chain. Therefore, we will not consider them.

For the matrix $\mathbb{P}^{[l,t]}_{(n\to m)}$ with $n = m$, it is easy to find the following stationary distributions:

$$\pi_{(n\to m)} = (\pi_{(n\to m),-1}, \pi_{(n\to m),0}, \pi_{(n\to m),1}).$$

Namely, we have:

$$\pi_{(3\to 3)} = \frac{1}{N}\left(\lambda u + \lambda^4 v, (\lambda + u + \lambda v)u, (\lambda^4 + \lambda u)v\right),$$

where N the normalizing factor, and:

$$\pi_{(2\to 2)} = \left(\frac{1}{2}, \frac{1}{2}\right).$$

Using the ergodic theorem (see [13]) for non-negative stochastic matrices and the above formulas for matrices and stationary distributions, we obtain.

Theorem 2. *In a stationary state of the set of DNAs, independently on $l \notin \mathbb{Z}$-path, a Holliday junction through l does not occur with the following probability (with respect to measure μ^*):*

$$\pi_{(3\to 3),0} = \pi^{(*)}_{(3\to 3),0} = \frac{1}{N}(2\lambda + u_*)u_*.$$

(Consequently, a Holliday junction occurs with probability $1 - \pi^{(*)}_{(3\to 3),0}$) where u_* are defined in Lemma 1.

It can be seen that $\pi^{(*)}_{(3\to 3),0}$ is a function only of temperature.

We now find the limits of the stationary distribution vectors $\pi_{(3\to 3)}$, $\pi_{(2\to 2)}$ (corresponding to the Markov chain generated by the Gibbs measure μ) as $T \to 0$ (as $\beta \to \infty$ and $\lambda \to 0$) and as $T \to +\infty$ (as $\beta \to 0$ and $\lambda \to 1$). To find the limits, we take the dependence of u_* on $T = 1/\beta$ into account.

Lemma 2. *We have the relations*:

$$\lim_{T\to 0} \pi^{(k)}_{(3\to 3)} = (0, 1, 0), \quad k = 2, 3, 4.$$

$$\lim_{T\to 0} \pi^{(k)}_{(2\to 2)} = \left(\frac{1}{2}, \frac{1}{2}\right), \quad k = 2, 3, 4.$$

in the low-temperature case $T \to 0$ and:

$$\lim_{T\to+\infty} \pi^{(2)}_{(3\to 3)} = \left(\frac{5}{34}, \frac{12}{17}, \frac{5}{34}\right) \approx (0.14705882, 0.70588235, 0.14705882),$$

$$\lim_{T\to+\infty} \pi^{(3)}_{(3\to 3)} = \left(\frac{5+\sqrt{41}}{41+7\sqrt{41}}, \frac{31+5\sqrt{41}}{41+7\sqrt{41}}, \frac{5+\sqrt{41}}{41+7\sqrt{41}}\right) \approx (0.13286968, 0.73426064, 0.13286968),$$

$$\lim_{T\to+\infty} \pi^{(4)}_{(3\to 3)} = (E, F, E) = (0.12195036, 0.75609928, 0.12195036),$$

$$\lim_{T\to+\infty} \pi^{(k)}_{(2\to 2)} = \left(\frac{1}{2}, \frac{1}{2}\right), \quad k = 2, 3, 4,$$

in the high-temperature case $T \to +\infty$, where:

$$E = \frac{36\sqrt{78} + 15(359+12\sqrt{78})^{\frac{2}{3}} + 147(359+12\sqrt{78})^{\frac{1}{3}} + 1077}{8145 + 144(359+12\sqrt{78})^{\frac{2}{3}} + (359+12\sqrt{78})^{\frac{4}{3}} + 784(359+12\sqrt{78})^{\frac{1}{3}} + 192\sqrt{78}} \approx 0.12195036,$$

$$F=\frac{5991+144(359+12\sqrt{78})^{\frac{2}{3}}+490(359+12\sqrt{78})^{\frac{1}{3}}+(359+12\sqrt{78})^{\frac{4}{3}}+120\sqrt{78}}{8145+144(359+12\sqrt{78})^{\frac{2}{3}}+(359+12\sqrt{78})^{\frac{4}{3}}+784(359+12\sqrt{78})^{\frac{1}{3}}+192\sqrt{78}}\approx 0.75609928.$$

By Lemma 2 we have the following structures of the DNA set:

- (i) In the case $T\to 0$, the DNA set has the following stationary states (configurations):

Case μ ($k=2,3,4$): For all neighboring DNA molecules, the Holliday junction does not occur. The sequence of ± 1 s, in a DNA on the $\mathbb{Z}$-path is free with independent identically distributed and equiprobable $(1/2)$ -1 and $+1$.

- (ii) In the case $T\to+\infty$, the DNA set has the following stationary states (configurations):

Case μ ($k=2$): All neighboring DNA molecules have Holliday junction with probability $5/17$ (more precisely, a junction via state -1 or $+1$ with equiprobable $5/34$) and no junction with probability $12/17$. The sequence of ± 1 s, in a DNA on the $\mathbb{Z}$-path is free with independent identically distributed and equiprobable $(1/2)$ -1 and $+1$.

Case μ ($k=3$): All neighboring DNA molecules have Holliday junction with probability 0.26573936 (more precisely, a junction via state -1 or $+1$ with equiprobable 0.13286968) and no junction with probability 0.73426064. The sequence of ± 1 s, in a DNA on the $\mathbb{Z}$-path is free with independent identically distributed and equiprobable $(1/2)$ -1 and $+1$.

Case μ ($k=4$): All neighboring DNA molecules have Holliday junction with probability 0.24390072 (more precisely, a junction via state -1 or $+1$ with equiprobable 0.12195036) and no junction with probability 0.75609928. The sequence of ± 1 s, in a DNA on the $\mathbb{Z}$-path is free with independent identically distributed and equiprobable $(1/2)$ -1 and $+1$.

4. Conclusions

On the Cayley tree, the results for DNA were obtained only for cases $k=2$. In this paper, the results are obtained for the case $k\geq 2$. Following [12] for the HC Blume–Capel model in "one case" in DNA on a Cayley tree of order $k\geq 2$, we proved that at a temperature $T>0$ there is a unique TIGM.

Since each such measure describes the phase of DNA recruitment. Our results refer to the Gibbs measure allowed us to study the distributions of Holliday junctions DNA compounds. In the previous section, for very high and very low temperatures, we gave stationary distributions and typical configurations of Holliday junctions.

Acknowledgements

The author thanks Professor U. A. Rozikov for his suggestions which were helpful to improve the readability of the paper.

References

[1] Alberts B., Johnson A., et al. *Molecular biology of the cell*, 4th edn., Garland Science, New York, 2002.
[2] Holliday R. A mechanism for gene conversion in fungi. *Genet Res.*, 1964, **5**, P. 282–304.
[3] Khatamov N.M. Holliday junctions in the Blume–Capel model of DNA. *Theoretical and Mathematical Physics*, 2021, **3** (206), P. 383–390.
[4] Rozikov U.A. Tree-hierarchy of DNA and distribution of Holliday junctions. *J. Math. Biol.*, 2017, **75**, P. 1715–1733.
[5] Rozikov U.A. Holliday junctions for the Potts model of DNA. *Algebra, Complex Analysis, and Pluripotential Theory*, 2018, **264**, P. 151–165.
[6] Rozikov U.A. Thermodynamics of interacting systems of DNA molecules. *Theoretical and Mathematical Physics*, 2021, **2** (206), P. 174–183.
[7] Rozikov U.A. Thermodynamics of DNA-RNA renaturation. *Inter. Jour. Geom. Methods Mod. Phys.*, 2021, **6** (18), 2150096.
[8] Cirillo E.N., Olivieri E. Metastabilty and nucleation for the Blume–Capel model.Different mechanisms of transition. *Journal of Statistical Physics*, 1996, **83**, P. 473–554.
[9] Khatamov N.M., Khakimov R.M. Translation-invariant Gibbs measures for the Blume–Capel model on a Cayley tree. *JMAG*, 2019, **2** (15), P. 239–255.
[10] Khatamov N.M. Translation-invariant extreme Gibbs measures for the Blume–Capel model with a wand on a Cayley tree. *Ukrains'kyi Matematychnyi Zhurnal*, 2020, **4** (72), P. 540–556.
[11] Rozikov U.A., Ishankulov F.T. Description of periodic p-harmonic functions on Cayley trees. *Nonlinear Diff. Equ. Appl.*, 2010, **2** (17), P. 153–160.
[12] Rozikov U.A. Gibbs measures on Cayley trees. World Scientific Publishing, Singapore, 2013.
[13] Georgii H.O. *Gibbs measures and phase transitions*. De Gruyter stadies in Math, Berlin, 1988.