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

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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.

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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].

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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 \( \Omega \). Configurations in \( L_n \) are defined similarly and the set of all configurations in \( L_n \) are denoted by \( \Omega_n \).

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 \( \sigma \) of a DNA set (see [4]):

\[
H(\sigma) = J \sum_{(l,t) \in L \times L} (\sigma(l) - \sigma(t))^2, \tag{1}
\]

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

Let \( \Omega_n^0 \) (respectively \( \Omega_n^1 \)) be the set of all admissible configurations on \( L_n \) (respectively \( L \)).

Let us introduce designations as [4]:

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

\[
\Omega_n^{l_o} = \text{the set of admissible configurations on } E_n.
\]

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

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

It is easy to see that:

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

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 \( \tilde{L}(G) \) be the set of “edge” of \( G \). We define adjacency matrix of \( G \) by \( A = A^G = (a_{ij})_{i,j=-1,0,1} \), i.e.:

\[
a_{ij} \equiv a^G_{ij} = \begin{cases} 1, & \text{if } (i, j) \in \tilde{L}(G), \\ 0, & \text{if } (i, j) \notin \tilde{L}(G). \end{cases}
\]

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:

\[
z_{0,l} = \frac{\alpha_{0,+1}z_{l_0} + \alpha_{0,-1}z_{l_0} + \alpha_{0,+1}z_{l_1} + \alpha_{0,-1}z_{l_1}}{\alpha_{-1,+1}z_{l_0} + \alpha_{-1,-1}z_{l_0} + \alpha_{-1,+1}z_{l_1} + \alpha_{-1,-1}z_{l_1}} \prod_{t \in S_0(l)} \frac{\alpha_{0,+1}z_{l_0} + \alpha_{0,-1}z_{l_0} + \alpha_{0,0}z_{0,t}}{\alpha_{-1,+1}z_{l_0} + \alpha_{-1,-1}z_{l_0} + \alpha_{-1,0}z_{0,t}}, \quad l \notin \mathbb{Z} \text{-path},
\]

\[
z_{1,l} = \frac{\alpha_{+1,+1}z_{l_0} + \alpha_{+1,-1}z_{l_0} + \alpha_{+1,+1}z_{l_1} + \alpha_{+1,-1}z_{l_1}}{\alpha_{-1,+1}z_{l_0} + \alpha_{-1,-1}z_{l_0} + \alpha_{-1,+1}z_{l_1} + \alpha_{-1,-1}z_{l_1}} \prod_{t \in S_0(l)} \frac{\alpha_{+1,+1}z_{l_0} + \alpha_{+1,-1}z_{l_0} + \alpha_{+1,0}z_{0,t}}{\alpha_{-1,+1}z_{l_0} + \alpha_{-1,-1}z_{l_0} + \alpha_{-1,0}z_{0,t}}, \quad l \notin \mathbb{Z} \text{-path},
\]

\[
z_{l} = \frac{\alpha_{+1,+1}z_{l_1} + \alpha_{+1,-1}z_{l_1}}{\alpha_{-1,+1}z_{l_1} + \alpha_{-1,-1}z_{l_1}} \prod_{t \in S_0(l)} \frac{\alpha_{+1,+1}z_{l_1} + \alpha_{+1,-1}z_{l_1} + \alpha_{+1,0}z_{0,t}}{\alpha_{-1,+1}z_{l_1} + \alpha_{-1,-1}z_{l_1} + \alpha_{-1,0}z_{0,t}} \quad l \in \mathbb{Z} \text{-path},
\]

where:

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

Moreover, this means that for any set of vectors \( z = \{z_{l_0,t}, z_{l_1,t}, z_t\}, l \notin \mathbb{Z} \text{-path}, t \in \mathbb{Z} \text{-path} \) satisfying the system of functional equations (2), there exists the only Gibbs measure \( \mu \) 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 \( z_t \) to the system of functional equations (2), which does not depend on \( l \), i.e.: \( z_{0,t} = u, \ z_{1,t} = v, \ \forall l \notin \mathbb{Z} \)-path; \( z_1 = w, \ \forall l \in \mathbb{Z} \)-path. (4)

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

\[
\begin{align*}
    u &= \left( \frac{\alpha_{0,1} + \lambda v + \alpha_{0,0} u}{\alpha_{-1,0} + \lambda v + \alpha_{-1,0} u} \right)^{k-2} \left( \frac{\alpha_{0,1} + \lambda w + \alpha_{0,0} \lambda}{\alpha_{-1,0} + \lambda w + \alpha_{-1,0} \lambda} \right)^{2}, \\
    v &= \left( \frac{\alpha_{0,1} + \lambda v + \alpha_{0,0} u}{\alpha_{-1,0} + \lambda v + \alpha_{-1,0} u} \right)^{k-2} \left( \frac{\alpha_{0,1} + \lambda w + \alpha_{0,0} \lambda}{\alpha_{-1,0} + \lambda w + \alpha_{-1,0} \lambda} \right)^{2}, \\
    w &= \left( \frac{\alpha_{0,1} + \lambda v + \alpha_{0,0} u}{\alpha_{-1,0} + \lambda v + \alpha_{-1,0} u} \right)^{k-1} \left( \frac{\alpha_{0,1} + \lambda w + \alpha_{0,0} \lambda}{\alpha_{-1,0} + \lambda w + \alpha_{-1,0} \lambda} \right),
\end{align*}
\]

Consider in “one case”:

\[
\begin{align*}
    \alpha_{-1,-1} &= 0, \quad \alpha_{-1,0} = 1, \quad \alpha_{-1,1} = 1, \\
    \alpha_{0,-1} &= 1, \quad \alpha_{0,0} = 1, \quad \alpha_{0,1} = 1, \\
    \alpha_{1,-1} &= 1, \quad \alpha_{1,0} = 1, \quad \alpha_{1,1} = 0,
\end{align*}
\]

then system (5) we obtain:

\[
\begin{align*}
    u &= \left( \frac{\lambda v + \lambda u}{\lambda^4 v + \lambda^4 u} \right)^{k-2} \left( \frac{\lambda w + \lambda}{\lambda^4 w} \right)^{2}, \\
    v &= \left( \frac{\lambda^4 + \lambda u}{\lambda^4 v + \lambda^4 u} \right)^{k-2} \left( \frac{1}{\lambda w^2} \right), \\
    w &= \left( \frac{\lambda^4 + \lambda u}{\lambda^4 v + \lambda^4 u} \right)^{k-1} \left( \frac{1}{\lambda w} \right).
\end{align*}
\]

We have the equation:

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

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:

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

For \( k \geq 2 \) true the following.

**Lemma 1.** If \( k \geq 2 \) and \( 0 < \lambda < 1 \), then system (7) has unique solution: \( z = (u, v, w) = (u_\ast, 1, 1) \), where \( u_\ast \) is solution of equation (9).

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

\[
u = f(u),
\]

where:

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

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

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

at the \( 0 < \lambda < 1 \), i.e. the function \( f(u) \) is decreasing for \( u > 0 \). Hence, equation (10) has a unique solution \( u_\ast \) for any \( \lambda \in (0, 1) \). Then system (7) has unique solution \( z = (u, v, w) = (u_\ast, 1, 1) \). 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:
\[
 u_{(2)}^{*} = \frac{4}{\lambda^6},
\]
i.e.,
\[
 z = (u, v, w) = (u_{(2)}^{*}, 1, 1).
\]
For $k = 3$ the system of equation (7) has unique solution for any $\lambda > 0$:
\[
 z = (u, v, w) = (u_{(3)}^{*}, 1, 1),
\]
where:
\[
 u_{(3)}^{*} = \sqrt{(\lambda^{10} - 4)^2 + 32\lambda^8 - (\lambda^{10} - 4)^2\lambda^7}. \tag{11}
\]
For $k = 4$ the system of equation (7) has unique solution:
\[
 z = (u, v, w) = (u_{(4)}^{*}, 1, 1),
\]
where:
\[
 u_{(4)}^{*}(\lambda) = \frac{1}{3\lambda^8} \left( \frac{2}{\sqrt{A + 6\sqrt{3B}}} + \frac{C}{\sqrt{A + 6\sqrt{3B}}} - 2\lambda^{11} + 4 \right), \tag{12}
\]
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 $\mu$ the Gibbs measure which, by (2), correspond to the solution $z$.
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

\[ T = \frac{J}{\ln \frac{1}{\lambda}} > 0 \]

there is unique translation-invariant Gibbs measure $\mu$.

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 $\{(z_{0,l}, z_{1,l}, z_{1,t}), l \notin \mathbb{Z}\text{-path}, t \in \mathbb{Z}\text{-path}\}$, i.e. solutions to the (2) system. This boundary law is normalized to $-1$, i.e., $z_{-1,l} = 1$. We have:
\[
 \mu(\sigma(l) = a, \sigma(t) = b) = \frac{1}{Z} z_{a,l} \exp(J\beta(a - b)^2) z_{b,t}, \quad a, b = -1, 0, +1,
\]
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]) $P[l,t] = \left( P_{ij}^{[l,t]} \right)$:
\[
 P[l,t] = P_{(3\to3)}^{[l,t]} = \begin{pmatrix}
 0 & \lambda u & \lambda^4 v \\
 \lambda & \frac{\lambda u + \lambda^4 v}{u} & \frac{\lambda u + \lambda^4 v}{\lambda v} \\
 \frac{\lambda^3 + \lambda u}{\lambda u + \lambda v} & \frac{\lambda^3 + \lambda u}{\lambda u + \lambda v} & \frac{\lambda^3 + \lambda u}{\lambda u + \lambda v}
\end{pmatrix}, \quad \text{if } l, t \notin \mathbb{Z}\text{-path}.
\]
\[
 P[l,t] = P_{(3\to2)}^{[l,t]} = \begin{pmatrix}
 0 & 0 & 1 \\
 1 & 0 & \frac{w}{1 + w} \\
 1 & 0 & 0
\end{pmatrix}, \quad \text{if } l \notin \mathbb{Z}\text{-path}, t \in \mathbb{Z}\text{-path}.
\]
find the limits, we take the dependence of $u$

Namely, we have:

$$
\begin{pmatrix}
0 & \lambda u & \lambda^4 v \\
\lambda u + \lambda^4 v & 0 & \lambda^4 v \\
\lambda^4 + \lambda^4 v & \lambda^4 + \lambda^4 v & 0
\end{pmatrix}, \quad \text{if } l \in \mathbb{Z}\text{-path, } t \notin \mathbb{Z}\text{-path,}
$$

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

$$
P_{11}^{l,t} = P_{12}^{l,t} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \text{if } l \in \mathbb{Z}\text{-path, } t \in \mathbb{Z}\text{-path.}
$$

Here, the matrix element $P_{ij}^{l,t}$ is the probability of the transition from the state $i$ on the edge $l$ to the state $j$ on the neighboring edge.

Matrices $P_{12}^{l,t}, P_{13}^{l,t}$ do not define standard Markov chain. Therefore, we will not consider them.

For the matrix $P_{n \rightarrow m}$ with $n = m$, it is easy to find the following stationary distributions:

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

Namely, we have:

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

where $N$ the normalizing factor, and:

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

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 $l \notin \mathbb{Z}\text{-path}$, a Holliday junction through $l$ does not occur with the following probability (with respect to measure $\mu^*$):

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

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

It can be seen that $\pi_{(3 \rightarrow 3),0}$ is a function only of temperature.

We now limit the stationary distribution vectors $\pi_{(3 \rightarrow 3)}, \pi_{(2 \rightarrow 2)}$ (corresponding to the Markov chain generated by the Gibbs measure $\mu$) 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:

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

$$
\lim_{T \to +\infty} \pi_{(3 \rightarrow 3)}^{(2)} = \left( \frac{5}{34}, \frac{12}{34}, \frac{5}{34} \right) \approx (0.14705882, 0.70588325, 0.14705882),
$$

$$
\lim_{T \to +\infty} \pi_{(3 \rightarrow 3)}^{(3)} = \left( \frac{5 + \sqrt{11}}{41 + 7\sqrt{11}}, \frac{31 + 5\sqrt{11}}{41 + 7\sqrt{11}}, \frac{5 + \sqrt{11}}{41 + 7\sqrt{11}} \right) \approx (0.13286968, 0.73426064, 0.13286968),
$$

$$
\lim_{T \to +\infty} \pi_{(3 \rightarrow 3)}^{(4)} = (E, E, E) = (0.12195036, 0.75609208, 0.12195036),
$$

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

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

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

in the high-temperature case $T \to +\infty,$ where:
\[ F = \frac{5991 + 144(359 + 12\sqrt{78})^\frac{2}{3} + 490(359 + 12\sqrt{78})^\frac{1}{3} + (359 + 12\sqrt{78})^\frac{1}{3} + 120\sqrt{78}}{8145 + 144(359 + 12\sqrt{78})^\frac{2}{3} + (359 + 12\sqrt{78})^\frac{1}{3} + 784(359 + 12\sqrt{78})^\frac{1}{3} + 192\sqrt{78}} \approx 0.75609928. \]

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

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