Combinatorial expressions of the solutions to initial value problems of the discrete and ultradiscrete Toda molecules

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Abstract

Combinatorial expressions are presented of the solutions to initial value problems of the discrete and ultradiscrete Toda molecules. For the discrete Toda molecule, a subtraction-free expression of the solution is derived in terms of non-intersecting paths, for which two results in combinatorics, Flajolet’s interpretation of continued fractions and Gessel–Viennot’s lemma on determinants, are applied. By ultradiscretizing the subtraction-free expression, the solution to the ultradiscrete Toda molecule is obtained. It is finally shown that the initial value problem of the ultradiscrete Toda molecule is exactly solved in terms of shortest paths on a specific graph. The behavior of the solution is also investigated in comparison with the box–ball system.

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1. Introduction

The Toda molecule [1] is a semi-infinite version of the Toda lattice [2]. As with the Toda lattice, the Toda molecule is known as a typical example of an integrable system which has, despite its nonlinearity, an exact solution in terms of Hankel determinants. The discrete Toda molecule is a discrete analogue of the Toda molecule, which was derived in [3] using the bilinear formalism. The discrete Toda molecule is a discrete integrable system which possesses a Hankel determinant solution analogous to the Toda molecule.

The discrete Toda molecule was also derived using the Lax formalism [4, 5], in which a connection with orthogonal polynomials is exploited to deduce the time evolution equations of the discrete Toda molecule:

\[ q_{n}^{(t+1)} + e_{n+1}^{(t+1)} = q_{n}^{(t)} + e_{n}^{(t)}, \]  
\[ q_{n}^{(t+1)} e_{n+1}^{(t+1)} = q_{n}^{(t)} e_{n+1}^{(t)} \]  

(1a)  

(1b)
for \( t \in \mathbb{Z} \). In the discrete Toda molecule, commonly, we consider the two types of boundary conditions: (a) on the semi-infinite lattice \( n \in \mathbb{N}_0 = \{0, 1, 2, \ldots\} \),
\[
e^{(t)}_0 = 0; \tag{1c}
\]
(b) on the finite lattice \( n = 0, \ldots, N, N \in \mathbb{N}_0 \),
\[
e^{(t)}_0 = e^{(t)}_{N+1} = 0. \tag{1d}
\]

In this paper, we examine the discrete Toda molecule both on the semi-infinite and finite lattices with the boundary conditions (1c) and (1d), respectively.

In numerical algorithms, equations (1) are known as recurrence equations of the \textit{qd algorithm}, which is used for computing Padé approximants of analytic functions (see, e.g., [6]) and for computing eigenvalues of tridiagonal matrices (see, e.g., [7]). In the study of pure combinatorics, Viennot [8] applied the \textit{qd} algorithm to a combinatorial problem of enumerating configurations of non-intersecting paths. From the viewpoint of dynamical systems, Viennot’s combinatorial result is observed as solving an initial value problem of the discrete Toda molecule (1) from a particular initial value.

In recent progress of investigating integrable systems, much attention has been given to ultradiscrete integrable systems, especially since the discovery of a direct connection between discrete integrable systems and soliton cellular automata [9]. A general method to derive an ultradiscrete integrable system from a discrete integrable system is called \textit{ultradiscretization}. For the discrete Toda molecule (1), \textit{ultradiscretization} is performed as follows [10]. Introduce new dependent variables \( Q^{(t)}_n, E^{(t)}_n \) by
\[
q^{(t)}_n = \exp(-Q^{(t)}_n/\varepsilon), \ e^{(t)}_n = \exp(-E^{(t)}_n/\varepsilon)
\]
with a parameter \( \varepsilon > 0 \), and take the limit \( \varepsilon \to 0 \). Equations (1) then tend to the \textit{ultradiscrete Toda molecule}
\[
Q^{(t+1)}_n = \min \left\{ \sum_{k=0}^{n} Q^{(t)}_k - \sum_{k=0}^{n-1} Q^{(t+1)}_k, E^{(t)}_{n+1} \right\}, \tag{2a}
\]
\[
E^{(t+1)}_{n+1} = Q^{(t)}_{n+1} - Q^{(t+1)}_n + E^{(t)}_{n+1}
\tag{2b}
\]
for \( t \in \mathbb{Z} \), with the boundary condition (a) on the semi-infinite lattice \( n \in \mathbb{N}_0 \)
\[
E^{(t)}_0 = +\infty, \tag{2c}
\]
or (b) on the finite lattice \( n = 0, \ldots, N \)
\[
E^{(t)}_0 = E^{(t)}_{N+1} = +\infty. \tag{2d}
\]

It is shown in [10] that the ultradiscrete Toda molecule (2) on the finite lattice describes the dynamics of a box–ball system. In section 4.3, we will discuss the box–ball system.

In this paper, we examine the initial value problems of the discrete and ultradiscrete Toda molecules, (1) and (2), for which the initial value is given at \( t = 0 \). Obviously, one can exactly solve the problems in the following sense. At any time \( t \in \mathbb{N}_0 \) and any site \( n \in \mathbb{N}_0 \), the exact value of each dependent variable can be calculated from the initial value in finitely many arithmetic and minimizing operations. However, it is still nontrivial how to formulate the solutions since the equations are nonlinear. The aim of this paper is to derive an exact expression of the solutions to the initial value problems purely in terms of the initial value. In order to formulate the solutions, we will utilize combinatorial objects, non-intersecting paths and shortest paths on a graph, in view of the combinatorial results on paths: Flajolet’s interpretation of continued fractions [11] and Gessel–Viennot’s lemma [12, 13] on determinants.

This paper is organized as follows. In section 2, we review a determinant solution to the discrete Toda molecule, based on which, in section 3, we combinatorially formulate an exact expression of the solution to the initial value problem of the discrete Toda molecule in terms
of non-intersecting paths. In section 4, we derive the solution to the initial value problem of the ultradiscrete Toda molecule by ultradiscretizing the solution to the discrete Toda molecule obtained in section 3. Further combinatorial observations lead us to a simpler expression of the solution in terms of shortest paths on a specific graph. Finally, we investigate the behavior of the solution obtained in terms of shortest paths in comparison with the box–ball system. Section 5 is devoted to concluding remarks.

2. Determinant solution to the discrete Toda molecule

In section 2, we give a brief review of a determinant solution to the discrete Toda molecule together with bilinear equations associated with the discrete and ultradiscrete Toda molecules. See, e.g., [10, 14] for detailed explanations. Based on the determinant solution, in the subsequent sections, we will examine initial value problems of the discrete and ultradiscrete Toda molecules.

We introduce a \textit{tau function} \( \tau_n^{(t)} \) of the discrete Toda molecule (1) by the variable transformation

\[
\begin{align*}
q_n^{(t)} &= \frac{\tau_n^{(t+1)} - \tau_n^{(t-1)}}{\tau_n^{(t+1)} - \tau_n^{(t)}}, \\
r_n^{(t)} &= \frac{\tau_n^{(t+1)} - \tau_n^{(t)}}{\tau_n^{(t+1)} - \tau_n^{(t-1)}},
\end{align*}
\]

(3)

where we assume \( \tau_0^{(t)} = 1 \) for normalization. We then obtain from (1) a bilinear equation of the discrete Toda molecule

\[
\tau_n^{(t+1)} \tau_n^{(t-1)} = \tau_{n-1}^{(t+1)} \tau_{n+1}^{(t-1)} + \tau_n^{(t)} \tau_n^{(t)},
\]

(4a)

with the boundary condition (a) on the semi-infinite lattice \( n \in \mathbb{N}_0 \)

\[
\tau_{-1}^{(t)} = 0
\]

(4b)

or (b) on the finite lattice \( n = 0, \ldots, N, N + 1 \)

\[
\tau_{-1}^{(t)} = \tau_{N+2}^{(t)} = 0.
\]

(4c)

To bilinear equation (4), we have an exact solution in the Hankel determinant of size \( n \):

\[
\tau_n^{(t)} = \det \left( f_j^{(i)} \right)_{j,k=0}^{n-1} = \begin{vmatrix}
\begin{array}{cccc}
\mathbf{f}_0^{(t)} & \mathbf{f}_1^{(t)} & \cdots & \mathbf{f}_{n-1}^{(t)} \\
\mathbf{f}_1^{(t)} & \mathbf{f}_2^{(t)} & \cdots & \mathbf{f}_n^{(t)} \\
\vdots & \vdots & \ddots & \vdots \\
\mathbf{f}_{n-1}^{(t)} & \mathbf{f}_n^{(t)} & \cdots & \mathbf{f}_{2n-2}^{(t)}
\end{array}
\end{vmatrix},
\]

(5a)

where \( f_n^{(t)} \) is an arbitrary function subject to the linear \textit{dispersion relation}

\[
f_n^{(t+1)} = f_n^{(t)}, \quad n \in \mathbb{N}_0.
\]

(5b)

(The determinant of size zero is assumed to be unity conventionally.) We can verify the solution (5) by means of Sylvester’s determinant identity. Substituting the determinant (5a) to (3), we obtain an exact solution to the discrete Toda molecule (1). Note that the dispersion relation (5b) should be satisfied for \( n \in \mathbb{N}_0 \) both on the semi-infinite lattice \( n \in \mathbb{N}_0 \) and on the finite lattice \( n = 0, \ldots, N, N + 1 \). On the semi-infinite lattice \( n \in \mathbb{N}_0 \), the solution (5a) is consistent with the boundary condition (4b) for every function \( f_n^{(t)} \) subject to (5b). However, on the finite lattice \( n = 0, \ldots, N, N + 1 \), the condition \( \tau_{N+2}^{(t)} = 0 \) in the boundary condition (4c) is not automatically fulfilled. Therefore, in order to derive a solution on the finite lattice, we should appropriately choose the function \( f_n^{(t)} \) so that the determinant \( \tau_{N+2}^{(t)} = \det \left( f_j^{(i)} \right)_{j+k=0}^{N-1} \) of size \( N + 2 \) vanishes for every \( t \).
We can derive a bilinear equation of the ultradiscrete Toda molecule (2) by ultradiscretizing the procedure for the discrete Toda molecule. Introducing a tau function $T_n^{(t)}$ by

$$ Q_n^{(t)} = T_n^{(t+1)} + T_{n+1}^{(t)} - T_n^{(t+1)} - T_{n+1}^{(t)}, $$

$$ E_n^{(t)} = T_{n-1}^{(t+1)} + T_{n+1}^{(t)} - T_n^{(t+1)} - T_{n+1}^{(t)}, $$

with $T_0^{(t)} = 0$, we then obtain from (2) a bilinear equation of the ultradiscrete Toda molecule,

$$ T_n^{(t+1)} + T_{n}^{(t-1)} = \min \{ T_{n-1}^{(t+1)} + T_{n+1}^{(t-1)}, 2T_n^{(t)} \} $$

with the boundary condition (a) on the semi-infinite lattice $n \in \mathbb{N}_0$

$$ T_n^{(t)} = +\infty $$

or (b) on the finite lattice $n = 0, \ldots, N, N+1$

$$ T_n^{(t)} = T_{N+2}^{(t)} = +\infty. $$

Equations (6) and (7) for the ultradiscrete Toda molecule are obtained by ultradiscretizing the corresponding (3) and (4) for the discrete Toda molecule. Assume that $q_n^{(t)} = \exp(-(Q_n^{(t)})/\varepsilon)$, $e_n^{(t)} = \exp(-E_n^{(t)}/\varepsilon)$, $\tau_n^{(t)} = \exp(-T_n^{(t)}/\varepsilon)$ with $\varepsilon > 0$ and take the limit $\varepsilon \to 0$. Then, equations (3), (4) tend to (6), (7), respectively. The limiting procedure in ultradiscretization replaces the operations $\times$, $/$ and $+$ with $\times$, $-$ and $\min$, respectively, for we have

$$ -\varepsilon \log(e^{-X/\varepsilon} \times e^{-Y/\varepsilon}) = X + Y, $$

$$ -\varepsilon \log(e^{-X/\varepsilon} / e^{-Y/\varepsilon}) = X - Y, $$

$$ -\varepsilon \log(e^{-X/\varepsilon} + e^{-Y/\varepsilon}) \to \min \{ X, Y \} \quad \text{as} \quad \varepsilon \to 0. $$

However, the counterpart of subtraction, $-$, does not exist since the limit of $\varepsilon \log(e^{-X/\varepsilon} - e^{-Y/\varepsilon})$ as $\varepsilon \to 0$ is undetermined. Commonly, we cannot ultradiscretize equations containing subtractions. In particular, we cannot directly ultradiscretize the determinant solution (5) because we may encounter subtractions in expanding the determinant. In section 3, we derive a subtraction-free expression of the determinant solution (5) to which ultradiscretization is directly applicable.

3. Initial value problem of the discrete Toda molecule

As an initial value problem of the discrete Toda molecule, we consider the following.

For the discrete Toda molecule (1), let us write the initial values at $t = 0$

$$ q_n^{(0)} = a_{2n}, \quad e_n^{(0)} = a_{2n+1} $$

(a) for $n \in \mathbb{N}_0$ on the semi-infinite lattice and (b) for $n = 0, \ldots, N$ on the finite lattice where $a_{2N+1} = 0$. Then, for each $t \in \mathbb{N}_0$ and $n$, find the exact value of $q_n^{(t)}$, $e_n^{(t)}$ uniquely determined from (1) in terms of the initial values $a_n$.

To the qd algorithm for Padé approximants whose recurrence equations are given by (1), a combinatorial interpretation was given by Viennot [8], in which a combinatorial expression of the determinant (5a) is formulated in terms of non-intersecting paths. The fundamental idea used in section 3 comes from Viennot’s approach to the qd algorithm.

The discrete Toda molecule (1) is linearized in the following sense. The nonlinear system (1) for $d_n^{(t)}$ and $e_n^{(t)}$ reduces into the linear system (5b) for $f_n^{(t)}$ through the dependent variable transformations (3) and (5a) via the tau function $\tau_n^{(t)}$. We can thus evaluate the time evolution
of the discrete Toda molecule by the dispersion relation (5b) whose initial value problem is exactly solved by
\[
f_n^t = f_n^0, \quad t, n \in \mathbb{N}_0.
\]

The initial value problem therefore amounts to the following two subproblems.

(i) Find the initial values \( f_n^0 \) of \( f_n^t \) at \( t = 0 \) in terms of \( a_n \) from (9), (3) and (5).

(ii) Find the value of the determinant (5a) to evaluate the tau function \( \tau_n^t \) for each \( t \in \mathbb{N}_0 \).

Note that the expression of the tau function \( \tau_n^t \) obtained in this way is surely exact despite that we need in subproblem (i) to determine infinitely many values \( f_n^0 \) for \( n \in \mathbb{N}_0 \). This is because, for each \( t, n \), the tau function \( \tau_n^t \) is given as a determinant of finitely many entries \( f_n^0, \ldots, f_{n+2n-1}^0 \). We can thus evaluate the value of \( \tau_n^t \) exactly in finitely many arithmetic operations from the initial values \( a_n \).

In section 3.1, we first examine the discrete Toda molecule on the semi-infinite lattice \( n \in \mathbb{N}_0 \), we then in section 3.2 consider it on the finite lattice \( n = 0, \ldots, N \).

3.1. Case of the semi-infinite lattice

In order to solve subproblem (i), we utilize Flajolet’s combinatorial interpretation of continued fractions [11]: Let us consider a path \( P \) in \( \mathbb{Z}^2 \) consisting of up steps \( U = (1, 1) \) and down steps \( D = (1, -1) \). We say that \( P \) is positive if \( P \) never goes beneath the x-axis, \( y = 0 \). (A positive path can touch the x-axis.) We say that \( P \) is grounded if both of the two ends, the initial and terminal points, of \( P \) are on the x-axis. Figure 1 shows an example of a positive grounded path \( P \). We label each step in \( P \) by \( a_i \) if the step is an up step ascending from the line \( y = n \) and by unity if a down step. We then define the weight \( w(P) \) of \( P \) by the product of the labels of all the steps in \( P \). For example, the path \( P \) in figure 1 weighs \( w(P) = a_2 a_1 a_2 \). We conventionally assume the weight of empty paths of no steps to be unity. We refer by \( D(P) \) to the number of down steps in \( P \).

Lemma 1 (Flajolet [11]). It holds that
\[
\sum_P w(P)^{D(P)} = \frac{1 - \frac{a_0 z}{1 - \frac{a_1 z}{1 - \frac{a_2 z}{1 - \ldots}}}}{1 - \frac{a_0 z}{1 - \frac{a_1 z}{1 - \frac{a_2 z}{1 - \ldots}}}},
\]
where the (formal) sum in the left-hand side is taken over all the positive grounded paths \( P \) whose initial point is fixed at \((0, 0)\).
the form called the Stieltjes–Rogers polynomial:

\[ f_n = \sum_{k_1=0}^{n} \sum_{k_2=0}^{k_1} \cdots \sum_{k_n=0}^{k_{n-1}+1} a_{k_1} a_{k_2} \cdots a_{k_n}. \]

The initial value \( f_n^{(0)} \) of \( f_n \) is thus found as a polynomial in \( a_k \) homogeneous of degree \( n \). The number of monomials in \( f_n^{(0)} \), which is equal to the number of positive grounded paths from \((0, 0)\) to \((2n, 0)\), is counted by the Catalan number \( C_n = \frac{1}{n+1} \binom{2n}{n} \). For details on the Catalan numbers, refer to the On-Line Encyclopedia of Integer Sequences [15] for Sequence A000108.

In order to solve subproblem (ii), we utilize Gessel–Viennot’s lemma on determinants [12, 13]. A general statement of Gessel–Viennot’s lemma is the following.

This observation on Padé approximants leads us to the solution to subproblem (i). Owing to lemma 1, with the normalization that \( f_0^{(0)} = 1 \),

\[ f_n^{(0)} = \sum_P w(P), \]

where the sum in the right-hand side is taken over all the positive grounded paths \( P \) whose two ends are fixed at \((0, 0)\) and \((2n, 0)\). For example, the first few \( f_n^{(0)} \) are

\[ f_0^{(0)} = 1, \]
\[ f_1^{(0)} = a_0, \]
\[ f_2^{(0)} = a_0^2 + a_0 a_1, \]
\[ f_3^{(0)} = a_0^3 + 2a_0^2 a_1 + a_0 a_1^2 + a_0 a_2 \cdot a_2. \]
Lemma 2 (Gessel–Viennot’s lemma, see, e.g., [13]). Let $X$ be a directed acyclic graph over which a (edge) weight function $w : E(X) \rightarrow \mathbb{C}$ is defined, where $E(X)$ denotes the set of edges in $X$. Let $u_1, \ldots, u_n$ and $v_1, \ldots, v_n$ be $n + n$ vertices in $X$. Suppose that, if $j < j'$ and $k > k'$, every two paths $P_{j,k}$ from $u_j$ to $v_k$ and $P_{j',k'}$ from $u_{j'}$ to $v_{k'}$ intersect at least one vertex in $G$, namely $P_{j,k} \cap P_{j',k'} \neq \emptyset$.

Then, with the normalization that

$$
\text{det} \left( \sum_{P_{j,k}} w(P_{j,k}) \right)_{j,k=1,\ldots,n} = \sum_{\{P_1, \ldots, P_n\}} w(P_1) \cdots w(P_n),
$$

(17)

where the $(j,k)$-entry of the determinant in the left-hand side is the sum of the weight of all the paths $P_{j,k}$ from $u_j$ to $v_k$: the sum in the right-hand side ranges over all $n$-tuples $(P_1, \ldots, P_n)$ of paths $P_j$ from $u_j$ to $v_j$, such that every two paths $P_j$ and $P_k$, $j \neq k$, are non-intersecting, namely $P_j \cap P_k = \emptyset$.

Due to (10) and (14), the $(j, k)$-entry of the determinant (5a), $f_{j+k}^{(t)} = f_{t+j+k}^{(0)}$, is shown to be equal to the sum of the weight $w(P)$ of all the positive grounded paths $P$ going from $(0, 0)$ to $(2t + 2j + 2k, 0)$ or equivalently going from $(-2j, 0)$ to $(2t + 2k, 0)$. Assuming the graph $X$ to be the union of all the positive grounded paths from $(-2n + 2, 0)$ to $(2t + 2n - 2, 0)$ as well as $u_{j+1} = (-2j, 0)$, $v_{j+1} = (2t + 2k, 0)$, we can thereby successfully apply Gessel–Viennot’s lemma to expand the determinant $\tau_n^{(0)} = \det(f_{t+j+k}^{(0)})_{j,k=0}^{t}$: For $t, n \in \mathbb{N}_0$, let $P(t, n)$ denote the collection of $n$-sets $P = \{P_0, \ldots, P_{n-1}\}$ of positive grounded paths $P_j$ satisfying the following conditions.

(a) The two ends of $P_j$ are fixed at $(-2j, 0)$ and $(2t + 2j, 0)$.
(b) The $n$ paths $P_0, \ldots, P_{n-1}$ are non-intersecting. Namely, every two distinct paths $P_j$ and $P_k$, $j \neq k$, never intersect at any points.

Then, with the normalization that $f_0^{(0)} = 1$, Gessel–Viennot’s lemma yields that

$$
\tau_n^{(0)} = \sum_{P \in P(t, n)} w(P) \quad \text{where } w(P) = w(P_0) \cdots w(P_{n-1}).
$$

(18)

As shown in figure 3, we can draw each $n$-set $P = \{P_0, \ldots, P_{n-1}\} \in P(t, n)$ as a diagram of $n$ positive grounded paths which are non-intersecting.

The value of $\tau_n^{(0)}$ is found as a polynomial in $a_t$ homogeneous of degree $2n + n - 1)/2$. The number of monomials in $\tau_n^{(0)}$, which is equal to the cardinality $\# P(t, n)$, is exactly evaluated in [8]

$$
\# P(t, n) = \prod_{1 \leq j \leq k < n} \frac{2n + j + k}{j + k}.
$$

(19)

We have solved subproblems (i) and (ii). The solution to the initial value problem of the discrete Toda molecule on the semi-infinite lattice $n \in \mathbb{N}_0$ is given as follows.

Theorem 3. The solution to the initial value problem of the discrete Toda molecule (1a), (1b) and (1c) on the semi-infinite lattice $n \in \mathbb{N}_0$ is given by (3) with the tau function

$$
\tau_n^{(t)} = \sum_{P \in P(t, n)} w(P), \quad t, n \in \mathbb{N}_0.
$$

(20)

For example, for $t = 2, n = 3$, the value of the tau function $\tau_3^{(2)}$ in theorem 3 is evaluated by

$$
\tau_3^{(2)} = a_0^3 a_1^3 a_2 a_3 a_4 a_5 + a_0^3 a_1^3 a_2 a_3 a_4 a_5 + a_0^3 a_1^3 a_2 a_3 a_4 a_5 + a_0^3 a_1^3 a_2 a_3 a_4 a_5.
$$

(21)
The $n$-sets $P = \{P_0, \ldots, P_{n-1}\} \in P(t, n)$ of positive grounded paths, where $t = 4, n = 3$. Each $n$-set $P$ can be drawn in a diagram of $n$ non-intersecting positive grounded paths $P_j$ such that $P_j$ goes from $(-2j, 0)$ to $(2t + 2j, 0)$.

Expression (20) of the tau function $\tau(t)$ is subtraction-free, namely contains no subtractions. That is why $\tau(t)$ is positive for every $t, n \in \mathbb{N}_0$ if and only if the initial value $a_n$ is positive for every $n \in \mathbb{N}_0$. Subtraction-free expression (20) of $\tau(t)$ is ultradiscretizable to obtain an exact solution to the ultradiscrete Toda molecule.

3.2. Case of the finite lattice

For the discrete Toda molecule on the finite lattice $n = 0, \ldots, N$, we can solve subproblems (i) and (ii) in much the same way as the semi-infinite lattice $n \in \mathbb{N}_0$ described in section 3.1. However, since we have finitely many initial values $a_0, \ldots, a_{2N}$ terminated by $a_{2N+1} = 0$, we should modify the discussion appropriately.

For a path $P$, let us refer by $H(P)$, the height of $P$, to the level (y-coordinate) of the highest points in $P$. For example, the height of the positive grounded path in figure 1 is $H(P) = 3$. The terminated version of Flajolet’s interpretation is the following.
Lemma 4 (Flajolet [11]). It holds for every \( K \in \mathbb{N}_0 \) that
\[
\sum_{H(P) \leq K+1} w(P) z^{D(P)} = \frac{1}{1 - a_0 z} - \frac{1}{1 - a_1 z} + \cdots - \frac{1}{1 - a_K z},
\]
where the (formal) sum on the left-hand side is taken over all the positive grounded paths \( P \) of height \( H(P) \leq K + 1 \) whose initial point is fixed at \((0, 0)\).

As a consequence of lemma 4, by solving (12) for \( n = 0, \ldots, N \), we obtain, instead of (14),
\[
f_{n}^{(0)} = \sum_{H(P) \leq 2N+1} w(P),
\]
where the sum in the right-hand side ranges over all positive grounded paths of height \( \leq 2N+1 \) going from \((0, 0)\) to \((2n, 0)\). The formula (23) is equivalent to (14) with \( a_k = 0 \) for all \( k > 2N \).

As an initial value problem of the ultradiscrete Toda molecule (2), we consider the totally ultradiscretizable As stated in theorem 5, the tau function \( \tau_n \) in (25) is consistent with the boundary condition (4e) on the finite lattice. Therefore, the tau function \( \tau_n \) solves the discrete Toda molecule on the finite lattice. Note that the formula (25) can be derived from (20) by assuming \( a_k = 0 \) for \( k > 2N \). Hence, the tau function \( \tau_n \) in (25) is also subtraction-free and ultradiscretizable.

4. Initial value problem of the ultradiscrete Toda molecule

As an initial value problem of the ultradiscrete Toda molecule (2), we consider the totally analogous problem to the discrete Toda molecule solved in section 3.

For the ultradiscrete Toda molecule (2), let us write the initial value at \( t = 0 \)
\[
Q_n^{(0)} = A_{2n}, \quad E_{n+1}^{(0)} = A_{2n+1}
\]

(26)
Let $P$ be a positive grounded path. We label each step in $P$ by $A_n$ if the step is an up step ascending from the line $y = n$ and by zero if a down step. We define the weight $W(P)$ by the sum of the labels of all the steps in $P$. The solution to the initial value problem of the ultradiscrete Toda molecule is then given by (6) with the tau functions
\[ T_n^{(t)} = \min_{P \in P(t,n)} W(P), \quad W(P) = W(P_0) + \cdots + W(P_{n-1}). \tag{27} \]

The support $P(t,n)$ of the minimum is much the same as the sum in (20).

Note that expression (27) applies not only to the semi-infinite lattice $n \in \mathbb{N}_0$ but also to the finite lattice $n = 0, \ldots, N$. Indeed, every path $P$ of height $H(P) > 2N + 1$ must contain an up step ascending from the line $y = 2N + 1$ which has the label $A_{2N+1} = +\infty$, and hence $W(P) = +\infty$. Hence, if $P \in P(t,n)$ contains a path $P_i$ of $H(P_i) > 2N + 1$, then $P$ does not contribute to the minimum in (27) since $W(P) = +\infty$. Hence,
\[ \min_{P \in P(t,n)} W(P) = \min_{P \in P(t,n,N)} W(P) \tag{28} \]
in which the right-hand side can be derived by ultradiscretizing the tau function (25) for the discrete Toda molecule on the finite lattice. In particular, $T_n^{(t)} = +\infty$ for the same reason that is consistent with the boundary condition $H_{N+1}$ on the finite lattice. The tau function $T_n^{(t)}$ in (27) therefore solves the initial value problem of the ultradiscrete Toda molecule $n \in \mathbb{N}_0$ both on the semi-infinite lattice and on the finite lattice $n = 0, \ldots, N$.

In following sections, 4.1 and 4.2, we will simplify expression (27) of the tau function $T_n^{(t)}$ by combinatorial observation. In section 4.3, we will investigate the behavior of the simplified expression from specific initial values in comparison with the box–ball system.

### 4.1. Solution in tabular paths

Let $P$ be a positive grounded path. We refer to two consecutive up–down steps and down–up steps, $UD$ and $DU$, in $P$ by a peak and a valley, respectively. We say that $P$ is tabular provided that, for some $k \in \mathbb{N}_0$, all the peaks and the valleys in $P$ reside in the strip of height one bordered by the two horizontal lines $y = k$ and $y = k + 1$.

For $t, n \in \mathbb{N}_0$, we define a subset $\hat{P}(t,n) \subseteq P(t,n)$ as the collection of $n$-sets $\hat{P} = \{P_0, \ldots, P_{n-1}\} \in P(t,n)$ in which every $P_i$ is tabular. For example, all the $n$-sets $P \in P(t,n)$ in figure 3, except the upper right one, belong to $\hat{P}(t,n)$ since each path in $P$ is tabular.

**Lemma 6.** There exists $\hat{P} \in \hat{P}(t,n)$ which takes the minimal weight: $W(\hat{P}) = \min_{P \in \hat{P}(t,n)} W(P)$.

**Proof.** We will prove the lemma by examining particular subpaths which we call hooks. Let $P$ be a positive grounded path. We call a subpath $H$ of $P$ an up hook (resp. a down hook) provided that $H$ is of at least four steps and that both the first and the last steps of $H$ are down steps (resp. up steps) and all the middle steps are up steps (resp. down steps). That is, each up hook (resp. down hook) is of the form $DU^kD$ (resp. $UD^kU$) for some integer $k \geq 2$. For example,
Figure 5. The hooks $H$ in a positive grounded path $P$. The path $P$ contains three up hooks, highlighted in dotted lines and two down hooks, in dashed lines.

Figure 6. The deformation by the maps $\varphi$ and $\psi$. The paths $\varphi(P)$ and $\psi(P)$ (depicted in solid lines) are obtained from the path $P$ (in dotted lines) in figure 5 by deforming each up hook in $P$ as indicated by an arrow.

see figure 5. Obviously, a positive grounded path $P$ is tabular if and only if $P$ contains no hooks.

Let us define two maps $\varphi$ and $\psi$ which deform a positive grounded path $P$ as follows: $\varphi(P)$ (resp. $\psi(P)$) denotes the positive grounded path obtained from $P$ by replacing each up hook in $P$, say $D Ud$, with $U_{j-1} Du$ (resp. with $Du U_{j-1}$), where $\varphi(P) = \psi(P) = P$ if $P$ contains no up hooks. See figure 6 which shows the deformed paths $\varphi(P)$ and $\psi(P)$ obtained from the positive grounded path $P$ in figure 5.

We can observe the following on the maps $\varphi$ and $\psi$. Let $P$ and $P'$ be positive grounded paths.

(a) $\varphi$ and $\psi$ never increase the number of up hooks in $P$ as well as the number of down hooks in $P$.

(b) If $P$ contains no up hooks to the right side of the line $x = j$ then $\varphi(P)$ so to $x = j - 2$.

Similarly, if $P$ contains no up hooks to the left side of $x = j$ then $\psi(P)$ so to $x = j + 2$.

(c) $\varphi$ and $\psi$ never move the location of the two ends of $P$.

(d) If $P$ and $P'$ are non-intersecting then so are $\varphi(P)$ and $\psi(P')$. That is also the case with $\varphi(P)$ and $\psi(P')$.

(e) The following 'mean' formula holds:

$$W(\varphi(P)) + W(\psi(P)) = 2W(P).$$

(29)

Now, let us prove lemma 6. Let $P = \{P_0, \ldots, P_{n-1}\} \in P(t, n)$. We can assume that $P$ takes the minimal weight, $W(P) = \min_{P \in P(t, n)} W(P')$, without any loss of generality.
For each \( k \in \mathbb{N}_0 \), let \( \varphi^k(P) = \{\varphi^k(P_0), \ldots, \varphi^k(P_{n-1})\} \) denote the \( n \)-sets of positive grounded paths obtained from \( P \) by applying the map \( \varphi \) iteratively \( k \) times to each path \( P_j \in P \). By induction with respect to \( k \in \mathbb{N}_0 \), we can show the following.

(i) Due to the observation (b), every path in \( \varphi^k(P) \) contains no up hooks to the right side of the line \( x = 2t - 2k - 1 \). That is because \( P \) contains no up hooks to the right side of \( x = 2t - 1 \).

(ii) Due to observations (c) and (d), \( \varphi^k(P) \in P(t, n) \).

(iii) Due to observation (e), \( W(\varphi^k(P)) = W(P) \). Indeed, if \( W(\varphi^k(P)) > W(\varphi^{k-1}(P)) \), formula (29) would lead to \( W(\psi \circ \varphi^{k-1}(P)) < W(\varphi^{k-1}(P)) \), which contradicts the minimality of \( W(P) \).

As a consequence of (i), (ii), (iii), we can deduce that \( \varphi^{-1}(P) \in P(t, n) \) contains no up hooks and has the minimal weight \( W(\varphi^{-1}(P)) = W(P) \).

In a similar way, we can show the existence of \( \tilde{P} \in P(t, n) \) containing no down hooks and having the minimal weight \( W(\tilde{P}) = W(P) \). From the discussion in the last paragraph, \( \varphi^{-1}(\tilde{P}) \) contains no up hooks and has the minimal weight \( W(\varphi^{-1}(\tilde{P})) = W(\tilde{P}) \). Further, due to observation (a), \( \varphi^{-1}(\tilde{P}) \) contains no down hooks. Therefore, \( \varphi^{-1}(\tilde{P}) \) having the minimal weight belongs to the set \( \tilde{P}(t, n) \). That completes the proof.

As a consequence of lemma 6, we can also solve the initial value problem of the ultradiscrete Toda molecule in the following way.

**Theorem 7.** The solution to the initial value problem of the ultradiscrete Toda molecule (2) is given by (6) with the tau function

\[
T_n^{(t)} = \min_{P \in P(t, n)} W(\tilde{P}).
\]

Expression (30) of the tau function \( T_n^{(t)} \) is supported by the set \( \tilde{P}(t, n) \) much smaller than \( P(t, n) \) in (27). In fact, the cardinality of \( \tilde{P}(t, n) \) is equal to the binomial number

\[
\#\tilde{P}(t, n) = \binom{t + n - 1}{t} = \prod_{1 \leq j \leq t} \frac{n + j}{j}
\]

which is much smaller than \( \#P(t, n) \) given by (19). In this sense, expression (30) gives a simpler expression of the tau function \( T_n^{(t)} \) than (27).

### 4.2. Solution in shortest paths on a graph

In section 4.2, based on theorem 7, we derive another combinatorial expression of the solution in terms of shortest paths on a graph.

Let \( G \) denote the (directed acyclic) graph in \( \mathbb{N}_0^2 \) consisting of the vertices at the points \( (j, k) \in \mathbb{N}_0^2, j \geq k \), connected by the two types of (directed) edges: east edges \( E_{j,k} = (2, 0) \) and south edges \( S_{j,k} = (0, -1) \). Here the subscripts \( j, k \) indicate that the initial points of \( E_{j,k} \) and \( S_{j,k} \) are at the vertex \( (j, k) \). As shown in figure 7, since the east edges \( E_{j,k} \) have length two, the graph \( G \) splits into two disjoint subgraphs.

We define the weight function \( W \) over the edges in \( G \) by

\[
W(E_{j,k}) = \sum_{t=0}^{j-k-1} A_t + kA_{j-k}, \quad W(S_{j,k}) = 0,
\]

where \( A_n \) are the initial values for the ultradiscrete Toda molecule. With respect to the Toda molecule on the finite lattice \( n = 0, \ldots, N \), we have \( A_{2N+1} = +\infty \), hence, we assume \( W(E_{j,k}) = +\infty \) if \( j - k \geq 2N + 1 \) when considering it on the finite lattice.
We think of the weight $W(e)$ of an edge $e$ as the length of $e$. For each path $Q$ on $G$, we then think of the weight $W(Q)$ as the length of $Q$, which is equal to the sum of the weight $W(e)$ of all the edges $e$ passed by $Q$. (The length $W(Q)$ may be negative due to the arbitrariness in $A_n$.)

For $t \in \mathbb{N}_0$, $t \geq 1$ and $n \in \mathbb{N}_0$, let $\bar{Q}(t, n)$ denote the collection of paths on $G$ between the two vertices $(t, t)$ and $(t + 2n, 1)$. We then have a one-to-one correspondence between $\bar{P} = \{P_0, \ldots, P_{n-1}\} \subseteq \bar{P}(t, n)$ and $\bar{Q} \in \bar{Q}(t, n)$. The tabular positive grounded path $\bar{P}$ has its peaks and valleys in the strip bordered by the lines $y = k - 2j$ and $y = k - 2j + 1$ if and only if the path $\bar{Q}$ on $G$ passes through the east edge $E_{t+2j-4}$. For example, in the $n$-sets $P \in P(t, n)$ of positive grounded paths in figure 3, the lower left one belongs to $\bar{P}(t, n)$ and is in one-to-one correspondence with the path $\bar{Q}$ in figure 7. Actually, the weight function $W$ on $G$ is defined in (32) so that $W(\bar{P}) = W(\bar{Q})$ for every pair of $\bar{P}$ and $\bar{Q}$ in one-to-one correspondence. We thereby have the identity

$$\min_{\bar{Q} \in \bar{Q}(t, n)} W(\bar{Q}) = \min_{P \in \bar{P}(t, n)} W(P).$$

(33)

For $t, n \in \mathbb{N}_0$, let us define $\bar{Q}(t, n)$ to be the collection of paths on $G$ between the two vertices $(t, t)$ and $(t + 2n, 0)$. We can then show that the identity (33) still holds even if we replace the support set $\bar{Q}(t, n)$ of the left-hand minimum with $\bar{Q}(t, n)$.

$$\min_{\bar{Q} \in \bar{Q}(t, n)} W(\bar{Q}) = \min_{P \in \bar{P}(t, n)} W(P),$$

(34)

for $W(E_{j,0}) = W(E_{j,1})$ for every $j \in \mathbb{N}_0, j \geq 1$. In addition, in that case, the identity (34) also takes place for $t = 0$.

Finally, combining theorem 7 and the identity (34), we obtain the following result.
Figure 8. Time evolution of the box–ball system. In each state, each ‘Φ’ and ‘1’ denote an empty box and a ball in a box, respectively. At each time $t$, $Q_n(t)$ denotes the size of the $(n + 1)$th soliton (a block of 1s) while $E_n(t)$ the distance between the $n$th and $(n + 1)$th solitons (the size of a block of 0s).

Theorem 8. The solution to the initial value problem of the ultradiscrete Toda molecule (2), both on the semi-infinite lattice $n \in \mathbb{N}_0$ and on the finite lattice $n = 0, \ldots, N$, is given by (6) with the tau function

$$T_n^{(t)} = \min_{Q \in \mathcal{Q}(t, n)} W(Q)$$

(35)

for $t \in \mathbb{Z}$, where the weight function $W$ on the graph $G$ is defined by (32).

The right-hand side of (35) denotes the length of the shortest paths on the graph $G$ between the two vertices $(t, t)$ and $(t + 2n, 0)$. It should be noted that Nakata [16] constructed a similar combinatorial expression in terms of shortest paths (called minimum weight flows in [16]) of a particular solution to the ultradiscrete Toda molecule on the finite lattice.

4.3. Examples of solutions and the box–ball system

In theorem 8, we obtained a combinatorial expression of the tau function $T_n^{(t)}$ of the ultradiscrete Toda molecule in terms of shortest paths on the graph $G$. The tau function $T_n^{(t)}$ is described in the initial values $A_n$ and solves the initial value problem of the ultradiscrete Toda molecule. In section 4.3, we examine the behavior of the combinatorial tau function from specific initial values $A_n$. In particular, we compare the results with the time evolution of the box–ball system [17].

At first, we will give a brief review of the box–ball system. The box–ball system is composed of an array of infinitely many boxes and finitely many balls put into the boxes. Each box can contain at most one ball. The time evolution of the box–ball system is described by the following rule. Given a state at the time $t$, move the leftmost ball to the right-nearest empty box. Next, in the balls not moved yet, move the leftmost one to the right-nearest empty box. Repeat this procedure until all the balls are moved. Then, we obtain the state at the next time $t + 1$. Figure 8 shows an example of the time evolution of the box–ball system from a specific initial state. In figure 8, each ‘Φ’ denotes an empty box while each ‘1’ a ball in a box.

It is well known that the ultradiscrete Toda molecule on the finite lattice describes the dynamics of the box–ball system [10, 18]. The ultradiscrete Toda molecule (2) on the finite lattice $n = 0, \ldots, N$ reads the box–ball system as follows. $Q_n^{(t)}$ denotes the size of the $(n + 1)$th soliton (from the left) at the time $t$ while $E_n^{(t)}$ the distance between the $n$th and $(n + 1)$th solitons, where a soliton means a block of balls. For example, in the state $t = 0$ in figure 8, we have three solitons (blocks of 1s) of size $Q_0^{(0)} = 2$, $Q_1^{(0)} = 1$ and $Q_2^{(0)} = 1$. The distance between the first and second solitons are given by $E_1^{(0)} = 2$, which is equal to the size of the block of empty boxes (0s) between the solitons. Similarly, the distance between the second and third solitons is $E_2^{(0)} = 2$. 

| time | state at the time $t$ | $Q_0^{(t)}$ | $E_1^{(t)}$ | $Q_1^{(t)}$ | $E_2^{(t)}$ | $Q_2^{(t)}$ |
|------|---------------------|------------|------------|------------|------------|------------|
| $t = 0$ | $\cdots 001100100100000000000 \cdots$ | $2$ | $2$ | $1$ | $2$ | $1$ |
| $1$ | $\cdots 000011010100000000000 \cdots$ | $2$ | $1$ | $1$ | $2$ | $1$ |
| $2$ | $\cdots 000000101101000000000 \cdots$ | $1$ | $1$ | $2$ | $1$ | $1$ |
| $3$ | $\cdots 000000001010110000000 \cdots$ | $1$ | $2$ | $1$ | $1$ | $2$ |
| $4$ | $\cdots 0000000000101001100000 \cdots$ | $1$ | $2$ | $1$ | $2$ | $2$ |
If the initial values $A_n$ at $t = 0$ are all positive integers, the ultradiscrete Toda molecule (2) on the finite lattice $n = 0, \ldots, N$ exactly describes the time evolution of the box–ball system of $(N + 1)$ solitons.

**Example 1.** We first observe the tau function $T^{(t)}_n$ on the finite lattice $n = 0, \ldots, N = 2$ from the initial values

$$A_0 = 2, \quad A_1 = 2, \quad A_2 = 1, \quad A_3 = 2, \quad A_4 = 1, \quad A_5 = +\infty, \quad \text{(36)}$$

which correspond to the initial state of the box–ball system in figure 8. We show in figure 9 the graph $G$ over which the length of each east edge $E_{jk}$ determined by (32) is written. (For simplicity, the two disjoint subgraphs of $G$ are drawn separately.) From theorem 8, we can determine the value of $T^{(t)}_n$ by finding the shortest path from $(t, t)$ to $(t + 2n, 0)$. For example, for $t = 4, n = 2$, the path $Q$ in figure 9 is the shortest path from $(4, 4)$ to $(8, 0)$ of length $W(Q) = 6 + 9 = 15$. Hence, $T_2^{(4)} = 15$. Similarly, for $t = 3, n = 3$, the path $Q'$ is the shortest path from $(3, 3)$ to $(9, 0)$ of length $W(Q') = 6 + 7 + 10 = 23$. Hence, $T_3^{(3)} = 23$. In a similar way, for $t = 0, \ldots, 5$ and $n = 0, 1, 2, 3$, we obtain

$$T_0^{(0)} = 0, \quad T_1^{(0)} = 0, \quad T_2^{(0)} = 4, \quad T_3^{(0)} = 11; \quad \text{(37a)}$$

$$T_0^{(1)} = 0, \quad T_1^{(1)} = 2, \quad T_2^{(1)} = 7, \quad T_3^{(1)} = 15; \quad \text{(37b)}$$

$$T_0^{(2)} = 0, \quad T_1^{(2)} = 4, \quad T_2^{(2)} = 10, \quad T_3^{(2)} = 19; \quad \text{(37c)}$$

$$T_0^{(3)} = 0, \quad T_1^{(3)} = 5, \quad T_2^{(3)} = 13, \quad T_3^{(3)} = 23; \quad \text{(37d)}$$

$$T_0^{(4)} = 0, \quad T_1^{(4)} = 6, \quad T_2^{(4)} = 15, \quad T_3^{(4)} = 27; \quad \text{(37e)}$$

$$T_0^{(5)} = 0, \quad T_1^{(5)} = 7, \quad T_2^{(5)} = 17, \quad T_3^{(5)} = 31. \quad \text{(37f)}$$
while $\hat{Q}$ southward to $\hat{Q}_1$. Substituting these values into (6), we obtain the values of $J$. Phys. A: Math. Theor. the time evolution of the box–ball system.

The initial values

\[ A_0 = 1, \quad A_1 = 2, \quad A_2 = 2, \quad A_3 = 2, \quad A_4 = 3, \quad A_5 = +\infty \]

yield the graph $G$ in figure 10, in which the path $\hat{Q}$ is the shortest path between (4, 4) and (8, 0) while $\hat{Q}'$ is the shortest path between (3, 3) and (9, 0). (Hence, $T_n^{(4)} = 15$ and $T_3^{(3)} = 22$.)

In general, if $A_n$ are weakly increasing, we have $W(E_{j,k}) = W(E_{j,k-1}) = (k-1)(A_{j-k} - A_{j-k+1}) \leq 0$. This implies that each east edge $E_{j,k}$ is shorter than any of the east edges below, $E_{j,k}', k' < k$. Hence, $\hat{Q}$ is shortest between $(t, t)$ and $(t + 2n, 0)$.

In the box–ball system, a corresponding initial state satisfies $Q_0^{(0)} \leq E_1^{(0)} \leq Q_1^{(0)} \leq \cdots \leq E_N^{(0)} \leq Q_N^{(0)}$. As shown in figure 11, such an initial state gives rise to the trivial time evolution in which each soliton independently goes right at the speed of its size. The initial values $A_n$ weakly increasing gives rise to trivial behaviors both in finding the shortest paths on $G$ and in the time evolution of the box–ball system.

Figure 10. The graph $G$ associated with the initial values $A_n$ weakly increasing. $A_0 \leq A_1 \leq \cdots$. Each east edge is shorter than all the east edges below itself. The paths $\hat{Q}$ and $\hat{Q}'$ on $G$ are the shortest paths between (4, 4) and (8, 0) and between (3, 3) and (9, 0), respectively.

Substituting these values into (6), we obtain the values of $Q_n^{(i)}$ and $E_n^{(i)}$.

\[
Q_0^{(0)} = 2, \quad E_1^{(0)} = 2, \quad Q_1^{(0)} = 1, \quad E_2^{(0)} = 2, \quad Q_2^{(0)} = 1; \quad (38a)
\]

\[
Q_0^{(1)} = 2, \quad E_1^{(1)} = 1, \quad Q_1^{(1)} = 1, \quad E_2^{(1)} = 2, \quad Q_2^{(1)} = 1; \quad (38b)
\]

\[
Q_0^{(2)} = 1, \quad E_1^{(2)} = 1, \quad Q_1^{(2)} = 2, \quad E_2^{(2)} = 1, \quad Q_2^{(2)} = 1; \quad (38c)
\]

\[
Q_0^{(3)} = 1, \quad E_1^{(3)} = 2, \quad Q_1^{(3)} = 1, \quad E_2^{(3)} = 1, \quad Q_2^{(3)} = 2; \quad (38d)
\]

\[
Q_0^{(4)} = 1, \quad E_1^{(4)} = 2, \quad Q_1^{(4)} = 1, \quad E_2^{(4)} = 2, \quad Q_2^{(4)} = 2. \quad (38e)
\]

Of course, the values of $Q_n^{(i)}$ and $E_n^{(i)}$ found in this way are equal to those in figure 8 which are determined from the time evolution of the box–ball system from the corresponding initial state.

Example 2. Case of $A_n$ increasing. Suppose that the initial values $A_n$ are weakly increasing: $A_0 \leq A_1 \leq A_2 \leq \cdots$. Then, we can readily find the shortest path from $(t, t)$ to $(t + 2n, 0)$: the path $\hat{Q}$ which departs from $(t, t)$, goes eastward to $(t + 2n, 0)$, turns south there and goes southward to $(t + 2n, 0)$.

For example, for $N = 2$, the initial values weakly increasing

\[
Q_0 = 1, \quad A_1 = 2, \quad A_2 = 2, \quad A_3 = 2, \quad A_4 = 3, \quad A_5 = +\infty \]

yields the graph $G$ in figure 10, in which the path $\hat{Q}$ is the shortest path between (4, 4) and (8, 0) while $\hat{Q}'$ is the shortest path between (3, 3) and (9, 0). (Hence, $T_n^{(4)} = 15$ and $T_3^{(3)} = 22$.)

In general, if $A_n$ are weakly increasing, we have $W(E_{j,k}) = W(E_{j,k-1}) = (k-1)(A_{j-k} - A_{j-k+1}) \leq 0$. This implies that each east edge $E_{j,k}$ is shorter than any of the east edges below, $E_{j,k}', k' < k$. Hence, $\hat{Q}$ is shortest between $(t, t)$ and $(t + 2n, 0)$.

In the box–ball system, a corresponding initial state satisfies $Q_0^{(0)} \leq E_1^{(0)} \leq Q_1^{(0)} \leq \cdots \leq E_N^{(0)} \leq Q_N^{(0)}$. As shown in figure 11, such an initial state gives rise to the trivial time evolution in which each soliton independently goes right at the speed of its size. The initial values $A_n$ weakly increasing gives rise to trivial behaviors both in finding the shortest paths on $G$ and in the time evolution of the box–ball system.
Figure 11. Time evolution of the box–ball system from an initial state such that $Q_0^{(0)} \leq E_1^{(0)} \leq Q_1^{(0)} \leq E_2^{(0)} \leq Q_2^{(0)}$. In this case, no interactions of solitons happen because every soliton cannot catch the solitons on the right side of itself.

Example 3. Case of $A_n$ weakly decreasing. Suppose that the initial values $A_n$ are weakly decreasing, $A_0 \geq \cdots \geq A_{2N}$ except for $A_{2N+1} = +\infty$. Also in this case, we can immediately find the shortest path from $(t, t)$ to $(t + 2n, 0)$ as follows. Let $\eta$ be a nonnegative integer $\leq t$ defined by $\eta = \min \{t, 2(N - n + 1)\}$. Then, the shortest is the path $\tilde{Q}$ which departs from $(t, t)$, goes southward to $(t, t - \eta)$, turns east there, goes eastward to $(t + 2n, \eta)$, turns south there and goes southward to $(t + 2n, 0)$. In other words, $\tilde{Q}$ is the southmost path from $(t, t)$ to $(t + 2n, 0)$ passing through no east edges of length $+\infty$. We can verify that $\tilde{Q}$ is shortest in the same idea as the case of $A_n$ weakly increasing discussed in example 2.

For example, for $N = 2$, the initial values weakly increasing $A_0 = 3$, $A_1 = 3$, $A_2 = 2$, $A_3 = 2$, $A_4 = 1$, $A_5 = +\infty$ (40) yields the graph $G$ in figure 12, in which the path $\tilde{Q}$ is the shortest path between $(4, 4)$ and $(8, 0)$ while $\tilde{Q}'$ is the shortest path between $(3, 3)$ and $(9, 0)$. (Hence, $T_2^{(4)} = 22$ and $T_3^{(3)} = 34$.)

In the box–ball system, a corresponding initial state satisfies $Q_0^{(0)} \geq E_1^{(0)} \geq Q_1^{(0)} \geq E_2^{(0)} \geq Q_2^{(0)} \geq \cdots \geq E_{N-1}^{(0)} \geq Q_N^{(0)}$. As shown in figure 13, such an initial state gives rise to interactions of solitons. Each soliton overtakes all the solitons on the right side of itself at the initial state. The initial values $A_n$ weakly decreasing gives rise to trivial behaviors in finding the shortest paths.
on \( G \). In contrast, the corresponding initial state of the box–ball system may lead to nontrivial interactions of solitons.

5. Concluding remarks

In this paper, we have investigated the discrete and ultradiscrete Toda molecules from a combinatorial viewpoint. To the tau function which solves an initial value problem of the discrete Toda molecule, we have given a combinatorial expression in terms of non-intersecting paths. In particular, in order to read the tau function in combinatorial words, we utilized Flajolet’s path interpretation of continued fractions and Gessel–Viennot’s lemma on determinants and non-intersecting paths. Due to the combinatorial expression, we have succeeded in deriving a subtraction-free expression of the tau function which is given in a Hankel determinant.

For an initial value problem of the ultradiscrete Toda molecule, we first obtained an exact solution by ultradiscretizing the tau function of the discrete Toda molecule. We next rewrote the tau function to derive a simpler expression in terms of shortest paths. As a result, we have shown that the tau function which solves the initial value problem of the ultradiscrete Toda molecule can be evaluated as the length of shortest paths on a specific graph in which the length of edges is determined by the initial value. We also observed the behavior of the tau function from specific initial values, especially weakly increasing or weakly decreasing, and compared with the time evolution of the box–ball system.

In this paper, we deduced combinatorial expressions of the tau functions with the help of a determinant solution to the discrete Toda molecule and the technique of ultradiscretization. For the tau functions (20) and (35) given in terms of combinatorial objects, however, it is expected to make combinatorial (or bijective) proofs to directly verify that the tau functions satisfy bilinear equations (4) and (7). For that purpose, the technique of alternating walks [19] for Schur symmetric functions would be useful.

The combinatorial idea used in this paper should be applicable to other discrete integrable systems associated with continued fractions, such as the \( R_I \) and \( R_{II} \) chains with \( R_I \)- and \( R_{II} \)-fractions [20, 21], the FST chain with Thiele-type continued fractions [22] and the matrix qd algorithm with the matrix S-fractions [23]. Those applications will be discussed in future works.

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