Uzbek Mathematical Journal
2021, Volume 65, Issue 1, pp.87-97
DOI: 10.29229/uzmj.2021-1-9

Holliday junctions for the HC (cycle) Blume-Capel model of DNA

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Abstract. In this article, we look at DNA as a configuration of the Blume-Capel model and insert it in the path of the Cayley tree. To study the thermodynamic properties of the DNA model, we describe the corresponding translational-invariant Gibbs measure (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 Holliday junctions.

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

MSC (2010): 92D20; 82B20; 60J10; 05C05.

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 G - C 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 [4] are a cruciform structure that forms during genetic recombination when two double-stranded DNA molecules split into four strands to exchange segments of genetic information.

In articles [10, 11] the Ising and Potts DNA models are considered for studying their thermodynamics. 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 [2, 5, 6].

In our model, we consider a set of DNAs that "live"on a tree graph. Let the l edge of this graph have a function $\sigma(l)$ with three possible values -1,0, 1 (an analog of the spin values in physical systems), in the case $\sigma(l) = 0$ it is said that the edge l does not belong to DNA. If this l separates two DNAs, then a value of $\sigma(l) = 1$ or $\sigma(l) = -1$ means that the two DNAs have a Holliday junction.

Now from the following [9, 10, 11], 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 is 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 y:

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

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

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

For any $x \in V$ denote

$$W_m(x) = \{y \in V : d(x, y) = m, m \geq 1\}.$$

Let $\mathbb{Z} = \{..., -2, -1, 0, 1, 2, ...\}$. It was proved in [8] 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 a Cayley tree. Consider function σ which assigns to each edge $l \in L$, values $\sigma(l) \in \{-1, 0, 1\}$. Value $\sigma(l) = -1$ (resp. $+1$) means that edge l is 'occupied' by -1 ="A with T"(resp. 1 ="C with G"), and $\sigma(l) = 0$ that l is 'vacant'.

A 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 analogously and the set of all configurations in L_n is denoted by Ω_n.

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

$$1) \ \ \sigma(l) \neq 0 \ \text{ for any } \ l \in \mathbb{Z} - path;$$

$$2) \ \ \{\sigma(l), \sigma(t)\} \in \{\{-1, 0\}, \{-1, +1\}, \{0, +1\}\};$$

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

The most common discrete models regard DNA as a set of rigid subunits that represent base pairs [12]. This description has long been used by chemists to characterize DNA crystal structures. We consider the following Blume-Capel model of energy configuration σ of a DNA set:

$$H(\sigma) = J \sum_{\langle l,t\rangle \in L\times L;} (\sigma(l) - \sigma(t))^2, \tag{1.2}$$

where $J > 0$ is a coupling constant, $\sigma(l) \in \{-1, 0, 1\}$ and $\langle l, t\rangle$ stands for the nearest neighbor edges, i.e. edges which have a common endpoint.

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

Denote

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

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

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

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

It is easy to see that

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

We denote

$$S_0(l) = S(l) \setminus \{l_0, l_1\}, l \notin \mathbb{Z} - path,$$

$$S_1(l) = S(l) \setminus \{l_1\}, l \in \mathbb{Z} - path.$$

Let $\widetilde{L}(G)$ be the set of "edge"of G. We define an 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 [9, 10, 11]), 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:

$$\begin{gathered} z_{0,l} = \frac{\alpha_{0,+1}\lambda z_{l_0} + \alpha_{0,-1}\lambda}{a_{-1,+1}\lambda^4 z_{l_0} + \alpha_{-1,-1}} \cdot \frac{\alpha_{0,+1}\lambda z_{l_1} + \alpha_{0,-1}\lambda}{\alpha_{-1,+1}\lambda^4 z_{l_1} + \alpha_{-1,-1}} \cdot \\ \prod_{t \in S_0(l)} \frac{\alpha_{0,+1}\lambda z_{+1,t} + \alpha_{0,-1}\lambda + \alpha_{0,0} z_{0,t}}{\alpha_{-1,+1}\lambda^4 z_{+1,t} + \alpha_{-1,-1} + \alpha_{-1,0}\lambda z_{0,t}}, l \notin \mathbb{Z} - path, \\ z_{1,l} = \frac{\alpha_{+1,+1} z_{l_0} + \alpha_{+1,-1}\lambda^4}{\alpha_{-1,+1}\lambda^4 z_{l_0} + \alpha_{-1,-1}} \cdot \frac{\alpha_{+1,+1} z_{l_1} + \alpha_{+1,-1}\lambda^4}{\alpha_{-1,+1}\lambda^4 z_{l_1} + \alpha_{-1,-1}} \cdot \\ \prod_{t \in S_0(l)} \frac{\alpha_{+1,+1} z_{+1,t} + \alpha_{+1,-1}\lambda^4 + \alpha_{+1,0}\lambda z_{0,t}}{\alpha_{-1,+1}\lambda^4 z_{+1,t} + \alpha_{-1,-1} + \alpha_{-1,0}\lambda z_{0,t}}, l \notin \mathbb{Z} - path, \\ z_l = \frac{\alpha_{+1,+1} z_l + \alpha_{+1,-1}\lambda^4}{\alpha_{-1,+1}\lambda^4 z_l + \alpha_{-1,-1}} \cdot \prod_{t \in S_1(l)} \frac{\alpha_{+1,+1} z_{+1,t} + \alpha_{+1,-1}\lambda^4 + \alpha_{+1,0}\lambda z_{0,t}}{\alpha_{-1,+1}\lambda^4 z_{+1,t} + \alpha_{-1,-1} + \alpha_{-1,0}\lambda z_{0,t}}, l \in \mathbb{Z} - path. \end{gathered} \tag{1.3}$$

Here

$$\lambda = exp(-J\beta). \tag{1.4}$$

Moreover, this implies that for any set of vectors $\mathbf{z} = \{(z_{0,l}, z_{1,l}, z_t), l \notin \mathbb{Z} - path, t \in \mathbb{Z} - path$ satisfying the system of functional equations (1.3), there exists the only Gibbs measure μ and vice versa. However, the analysis of solutions (1.3) is not easy. Here are some solutions (1.3).

2 Translation Invariant Gibbs Measures of the Set of DNAs

A translation invariant Gibbs measure corresponds a solution $\mathbf{z}_l$ of the system of functional equations (1.3), which does not depend on l, i.e.,

$$z_{0,l} = u, z_{1,l} = v, \forall l \notin \mathbb{Z} - path; z_l = w, \forall l \in \mathbb{Z} - path. \tag{2.1}$$

where $u, v, w > 0$ (by (1.3)) satisfy

$$u = \left(\frac{\alpha_{0,+1}\lambda v + \alpha_{0,-1}\lambda + \alpha_{0,0}u}{\alpha_{-1,+1}\lambda^4 v + \alpha_{-1,-1} + \alpha_{-1,0}\lambda u}\right)^{k-2} \left(\frac{\alpha_{0,+1}\lambda w + \alpha_{0,-1}\lambda}{\alpha_{-1,+1}\lambda^4 w + \alpha_{-1,-1}}\right)^2,$$

$$v = \left(\frac{\alpha_{+1,+1}v + \alpha_{+1,-1}\lambda^4 + \alpha_{+1,0}\lambda u}{\alpha_{-1,+1}\lambda^4 v + \alpha_{-1,-1} + \alpha_{-1,0}\lambda u}\right)^{k-2} \left(\frac{\alpha_{+1,+1}w + \alpha_{+1,-1}\lambda^4}{\alpha_{-1,+1}\lambda^4 w + \alpha_{-1,-1}}\right)^2,$$

$$w = \left(\frac{\alpha_{+1,+1}v + \alpha_{+1,-1}\lambda^4 + \alpha_{+1,0}\lambda u}{\alpha_{-1,+1}\lambda^4 v + \alpha_{-1,-1} + \alpha_{-1,0}\lambda u}\right)^{k-1} \left(\frac{\alpha_{+1,+1}w + \alpha_{+1,-1}\lambda^4}{\alpha_{-1,+1}\lambda^4 w + \alpha_{-1,-1}}\right). \tag{2.2}$$

Consider the case of cycle:

$$\alpha_{-1,-1} = 0, \quad \alpha_{-1,0} = 1, \quad \alpha_{-1,+1} = 1,$$

$$\alpha_{0,-1} = 1, \quad \alpha_{0,0} = 0, \quad \alpha_{0,+1} = 1,$$

$$\alpha_{+1,-1} = 1, \quad \alpha_{+1,0} = 1, \quad \alpha_{+1,+1} = 0, \tag{2.3}$$

then system (2.2) we obtain

$$u = \left(\frac{v+1}{\lambda^3 v + u}\right)^{k-2} \cdot \left(\frac{w+1}{\lambda^3 w}\right)^2,$$

$$v = \left(\frac{\lambda^3 + u}{\lambda^3 v + u}\right)^{k-2} \cdot \frac{1}{w^2},$$

$$w = \left(\frac{\lambda^3 + u}{\lambda^3 v + u}\right)^{k-1} \cdot \frac{1}{w}. \tag{2.4}$$

We have the equation

$$w^2 = \left(\frac{\lambda^3 + u}{\lambda^3 v + u}\right)^{k-1} \tag{2.5}$$

from the last equation of the system (2.4). Then, from the second equation of the system (2.4), $v = 1$. From equation (2.5) we obtain $w = 1$. If we put them to the first equation of the system (2.4), then we have

$$u = \frac{4}{\lambda^6} \cdot \left(\frac{2}{\lambda^3 + u}\right)^{k-2}. \tag{2.6}$$

At $k = 2$, the equation (2.6) has a unique solution

$$u = \frac{4}{\lambda^6}$$

for any $\lambda > 0$. Then, the system of the equation (2.4) has for $k = 2$ a unique solution for any $\lambda > 0$ too,

$$\mathbf{z} = (u, v, w) = (\frac{4}{\lambda^6}, 1, 1).$$

For $k \geq 2$ true the following.

Lemma 2.1. *If* $k \geq 2$ *and* $0 < \lambda < 1$, *then the system* (2.4) *has a unique solution*

$$z = (u, v, w) = (u_*, 1, 1),$$

where u_* *is a solution of the equation* (2.6).

Proof. We have seen above that at $k = 2$, the equation (2.6) has a unique solution. Let $k > 2$. Denote

$$u = \frac{x^{k-2}}{\lambda^6}, x > 0. \tag{2.7}$$

Then the equation (2.6) has the form

$$x^{k-1} + \lambda^9 x - 2^{\frac{k}{k-2}} \lambda^6 = 0. \tag{2.8}$$

Note that the signs of the coefficients of this equation change only once. Then by the well-known property [7] that the number of positive roots of a polynomial does not exceed the number of changes in the signs of its coefficients, we obtain that the equation (2.8) has a unique positive solution. According to (2.7) equation (2.6) also has a unique positive solution. From this and the above comments (2.4) it follows that the system has a unique solution. Lemma 2.1 is proved.

For some values of k one can give explicit form of the unique solution to (2.6). For example, if $k = 2$ then the unique solution of equation (2.4) is with

$$u_*^{(2)} = \frac{4}{\lambda^6} \tag{2.9}$$

i.e.,

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

For $k = 3$ the system of equation (2.4) has a unique solution for any $\lambda > 0$

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

where

$$u_*^{(3)} = \frac{\sqrt{\lambda^{12} + 32} - \lambda^6}{2\lambda^3}. \tag{2.10}$$

For $k = 4$ the system of equation (2.4) has a unique solution

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

where

$$u_*^{(4)} = \frac{\sqrt[3]{\lambda^{15} + 216 + 12\sqrt{3\lambda^{15} + 324}} + \frac{\lambda^{10}}{\sqrt[3]{\lambda^{15}+216+12\sqrt{3\lambda^{15}+324}}} - 2\lambda^5}{3\lambda^2}. \tag{2.11}$$

On the cases $k > 4$, it is not possible to find an explicit form of the solution to equation (2.6).

Denote by μ the Gibbs measure which, by (1.3), correspond to the solution $\mathbf{z}$.

Thus we obtain the following.

Theorem 2.2. *For the HC (cycle) Blume-Capel model of DNAs on the Cayley tree of order $k \geq 2$ at the $T = \frac{J}{ln\frac{1}{\lambda}} > 0$ there is a unique translation-invariant Gibbs measure μ.*

3 Markov Chains of TIGMs and Holliday Junction of DNA

For marginals on the two-edge sets which consist of two neighbor edges l, t, considering a boundary law $\{(z_{0,l}, z_{1,l}, z_t, l \notin \mathbb{Z} - path, t \in \mathbb{Z} - path)\}$, i.e., the solutions of system (1.3). This boundary law is normalized at -1, i.e., $z_{-1,l} = 1$, that is $h_{-1,l} = 0$. We have

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

where Z is normalizing factor.

Hence, the connection between the boundary law and the transition matrix for the associated tree-indexed Markov chain (Gibbs measure) is immediately obtained from the conditional probability formula. Indeed, if we have $h_{a,l}$ (given in formula (1.3)) which does not depend on l , we define a (inhomogeneous) Markov chain indexed by a tree (inhomogeneous) with states $\{-1, 0, +1\}$ with transition matrix $\mathbb{P}^{[l,t]} = \left(P_{ij}^{[l,t]}\right)$, depending on $\langle l, t\rangle$ with

$$P_{ij}^{[l,t]} = \begin{cases} \frac{\alpha_{i,j} exp(-J\beta(i-j)^2+h_j)}{\alpha_{i,-1} exp(-J\beta(i+1)^2+h_{-1})+\alpha_{i,0} exp(-J\beta i^2+h_0)+\alpha_{i,+1} exp(-J\beta(i-1)^2+h_1)}, \\ if l, t \notin \mathbb{Z}-path, i, j = -1, 0, 1 \\ \frac{\alpha_{i,j} exp(-J\beta(i-j)^2+h_j)}{\alpha_{i,-1} exp(-J\beta(i+1)^2+h_{-1})+\alpha_{i,+1} exp(-J\beta(i-1)^2+h_1)}, \\ if l \notin \mathbb{Z}-path, t \in \mathbb{Z}-path, i = -1, 0, 1; j = -1, 1 \\ \frac{\alpha_{i,j} exp(-J\beta(i-j)^2+h_j)}{\alpha_{i,-1} exp(-J\beta(i+1)^2+h_{-1})+\alpha_{i,0} exp(-J\beta i^2+h_0)+\alpha_{i,+1} exp(-J\beta(i-1)^2+h_1)}, \\ if l \in \mathbb{Z}-path, t \notin \mathbb{Z}-path, i = -1, 1; j = -1, 0, 1 \\ \frac{\alpha_{i,j} exp(-J\beta(i-j)^2+h_j)}{\alpha_{i,-1} exp(-J\beta(i+1)^2+h_{-1})+\alpha_{i,+1} exp(-J\beta(i-1)^2+h_1)}, \\ if l, t \in \mathbb{Z}-path, i, j = -1, 1 \end{cases}$$

Here $P_{ij}^{[l,t]}$ is the probability to go from a state i at edge l to a state j at the neighbor edge t.

From this, using formulas (1.4) and (2.1) for solutions (u, v, w) to (2.4) we write the matrices of the tree-indexed Markov chains (related to Gibbs measures, see [3]) $\mathbb{P}^{[l,t]} = \left(P_{ij}^{[l,t]}\right)$:

$$\mathbb{P}^{[l,t]} = \mathbb{P}^{[l,t]}_{(3\to 3)} = \begin{pmatrix} 0 & \frac{u}{u+\lambda^3 v} & \frac{\lambda^3 v}{u+\lambda^3 v} \\ \frac{1}{1+v} & 0 & \frac{v}{1+v} \\ \frac{\lambda^3}{\lambda^3+u} & \frac{u}{\lambda^3+u} & 0 \end{pmatrix}, \ if\ l, t \notin \mathbb{Z}-path.$$

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

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

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

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

We note that each matrix $\mathbb{P}^{[l,t]}_{(n\to m)}, n, m = 2, 3$ is homogenous on the corresponding set of neighbor edges $\langle l, t\rangle$ where it is given, i.e., $\mathbb{P}^{[l,t]}_{(n\to m)}$ does not depend on $\langle l, t\rangle$ itself but only depends on its relation with $\mathbb{Z}-path$.

It is easy to find the following stationary distributions

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

of the matrix $\mathbb{P}^{[l,t]}_{(n\to m)}, n=m$.

$$\pi_{(3\to 3)}=\frac{1}{N}\begin{pmatrix}(\lambda u+\lambda^4 v)\\(\lambda+\lambda v)u\\(\lambda^4+\lambda u)v\end{pmatrix}^t,$$

where N is the normalizing factor

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

Using the ergodic theorem (see [3]) for positive stochastic matrices and the above formulas for matrices and stationary distributions, we obtain.

Theorem 3.1. *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^*)*

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

(Consequently, a Holliday junction occurs with probability $1-\pi^{(*)}_{(3\to 3),0}$) where u_* is defined in Lemma 2.1.

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

Now we are interested to calculate the limit of stationary distribution vectors $\pi_{(3\to 3)}$, $\pi_{(2\to 2)}$ (which correspond to the Markov chain generated by the Gibbs measure μ) in case when temperature $T\to 0$ (i.e. $\beta\to\infty$ and $\lambda\to 0$) and when temperature $T\to+\infty$ (i.e. $\beta\to 0$ and $\lambda\to 1$). To calculate the limit observe that value u_* varies with $T=1/\beta$.

Lemma 3.2. *The following equalities hold on $k=2,3,4$*

- The case of low temperature:

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

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

-The case of high temperature:

$$\lim_{T\to+\infty}\pi^{(2)}_{(3\to 3)}=\left(\frac{5}{18},\frac{4}{9},\frac{5}{18}\right)\approx(0.277777778,0.444444444,0.277777778),$$

$$\lim_{T\to+\infty}\pi^{(3)}_{(3\to 3)}=\left(\frac{\sqrt{33}}{132}+\frac{1}{4},\frac{1}{2}-\frac{\sqrt{33}}{66},\frac{\sqrt{33}}{132}+\frac{1}{4}\right)\approx$$

$$\approx (0.293519414, 0.412961172, 0.293519414)\,,$$

$$\lim_{T\to+\infty} \pi^{(4)}_{(3\to 3)} = (A, B, A) = (0.302059899, 0.395880202, 0.302059899)\,,$$

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

where

$$A = \frac{(12\sqrt{327}+217)^{\frac{2}{3}} + (12\sqrt{327}+217)^{\frac{1}{3}} + 1}{4(12\sqrt{327}+217)^{\frac{2}{3}} - 2(12\sqrt{327}+217)^{\frac{1}{3}} + 4} \approx 0.302059899,$$

$$B = \frac{(12\sqrt{327}+217)^{\frac{2}{3}} - (12\sqrt{327}+217)^{\frac{1}{3}} + 1}{2(12\sqrt{327}+217)^{\frac{2}{3}} - (12\sqrt{327}+217)^{\frac{1}{3}} + 2} \approx 0.395880202.$$

By Lemma 3.2 we have the following structures of the set of DNAs:

(i) In case $T \to 0$ the set of DNAs have the following stationary states (configurations):

Case μ **(**$k = 2, 3, 4$**).** All neighboring DNAs have Holliday junction with probability 1/2 (more precisely, a junction through state −1 or +1 with equiprobable 1/4) and no junction with probability 1/2. The sequence of ±1*s*, in a DNA on the $\mathbb{Z} - path$, is free, with iid and equiprobable (= 1/2), of −1 and +1*s*.

(ii) In case $T \to +\infty$ the set of DNAs have the following stationary states (configurations):

Case μ **(**$k = 2$**).** All neighboring DNAs have Holliday junction with probability 0.555555556 (more precisely, a junction through state −1 or +1 with equiprobable 0.277777778) and no junction with probability 0.444444444. The sequence of ±1*s*, in a DNA on the $\mathbb{Z} - path$, is free, with iid and equiprobable (= 1/2), of −1 and +1*s*.

Case μ **(**$k = 3$**).** All neighboring DNAs have Holliday junction with probability 0.587038828 (more precisely, a junction through state −1 or +1 with equiprobable 0.293519414) and no junction with probability 0.412961172. The sequence of ±1*s*, in a DNA on the $\mathbb{Z} - path$, is free, with iid and equiprobable (= 1/2), of −1 and +1*s*.

Case μ **(**$k = 4$**).** All neighboring DNAs have Holliday junction with probability 0.604119798 (more precisely, a junction through state −1 or +1 with equiprobable 0.302059899) and no junction with probability 0.395880202. The sequence of ±1*s*, in a DNA on the $\mathbb{Z} - path$, is free, with iid and equiprobable (= 1/2), of −1 and +1*s*.

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 [10] for the HC (cycle) Blume-Capel model 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 readability of the paper.

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