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Heat kernel expansions on the integers and the Toda lattice hierarchy

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Abstract. We consider the heat equation $u_t = Lu$ where L is a second-order difference operator in a discrete variable n. The fundamental solution has an expansion in terms of the Bessel functions of imaginary argument. The coefficients $\alpha_k(n,m)$ in this expansion are analogs of Hadamard's coefficients for the (continuous) Schrödinger operator.

We derive an explicit formula for α_k in terms of the wave and the adjoint wave functions of the Toda lattice hierarchy. As a first application of this result, we prove that the values of these coefficients on the diagonals $n = m$ and $n = m + 1$ define a hierarchy of differential-difference equations which is equivalent to the Toda lattice hierarchy. Using this fact and the correspondence between commutative rings of difference operators and algebraic curves we show that the fundamental solution can be summed up, giving a finite formula involving only two Bessel functions with polynomial coefficients in the time variable t, if and only if the operator L belongs to the family of bispectral operators constructed in [18].

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Contents

1. Introduction

The fundamental solution of the heat equation

$$u_t = u_{xx} + V(x)u, \qquad u(x,0) = \delta_y(x),$$

has an asymptotic expansion of the form

$$u(x,y,t) \sim \frac{e^{-(x-y)^2/4t}}{\sqrt{4\pi t}}\Big(1 + \sum_{k=1}^{\infty} H_k(x,y)t^n\Big) \quad \text{as } t \to 0+,$$

where Hadamard's coefficients $H_n(x,y)$ are defined in a neighborhood of the diagonal $x = y$. Restricted to the diagonal, the coefficients $H_n(x,x)$ become differential polynomials of the potential $V(x)$ and can be used to define the Korteweg–de Vries (for short KdV) hierarchy. There are several proofs and applications of this fact; see for instance [4, 25, 29, 31] and the references therein. One of the important steps in these papers is to use the connection between the heat kernel and the resolvent of the corresponding Schrödinger operator and the work of Gelfand and Dickey [12]. In particular, this construction was used to obtain explicit formulas for the higher KdV equations exploring different properties of Hadamard's coefficients.

On the other hand, after the works [9, 30, 32], we have a much better understanding of the KdV hierarchy and the parametrization of its solutions. Therefore it seems natural to reexamine the connection between the heat kernel and the KdV hierarchy within the framework of Sato's theory and to use the soliton technology as a tool to investigate the heat expansions. This idea was developed in [21] and it led to a new formula for Hadamard's coefficients in terms of the τ-function (or equivalently the wave and adjoint wave functions) of the KdV hierarchy. This formula made transparent some of the basic properties of Hadamard's coefficients such as the symmetry about the diagonal, or the connection between $H_n(x,x)$ and the KdV flows. We also used this formula in [22] to prove that heat kernel is finite (i.e. $H_n(x,y) = 0$ for n large enough) if and only if the potential $V(x)$ is among the rational solutions of the KdV hierarchy (for specific values of the time variables) studied in [2, 3]. These operators also appear as solutions of the bispectral problem [11, 13]. For multivariable versions of the heat kernel and interesting connections with the bispectral problem and Huygens' principle see [5–8].

It is natural then to ask if one can use the soliton technology to study heat kernel expansions where very little or even nothing is known. The aim of the present paper is to show that there is a very close connection between the heat kernel expansion on the integers and the Toda lattice hierarchy. Some partial results in this direction were already established in [14–16], mainly in connection with the bispectral problem. Jointly with F. A. Grünbaum [15] we studied the heat kernel for specific second-order difference operators which were introduced in [18] as solutions of a difference-differential version of the bispectral problem. These second-order difference operators depend on free parameters and, appropriately normalized, they provide rational solutions of the Toda lattice hierarchy. The main result in [15] is that the fundamental solution corresponding to these operators can be written as a finite sum of Bessel functions of imaginary argument, which is a discrete analog of the finiteness property mentioned above for the continuous Schrödinger operator. The case when the operator L corresponds to a soliton solution of the Toda lattice was considered in [16]. Both papers rely on the fact that the second-order operators belong to rank one commutative rings with spectral curves having specific singularities, which prevents their use for arbitrary L. The goal of this work is to derive a general formula for the analogs of Hadamard's coefficients in terms of the wave and adjoint wave functions for the Toda lattice hierarchy and to present a few applications. In order to state the main results, let me first introduce some basic notations and define the analogs of Hadamard's coefficients in the discrete case.

We denote by E the customary shift operator acting on functions $f(n) = f_n$ of a discrete variable $n \in \mathbb{Z}$ by

$$Ef(n) = f(n+1).$$

For a second-order difference operator L of the form

$$L = E + b_n \mathrm{Id} + a_n E^{-1}, \tag{1.1}$$

the fundamental solution (or the discrete heat kernel) is the solution $u(n,m;t)$ of the heat equation

$$\frac{\partial u}{\partial t} = Lu \tag{1.2}$$

with initial condition

$$u(n,m;0) = \delta_{n,m}. \tag{1.3}$$

The papers [14–16] suggest looking for a solution of (1.2)–(1.3) of the form

$$u(n,m;t) = \sum_{k=0}^{\infty} \alpha_k(n,m) I_{n-m-k}(2t), \tag{1.4}$$

where $I_j(2t)$ is the Bessel function of imaginary argument. The coefficients $\alpha_k(n,m)$ are the analogs of Hadamard's coefficients $H_k(x,y)$. Plugging (1.4) in (1.2), using the identity

$$\partial_t I_k(2t) = I_{k+1}(2t) + I_{k-1}(2t)$$

and comparing the coefficients of $I_{n-m-k+1}(2t)$ we get

$$\begin{aligned}\alpha_k(n,m) &+ \alpha_{k-2}(n,m) \\ &= \alpha_k(n+1,m) + b_n\alpha_{k-1}(n,m) + a_n\alpha_{k-2}(n-1,m),\end{aligned} \tag{1.5}$$

with the convention that $\alpha_i(n,m) = 0$ if $i < 0$. From (1.4) and using the fact that $I_j(0) = \delta_{j,0}$ we obtain

$$u(n,m;0) = \begin{cases} 0 & \text{if } n < m, \\ \alpha_{n-m}(n,m) & \text{if } n \geq m, \end{cases}$$

which combined with (1.3) leads to

$$\alpha_{n-m}(n,m) = \delta_{n,m} \quad \text{for every } n \geq m. \tag{1.6}$$

It is clear that the system of equations (1.5)–(1.6) has a unique solution. Indeed, for $k = 0$ equation (1.5) gives $\alpha_0(n,m) = \alpha_0(n+1,m)$, which essentially means that $\alpha_0(n,m) = \beta_m$ is independent of n. On the other hand, from equation (1.6) we see that $\alpha_0(m,m) = 1$, which shows that $\alpha_0(n,m) = 1$. Similarly, for $k = 1$ we obtain the system

$$\begin{aligned}&\alpha_1(n,m) = \alpha_1(n+1,m) + b_n, \\ &\alpha_1(m+1,m) = 0,\end{aligned}$$

which uniquely determines $\alpha_1(n,m)$. Next we can compute $\alpha_2(n,m)$, $\alpha_3(n,m)$, etc. We want to stress at this point that although the system (1.5)–(1.6) has a unique solution, the coefficients in the expansion (1.4) are uniquely determined from $u(n,m;t)$ only if $n \leq m$. Indeed, for $r \in \mathbb{N}_0$ we have

$$I_r(2t) = I_{-r}(2t) = \sum_{j=0}^{\infty} \frac{t^{r+2j}}{j!(r+j)!}. \tag{1.7}$$

If $n \leq m$ then the $\alpha_k(n,m)$ are uniquely determined by comparing the coefficients of the different powers of t in (1.4). However, for $n > m$ the expansion will contain both $I_r(2t)$ and $I_{-r}(2t)$ for $r = 1,\ldots,n-m$ and therefore only the sum of these two coefficients is uniquely determined by $u(n,m;t)$. If we want to make the expansion unique, we can rearrange it so that the sum (1.4) contains only terms I_j with $j \leq 0$. However, this would complicate the recurrence relation (1.5) significantly by introducing different cases when $n > m$ and $n \leq m$. Therefore we will keep the form (1.4) with $\alpha_k(n,m)$ uniquely determined by (1.5)–(1.6).

Let me now briefly describe the main results of the paper. In the next section we collect some basic facts about the Toda lattice hierarchy. In Section 3 we derive simple formulas for the coefficients $\alpha_k(n,m)$ in terms of the wave and adjoint wave functions for the Toda lattice hierarchy (or equivalently the τ-function). In other words, the soliton technology allows us to integrate equations (1.5)–(1.6) explicitly and write $\alpha_k(n,m)$ in closed form. As a first application of this formula, we show in Section 4 that $\alpha_k(n,n)$ and $\alpha_{k+1}(n,n-1)$ generate a hierarchy which is equivalent to the Toda lattice hierarchy (notice that we need two coefficients in order to generate two equations for a_n and b_n). This provides a discrete analog of the connection between Hadamard's coefficients $H_n(x,x)$ and the KdV hierarchy. It would be interesting to see if some of the proofs in the continuous case can be adapted to this situation. We note, however, that the situation in the discrete case is a little more complicated because the k-th vector field of the Toda lattice $\mathbb{X}_k$ is not equal to the vector field $\mathbb{X}'_k$ generated by $\alpha_k(n,n)$ and $\alpha_{k+1}(n,n-1)$, but we have $\mathbb{X}'_k = \mathbb{X}_k +$ a linear combination of $\mathbb{X}_{k-2j}$ with $2j < k$ (see Theorem 4.4). All this follows easily from the explicit formula for $\alpha_k(n,m)$ derived here, but clearly a direct approach should be carefully constructed in order to capture the lower-order vector fields that appear.

Next we prove that the heat kernel can be written as

$$(1 + p_1(n,m;t))I_{n-m}(2t) + p_2(n,m;t)I_{n-m-1}(2t), \tag{1.8}$$

where $p_1(n,m;t)$ and $p_2(n,m;t)$ are polynomials in t with coefficients depending on n and m, such that $p_1(n,m;0) = p_2(n,m;0) = 0$ if and only if the operator L belongs to the family of bispectral operators constructed in [18]. The "if" part is essentially the main result in [15] (see Section 6 for more details). In order to prove the "only if" part, we first discuss in Section 5 the operators constructed in [18] and we show that they can be characterized by the vanishing of a specific linear combination of the Toda flows, after a particular point. The heart of the proof is to show that if this specific linear combination of the Toda flows vanishes after a particular point, then the operator L belongs to a rank one commutative ring with spectral curve of the form $v^2 = (u-2)^{2N_1+1}(u+2)^{2N_2+1}$, which leads to the operators introduced in [18]. Using this result and the connection between the heat coefficients and the Toda flows, we establish the "only if" part in Subsection 6.2.

The results in the last section deepen the mystery surrounding the bispectral problem and its connection with the heat equation. The finiteness property of the heat kernel provides one more reason to believe that the operators constructed in [18] are the discrete analogs of the Adler–Moser operators [2]. It would be interesting to see if some of the recent developments [19, 20] in the purely continuous version of the bispectral problem can be extended to the operators in [18], or to the more general (higher-order) bispectral operators in [17], which we constructed in collaboration with L. Haine, inspired by Wilson's work [34, 35].

2. The Toda lattice hierarchy

In this section we briefly recall the construction of the Toda lattice hierarchy, its wave and adjoint wave functions. For more details we refer the reader to the paper [33], or to the more recent contributions [1, 26].

Let us first introduce some notations, which will be used throughout the paper. We denote by Δ and ∇ the customary forward and backward difference operators, acting on a function $f(n) = f_n$ as follows:

$$\Delta f(n) = f(n+1) - f(n) = (E - \mathrm{Id})f(n),$$
$$\nabla f(n) = f(n) - f(n-1) = (\mathrm{Id} - E^{-1})f(n).$$

Sometimes, we will write Δ_n and ∇_n if the operators are applied to functions depending on several variables to indicate that Δ and ∇ act in the variable n.

When we work with pseudo-difference operators of the form

$$M = \sum_{k=-\infty}^{d} c_k(n)E^k$$

we will denote by $M_+ = \sum_{k=0}^{d} c_k(n)E^k$ (resp. $M_- = \sum_{k=-\infty}^{-1} c_k(n)E^k$) the non-negative (resp. negative) difference part of M.

For a second-order difference operator $L = E + b_n\mathrm{Id} + a_nE^{-1}$, the Toda lattice hierarchy is defined by the Lax equations

$$\frac{\partial L}{\partial s_j} = [(L^j)_+, L] \quad \text{for } j = 1, 2, \ldots. \tag{2.1}$$

It is well-known that the vector fields $\mathbb{X}_j(L) = [(L^j)_+, L]$ commute with each other, that is, each of the equations (2.1) defines a symmetry of any other equation. For this reason, the family of equations (2.1) is called a *hierarchy*. The first equation, corresponding to $j = 1$, is the well-known Toda lattice equation.

We denote by $W_n = 1 + \sum_{k=1}^{\infty} \psi_k(n)E^{-k}$ the *wave operator*, i.e. the operator which conjugates L to E:

$$L = W_nEW_n^{-1}. \tag{2.2}$$

The flows (2.1) can be extended on W_n by

$$\frac{\partial W_n}{\partial s_j} = -(L^j)_-W_n. \tag{2.3}$$

The *wave function* $\Psi_n(z; s)$ and the *adjoint wave function* $\Psi_n^*(z; s)$ are defined by the formulas

$$\begin{aligned}\Psi_n(z; s) &= W_nz^n \exp\Big(\sum_{j=1}^{\infty} s_jz^j\Big)\\ &= \Big(1 + \sum_{k=1}^{\infty} \frac{\psi_k(n; s)}{z^k}\Big)z^n \exp\Big(\sum_{j=1}^{\infty} s_jz^j\Big)\end{aligned} \tag{2.4a}$$

and

$$\begin{aligned}\Psi_n^*(z; s) &= (W_{n-1}^{-1})^*z^{-n} \exp\Big(-\sum_{j=1}^{\infty} t_jz^j\Big)\\ &= \Big(1 + \sum_{k=1}^{\infty} \frac{\psi_k^*(n; s)}{z^k}\Big)z^{-n} \exp\Big(-\sum_{j=1}^{\infty} s_jz^j\Big),\end{aligned} \tag{2.4b}$$

where $E^* = E^{-1}$. With these definitions we have

$$L\Psi_n(z;s) = z\Psi_n(z;s) \quad \text{and} \quad \frac{\partial \Psi_n(z;s)}{\partial s_j} = (L^j)_+\Psi_n(z;s). \tag{2.5}$$

We denote by $\bar{\Psi}_n(z;s)$ and $\bar{\Psi}^*_n(z;s)$ the reduced wave function and the reduced adjoint wave function obtained from $\Psi_n(z;s)$ and $\Psi^*_n(z;s)$, respectively, by omitting the exponential factors, i.e.

$$\bar{\Psi}_n(z;s) = 1 + \sum_{k=1}^{\infty} \frac{\psi_k(n;s)}{z^k} \quad \text{and} \quad \bar{\Psi}^*_n(z;s) = 1 + \sum_{k=1}^{\infty} \frac{\psi^*_k(n;s)}{z^k}. \tag{2.6}$$

In order to simplify the notations, we will often omit the s-dependence, e.g. we will write simply $\Psi_n(z)$ instead of $\Psi_n(z;s)$, etc. Notice that the first equation in (2.5) is equivalent to the following equation for the reduced wave function:

$$z\bar{\Psi}_{n+1}(z) + b_n\bar{\Psi}_n(z) + a_n\frac{\bar{\Psi}_{n-1}(z)}{z} = z\bar{\Psi}_n(z). \tag{2.7}$$

For series $\sum_k c_k z^k$ and for formal pseudo-difference operators $\sum_k d_k E^k$ we define

$$\operatorname{res}_z\Big(\sum_k c_k z^k\Big) = c_{-1} \quad \text{and} \quad \operatorname{res}_E\Big(\sum_k d_k E^k\Big) = d_{-1}.$$

It is easy to see that for pseudo-difference operators $P_n = \sum_k d_k(n)E^k$ and $Q_n = \sum_k c_k(n)E^k$ we have

$$\operatorname{res}_z((P_n z^n)(Q^*_{n-1}z^{-n})) = \operatorname{res}_E(P_nQ_n). \tag{2.8}$$

From this equality it follows that $\Psi_n(z;s)$ and $\Psi^*_n(z;s)$ satisfy the bilinear identities

$$\operatorname{res}_z((\partial_1^{k_1}\cdots\partial_j^{k_j}\Psi_{n+k_0}(z;s))\Psi^*_n(z;s)) = 0, \tag{2.9}$$

where $k_0, k_1, \dots, k_j \in \mathbb{N}_0$ and $\partial_j = \partial/\partial s_j$. Indeed, from the second equation in (2.5) we see that it is enough to prove (2.9) for $k_1 = \cdots = k_j = 0$. Using now (2.8) we get

$$\begin{aligned}\operatorname{res}_z(\Psi_{n+k_0}(z;s))\Psi^*_n(z;s)) &= \operatorname{res}_z((E^{k_0}W_nz^n)((W^{-1}_{n-1})^*z^{-n}))\\ &= \operatorname{res}_E(E^{k_0}) = 0,\end{aligned}$$

which establishes (2.9).

For example, for $k_0 = 0$ and $k_0 = 1$ with $k_j = 0$ for $j \geq 1$, the identity (2.9) gives

$$\psi_1(n) + \psi^*_1(n) = 0, \tag{2.10a}$$
$$\psi_2(n+1) + \psi_1(n+1)\psi^*_1(n) + \psi^*_2(n) = 0. \tag{2.10b}$$

From (2.2) and (2.4) we can express b_n and a_n in terms of the coefficients of $\Psi_n(z;s)$ and $\Psi^*_n(z;s)$:

$$b_n = \psi_1(n) + \psi^*_1(n+1), \tag{2.11a}$$
$$a_n = \psi_2(n) + \psi_1(n)\psi^*_1(n) + \psi_2(n). \tag{2.11b}$$

Remark 2.1. If we fix n and take $k_0 = 0$, then the bilinear identities (2.9) show that $\Psi_n(z;s)z^{-n}$ and $\Psi^*_n(z;s)z^n$ are the wave and adjoint wave functions of the Kadomtsev–Petviashvili (KP) hierarchy. Thus, by the classical theory (see [9], [10, Theorem 6.3.8, p. 97]), there exists a τ-function $\tau_n(s)$ such that

$$\bar{\Psi}_n(z;s) = \frac{\tau_n(s-[z^{-1}])}{\tau_n(s)} \quad \text{and} \quad \bar{\Psi}^*_n(z;s) = \frac{\tau_n(s+[z^{-1}])}{\tau_n(s)},$$

where $[z] = (z, z^2/2, z^3/3, \dots)$. This function plays a central role in the KP and the Toda lattice hierarchies. Since we are not going to make an explicit use of it in the present paper, we stop the discussion here. Notice that the last formulas allow us to express the coefficients of $\bar{\Psi}_n(z;s)$ and $\bar{\Psi}^*_n(z;s)$ in terms of $\tau_n(s)$. In particular, this means that all formulas involving $\bar{\Psi}_n(z;s)$ and $\bar{\Psi}^*_n(z;s)$ that follow can be rewritten as formulas involving only $\tau_n(s)$.

3. Explicit formulas for the heat coefficients $\alpha_k(n,m)$

In this section we show that, using the notations in the previous section, we can "integrate" equation (1.5) for all $k \in \mathbb{N}$ and obtain simple formulas for $\alpha_k(n,m)$ in terms of the wave and adjoint wave functions of the Toda lattice hierarchy. Before we present and prove the general formula, we illustrate how the method works for $\alpha_1(n,m)$ and $\alpha_2(n,m)$. This will help the reader understand the nature of these formulas and the importance of the bilinear identity (2.9).

Plugging $k = 1$ in (1.5) and using (2.11) we get

$$\alpha_1(n,m) = \alpha_1(n+1,m) + \psi_1(n) + \psi^*_1(n+1).$$

Using (2.10a) we can rewrite this as

$$\alpha_1(n,m) - \psi_1(n) = \alpha_1(n+1,m) - \psi_1(n+1),$$

which shows that $\alpha_1(n,m) - \psi_1(n) = \beta_1(m)$ is a function independent of n. From (1.6) we see that $\alpha_1(m+1,m) = 0$, which gives $\beta_1(m) = -\psi(m+1) = \psi^*_1(m+1)$. Thus we have

$$\alpha_1(n,m) = \psi_1(n) + \psi^*_1(m+1) = \mathrm{res}_z[\bar{\Psi}_n(z)\bar{\Psi}^*_{m+1}(z)]. \tag{3.1}$$

Similarly, for $k = 2$ we obtain the following equation for $\alpha_2(n,m)$:

$$\begin{aligned} \alpha_2(n,m) + 1 = \alpha_2(n+1,m) &+ [\psi_1(n) + \psi^*_1(n+1)][\psi_1(n) + \psi^*_1(n+1)] \\ &+ \psi_2(n) + \psi_1(n)\psi^*_1(n) + \psi^*_2(n). \end{aligned} \tag{3.2}$$

Using now both equations in (2.10) one can check that (3.2) is equivalent to

$$\Delta_n(\alpha_2(n,m) - \psi_2(n) - \psi_1(n)\psi^*_1(m+1) - n) = 0,$$

which means that $\alpha_2(n,m) = \psi_2(n) + \psi_1(n)\psi^*_1(m+1) + n + \beta_2(m)$, where $\beta_2(m)$ depends only on m. From (1.6) we see that $\alpha_2(m+2,m) = 0$, leading to $\beta_2(m) =$

$-\psi_2(m+2) - \psi_1(m+2)\psi_1^*(m+1) - m - 2 = \psi_2^*(m+1) - m - 2$, where in the last equality we used again (2.10b). Thus we obtain

$$\begin{aligned}\alpha_2(n,m) &= \psi_2(n) + \psi_1(n)\psi_1^*(m+1) + \psi_2^*(m+1) + (n-m-2)\\ &= \mathrm{res}_z\left[(z^2+n-m-2)\frac{\bar{\Psi}_n(z)\bar{\Psi}^*_{m+1}(z)}{z}\right]. \qquad (3.3)\end{aligned}$$

The point is that this process can be successfully iterated, providing simple formulas for $\alpha_k(n,m)$ for every $k \in \mathbb{N}$. Below we introduce the necessary functions which are needed to state and prove the general formula, extending (3.1) and (3.3).

Let us define monic polynomials $Q_k^\beta(z)$ by the formula

$$Q_k^\beta(z) = z^k + (\beta - 2k)\sum_{j=0}^{k-1}\binom{\beta-2j-1}{k-j-1}\frac{z^j}{k-j}. \qquad (3.4)$$

From (3.4) it is easy to see that

$$Q_k^\beta(z) - zQ_{k-1}^{\beta-2}(z) = \frac{\beta-2k}{k}\binom{\beta-1}{k-1} \qquad (3.5)$$

and

$$Q_k^\beta(z) + Q_{k-1}^\beta(z) - zQ_{k-1}^{\beta-1}(z) = \frac{\beta-2k+1}{k}\binom{\beta}{k-1}. \qquad (3.6)$$

Let us define

$$g_k(n,m;z) = \begin{cases} Q_{k/2}^{n-m}(z^2) & \text{if } k \text{ is even,}\\ zQ_{(k-1)/2}^{n-m-1}(z^2) & \text{if } k \text{ is odd.}\end{cases} \qquad (3.7)$$

It is clear that $g_k(n,m;z)$ is a monic polynomial in z of degree k, and it is an even polynomial when k is even and an odd polynomial when k is odd. From the defining relation (3.7) and equation (3.5) one sees immediately that

$$g_k(n,m;z) - zg_{k-1}(n-1,m;z) = 0 \qquad \text{if } k \text{ is odd} \qquad (3.8a)$$

and

$$\begin{aligned}g_k(n,m;z) - zg_{k-1}(n-1,m;z) &= g_k(n,m;z) - z^2 g_{k-2}(n-2,m;z)\\ &= \frac{2(n-m-k)}{k}\binom{n-m-1}{k/2-1} \qquad \text{if } k \text{ is even.} \qquad (3.8b)\end{aligned}$$

Now we are ready to formulate the main result in this section which gives an explicit formula for $\alpha_k(n,m)$ in terms of $\bar{\Psi}_n(z)$ and $\bar{\Psi}_n^*(z)$.

Theorem 3.1. *The coefficients $\alpha_k(n,m)$ in the expansion* (1.4) *of the fundamental solution of the discrete heat equation* (1.2) *can be expressed in terms of the reduced wave function $\bar{\Psi}_n(z)$ and the reduced adjoint wave function $\bar{\Psi}_n^*(z)$ as follows:*

$$\alpha_k(n,m) = \mathrm{res}_z\left[g_k(n,m;z)\frac{\bar{\Psi}_n(z)\bar{\Psi}^*_{m+1}(z)}{z}\right], \qquad (3.9)$$

where $g_k(n,m;z)$ is the polynomial defined by (3.4) *and* (3.7).

Proof. We need to check that the functions defined by formula (3.9) satisfy the difference equation (1.5) and the initial conditions (1.6). Let us first establish that equation (1.5) holds. We denote by RHS (resp. LHS) the right-hand side (resp. the left-hand side) of equation (1.5). Plugging (3.9) in (1.5) leads to

$$\begin{aligned}
\mathrm{RHS} &= \alpha_k(n+1,m) + b_n\alpha_{k-1}(n,m) + a_n\alpha_{k-2}(n-1,m)\\
&= \mathrm{res}_z\Bigg[g_k(n+1,m;z)\frac{\bar\Psi_{n+1}(z)\bar\Psi^*_{m+1}(z)}{z} + b_n g_{k-1}(n,m;z)\frac{\bar\Psi_{n}(z)\bar\Psi^*_{m+1}(z)}{z}\\
&\quad + a_n g_{k-2}(n-1,m;z)\frac{\bar\Psi_{n-1}(z)\bar\Psi^*_{m+1}(z)}{z}\Bigg]\\
&= \mathrm{res}_z\Bigg[((z^2-zb_n)g_{k-2}(n-1,m;z) + b_n g_{k-1}(n,m;z))\frac{\bar\Psi_{n}(z)\bar\Psi^*_{m+1}(z)}{z}\\
&\quad + (g_k(n+1,m;z) - z^2 g_{k-2}(n-1,m;z))\frac{\bar\Psi_{n+1}(z)\bar\Psi^*_{m+1}(z)}{z}\Bigg],
\end{aligned}$$

where in the last equality we eliminated $\bar\Psi_{n-1}(z)$ using (2.7).

Now we consider two cases depending on whether k is even or odd.

Case 1. Let k be even (hence $k-1$ is odd). Using (3.8) we see that

$$(z^2-zb_n)g_{k-2}(n-1,m;z) + b_n g_{k-1}(n,m;z) = z^2 g_{k-2}(n-1,m;z)$$

and

$$g_k(n+1,m;z) - z^2 g_{k-2}(n-1,m;z) = \frac{2(n+1-m-k)}{k}\binom{n-m}{k/2-1},$$

which leads to the following expressions for RHS and LHS:

$$\begin{aligned}
\mathrm{RHS} = \mathrm{res}_z&\left[z^2 g_{k-2}(n-1,m;z)\frac{\bar\Psi_{n}(z)\bar\Psi^*_{m+1}(z)}{z}\right]\\
&+ \frac{2(n+1-m-k)}{k}\binom{n-m}{k/2-1}
\end{aligned}$$

and

$$\mathrm{LHS} = \mathrm{res}_z\left[(g_k(n,m;z) + g_{k-2}(n,m;z))\frac{\bar\Psi_{n}(z)\bar\Psi^*_{m+1}(z)}{z}\right].$$

Using now equation (3.6) we get

$$\begin{aligned}
&g_k(n,m;z) + g_{k-2}(n,m;z) - z^2 g_{k-2}(n-1,m;z)\\
&\quad = Q^{n-m}_{k/2}(z^2) + Q^{n-m}_{k/2-1}(z^2) - z^2 Q^{n-m-1}_{k/2-1}(z^2) = \frac{2(n+1-m-k)}{k}\binom{n-m}{k/2-1},
\end{aligned}$$

which shows that RHS = LHS and establishes (1.5).

Case 2. Let k be odd (hence $k-1$ is even). Using again (3.8) we obtain

$$\begin{aligned} g_k(n+1,m;z) - z^2 g_{k-2}(n-1,m;z) &= z(g_{k-1}(n,m;z) - z^2 g_{k-3}(n-2,m;z)) \\ &= \frac{2(n-m-k+1)}{k-1}\binom{n-m-1}{(k-1)/2-1} z \end{aligned}$$

and

$$\begin{aligned} &(z^2 - zb_n)g_{k-2}(n-1,m;z) + b_n g_{k-1}(n,m;z) \\ &\quad = (z^2 - zb_n) z g_{k-3}(n-2,m;z) + b_n g_{k-1}(n,m;z) \\ &\quad = b_n(g_{k-1}(n,m;z) - z^2 g_{k-3}(n-2,m;z)) + z^3 g_{k-3}(n-2,m;z) \\ &\quad = b_n \frac{2(n-m-k+1)}{k-1}\binom{n-m-1}{(k-1)/2-1} + z^3 g_{k-3}(n-2,m;z). \end{aligned}$$

Thus

$$\begin{aligned} \mathrm{RHS} = \operatorname{res}_z \Bigg[&\frac{2(n-m-k+1)}{k-1}\binom{n-m-1}{(k-1)/2-1}(z\bar\Psi_{n+1}(z) + b_n\bar\Psi_n(z))\frac{\bar\Psi^*_{m+1}(z)}{z} \\ &+ z^3 g_{k-3}(n-2,m;z)\frac{\bar\Psi_n(z)\bar\Psi^*_{m+1}(z)}{z}\Bigg] \\ = \operatorname{res}_z \Bigg[&\left(\frac{2(n-m-k+1)}{k-1}\binom{n-m-1}{(k-1)/2-1} + z^2 g_{k-3}(n-2,m;z)\right) \\ &\times \bar\Psi_n(z)\bar\Psi^*_{m+1}(z)\Bigg], \end{aligned}$$

where in the last equality we used (2.7) to eliminate $z\bar\Psi_{n+1}(z) + b_n\bar\Psi_n(z)$. On the other hand, we have

$$\mathrm{LHS} = \operatorname{res}_z[(g_{k-1}(n-1,m;z) + g_{k-3}(n-1,m;z))\bar\Psi_n(z)\bar\Psi^*_{m+1}(z)],$$

and applying the definition (3.7) and equation (3.6) we get

$$\begin{aligned} &g_{k-1}(n-1,m;z) + g_{k-3}(n-1,m;z) - z^2 g_{k-3}(n-2,m;z) \\ &\qquad = Q^{n-m-1}_{(k-1)/2}(z^2) + Q^{n-m-1}_{(k-1)/2-1}(z^2) - z^2 Q^{n-m-2}_{(k-1)/2-1}(z^2) \\ &\qquad = \frac{2(n-m-k+1)}{k-1}\binom{n-m-1}{(k-1)/2-1}, \end{aligned}$$

which shows that RHS = LHS and completes the proof of the difference equation (1.5).

It remains to check that the initial condition (1.6) holds, i.e. we need to show that for every $k \in \mathbb{N}$, $\alpha_k(m+k,k) = 0$. Using the defining relations (3.4) and (3.7) one can easily see that

$$g_k(m+k,m;z) = z^k.$$

Thus (3.9) gives

$$\alpha_k(m+k,m) = \mathrm{res}_z\left[z^k \frac{\bar\Psi_{m+k}(z)\bar\Psi^*_{m+1}(z)}{z}\right] = \mathrm{res}_z[\Psi_{m+k}(z)\Psi^*_{m+1}(z)] = 0,$$

where in the last equality we used the bilinear identity (2.9). □

4. Generating the Toda flows with the heat coefficients

As a first application of formula (3.9) we show in this section that $\Delta_n\alpha_{k+1}(n,n-1)$ and $a_n\nabla_n\alpha_k(n,n)$ generate the Toda lattice hierarchy. This is a discrete analog of the remarkable connection between the restriction of Hadamard's coefficients on the diagonal and the Korteweg–de Vries hierarchy. Before we prove this, we establish some auxiliary facts.

Proposition 4.1. *Define*

$$\mathfrak{r}_k(n) = \mathrm{res}_z(z^k\bar\Psi_n(z)\bar\Psi^*_n(z)), \tag{4.1a}$$

$$\mathfrak{l}_k(n) = \mathrm{res}_z(z^{k-1}\bar\Psi_{n-1}(z)\bar\Psi^*_n(z)). \tag{4.1b}$$

Then the Toda lattice hierarchy (2.1) *is equivalent to the equations*

$$\frac{\partial b_n}{\partial s_k} = \mathfrak{r}_k(n+1) - \mathfrak{r}_k(n), \tag{4.2a}$$

$$\frac{\partial a_n}{\partial s_k} = a_n(\mathfrak{l}_k(n+1) - \mathfrak{l}_k(n)). \tag{4.2b}$$

Proof. Notice that equation (2.4b) implies

$$W_n^{-1} = 1 + \sum_{j=1}^{\infty} E^{-j}\cdot\psi^*_j(n+1),$$

and therefore, using (2.2) and (2.4a), we get

$$L^k = W_nE^kW_n^{-1} = \sum_{m=0}^{\infty}\Big[\sum_{j=0}^{m}\psi_{m-j}(n)\psi^*_j(n+1+k-m)\Big]E^{k-m},$$

where $\psi_0(n) = \psi^*_0(n) = 1$. From the above equation it is clear that the coefficients of E^0 and E^{-1} in the operator L^k are $\mathfrak{l}_k(n+1)$ and $\mathfrak{r}_k(n)$ respectively. This shows that

$$\begin{aligned}[(L^k)_+, L] = [L,(L^k)_-] &= [E + b_n\mathrm{Id} + a_nE^{-1}, \mathfrak{r}_k(n)E^{-1} + O(E^{-2})]\\ &= (\mathfrak{r}_k(n+1) - \mathfrak{r}_k(n))\mathrm{Id} + O(E^{-1}),\end{aligned}$$

which gives (4.2a). A similar computation shows that the coefficient of E^{-1} in $[(L^k)_+, L]$ is $a_n(\mathfrak{l}_k(n+1) - \mathfrak{l}_k(n))$, completing the proof. □

Lemma 4.2. *Let $k \in \mathbb{N}_0$ and $j \in \mathbb{Z}$ be fixed. Then*

$$\alpha_k(n, n+j) \in \mathbb{C}[a_n, b_n, a_{n\pm1}, b_{n\pm1}, a_{n\pm2}, b_{n\pm2}, \dots],$$

i.e. $\alpha_k(n, n+j)$ is a polynomial of finitely many of $\{a_n, b_n, a_{n\pm1}, b_{n\pm1}, \dots\}$.

Proof. The proof can be easily obtained by induction on k and $|k + j|$, using (1.5)–(1.6). □

Example 4.3. We list the values of the first few heat coefficients in a neighborhood of the diagonal $n = m$:

$$\begin{aligned}
&\alpha_1(n, n) = b_n,\\
&\alpha_1(n, n-1) = 0,\\
&\alpha_1(n, n+1) = b_n + b_{n+1}\\
&\alpha_2(n, n) = a_{n+1} + a_n + b_n^2 - 2,\\
&\alpha_2(n, n-1) = a_n - 1,\\
&\alpha_2(n, n+1) = a_n + a_{n+1} + a_{n+2} + b_n^2 + b_{n+1}^2 + b_n b_{n+1} - 3.
\end{aligned}$$

The main result in this section is the following theorem.

Theorem 4.4. *The system of differential-difference equations*

$$\frac{\partial b_n}{\partial s'_k} = \alpha_{k+1}(n+1, n) - \alpha_{k+1}(n, n-1) = \Delta_n \alpha_{k+1}(n, n-1), \tag{4.3a}$$

$$\frac{\partial a_n}{\partial s'_k} = a_n(\alpha_k(n, n) - \alpha_k(n-1, n-1)) = a_n \nabla_n \alpha_k(n, n), \tag{4.3b}$$

where $k \in \mathbb{N}$, forms a hierarchy. Moreover, if denote by $\mathbb{X}_k$ and $\mathbb{X}'_k$ the vector fields corresponding to the flows $\partial/\partial s_k$ and $\partial/\partial s'_k$ given by (2.1) *and* (4.3) *respectively, then*

$$\mathbb{X}'_k = k \sum_{i=0}^{\lfloor (k-1)/2 \rfloor} \frac{(-1)^i}{k-2i} \binom{k-i-1}{i} \mathbb{X}_{k-2i}, \tag{4.4}$$

where $\lfloor x \rfloor$ denotes the greatest integer less than or equal to x.

Remark 4.5. Notice that according to Lemma 4.2, for every $k \in \mathbb{N}$ the right-hand sides of equations (4.3) are polynomials of finitely many of $\{a_{n+j}, b_{n+j}\}_{j\in\mathbb{Z}}$, i.e. (4.3) is a well-defined system of differential equations for a_n and b_n. The above theorem essentially says that the hierarchy of equations (4.3) is equivalent to the Toda lattice hierarchy (2.1) modulo a simple (linear) change of variables given by (4.4). Below we also write the explicit linear combination that gives $\mathbb{X}_k$ in terms of $\{\mathbb{X}'_j\}$, which will be needed later. First we show that for every $k \in \mathbb{N}$ and $m \in \mathbb{N}_0$ satisfying $m \leq \lfloor (k-1)/2 \rfloor$ the identity

$$k \sum_{i=0}^{m} \frac{(-1)^i}{k-2i} \binom{k-i-1}{i} \binom{k-2i}{m-i} = \delta_{m,0} \tag{4.5}$$

holds. Indeed, if $m = 0$ then (4.5) is obvious. For $m \geq 1$ we can rewrite the left-hand side of (4.5) as

$$\frac{k}{m}\sum_{i=0}^{m}(-1)^i\binom{k-1-i}{m-1}\binom{m}{i} = \frac{k}{m}\binom{k-1-m}{k-m} = 0.$$

In the first equality we used the well-known binomial identity

$$\sum_{i=0}^{m}(-1)^i\binom{k-i}{r}\binom{m}{i} = \binom{k-m}{k-r}, \tag{4.6}$$

which can be easily proved by applying the principle of inclusion and exclusion to the following problem: In how many ways can one select r of given k distinct objects so that each selection includes some particular m of the k objects?

Combining (4.4) and (4.5) one can deduce that

$$\mathbb{X}_k = \sum_{j=0}^{\lfloor (k-1)/2\rfloor}\binom{k}{j}\mathbb{X}'_{k-2j}. \tag{4.7}$$

Proof of Theorem 4.4. It is enough to prove (4.4), because this formula and the fact that $\{\mathbb{X}_k\}$ commute will imply that $\{\mathbb{X}'_k\}$ commute, i.e. the equations (4.3) form a hierarchy.

Using (3.4) and (3.7) one can easily check that

$$g_{k+1}(n,n-1;z) = z^{k+1} + k\sum_{i=1}^{\lfloor (k+1)/2\rfloor}\frac{(-1)^i}{i}\binom{k-i-1}{i-1}z^{k+1-2i}, \tag{4.8}$$

which combined with (3.9) and (4.1a) gives

$$\alpha_{k+1}(n,n-1) = \mathfrak{r}_k(n) + k\sum_{i=1}^{\lfloor (k+1)/2\rfloor}\frac{(-1)^i}{i}\binom{k-i-1}{i-1}\mathfrak{r}_{k-2i}(n). \tag{4.9}$$

On the other hand, from equations (3.8) it follows that

$$g_{k+1}(n,n-1;z) = zg_k(n-1,n-1;z) - \delta_{k,1},$$

which shows that

$$g_k(n-1,n-1;z) = z^k + k\sum_{i=1}^{\lfloor (k+1)/2\rfloor}\frac{(-1)^i}{i}\binom{k-i-1}{i-1}z^{k-2i} + \frac{\delta_{k,1}}{z}, \tag{4.10}$$

and therefore, using (3.9) and (4.1b) we get

$$\alpha_k(n-1,n-1) = \mathfrak{l}_k(n) + k\sum_{i=1}^{\lfloor (k+1)/2\rfloor}\frac{(-1)^i}{i}\binom{k-i-1}{i-1}\mathfrak{l}_{k-2i}(n). \tag{4.11}$$

The proof now follows from (4.9), (4.11), Proposition 4.1 and the fact that $\mathfrak{r}_0(n) = 0$, $\mathfrak{r}_{-1}(n) = 1$, $\mathfrak{l}_0(n) = 1$, $\mathfrak{l}_{-1}(n) = 0$ are independent of n. $\square$

5. Darboux transformations from $L_0 = E + E^{-1}$ at the end points of the spectrum

In this section we focus on certain second-order difference operators L_{N_1,N_2}, which were introduced in [18] in connection with a difference-differential version of the bispectral problem [11]. These operators can be defined by successive Darboux transformations from the operator $L_0 = E + E^{-1}$ at the end points ± 2 of the spectrum. Recall (see [24]) that the Darboux transformation of a second-order operator L at a point c_0 consists of factorizing $L - c_0\mathrm{Id}$ as a product of first-order operators and producing a new operator $\hat{L}$ by exchanging the factors, i.e. if we write $L - c_0\mathrm{Id} = \mathcal{P}\mathcal{Q}$, then $\hat{L}$ is defined by $\hat{L} - c_0\mathrm{Id} = \mathcal{Q}\mathcal{P}$. The main result in this section is a characterization of these operators in terms of the vector fields of the Toda lattice hierarchy. This is needed in the next section where we prove that the heat kernel expansion for these operators can be written as a sum of only two Bessel functions with polynomial coefficients (in the time variable t), and that this property completely characterizes the operators L_{N_1,N_2}.

5.1. Constructing the operators L_{N_1,N_2}

The operators L_{N_1,N_2} are obtained by the following sequence of Darboux transformations:

$$\begin{aligned} L_0 - 2\,\mathrm{Id} = \mathcal{P}_0\mathcal{Q}_0 \curvearrowright L_{1,0} - 2\,\mathrm{Id} = \mathcal{Q}_0\mathcal{P}_0 = \mathcal{P}_1\mathcal{Q}_1 \curvearrowright \cdots \\ \curvearrowright L_{N_1,0} - 2\,\mathrm{Id} = \mathcal{Q}_{N_1-1}\mathcal{P}_{N_1-1}, \\ L_{N_1,0} + 2\,\mathrm{Id} = \mathcal{P}_{N_1}\mathcal{Q}_{N_1} \curvearrowright L_{N_1,1} + 2\,\mathrm{Id} = \mathcal{Q}_{N_1}\mathcal{P}_{N_1} = \mathcal{P}_{N_1+1}\mathcal{Q}_{N_1+1} \curvearrowright \cdots \\ \curvearrowright L_{N_1,N_2} + 2\,\mathrm{Id} = \mathcal{Q}_{N_1+N_2-1}\mathcal{P}_{N_1+N_2-1}. \end{aligned} \tag{5.1}$$

At each step, the factorization of the operator $L_{i_1,i_2} \pm 2\,\mathrm{Id}$ depends on one free parameter. Thus, the operator L_{N_1,N_2} will depend on N_1+N_2 free parameters. The operator L_{N_1,N_2} belongs to a rank one commutative ring of difference operators, i.e. we can apply the correspondence between commutative rings of difference operators and algebraic curves developed in the papers [23, 27, 28]. We first sketch the main steps of this construction with an emphasis on the operators obtained by the Darboux process (5.1) and refer the reader to [17, 18] for more details.

Following [28], we call a difference operator $M = \sum_{k=K_-}^{K_+} \mu_k(n)E^k$ *properly bordered* if $\mu_{K_-}(n) \neq 0$ and $\mu_{K_+}(n) \neq 0$ for all $n \in \mathbb{Z}$; the interval $[K_-, K_+]$ is the *support* of M. A commutative ring $\mathcal{A}$ of difference operators is called *rank one* if it contains two properly bordered difference operators M' and M'' with supports $[K'_-, K'_+]$ and $[K''_-, K''_+]$ such that $\gcd(K'_-, K''_-) = 1$, $\gcd(K'_+, K''_+) = 1$ and $K'_-K''_+ < K'_+K''_-$. In that case, $\mathrm{Spec}(\mathcal{A})$ is an irreducible complex affine curve that completes by adding two nonsingular points $Q^{\pm}_{\infty}$ at infinity.

Starting with a properly bordered second-order difference operator $L = E + b_n\mathrm{Id} + a_nE^{-1}$ we denote by $\mathcal{A}_L$ the ring of all difference operators commuting with L, i.e.

$$\mathcal{A}_L = \Big\{ M = \sum_{k=K_-}^{K_+} \mu_k(n) E^k : [M, L] = 0 \Big\}.$$

One can show that $\mathcal{A}_L$ is in fact a commutative ring consisting of properly bordered difference operators, and it is a rank one ring if and only if $\mathcal{A}_L$ contains an operator which is not a polynomial of L. For every $M \in \mathcal{A}_L$ the operators L and M satisfy an algebraic relation of the form

$$M^2 = MT_1(L) + T_2(L),$$

where T_1 and T_2 are some polynomials. This equation defines an affine curve $f_{L,M}(u,v) = v^2 - vT_1(u) - T_2(u) = 0$. It is easy to see that for every $M \in \mathcal{A}_L$ there exists a unique polynomial g_M such that $g_M(0) = 0$ and the operator $M - g_M(L)$ contains only nonnegative powers of E, i.e. $M = g_M(L) + \sum_{j=0}^{\nu(M)} c_k(n) E^k$. From this, it follows that the ring $\mathcal{A}_L$ is generated by two operators $\{L, M\}$ where M is chosen so that $\nu(M) > 0$ is minimal. The *spectral curve* $\mathrm{Spec}(\mathcal{A}_L)$ is $f_{L,M}(u,v) = 0$ and the *complete curve* is $X_L = \mathrm{Spec}(\mathcal{A}_L) \cup \{Q_\infty^+, Q_\infty^-\}$.

The *Baker function* Ψ_n for $\mathcal{A}_L$ is the unique (up to a factor independent of n) eigenfunction for the operators from $\mathcal{A}_L$. If we denote by A_L the ring of functions meromorphic on X with poles only at $Q_\infty^\pm$, then for every $M \in \mathcal{A}_L$ we have

$$M\Psi_n(P) = h_M(P)\Psi_n(P), \qquad \text{where } h_M(P) \in A_L.$$

Moreover, if the support of M is $[K_-, K_+]$ then $h_M(P)$ has poles of orders K_+ and K_- at Q_∞^+ and Q_∞^-, respectively.

Let us denote by $\mathcal{A}_{N_1,N_2} = \mathcal{A}_{L_{N_1,N_2}}$ the ring of all difference operators commuting with L_{N_1,N_2}. In [18] it was shown that $\mathcal{A}_{N_1,N_2}$ is a rank one commutative ring of difference operators, which is isomorphic to the ring

$$A_{N_1,N_2} = A_{L_{N_1,N_2}} = \mathbb{C}[x + x^{-1}, f_{N_1,N_2}(x)] \subset \mathbb{C}[x, x^{-1}],$$

where

$$f_{N_1,N_2}(x) = \frac{(x-1)^{2N_1+1}(x+1)^{2N_2+1}}{x^{N_1+N_2+1}}. \tag{5.2}$$

In other words, if Ψ_n is the Baker function for $\mathcal{A}_{N_1,N_2}$ then

$$L_{N_1,N_2}\Psi_n(x) = (x + x^{-1})\Psi_n(x), \tag{5.3a}$$

$$M_{N_1,N_2}\Psi_n(x) = f_{N_1,N_2}(x)\Psi_n(x), \tag{5.3b}$$

for some $M_{N_1,N_2} \in \mathcal{A}_{N_1,N_2}$, and the ring $\mathcal{A}_{N_1,N_2}$ is generated by L_{N_1,N_2} and M_{N_1,N_2}. The spectral curve is given by the equation

$$\mathrm{Spec}(\mathcal{A}_{N_1,N_2}): \quad v^2 = (u-2)^{2N_1+1}(u+2)^{2N_2+1}. \tag{5.4}$$

Clearly, $\mathrm{Spec}(\mathcal{A}_{N_1,N_2})$ is rational and has a cusp at $u = 2$ (resp. $u = -2$) when $N_1 > 0$ (resp. $N_2 > 0$). Another property, which we will need later, is that for every $j \in \mathbb{Z}$ we have

$$x^j f_{N_1,N_2}(x) \in A_{N_1,N_2} \tag{5.5}$$

(see [18, proof of Theorem 4.2]; note that x here corresponds to $z+1$ in [18]).

Conversely, let $L = E + b_n\mathrm{Id} + a_nE^{-1}$ be a properly bordered second-order difference operator whose spectral curve is given by equation (5.4). From the correspondence in [28] we can conclude that $\mathcal{A}_L$ is obtained from $\mathcal{A}_{N_1,N_2}$ for a specific choice of the free parameters in the Darboux steps, up to a conjugation by a nonzero function g_n, i.e.

$$\mathcal{A}_L = \{g_n^{-1}Mg_n : M \in \mathcal{A}_{N_1,N_2}\}. \tag{5.6}$$

If L is nonconstant (i.e. at least one of the functions a_n and b_n is not a constant), then it is easy to see that all second-order operators operators in $\mathcal{A}_L$ with support $[-1,1]$ must have the form $\gamma_1L + \gamma_2\mathrm{Id}$ for some constants γ_1,γ_2. From this, it follows that the only possible functions g_n in (5.6) are $g_n = c^n$, and we must have

$$L = c^{-n-1}L_{N_1,N_2}c^n + d\,\mathrm{Id} \tag{5.7}$$

for some constants $c \neq 0$ and d.

One possible way to eliminate this freedom and characterize precisely the operators L_{N_1,N_2} is to consider properly bordered second-order difference operators of the form $L = E+b_n\mathrm{Id}+a_nE^{-1}$ with spectral curve given in (5.4) and coefficients satisfying

$$\lim_{n\to\infty} b_n = 0, \qquad \lim_{n\to\infty} a_n = 1. \tag{5.8}$$

Indeed, if $L = L_{N_1,N_2}$ then the coefficients b_n, a_n can be computed from the formulas

$$b_n = \frac{\partial}{\partial s_1}\log\frac{\bar{\tau}_{n+1}(s)}{\bar{\tau}_n(s)}, \quad a_n = \frac{\bar{\tau}_{n+1}(s)\bar{\tau}_{n-1}(s)}{\bar{\tau}_n(s)^2},$$

where $\bar{\tau}_n(s)$ is a polynomial in n, which makes (5.8) obvious. We note, however, that $\bar{\tau}_n(s)$ in the last formulas differs from the τ-function introduced in Section 2 (due to the different approach in the papers [17, 18]). Conversely, if L is a nonconstant coefficient operator which belongs to a rank one commutative ring of difference operators whose spectral curve is given by (5.4), then (5.7) must hold, which combined with (5.8) shows that $c = \pm 1$ and $d = 0$. Conjugating L_{N_1,N_2} by $(-1)^n$ essentially exchanges the roles of $+2$ and -2 in (5.1) (or, equivalently, the roles of N_1 and N_2). Thus, we have $L = L_{N_1,N_2}$ or $L = L_{N_2,N_1}$, completing the proof in this case. Finally, if a_n and b_n are constants, then (5.8) implies that $L = L_0$.

Next, we establish several new facts needed for the characterization of the operators L_{N_1,N_2} in terms of the Toda vector fields, proved at the end of this section.

Lemma 5.1. *Let A be a ring of Laurent polynomials in x such that $A_{N_1,N_2} \subset A$ for some $N_1, N_2 \in \mathbb{N}_0$. If A contains a polynomial $p(x)$ such that $0 < \deg(p(x)) \leq N_1 + N_2$ then one of the following must hold:*

(i) $N_1 \geq 1$ *and* $f_{N_1-1,N_2}(x) \in A$;
(ii) $N_2 \geq 1$ *and* $f_{N_1,N_2-1}(x) \in A$.

Proof. Assume that $p(x) \in A \cap \mathbb{C}[x]$ is such that $0 < \deg(p(x)) \leq N_1 + N_2$. Since $x + x^{-1} \in A$, it is clear that $p(x) + p(1/x) \in A$, which combined with $p(x) \in A$ shows that $f(x) = p(x) - p(1/x) \in A$. Notice that $f(1/x) = -f(x)$ and therefore we can write $f(x)$ in the form

$$f(x) = \left(x - \frac{1}{x}\right)^{2l+1} \tilde{f}(x), \tag{5.9}$$

where $\tilde{f}(x) \in \mathbb{C}[x, x^{-1}]$ is not divisible by $x - 1/x$ (i.e. $\tilde{f}(-1) \neq 0$ or $\tilde{f}(1) \neq 0$) and $2l + 1 \leq N_1 + N_2$.

Let us define $T = \min(N_1, N_2)$ and $T' = \max(N_1, N_2) > 0$. Choosing $\epsilon = 1$ if $T' = N_2$ and $\epsilon = -1$ otherwise we can rewrite $f_{N_1,N_2}(x)$ as

$$f_{N_1,N_2}(x) = \frac{(x+\epsilon)^{2T'+1}(x-\epsilon)^{2T+1}}{x^{T'+T+1}} = \left(x - \frac{1}{x}\right)^{2T+1} \left[x + 2\epsilon + \frac{1}{x}\right]^{T'-T}.$$

Below we consider separately the cases $l \leq T - 1$ and $l \geq T$.

Case 1: $l \leq T - 1$. Let us write $\tilde{f}(x)$ in (5.9) as follows:

$$\tilde{f}(x) = \sum_{j=0}^{S} f_j \left(x + 2\epsilon + \frac{1}{x}\right)^j.$$

Case 1.a. Assume first that $f_0 \neq 0$ and $T' > T$. Then we can multiply $f(x)$ by

$$\left(x - \frac{1}{x}\right)^{2(T-l)} \left(x + 2\epsilon + \frac{1}{x}\right)^{T'-T-1} \in A$$

to get

$$\sum_{j=0}^{S} f_j \left(x - \frac{1}{x}\right)^{2T+1} \left(x + 2\epsilon + \frac{1}{x}\right)^{j+T'-T-1} \in A.$$

Notice that for $j \geq 1$ the terms in the above sum are multiples of f_{N_1,N_2} and therefore belong to A by (5.5). Thus, the term corresponding to $j = 0$ also belongs to A and since $f_0 \neq 0$ we obtain

$$\left(x - \frac{1}{x}\right)^{2T+1} \left(x + 2\epsilon + \frac{1}{x}\right)^{T'-T-1} = \frac{(x+\epsilon)^{2T'-1}(x-\epsilon)^{2T+1}}{x^{T'+T}} \in A,$$

which is what we wanted to show.

Case 1.b. Assume now that $f_0 \neq 0$ but $T' = T$ (hence $\epsilon = 1$), and let us multiply $f(x)$ by

$$\left(x - \frac{1}{x}\right)^{2(T-l-1)} \left(x - 2 + \frac{1}{x}\right) \in A.$$

We have

$$\sum_{j=0}^{m} f_j \left(x - \frac{1}{x}\right)^{2T-1} \left(x + 2 + \frac{1}{x}\right)^j \left(x - 2 + \frac{1}{x}\right) \in A.$$

Again all terms for $j \geq 1$ in the sum above are in A and therefore, since $f_0 \neq 0$, we get

$$\left(x - \frac{1}{x}\right)^{2T-1}\left(x - 2 + \frac{1}{x}\right) = \frac{(x+1)^{2T-1}(x-1)^{2T+1}}{x^{2T}} \in A.$$

Case 1.c. Let now $f_0 = 0$, i.e. $\tilde{f}(-\epsilon) = 0$. This implies that $\tilde{f}(\epsilon) \neq 0$, because otherwise $x - 1/x$ will divide $\tilde{f}(x)$ contrary to our factorization in (5.9). Thus we can write $\tilde{f}(x)$ as

$$\tilde{f}(x) = \sum_{j=0}^{m} \tilde{f}_j \left(x - 2\epsilon + \frac{1}{x}\right)^j, \tag{5.10}$$

with $\tilde{f}_0 \neq 0$. Using now (5.10) and multiplying $f(x)$ by

$$\left(x - 2\epsilon + \frac{1}{x}\right)^{T-l-1}\left(x + 2\epsilon + \frac{1}{x}\right)^{T'-l} \in A$$

we get

$$\sum_{j=0}^{m} \tilde{f}_j \left(x - \frac{1}{x}\right)^{2l+1}\left(x - 2\epsilon + \frac{1}{x}\right)^{j+T-l-1}\left(x + 2\epsilon + \frac{1}{x}\right)^{T'-l} \in A.$$

For $j \geq 1$, the j-th term in the above sum is

$$\left(x - 2\epsilon + \frac{1}{x}\right)^{j-1}\frac{(x-\epsilon)^{2T+1}(x+\epsilon)^{2T'+1}}{x^{T+T'+1}} \in A,$$

and therefore for $j = 0$ we have

$$\frac{(x-\epsilon)^{2T-1}(x+\epsilon)^{2T'+1}}{x^{T+T'}} \in A.$$

Case 2. Finally, if $l \geq T$ we can write $f(x)$ as

$$f(x) = \left(x - \frac{1}{x}\right)^{2T+1}\sum_{j=j_0}^{S} h_j \left(x + 2\epsilon + \frac{1}{x}\right)^j, \tag{5.11}$$

with $h_{j_0} \neq 0$ and $S \leq T' - T - 1$. Multiplying (5.11) by $(x + 2\epsilon + 1/x)^{T'-T-1-j_0} \in A$ we see as before that

$$\frac{(x-\epsilon)^{2T+1}(x+\epsilon)^{2T'-1}}{x^{T+T'}} \in A,$$

which completes the proof of the lemma. □

Corollary 5.2. *If A is a ring of Laurent polynomials in x such that $A_{N,N} \subset A$ for some $N \in \mathbb{N}_0$, then $A = A_{N_1,N_2}$ for some $N_1, N_2 \in \mathbb{N}_0$.*

Proof. For every $f(x) \in A$ there exists a unique polynomial $p(x)$ such that $p(0) = 0$ and $f(x) - p(x) \in \mathbb{C}[x + x^{-1}]$. Since $x + x^{-1} \in A$ we see that A is generated by $x + x^{-1}$ and the polynomial of minimal positive degree in $A \cap \mathbb{C}[x]$. The proof now follows immediately from Lemma 5.1. □

Let us denote by $q_k(x)$ the odd polynomial of degree $2k+1$ given by

$$q_k(x) = \sum_{j=0}^{k} \binom{2k+1}{j} (-1)^j x^{2k-2j+1}. \tag{5.12}$$

Then

$$f_{k,k}(x) = \left(x - \frac{1}{x}\right)^{2k+1} = q_k(x) - q_k(1/x). \tag{5.13}$$

If we put $u = x + x^{-1}$ then from (5.12) and (5.13) it is easy to see that

$$q_{k+1}(x) = (u^2 - 4)q_k(x) + (-1)^{k+1}\binom{2k+1}{k} u. \tag{5.14}$$

Using the last relation, one can deduce by induction on k that

$$q_k(x) + q_k(1/x) = P_k(u), \tag{5.15}$$

where

$$\begin{aligned} P_k(u) &= \sum_{j=0}^{k} \frac{(-2)^j}{j!} \frac{(2k+1)!!}{(2k+1-2j)!!} u^{2k-2j+1} \\ &= \frac{(2k+1)!}{k!} \sum_{j=0}^{k} \frac{(-1)^j}{j!} \frac{(k-j)!}{(2k+1-2j)!} u^{2k-2j+1}, \end{aligned} \tag{5.16}$$

and $(2j+1)!! = 1 \cdot 3 \cdots (2j+1)$.

Proposition 5.3. *Let L_{N_1,N_2} be the second-order difference operator constructed in* (5.1) *and $N = \max(N_1, N_2)$. Then for every $k \geq N$ we have*

$$P_k(L_{N_1,N_2})_+ \in \mathcal{A}_{N_1,N_2} \quad \text{and} \quad (L_{N_1,N_2} P_k(L_{N_1,N_2}))_+ \in \mathcal{A}_{N_1,N_2}. \tag{5.17}$$

Proof. Clearly $P_k(L_{N_1,N_2}) \in \mathcal{A}_{N_1,N_2}$. From (5.2), (5.5) and (5.13) it follows that $q_k(x) \in A_{N_1,N_2}$ for every $k \geq N$. This combined with equations (5.15) and (5.3a) shows that $P_k(L_{N_1,N_2})_+ \in \mathcal{A}_{N_1,N_2}$. A similar argument gives the second statement in (5.17). Indeed, using the fact that

$$(x + 1/x) f_{k,k} \in A_{N_1,N_2} \quad \text{for every } k \geq N,$$

and (5.13) one can deduce that $(x+1/x)q_k(x) \in A_{N_1,N_2}$ for all $k \geq N$, which combined with $uP_k(u) = (x+1/x)q_k(x) + (-1)^k\binom{2k+1}{k} + O(1/x)$ gives the second part of (5.17). □

5.2. Characterization of L_{N_1,N_2} in terms of the Toda flows

In this subsection we prove that the operators L_{N_1,N_2} can be characterized by the property (5.17), or equivalently by the vanishing of an appropriate linear combination of the Toda flows after a particular point. This is a discrete analog of the well-known fact that the rational solutions of the Korteweg–de Vries hierarchy are precisely the second-order differential operators which are stationary under the KdV flows, after a particular point.

Theorem 5.4. *Let $L = E + b_n\mathrm{Id} + a_nE^{-1}$ be a nonconstant properly bordered second-order difference operator. Then the following conditions are equivalent.*

(i) *The operator L can be obtained by a sequence of Darboux transformations from the operator $L_0 = E + E^{-1}$ at the end points ± 2 of the spectrum, i.e. $L = L_{N_1,N_2}$ for some $N_1, N_2 \in \mathbb{N}_0$ with $N_1 + N_2 > 0$ and for specific values of the free parameters in the Darboux process* (5.1).

(ii) *There exists $N \in \mathbb{N}$ such that*

$$[P_k(L)_+, L] = [(LP_k(L))_+, L] = 0 \quad \text{for every } k \geq N, \tag{5.18}$$

where $P_k(u)$ is the polynomial defined by (5.16).

Proof. The implication (i)⇒(ii) follows immediately from Proposition 5.3. Assume now that (5.18) holds for every $k \geq N$. Then L belongs to a rank-one commutative ring of difference operators $\mathcal{A}_L$ and $P_k(L)_+$, $(LP_k(L))_+ \in \mathcal{A}_L$ for $k \geq N$. Let Ψ_n be the Baker function and $X = \mathrm{Spec}(\mathcal{A}) \cup \{Q_\infty^+, Q_\infty^-\}$ be the complete curve. Then there exists a function $\mathfrak{f}(P)$ on X with simple poles at Q_∞^+ and Q_∞^- such that

$$L\Psi_n(P) = \mathfrak{f}(P)\Psi_n(P). \tag{5.19}$$

Let us pick local parameters x^{-1} and y^{-1} near Q_∞^+ and Q_∞^-, respectively, such that

$$\mathfrak{f}(P) = \begin{cases} x + 1/x & \text{when } P \text{ is in a neighborhood of } Q_\infty^+, \\ y + 1/y & \text{when } P \text{ is in a neighborhood of } Q_\infty^-. \end{cases} \tag{5.20}$$

Then for each $k \geq N$ there exist functions $\mathfrak{f}_{2k+1}(P)$ and $\mathfrak{f}_{2k+2}(P)$ with poles only at Q_∞^+ such that

$$P_k(L)_+\Psi_n(P) = \mathfrak{f}_{2k+1}(P)\Psi_n(P), \tag{5.21a}$$

$$(LP_k(L))_+\Psi_n(P) = \mathfrak{f}_{2k+2}(P)\Psi_n(P). \tag{5.21b}$$

From (5.20) and (5.15) it follows that near Q_∞^+ and Q_∞^- these functions have the following expansions:

$$\mathfrak{f}_{2k+1}^+(x) = q_k(x) + \sum_{j=1}^{\infty} \frac{\delta_j^k}{x^j}, \tag{5.22a}$$

$$\mathfrak{f}_{2k+1}^-(y) = \sum_{j=0}^{\infty} \frac{\delta_j'^k}{y^j}, \tag{5.22b}$$

and

$$\mathfrak{f}_{2k+2}^+(x) = \left(x + \frac{1}{x}\right)q_k(x) + (-1)^k \binom{2k+1}{k} + \sum_{j=1}^{\infty} \frac{\gamma_j^k}{x^j}, \tag{5.23a}$$

$$\mathfrak{f}_{2k+2}^-(y) = \sum_{j=0}^{\infty} \frac{\gamma_j'^k}{y^j}. \tag{5.23b}$$

Let us now consider the function

$$\mathfrak{g}_k = \mathfrak{f}_{2k+1}\mathfrak{f} - \mathfrak{f}_{2k+2} \in A_L.$$

A straightforward computation using (5.20), (5.22) and (5.23) shows that near Q_∞^+ and Q_∞^- we have

$$\mathfrak{g}_k^+(x) = \delta_1^k + (-1)^k \binom{2k+1}{k} + O(1/x), \tag{5.24a}$$

$$\mathfrak{g}_k^-(y) = \delta_0'^k y + (\delta_1'^k - \gamma_0'^k) + O(1/y). \tag{5.24b}$$

If $\delta_0'^k \neq 0$, the function $\mathfrak{g}_k$ will correspond to a difference operator from $\mathcal{A}_L$ with support $[-1,0]$, which would imply that L is a constant coefficient operator, contrary to our assumption. Thus

$$\delta_0'^k = 0 \tag{5.25}$$

and $\mathfrak{g}_k(P)$ is a constant (depending on k). Next, we define

$$\mathfrak{h}_k = \mathfrak{f}_{2k+3} - (\mathfrak{f}^2 - 4)\mathfrak{f}_{2k+1} + (-1)^k \binom{2k+1}{k} \mathfrak{f} \in A_L.$$

We have

$$\mathfrak{h}_k^+(x) = -\delta_1^k x - \delta_2^k + O(1/x), \tag{5.26a}$$

$$\mathfrak{h}_k^-(y) = \left(-\delta_1'^k + (-1)^k \binom{2k+1}{k}\right) y - \delta_2'^k + O(1/y), \tag{5.26b}$$

and the same argument as above shows that $\mathfrak{h}_k + \delta_1^k \mathfrak{f} + \delta_2^k = 0$, i.e.

$$\mathfrak{f}_{2k+3} - (\mathfrak{f}^2 - 4)\mathfrak{f}_{2k+1} + (-1)^k \binom{2k+1}{k} \mathfrak{f} + \delta_1^k \mathfrak{f} + \delta_2^k = 0. \tag{5.27}$$

In particular, this equality implies that

$$\delta_1^k = \delta_1'^k + (-1)^{k+1} \binom{2k+1}{k}, \tag{5.28}$$

$$\delta_2^k = \delta_2'^k. \tag{5.29}$$

We want to show now that for every $k \geq N$, around Q_∞^- we have

$$\mathfrak{f}_{2k+1}^-(y) = q_k(1/y) + \sum_{j=1}^{\infty} \frac{\delta_j^k}{y^j}. \tag{5.30}$$

From equations (5.14), (5.20), (5.22a) and (5.27) we deduce that the coefficients δ_j^k in the expansion of the function $\mathfrak{f}_{2k+1}^+(x) - q_k(x) = \sum_{j=1}^{\infty} \delta_j^k / x^j$ satisfy the following recurrence relations:

$$\delta_3^k = \delta_1^{k+1} + 3\delta_1^k, \tag{5.31a}$$

$$\delta_{j+2}^k = \delta_j^{k+1} + 2\delta_j^k - \delta_{j-2}^k \quad \text{for } j \geq 2. \tag{5.31b}$$

The same argument shows that the same relations will be satisfied by the coefficients in the expansion of the function $\mathfrak{f}_{2k+1}^-(y) - q_k(1/y)$. Thus, to prove that (5.30) holds, it is enough to show that the coefficient of $1/x^j$ in $\mathfrak{f}_{2k+1}^+(x) - q_k(x)$ is equal to the coefficient of $1/y^j$ in $\mathfrak{f}_{2k+1}^-(y) - q_k(1/y)$ for $j = 0, 1, 2$ and every

$k \geq N$. It is easy to see that the equality of these three coefficients is equivalent to equations (5.25), (5.28) and (5.29), completing the proof of (5.30).

Next, we define

$$\mathfrak{p}_k = 2\mathfrak{f}_{2k+1} - P_k(\mathfrak{f}) \in A_L.$$

Using equations (5.13), (5.15), (5.22a) and (5.30) we see that $\mathfrak{p}_k(P)$ has the following expansions near Q_∞^+ and Q_∞^-:

$$\mathfrak{p}_k^+(x) = q_k(x) - q_k(1/x) + 2\sum_{j=1}^{\infty} \frac{\delta_j^k}{x^j} = \left(x - \frac{1}{x}\right)^{2k+1} + 2\sum_{j=1}^{\infty} \frac{\delta_j^k}{x^j}, \tag{5.32a}$$

$$\mathfrak{p}_k^-(y) = -q_k(y) + q_k(1/y) + 2\sum_{j=1}^{\infty} \frac{\delta_j^k}{y^j} = -\left(y - \frac{1}{y}\right)^{2k+1} + 2\sum_{j=1}^{\infty} \frac{\delta_j^k}{y^j}. \tag{5.32b}$$

We now use the fact that $\mathfrak{p}_k$ and $\mathfrak{f}$ satisfy an algebraic relation of the form

$$\mathfrak{p}_k^2 = \mathfrak{p}_k T_1(\mathfrak{f}) + T_2(\mathfrak{f}) \tag{5.33}$$

for some polynomials T_1 and T_2. It is easy to show that $T_1(\mathfrak{f}) = 0$. Indeed, if we assume that $T_1(\mathfrak{f}) = r\mathfrak{f}^s + \cdots$ for some nonzero constant r, then the function $\mathfrak{p}_k T_1(\mathfrak{f})$ has the following expansions near Q_∞^+ and Q_∞^-:

$$\mathfrak{p}_k T_1(\mathfrak{f}) = \begin{cases} rx^{2k+1+s} + O(x^{2k+s}) & \text{in a neighborhood of } Q_\infty^+, \\ -ry^{2k+1+s} + O(y^{2k+s}) & \text{in a neighborhood of } Q_\infty^-. \end{cases}$$

On the other hand, from equations (5.32) it is clear that if

$$\mathfrak{p}_k^2 - T_2(\mathfrak{f}) = \begin{cases} rx^l + O(x^{l-1}) & \text{in a neighborhood of } Q_\infty^+, \\ -ry^l + O(y^{l-1}) & \text{in a neighborhood of } Q_\infty^-, \end{cases}$$

for some nonzero constant r; then $l \leq 2k$, leading to a contradiction. Thus $T_1(\mathfrak{f}) = 0$ and therefore (5.33) reduces to

$$\mathfrak{p}_k^2 = T_2(\mathfrak{f}). \tag{5.34}$$

We can now show that $\delta_j^k = 0$ for all $j \in \mathbb{N}$, which implies that $T_2(\mathfrak{f}) = (\mathfrak{f}^2 - 4)^{2k+1}$. Indeed, let $\delta_{j_0}^k \neq 0$ for some $j_0 \in \mathbb{N}$ and let j_0 be the minimal possible. Then we can rewrite (5.34) as

$$\mathfrak{p}_k^2 - (\mathfrak{f}^2 - 4)^{2k+1} = T_2(\mathfrak{f}) - (\mathfrak{f}^2 - 4)^{2k+1}. \tag{5.35}$$

The left-hand side of (5.35) has the following expansions near Q_∞^+ and Q_∞^-:

$$\mathfrak{p}_k^2 - (\mathfrak{f}^2 - 4)^{2k+1} = \begin{cases} 4\delta_{j_0}^k x^{2k+1-j_0} + O(x^{2k-j_0}) & \text{in a neighborhood of } Q_\infty^+, \\ -4\delta_{j_0}^k y^{2k+1-j_0} + O(y^{2k-j_0}) & \text{in a neighborhood of } Q_\infty^-. \end{cases}$$

Again we get a contradiction because clearly the highest coefficients in the expansions of $T_2(\mathfrak{f}) - (\mathfrak{f}^2 - 4)^{2k+1}$ near Q_∞^+ and Q_∞^- must be equal. Thus (5.34) becomes

$$\mathfrak{p}_k^2 = (\mathfrak{f}^2 - 4)^{2k+1}. \tag{5.36}$$

Notice that the curve given by the last equation is exactly the spectral curve $\mathrm{Spec}(\mathcal{A}_{k,k})$ in (5.4). Thus, we conclude that the spectral curve X is rational and choosing an appropriate parametrization we have

$$A_{N,N} \subset A_L \subset \mathbb{C}[x, x^{-1}].$$

From Corollary 5.2 it follows that $A = A_{N_1,N_2}$ for some $N_1, N_2 \in \mathbb{N}_0$ with $N_1 + N_2 > 0$ (because L is nonconstant). Moreover, as we saw at the beginning of the section, equation (5.7) must hold. Let $\Psi_n(x)$ be the Baker function for $\mathcal{A}_{N_1,N_2}$, i.e. the function in formulas (5.3a)–(5.3b). Then the Baker function for $\mathcal{A}_L$ is $\tilde{\Psi}_n(x) = c^{-n}\Psi_n(x)$. Thus

$$L\tilde{\Psi}_n(x) = \left(\frac{1}{c}\left(x + \frac{1}{x}\right) + d\right)\tilde{\Psi}_n(x).$$

Equation (5.36) shows that for k large enough the function

$$\left[\left(\frac{1}{c}\left(x + \frac{1}{x}\right) + d\right)^2 - 4\right]^{2k+1}$$

must be the square of a rational function. It is easy to see that this can only happen when $d = 0$ and $c = \pm 1$, which means that $L = L_{N_1,N_2}$ or $L = L_{N_2,N_1}$, finishing the proof. □

Remark 5.5. We can easily reformulate Theorem 5.4 in terms of the vector fields $\mathbb{X}_k$ of the Toda lattice hierarchy (2.1). For every $k \in \mathbb{N}$ let

$$\varepsilon_k = \begin{cases} 0 & \text{if } k \text{ is odd,} \\ 1 & \text{if } k \text{ is even,} \end{cases} \tag{5.37}$$

and let us define

$$\mathbb{Y}_k(L) = \frac{(k - \varepsilon_k)!}{(\lfloor (k-1)/2 \rfloor)!} \sum_{j=0}^{\lfloor (k-1)/2 \rfloor} \frac{(-1)^j}{j!} \frac{(\lfloor (k-1)/2 \rfloor - j)!}{(k - \varepsilon_k - 2j)!} \mathbb{X}_{k-2j}(L), \tag{5.38}$$

where $\mathbb{X}_j(L) = [(L^j)_+, L]$. Then the operators L_{N_1,N_2} with $N_1 + N_2 > 0$ can be characterized as the only nonconstant properly bordered second-order difference operators of the form $L = E + b_n \mathrm{Id} + a_n E^{-1}$ satisfying the constraints

$$\mathbb{Y}_k(L) = 0 \quad \text{for every } k \text{ large enough.} \tag{5.39}$$

We end this section by giving an explicit formula for $\mathbb{Y}_k$ in terms of the vector fields $\mathbb{X}'_j$ defined in Theorem 4.4. The proposition below will be needed in the next section when we want to characterize the operators having specific heat kernel expansions.

Proposition 5.6. *The vector fields* $\mathbb{Y}_k$ *defined by* (5.38) *can be rewritten as a linear combination of the vector fields* $\mathbb{X}'_k$, *corresponding to the flows of the system* (4.3), *as follows:*

$$\mathbb{Y}_k = \sum_{l=0}^{\lfloor (k-1)/2 \rfloor} (-1)^l \left(1 - \frac{2l}{k}\varepsilon_k\right) \binom{k}{l} \mathbb{X}'_{k-2l}, \tag{5.40}$$

where ε_k *is defined in* (5.37).

Proof. Using (4.7) and (5.38) we get

$$\begin{aligned}\mathbb{Y}_k &= \frac{(k-\varepsilon_k)!}{(\lfloor (k-1)/2 \rfloor)!} \sum_{j=0}^{\lfloor (k-1)/2 \rfloor} \frac{(-1)^j}{j!} \frac{(\lfloor (k-1)/2 \rfloor - j)!}{(k-\varepsilon_k-2j)!} \\ &\quad \times \sum_{i=0}^{\lfloor (k-1)/2 \rfloor - j} \binom{k-2j}{i} \mathbb{X}'_{k-2i-2j} \\ &= \sum_{l=0}^{\lfloor (k-1)/2 \rfloor} R_{k,l} \mathbb{X}'_{k-2l},\end{aligned}$$

where

$$R_{k,l} = \frac{(k-\varepsilon_k)!}{(\lfloor (k-1)/2 \rfloor)!} \sum_{j=0}^{l} \frac{(-1)^j}{j!} \frac{(\lfloor (k-1)/2 \rfloor - j)!(k-2j)!}{(k-\varepsilon_k-2j)!(l-j)!(k-l-j)!}. \tag{5.41}$$

We now consider separately the cases when k is odd or even.

Case 1. Assume first that k is odd, i.e. $k = 2s+1$. Then $\varepsilon_k = 0$ and equation (5.41) gives

$$\begin{aligned}R_{2s+1,l} &= \frac{(2s+1)!}{s!} \sum_{j=0}^{l} \frac{(-1)^j}{j!} \frac{(s-j)!}{(l-j)!(2s+1-l-j)!} \\ &= \binom{2s+1}{l} {}_2F_1\left(\begin{matrix} -l, -2s-1+l \\ -s \end{matrix}; 1\right) \\ &= \binom{2s+1}{l} \frac{(s+1-l)_l}{(-s)_l} = (-1)^l \binom{2s+1}{l},\end{aligned}$$

where in the last line we used the Chu–Vandermonde formula to evaluate the ${}_2F_1$, and $(a)_l = a(a+1)\cdots(a+l-1)$ denotes the shifted factorial. This completes the proof in the case when k is odd.

Case 2. Assume now that k is even, i.e. $k = 2s+2$ and therefore $\varepsilon_k = 1$. A similar computation gives

$$\begin{aligned} R_{2s+2,l} &= 2\frac{(2s+1)!}{s!}\sum_{j=0}^{l}\frac{(-1)^j}{j!}\frac{(s+1-j)!}{(l-j)!(2s+2-l-j)!} \\ &= \binom{2s+2}{l}{}_2F_1\left(\begin{matrix}-l,-2s-2+l\\ -s-1\end{matrix};1\right) \\ &= \binom{2s+2}{l}\frac{(s+1-l)_l}{(-s-1)_l} = (-1)^l\,\frac{s-l+1}{s+1}\binom{2s+2}{l}, \end{aligned}$$

which completes the proof. □

6. Finite heat kernel expansions

In this section we prove that the operators L_{N_1,N_2} constructed in the previous section can be characterized as the only operators for which the heat kernel can be written as a sum of only two Bessel functions with polynomial (in t) coefficients.

We work below with series of the form

$$\sum_{r\leq k} p(r)I_r(2t), \tag{6.1}$$

where $p(r)$ is a polynomial in r, and before we state the main result, we establish several properties of the series (6.1). Using (1.7) we see that for $r \geq 0$ we have

$$|I_{-r}(2t)| \leq \frac{|t|^r}{r!}\sum_{j=0}^{\infty}\frac{|t|^{2j}}{j!} \leq \frac{|t|^r}{r!}e^{|t|^2}.$$

Thus if $|t| \leq T$, then $|I_{-r}(2t)| \leq (|T|^r/r!)e^{|T|^2}$. Since for every polynomial $p(r)$ and every positive constant T the series $\sum_{r=0}^{\infty}(|p(-r)|/r!)T^r$ converges we conclude that (6.1) converges absolutely and uniformly on bounded sets.

The next lemma allows us to identify polynomials $p(r)$ for which the sum of the series (6.1) can be written in a simple closed form.

Lemma 6.1. *For every $m \in \mathbb{N}$ and $k \in \mathbb{Z}$ we have*

$$t^m I_k(2t) = (-1)^m \sum_{\substack{i\leq k\\ i\equiv k+m \pmod 2}} A_i^{m,k}\, I_i(2t), \tag{6.2}$$

where

$$A_i^{m,k} = \frac{i}{4^{m-1}(m-1)!}\prod_{\substack{|j|<m\\ j\equiv m \pmod 2}}((k+j)^2-i^2). \tag{6.3}$$

Proof. The proof can be obtained by induction on m using the identity

$$t(I_{k-1}(2t)-I_{k+1}(2t)) = kI_k(2t).$$ □

Notice that $A_i^{m,k}$ is an odd polynomial in i of degree $2m-1$. Thus, as an immediate application of the above lemma, we obtain the following corollary.

Corollary 6.2. *Let $p(i)$ be a function which is an odd polynomial in i when i is even or odd.*[1] *Then*

$$\sum_{i<k} p(i)I_i(2t) = p_1(t)I_k(2t) + p_2(t)I_{k-1}(2t),$$

where $p_1(t)$ and $p_2(t)$ are polynomials of t such that $p_1(0) = p_2(0) = 0$.

We can now formulate and prove the main result in this section.

Theorem 6.3. *Let $L = E + b_n\mathrm{Id} + a_nE^{-1}$ be a properly bordered second-order difference operator. Then the following conditions are equivalent.*

(i) *The operator L can be obtained by a sequence of Darboux transformations from the operator $L_0 = E + E^{-1}$ at the end points ± 2 of the spectrum, i.e. $L = L_{N_1,N_2}$ for some $N_1, N_2 \in \mathbb{N}_0$ and for some specific values of the free parameters in the Darboux process* (5.1).

(ii) *The fundamental solution of the discrete heat equation* (1.2) *can be written as*

$$u(n,m;t) = (1 + p_1(n,m;t))I_{n-m}(2t) + p_2(n,m;t)I_{n-m-1}(2t), \tag{6.4}$$

where $p_1(n,m;t)$ and $p_2(n,m;t)$ are polynomials in t with coefficients depending on n and m, such that $p_1(n,m;0) = p_2(n,m;0) = 0$.

6.1. Finiteness of the heat kernel for the operators L_{N_1,N_2}

The implication (i)⇒(ii) is essentially proved in [15], except the fact that exactly two Bessel functions (I_{n-m} and I_{n-m-1}) are enough. This can be deduced from the arguments given there combined with Corollary 6.2. We explain below the main steps of the proof together with the essential ingredients from [15, 18].

We consider the operator L_{N_1,N_2} obtained by the sequence of Darboux transformations (5.1) and the corresponding maximal commutative ring $\mathcal{A}_{N_1,N_2}$ of difference operators that contains L_{N_1,N_2}. From (5.1) one can deduce that L_{N_1,N_2} and $L_0 = E + E^{-1}$ are related by the intertwining relation

$$QL_0 = L_{N_1,N_2}Q, \tag{6.5}$$

where

$$Q = \mathcal{Q}_{N_1+N_2-1}\cdots\mathcal{Q}_1\mathcal{Q}_0.$$

Equation (6.5) implies that $\ker Q$ is preserved by L_0, i.e. $L_0(\ker Q) \subset \ker Q$. Conversely, one can show by induction on the order of Q that if two operators L_0 and $L = L_{N_1,N_2}$ are related by (6.5) for some difference operator Q, then L can be obtained by a sequence of Darboux transformations from L_0. The fact that we iterate the Darboux transformation only at ± 2 means that the operator L_0 restricted to $\ker Q$ has 2 and -2 as eigenvalues with multiplicities N_1 and N_2,

[1] Equivalently, we can say that $p(i) = \tilde{p}(i) + (-1)^i\hat{p}(i)$, where $\tilde{p}(i)$ and $\hat{p}(i)$ are odd polynomials in i.

respectively. This allows us to reconstruct Q explicitly from its kernel as follows. We define functions $\phi_1^+,\dots,\phi_{N_1}^+$ and $\phi_1^-,\dots,\phi_{N_2}^-$ such that

$$\begin{aligned}(L_0-2\,\mathrm{Id})\phi_j^+ &= \phi_{j-1}^+ \quad \text{for } j=1,\dots,N_1,\\ (L_0+2\,\mathrm{Id})\phi_j^- &= \phi_{j-1}^- \quad \text{for } j=1,\dots,N_2,\end{aligned}$$

with the convention that $\phi_0^+=\phi_0^-=0$. Let Wr_Δ denote the discrete Wronskian (Casorati determinant) with respect to the variable n,

$$\mathrm{Wr}_\Delta(f_1,\dots,f_k)=\det(\Delta^{i-1}f_j)_{1\le i,j\le k}.$$

Then the operator Q, normalized to be monic, is defined by,

$$Q(f)=\frac{\mathrm{Wr}_\Delta(\phi_1^+,\dots,\phi_{N_1}^+,\phi_1^-,\dots,\phi_{N_2}^-,f)}{\mathrm{Wr}_\Delta(\phi_1^+,\dots,\phi_{N_1}^+,\phi_1^-,\dots,\phi_{N_2}^-)}. \tag{6.6}$$

The Baker function for the ring $\mathcal{A}_{N_1,N_2}$ can be written in terms of the operator Q by

$$\Psi_n(x)=\frac{1}{(x-1)^{N_1}(x+1)^{N_2}}Q(x^n). \tag{6.7}$$

Using the explicit form of the functions $\phi_j^\pm$ and equations (6.6) and (6.7) one can show that $\Psi_n(1/x)$ and $x\Psi_{n+1}^*(x)$ are equal up to a multiplicative constant independent of x, i.e.

$$\Psi_n(1/x)=c_nx\Psi_{n+1}^*(x). \tag{6.8}$$

Finally, we can use the above information to prove that $\Psi_n(x)$ and $\Psi_n^*(x)$ satisfy the orthogonality relation

$$\frac{1}{2\pi i}\oint_C \Psi_n(x)\Psi_{m+1}^*(x)\,dx=\delta_{n,m}, \tag{6.9}$$

where C is a simple closed contour around the origin, avoiding the points $x=\pm1$. The proof of (6.9) can be obtained as follows. Notice first that $\Psi_n(x)$ and $\Psi_{m+1}^*(x)$ have poles only at ±1. However, the spectral curve has cusps at these points and since the differential $\Psi_n(x)\Psi_{m+1}^*(x)\,dx$ is regular on the affine curve $\mathrm{Spec}(\mathcal{A}_{N_1,N_2})$ we deduce that the residues at $x=\pm1$ are equal to zero. Using the explicit formulas for $\Psi_n(x)$ and $\Psi_{m+1}^*(x)$ we see that expanding around $x=0$ for $m\le n$ we have

$$\Psi_n(x)\Psi_{m+1}^*(x)=\frac{1}{x}(\delta_{n,m}+O(x)),$$

which establishes (6.9) for $m\le n$. When $m>n$ we replace x by $1/x$ in (6.9), and applying (6.8) we obtain zero by the bilinear identity (2.9). We refer the reader to [18] for detailed proofs of all statements in the above construction.

From (5.3a) and (6.9) it follows that the fundamental solution for L_{N_1,N_2} can be written as

$$u(n,m;t)=\frac{1}{2\pi i}\oint_C e^{t(x+1/x)}\Psi_n(x)\Psi_{m+1}^*(x)\,dx. \tag{6.10}$$

Since

$$e^{t(x+1/x)} = \sum_{k\in\mathbb{Z}} x^k I_k(2t)$$

we can deduce from (6.10) that

$$u(n,m;t) = \sum_{k=0}^{\infty} \alpha_k(n,m) I_{n-m-k}(2t),$$

where

$$\alpha_k(n,m) = \frac{1}{2\pi i}\oint_C x^{k-n+m}\Psi_n(x)\Psi^*_{m+1}(x)\,dx. \tag{6.11}$$

Using the last formula, we prove that for $k \geq 1$ running over the even or the odd integers, $\alpha_k(n,m)$ is an odd function of $n-m-k$ with coefficients depending on n and m. The statement will then follow from Corollary 6.2.

The idea of the proof is to write x^{k-n+m} in (6.11) as $[x^{k-n+m} - p(x, n-m-k)] + p(x, n-m-k)$ for appropriate $p(x, n-m-k)$ which is a Laurent polynomial of x, and an odd polynomial of $n-m-k$. We want to pick $p(x, n-m-k)$ so that $f(x) = x^{k-n+m} - p(x, n-m-k) \in A_{N_1,N_2}$. Then there exists a difference operator $L_f = \sum_{l=K_-}^{K_+} \mu_l(n) E^l \in \mathcal{A}_{N_1,N_2}$ and therefore

$$f(x)\Psi_n(x) = L_f\Psi_n(x) = \sum_{l=K_-}^{K_+} \mu_l(n)\Psi_{n+l}(x).$$

If the interval $[n+K_-, n+K_+]$ does not contain m we deduce from (6.9) that

$$\frac{1}{2\pi i}\oint_C f(x)\Psi_n(x)\Psi^*_{m+1}(x)\,dx = 0,$$

and therefore formula (6.11) will give

$$\alpha_k(n,m) = \frac{1}{2\pi i}\oint_C p(x, n-m-k)\Psi_n(x)\Psi^*_{m+1}(x)\,dx,$$

completing the proof. The main problem now is to construct a class of Laurent polynomials in A_{N_1,N_2} which allows implementing the above idea. The key ingredient is the following proposition established in [15].

Proposition 6.4. *Let $N \geq \max(N_1, N_2)$, and let $l_0, l_1, \ldots, l_N$ be distinct nonzero integers such that $l_j \equiv l_k \pmod 2$ and $l_j + l_k \neq 0$ for $0 \leq j, k \leq N$. Then*

$$\sum_{k=0}^{N} \frac{x^{l_k}}{l_k \prod_{j\neq k}(l_k^2 - l_j^2)} \in A_{N_1,N_2}. \tag{6.12}$$

To complete the proof, we fix n and m, and we choose $\epsilon = 1$ or $\epsilon = 2$ so that $k \equiv \epsilon \pmod 2$. Let $N = \max(N_1, N_2)$ and define

$$h^s_J(j) = \frac{j}{J+2s}\prod_{\substack{l=0\\ l\neq s}}^{N-1} \frac{j^2 - (J+2l)^2}{(J+2s)^2 - (J+2l)^2}.$$

Clearly, $h_J^s(j)$ is an odd polynomial of j. Now we can rewrite (6.11) as follows:

$$\alpha_k(n,m) = \frac{1}{2\pi i}\oint_C \Big(x^{k-n+m} - \sum_{s=0}^{N-1} h_J^s(k-n+m)x^{J+2s}\Big)\Psi_n(x)\Psi^*_{m+1}(x)\,dx$$
$$+ \sum_{s=0}^{N-1}\frac{h_J^s(k-n+m)}{2\pi i}\oint_C x^{J+2s}\Psi_n(x)\Psi^*_{m+1}(x)\,dx. \tag{6.13}$$

We need to define J depending only on n and m so that

$$\frac{1}{2\pi i}\oint_C \Big(x^{k-n+m} - \sum_{s=0}^{N-1} h_J^s(k-n+m)x^{J+2s}\Big)\Psi_n(x)\Psi^*_{m+1}(x)\,dx = 0 \tag{6.14}$$

for every k, because then the right-hand side of equation (6.13) will clearly be an odd polynomial of $n-m-k$ with coefficients depending on n and m.

Assume first that $n \le m$ and take $J = m-n+\epsilon$. If $1 \le k \le 2N$, then $k-n+m = J+2s$ for some $s \in \{0,1,\dots,N-1\}$ and (6.14) is obvious because the polynomial

$$f(x) = x^{k-n+m} - \sum_{s=0}^{N-1} h_J^s(k-n+m)x^{J+2s}$$

is identically zero. If $k > 2N$, then $f(x) \in A_{N_1,N_2}$ by Proposition 6.4 and therefore $f(x)\Psi_n(x)$ can be written as a linear combination of

$$\{\Psi_{k+m}(x), \Psi_{k+m-1}(x), \dots, \Psi_{m+\epsilon}(x)\}$$

and thus (6.14) follows from (6.9).

If $n > m$ we can use a similar argument by taking $J = n-m+\epsilon$. This completes the proof of the implication (i)⇒(ii). □

6.2. Characterization of L_{N_1,N_2} in terms of the heat kernel

In this subsection we prove that (ii) implies (i) in Theorem 6.3. Assume first that L is a nonconstant second-order difference operator. The strategy of the proof is to show that (5.39) holds using (5.40) and then apply Theorem 5.4 and Remark 5.5.

From (6.4) we see that

$$u(n,n;t) = I_0(2t) + p_1(n,n;t)I_0(2t) + p_2(n,n;t)I_{-1}(2t). \tag{6.15}$$

On the other hand, (1.4) gives

$$u(n,n;t) = I_0(2t) + \sum_{k=1}^{\infty}\alpha_k(n,n)I_{-k}(2t). \tag{6.16}$$

Using equations (6.15)–(6.16), the fact that the coefficients $\alpha_k(n,n)$ in the expansion (6.16) are uniquely determined by $u(n,n;t)$ and Lemma 6.1 we see that for $k \ge 1$ running over the even or the odd integers, $\alpha_k(n,n)$ is an odd polynomial in k with coefficients depending on n. Similarly, using again (6.4) and writing $u(n+1,n;t)$ as

$$u(n+1,n;t) = I_1(2t) + p_2(n+1,n;t)I_0(2t) + p_1(n+1,n;t)I_{-1}(2t),$$

we conclude that for $k \geq 1$ running over the even or the odd integers, $\alpha_{k+1}(n+1,n)$ is an odd polynomial in k with coefficients depending on n.

Let $2N-1$ be the maximal degree of the four polynomials of k: $\alpha_k(n,n)$ when k is odd/even and $\alpha_{k+1}(n+1,n)$ when k is odd/even. We show below that $\mathbb{Y}_k(L) = 0$ for all $k \geq 2N+1$. From (5.40) and (4.3) it follows that it suffices to prove that if $f(x)$ is an odd polynomial of degree at most $2N-1$, then

$$\sum_{l=0}^{\lfloor (k-1)/2 \rfloor} (-1)^l \left(1 - \frac{2l}{k}\varepsilon_k\right)\binom{k}{l} f(k-2l) = 0 \tag{6.17}$$

for every $k \geq 2N+1$, where ε_k is defined by (5.37).

If k is odd, i.e. $k = 2s+1$, equation (6.17) reduces to

$$\sum_{l=0}^{s} (-1)^l \binom{2s+1}{l} f(2s+1-2l) = 0. \tag{6.18}$$

Since f is odd, we see that the left-hand side of (6.18) is equal to

$$\frac{1}{2}\sum_{l=0}^{2s+1} (-1)^l \binom{2s+1}{l} f(2s+1-2l)$$

and therefore (6.18) is equivalent to

$$\sum_{l=0}^{2s+1} (-1)^l \binom{2s+1}{l} f(2s+1-2l) = 0. \tag{6.19}$$

Equation (6.19) will follow immediately if we can show that for every polynomial $F(x)$ of degree less than j, we have

$$\sum_{l=0}^{j} (-1)^l \binom{j}{l} F(l) = 0. \tag{6.20}$$

The proof of the last identity is straightforward:

$$\sum_{l=0}^{j} (-1)^l \binom{j}{l} F(l) = \left[F(\partial_z) \sum_{l=0}^{j} (-1)^l \binom{j}{l} e^{lz} \right]\Bigg|_{z=0} = [F(\partial_z)(1-e^z)^j]|_{z=0} = 0.$$

If k is even, i.e. $k = 2s+2$, then (6.17) is equivalent to

$$\begin{aligned} &\sum_{l=0}^{s} (-1)^l \binom{2s+2}{l} (2s+2-2l) f(2s+2-2l) \\ &\qquad = \frac{1}{2}\sum_{l=0}^{2s+2} (-1)^l \binom{2s+2}{l} (2s+2-2l) f(2s+2-2l) = 0, \end{aligned}$$

which follows again from (6.20).

It remains to prove the statement when L has constant coefficients, i.e. $L = E + b\,\mathrm{Id} + aE^{-1}$, where a and b are constants and $a \neq 0$. In this case, we can write an explicit formula for $u(n, m; t)$ and calculate $\alpha_k(n, m)$. For the fundamental solution we obtain

$$u(n, m; t) = \frac{1}{2\pi i} \oint_C e^{(z+b+a/z)t} z^{n-m-1} dz, \tag{6.21}$$

where C is a simple closed contour around the origin. Let w be such that $z + b + a/z = w + 1/w$ and $w \to 0$ as $z \to 0$. A short computation using (6.21) shows that

$$\alpha_k(0, 0) = \mathrm{res}_{w=0}\left(\frac{(1 - w^2)w^{-1-k}}{\sqrt{\mathfrak{q}(w)}}\right), \tag{6.22}$$

where

$$\mathfrak{q}(w) = 1 - 2bw + (2 + b^2 - 4a)w^2 - 2bw^3 + w^4.$$

In other words, the $\alpha_k(0, 0)$ are the coefficients in the expansion of the function $(1 - w^2)/\sqrt{\mathfrak{q}(w)}$ around $w = 0$. We know from Lemma 6.1 that if (6.4) holds for $m = n = 0$ then $\alpha_k(0, 0)$ must be an odd polynomial in k for k odd or even. Let

$$\alpha_k(0, 0) = \begin{cases} \beta_1(k) & \text{when } k \text{ is odd,} \\ \beta_2(k) & \text{when } k \text{ is even.} \end{cases}$$

Then

$$\begin{aligned}\sum_{k=1}^{\infty} \alpha_k(0, 0)w^k &= \beta_1(w\partial_w) \sum_{j=1}^{\infty} w^{2j-1} + \beta_2(w\partial_w) \sum_{j=1}^{\infty} w^{2j} \\ &= \beta_1(w\partial_w)\frac{w}{1 - w^2} + \beta_2(w\partial_w)\frac{w^2}{1 - w^2} = \frac{\text{polynomial of } w}{(1 - w^2)^K},\end{aligned}$$

showing that $\sum_{k=1}^{\infty} \alpha_k(0, 0)w^k$ must be a rational function of w with denominator having zeros only at $w = \pm 1$. This implies that the only possible choices for $\mathfrak{q}(w)$ in (6.22) are $(1-w)^4$, $(1+w)^4$ and $(1-w^2)^2$. But the first two are clearly impossible (because $\alpha_k(0, 0)$ become nonzero constants when k is even or odd), leading to $\mathfrak{q}(w) = (1 - w^2)^2$, which is equivalent to $b = 0$, $a = 1$. Thus $L = L_0$, completing the proof. □

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