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# SOME ASPECTS OF THE TODA MOLECULE

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**Abstract.** A $q$-discrete analog of the Toda molecule equation and its $N$-soliton solution are constructed by using the bilinear method. The solution is expressed in the Casorati determinant form whose elements are given in terms of the $q$-orthogonal polynomials.

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**1. Introduction.** Recently the discrete integrable systems have attracted lots of interest since their deep relations with various physical problems and numerical schemes have been found. For example, the discrete Toda equation is nothing but the scheme of qd-algorithm for computing poles of meromorphic functions [**1**, **2**]. One of the interesting features of a Toda equation is that it allows several types of determinant expressions of solutions according to the boundary conditions. The infinite Toda lattice has the soliton solutions which are expressed by Wronski or Gram determinant, while in the finite or semi-infinite lattice case, i.e., the so-called Toda molecule case, the general solution is given in terms of a Wronski determinant. In 1998, Nakamura [**3**] showed that even in the molecule case, the soliton solutions do exist and he obtained their Gram and Casorati determinant expressions whose elements are given by the Gauss hypergeometric functions. The nontrivial vacuum solution plays the essential role for the soliton solutions to satisfy the boundary condition. It is known that the nontrivial vacuum is also crucial for the similarity reduction to nonautonomous systems. In the case of discrete soliton equations, such vacuum solutions and soliton solutions constructed from the vacuum have not yet been studied in depth. So far only a few examples of solutions of nonautonomous partial difference equations are known [**4**, **5**].

The purpose of this article is to construct a discrete analog of the $N$-soliton solution for the Toda molecule equation. We take an appropriate vacuum and show how the vacuum solution works to satisfy the boundary condition and which type of special function appears to express the soliton solution. There are many possibilities for the choice of vacuum solution. In this paper we consider the $q$-discrete case by choosing a trigonometric vacuum and give the Casorati determinant expression of soliton solutions. We should comment that very recently Nakamura obtained the same results independently and he derived the Gram determinant expression in [**6**]. In Section 2, we briefly summarize the known results about the Wronski and Casorati determinant solutions for Toda equations. The main results are given in Section 3. By a suitable choice of the vacuum solution, a natural $q$-analog of the soliton solution of the Toda molecule equation comes out. In Section 4, we give a proof of the results based on the bilinear technique of soliton theory. Concluding remarks are given in Section 5.

**2. Toda lattice and Toda molecule.** It is well known that the Toda lattice equation

$$(\log V_n)_{tt} = V_{n+1} - 2V_n + V_{n-1}$$

is transformed into the bilinear form

$$D_t^2 \tau_n \cdot \tau_n = 2\left(\tau_{n+1}\tau_{n-1} - \tau_n{}^2\right) \tag{1}$$

through the dependent variable transformation

$$V_n = 1 + (\log \tau_n)_{tt}.$$

Also the $N$-soliton solution is given in terms of the Wronski determinant

$$\tau_n = \det\left(p_i^{n+j} e^{p_i t + \xi_i} + \frac{1}{p_i^{n+j}} e^{\frac{t}{p_i}}\right)_{i,j=1}^{N},$$

where $p_i$ and $\xi_i$ are the wave number and phase constant of $i$-th soliton, respectively [**7**]. In this determinant expression, the determinant size $N$ stands for the number of solitons and the lattice site number $n$ appears as a parameter in the elements of the determinant.

On the other hand, the Toda molecule equation is written as

$$\begin{aligned} (\log V_n)_{tt} &= V_{n+1} - 2V_n + V_{n-1} \qquad (n \geq 2), \\ (\log V_1)_{tt} &= V_2 - 2V_1, \end{aligned}$$

which is in fact the simultaneous equation of the Toda lattice equation and boundary condition $V_0 = 0$. The variable transformation

$$V_n = (\log \tau_n)_{tt} \qquad (n \geq 0)$$

leads to the bilinear equation

$$D_t^2 \tau_n \cdot \tau_n = 2\tau_{n+1}\tau_{n-1} \qquad (n \geq 1)$$

with the boundary condition $\tau_0 = 1$. In this case the general solution is given in the form of the Wronski determinant

$$\tau_n = \det\left(\partial_t^{i+j-2} w\right)_{i,j=1}^{n} \qquad (n \geq 0),$$

where $w$ is an arbitrary function of $t$ [**7**, **8**]. Here the determinant size $n$ stands for the lattice site number.

Now a natural question arises: what is the relation between the determinant solutions of Toda lattice and Toda molecule? The molecule can be derived as a special

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case of the lattice by imposing the boundary condition. On the other hand the lattice can be regarded as a special case of the molecule by moving the boundary of the molecule to $-\infty$. However it is not clear how the determinant solutions relate to each other. In the case of continuous Toda, Nakamura [**3**] gave an answer to this question by constructing the explicit $N$-soliton solutions for the Toda molecule equation in terms of the Casorati and Gram determinants whose elements are given by the hypergeometric functions. The Casorati determinant solution for the Toda molecule of finite size is obtained as follows. For the Toda molecule equation

$$\begin{aligned}&(\log V_n)_{tt} = V_{n+1} - 2V_n + V_{n-1} \qquad (1 \le n \le M-1),\\ &V_0 = V_M = 0,\end{aligned}$$

by applying the variable transformation

$$V_n = U_n + (\log \tau_n)_{tt} \qquad (0 \le n \le M),$$

we get the bilinear equation

$$D_t^2 \tau_n \cdot \tau_n = 2U_n \left(\tau_{n+1}\tau_{n-1} - {\tau_n}^2\right) \qquad (0 \le n \le M). \tag{2}$$

Here $U_n$ is a vacuum solution of the Toda molecule equation itself; that is, $U_n$ satisfies the same equation

$$\begin{aligned}&(\log U_n)_{tt} = U_{n+1} - 2U_n + U_{n-1} \qquad (1 \le n \le M-1),\\ &U_0 = U_M = 0.\end{aligned}$$

The bilinear form (2) can be regarded as the equation of the Darboux transformation of the Toda lattice. In the case of the usual soliton solution of infinite lattice (1), we choose the trivial vacuum $U_n = 1$. For the nontrivial vacuum $U_n$, we get the nonautonomous bilinear equation for the $\tau$ function, whose solutions are normally no longer given by the exponential polynomial. From the above bilinear equation, $V_n$ is written as

$$V_n = U_n \frac{\tau_{n+1}\tau_{n-1}}{{\tau_n}^2} \qquad (0 \le n \le M).$$

Thus when $U_n$ satisfies the boundary condition, so does $V_n$. By taking the nontrivial vacuum as

$$U_n = n(M-n)(\log(1+e^t))_{tt} = \frac{n(M-n)}{\left(e^{t/2} + e^{-t/2}\right)^2} \qquad (0 \le n \le M), \tag{3}$$

the bilinear equation (2) admits the $N$-soliton solution which is given in the Casorati determinant form

$$\tau_n = (1+e^t)^{-\frac{N(N-1)}{2}} \det\left({}_2F_1\left(\begin{matrix}-n-j+1, p_i\\ -M-N+1\end{matrix}; 1+e^t\right)\right)_{i,j=1}^{N} \qquad (0 \le n \le M),$$

where ${}_2F_1$ is the Gauss hypergeometric function and $p_i$ is the wave number of $i$-th soliton chosen as

$$p_i \in \{0, -1, -2, \cdots, -M-N+1\} \qquad (1 \le i \le N).$$

Here the determinant size $N$ corresponds to the number of solitons and the lattice site number $n$ appears as a parameter in the elements of the determinant. In the next

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section we give a $q$-discrete analog of this Casorati determinant solution for the Toda molecule equation.

**3. Discrete Toda molecule and its soliton solution.** A discrete analog of the Toda molecule equation is given by

$$\frac{V_n(t+1)V_n(t-1)}{V_n(t)^2} = \frac{(1+V_{n+1}(t))(1+V_{n-1}(t))}{(1+V_n(t))^2} \qquad (1 \le n \le M-1),$$
$$V_0(t) = V_M(t) = 0,$$

which is bilinearized as

$$\tau_n(t+1)\tau_n(t-1) - \tau_n(t)^2 = \frac{U_n(t)}{1+U_n(t)}(\tau_{n+1}(t)\tau_{n-1}(t) - \tau_n(t)^2) \qquad (0 \le n \le M) \qquad (4)$$

through the dependent variable transformation

$$V_n(t) = (1+U_n(t))\frac{\tau_n(t+1)\tau_n(t-1)}{\tau_n(t)^2} - 1 \qquad (0 \le n \le M),$$

where $U_n(t)$ is the vacuum solution of the discrete Toda molecule equation satisfying

$$\frac{U_n(t+1)U_n(t-1)}{U_n(t)^2} = \frac{(1+U_{n+1}(t))(1+U_{n-1}(t))}{(1+U_n(t))^2} \qquad (1 \le n \le M-1),$$
$$U_0(t) = U_M(t) = 0.$$

By using the above bilinear equation (4), $V_n(t)$ is rewritten as

$$V_n(t) = U_n(t)\frac{\tau_{n+1}(t)\tau_{n-1}(t)}{\tau_n(t)^2} \qquad (0 \le n \le M).$$

There are many possible choices for the vacuum solution $U_n(t)$. In this article we consider a $q$-discrete Toda molecule equation. By choosing

$$U_n(t) = \frac{\left(q^{n/2} - q^{-n/2}\right)\left(q^{(M-n)/2} - q^{-(M-n)/2}\right)}{\left(q^{(t+n)/2} + q^{-(t+n)/2}\right)\left(q^{(t+M-n)/2} + q^{-(t+M-n)/2}\right)} \qquad (0 \le n \le M),$$

the bilinear equation (4) is written as

$$\tau_n(t+1)\tau_n(t-1) - \tau_n(t)^2 = \frac{\left(q^{n/2} - q^{-n/2}\right)\left(q^{(M-n)/2} - q^{-(M-n)/2}\right)}{\left(q^{t/2} + q^{-t/2}\right)\left(q^{(t+M)/2} + q^{-(t+M)/2}\right)}$$
$$\times(\tau_{n+1}(t)\tau_{n-1}(t) - \tau_n(t)^2) \qquad (0 \le n \le M).$$

In the limit $q \to 1$, this recovers the continuous case (2) with (3). The above bilinear equation is solved by the Casorati determinant

$$\tau_n(t) = \frac{1}{\prod_{k=0}^{N-2}(1+q^{t-N+1+k})^{N-1-k}} \det\left({}_3\phi_2\left(\begin{matrix} q^{-n-j+1}, p_i, -q^{t-N+1} \\ q^{-M-N+1}, 0 \end{matrix}; q, q\right)\right)_{i,j=1}^{N}$$
$$(0 \le n \le M),$$

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where ${}_3\phi_2$ is the $q$-hypergeometric function [9], which is given as

$$ {}_3\phi_2\left(\begin{matrix} a_0, a_1, a_2 \\ b_1, b_2 \end{matrix}; q, x\right) = \sum_{k=0}^{\infty} \frac{(a_0;q)_k (a_1;q)_k (a_2;q)_k}{(q;q)_k (b_1;q)_k (b_2;q)_k} x^k, $$

where $(a;q)_k$ is the $q$-shifted factorial defined by

$$ (a;q)_k = \prod_{i=0}^{k-1} (1 - aq^i) \qquad (k \geq 0) $$

and $p_i$ is the wave number of $i$-th soliton chosen as

$$ p_i \in \{1, q^{-1}, q^{-2}, \ldots, q^{-M-N+1}\} \qquad (1 \leq i \leq N). $$

The determinant size $N$ corresponds to the number of solitons. We note that this is not the general solution of the discrete Toda molecule equation although the general solution can be expressed in terms of another type of Casorati determinant [7].

**4. Proof of results.** For a positive integer $m$, the $q$-orthogonal polynomials

$$ \varphi_i^n(x) = {}_3\phi_2\left(\begin{matrix} q^{-n}, p_i, x \\ q^{-m}, 0 \end{matrix}; q, q\right) = \sum_{k=0}^{n} \frac{(q^{-n};q)_k (p_i;q)_k (x;q)_k}{(q^{-m};q)_k (q;q)_k} q^k \qquad (0 \leq n \leq m) $$

satisfy the contiguous relations

$$ (1-x)\varphi_i^0(x) = (1-x)\varphi_i^0(xq), $$

$$ (1 - xq^n)\varphi_i^n(x) - (1-q^n)x\varphi_i^{n-1}(x) = (1-x)\varphi_i^n(xq) \qquad (1 \leq n \leq m), $$

$$ \left(1 - \frac{q^{n-m}}{x}\right)\varphi_i^n(x) - \frac{1-q^{n-m}}{x}\varphi_i^{n+1}(x) = p_i\left(1 - \frac{1}{x}\right)\varphi_i^n(xq) \qquad (0 \leq n \leq m-1), $$

$$ \left(1 - \frac{1}{x}\right)\varphi_i^m(x) = p_i\left(1 - \frac{1}{x}\right)\varphi_i^m(xq) - \frac{(p_i;q)_{m+1}(x;q)_{m+1}}{(q;q)_m x}. $$

Thus for $1 \leq N \leq m+1$, the $\tau$ function

$$ \tau_n(x) = \begin{vmatrix} \varphi_1^n(x) & \varphi_1^{n+1}(x) & \cdots & \varphi_1^{n+N-1}(x) \\ \varphi_2^n(x) & \varphi_2^{n+1}(x) & \cdots & \varphi_2^{n+N-1}(x) \\ \vdots & \vdots & & \vdots \\ \varphi_N^n(x) & \varphi_N^{n+1}(x) & \cdots & \varphi_N^{n+N-1}(x) \end{vmatrix} \qquad (0 \leq n \leq m-N+1) $$

satisfies the difference formulas

$$\frac{(xq^{n+1};q)_{N-1}}{(1-x)^{N-1}}\tau_n(x) = \left|\varphi_i^n(x) \quad \varphi_i^{n+1}(xq) \quad \varphi_i^{n+2}(xq) \quad \cdots \quad \varphi_i^{n+N-1}(xq)\right| \qquad (0 \le n \le m-N+1)$$

$$(1-q^n)x\frac{(xq^{n+1};q)_{N-2}}{(1-x)^{N-1}}\tau_{n-1}(x) = \left|\varphi_i^n(x) \quad \varphi_i^n(xq) \quad \varphi_i^{n+1}(xq) \quad \cdots \quad \varphi_i^{n+N-2}(xq)\right| \qquad (1 \le n \le m-N+2,\ N \ge 2)$$

$$\frac{\left(\dfrac{q^{n-m}}{x};q\right)_{N-1}}{\left(1-\dfrac{1}{x}\right)^{N-1}\displaystyle\prod_{i=1}^{N}p_i}\tau_n(x) = \left|\varphi_i^n(xq) \quad \varphi_i^{n+1}(xq) \quad \cdots \quad \varphi_i^{n+N-2}(xq) \quad \frac{1}{p_i}\varphi_i^{n+N-1}(x)\right| \qquad (0 \le n \le m-N+1)$$

$$\begin{aligned}&\frac{1-q^{n+N-m-1}}{x}\frac{\left(\dfrac{q^{n-m+1}}{x};q\right)_{N-2}}{\left(1-\dfrac{1}{x}\right)^{N-1}\displaystyle\prod_{i=1}^{N}p_i}\tau_{n+1}(x)\\ &\quad= \left|\varphi_i^{n+1}(xq) \quad \varphi_i^{n+2}(xq) \quad \cdots \quad \varphi_i^{n+N-1}(xq) \quad \frac{1}{p_i}\varphi_i^{n+N-1}(x)\right| \qquad (-1 \le n \le m-N,\ N \ge 2)\end{aligned}$$

$$\begin{aligned}&q^{n+N-1}\left(1-\frac{1}{xq^m}\right)\frac{(xq^{n+1};q)_{N-2}\left(\dfrac{q^{n-m+1}}{x};q\right)_{N-2}}{(1-x)^{N-2}\left(1-\dfrac{q}{x}\right)^{N-1}\displaystyle\prod_{i=1}^{N}p_i}\tau_n\left(\frac{x}{q}\right)\\ &\quad= \left|\varphi_i^n(x) \quad \varphi_i^{n+1}(xq) \quad \cdots \quad \varphi_i^{n+N-2}(xq) \quad \frac{1}{p_i}\varphi_i^{n+N-1}(x)\right| \qquad (0 \le n \le m-N+1,\ N \ge 2).\end{aligned}$$

By using the Plücker relation, we can verify the bilinear equation for the $\tau$ function

$$\begin{aligned}&q^n\left(1-\frac{1}{xq^m}\right)\frac{(1-x)^N}{\left(1-\dfrac{x}{q}\right)^{N-1}}\tau_n(xq)\tau_n\left(\frac{x}{q}\right) - (1-xq^{n+N-1})\left(1-\frac{q^{n-m}}{x}\right)\tau_n(x)^2\\ &= \begin{cases} 0 & (n=0),\\ -(1-q^n)(1-q^{n+N-m-1})\tau_{n+1}(x)\tau_{n-1}(x) & (1 \le n \le m-N),\\ (1-q^{m-N+1})\dfrac{(x;q)_{m+1}}{(q;q)_m}\tau_{m-N}(x) & \\ \quad\times\left|\varphi_i^{m-N+2}(x) \quad \varphi_i^{m-N+3}(x) \cdots \varphi_i^m(x) \quad (p_i;q)_{m+1}\right| & (n=m-N+1).\end{cases}\end{aligned}$$

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By the gauge transformation

$$\sigma_n(x) = \frac{\tau_n(x)}{\prod_{k=0}^{N-2}(1-xq^k)^{N-1-k}} \qquad (0 \le n \le m-N+1)$$

the above bilinear equation is rewritten as

$$\sigma_n(xq)\sigma_n\left(\frac{x}{q}\right) - \sigma_n(x)^2 = \begin{cases} 0 & (n=0) \\ \dfrac{(1-q^n)(1-q^{m-N+1-n})}{(1-xq^m)\left(1-\dfrac{1}{xq^{N-1}}\right)}(\sigma_{n+1}(x)\sigma_{n-1}(x)-\sigma_n(x)^2) & \\ & (1 \le n \le m-N) \\ \dfrac{1-q^{m-N+1}}{(1-xq^m)\left(1-\dfrac{1}{xq^{N-1}}\right)}\dfrac{(x;q)_{m+1}}{(q;q)_m}\dfrac{\sigma_{m-N}(x)}{\prod_{k=0}^{N-2}(1-xq^k)^{N-1-k}} & \\ \quad \times\left|\varphi_i^{m-N+2}(x) \quad \varphi_i^{m-N+3}(x) \quad \cdots \quad \varphi_i^m(x) \quad (p_i;q)_{m+1}\right| & \\ & (n=m-N+1). \end{cases}$$

If we choose the parameters $p_i$ as

$$p_i \in \{1, q^{-1}, q^{-2}, \dots, q^{-m}\} \qquad (1 \le i \le N),$$

then we get

$$\sigma_n(xq)\sigma_n\left(\frac{x}{q}\right) - \sigma_n(x)^2 = \begin{cases} 0 & (n=0) \\ \dfrac{(1-q^n)(1-q^{m-N+1-n})}{(1-xq^m)\left(1-\dfrac{1}{xq^{N-1}}\right)}(\sigma_{n+1}(x)\sigma_{n-1}(x)-\sigma_n(x)^2) & \\ & (1 \le n \le m-N) \\ 0 & (n=m-N+1). \end{cases}$$

Defining the vacuum solution by

$$U_n(x) = \frac{(1-q^n)(1-q^{m-N+1-n})}{q^n(1-xq^{m-n})\left(1-\dfrac{1}{xq^{N+n-1}}\right)} \qquad (0 \le n \le m-N+1)$$

which satisfies the $q$-discrete Toda molecule equation

$$\frac{U_n(xq)U_n\left(\dfrac{x}{q}\right)}{U_n(x)^2} = \frac{(1+U_{n+1}(x))(1+U_{n-1}(x))}{(1+U_n(x))^2} \qquad (1 \le n \le m-N)$$

$$U_0(x) = U_{m-N+1}(x) = 0$$

we finally obtain

$$\sigma_n(xq)\sigma_n\left(\frac{x}{q}\right) - \sigma_n(x)^2 = \begin{cases} 0 & (n=0) \\ \dfrac{U_n(x)}{1+U_n(x)}(\sigma_{n+1}(x)\sigma_{n-1}(x) - \sigma_n(x)^2) & (1 \leq n \leq m-N) \\ 0 & (n = m-N+1). \end{cases}$$

By rewriting $m = M + N - 1$, $x = -q^{t-N+1}$, $\sigma_n(x) \to \tau_n(t)$ and $U_n(x) \to U_n(t)$, we recover the results in the previous section.

**5. Concluding remarks.** The Bäcklund and Darboux transformations enable us to construct a class of solutions starting from a vacuum solution. In order to satisfy some extra conditions such as the boundary condition and the condition of similarity reduction, the choice of vacuum solution is crucial. Investigating the solutions of nonautonomous discrete nonlinear integrable systems by choosing appropriate vacuum solutions would be an interesting subject. In this article we considered only the $q$-discrete analog of the Toda molecule equation by using the trigonometric vacuum solution. Recently the elliptic discrete equations and their solutions have been studied from several view points [**10**, **11**, **12**]. The method of vacuum solution is applicable to various types of discretization, and the elliptic function type vacuum is a future subject to be studied. It is known that the hypergeometric functions appear in the $\tau$ function of KP hierarchy [**13**]. Investigating the relation between the solutions derived from vacuum and the theories of matrix integral and fermionic representation of the solutions is also another direction of future study.

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