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Decio Levi
Raphaël Rebelo
Pavel Winternitz *Editors*

Symmetries and Integrability of Difference Equations

Lecture Notes of the Abecederian School of SIDE 12, Montreal 2016

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Preface

This volume is based on nine series of lectures presented at the Abecedarian School on Symmetries and Integrability of Difference Equations (ASIDE). The school took place at the Centre de recherches mathématiques, Université de Montréal, June 27–July 1, 2016. It was followed by an international meeting on the same subject, SIDE 12, held in Sainte-Adèle, Québec, Canada, July 33–9, 2016.

The SIDE meetings take place every two years since 1994 and it has become a tradition that a school precedes these meetings. The school is aimed at graduate students, postdoctoral fellows and other early career researchers (ECRs) to prepare them for full participation in the actual meeting.

Lecturers at summer schools are usually famous or at least distinguished senior scientists; the participants are usually ECRs. The ASIDE schools break with this tradition. The lecturers and the students at the school were ECRs. The idea, originally proposed by ECRs at the SIDE 8 meeting in 2008, was that this would encourage a more informal atmosphere, make it easier to ask questions and have in-depth discussions. A previous ASIDE school together with the SIDE 10 meeting took place near Shanghai in 2012. This is the first time that ASIDE lectures are published. They were carefully refereed by experts in the field.

The topics treated in each of the nine lecture series coincide with those treated in the nine sessions of SIDE 12. The ASIDE lecturers were proposed by the session organizers and were usually current or former graduate students or postdoctoral fellows of the session organizers. Thus they all had in-depth and up-to-date knowledge of the field they were lecturing on. The fact that their knowledge was recently acquired meant that the lecturers were well aware of the difficulties they had encountered. This was a great advantage from the pedagogical point of view.

The consensus was that the ASIDE experiment was a successful one. Most of the participants stayed for the SIDE 12 meeting and contributed to and benefitted from both events.

There were 95 participants at SIDE 12, 56 at ASIDE with a large overlap between the two. Both SIDE 12 and ASIDE were made possible by generous support from the NSF, the CRM and the UMI/CRNS.

Each of these lectures is an introduction to the corresponding SIDE session and we are sure that they are of permanent value. The volume should be useful both to beginners entering into the field and to seasoned practitioners.

Roma, Italy — Decio Levi
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February 2017

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Continuous, Discrete and Ultradiscrete Painlevé Equations

Nobutaka Nakazono, Yang Shi, and Masataka Kanki

Abstract We give an introductory lecture on the theory of Painlevé equations, which are one of the most important objects in the theory of integrable systems, and their discrete counterparts. The lecture is divided into three parts: the Painlevé equations, discrete Painlevé equations and ultradiscrete Painlevé equations.

1 Introduction

Before going into the details, let us briefly introduce Prof. Paul Painlevé. He was the first mathematician to board an airplane and also Wilbur Wright's first airplane passenger. He later turned to politics and became the French Prime Minister twice in 1917 and in 1925. In this lecture, we study the theory of Painlevé equations, which are six ordinary differential equations listed in Sect. 2.1 and found by P. Painlevé and his student B. Gambier. Moreover, we also study their discrete counterparts.

This lecture note is divided into three topics: (Sect. 2) the Painlevé equations, (Sect. 3) the discrete Painlevé equations, which are discrete analogues of the Painlevé equations, and (Sect. 4) the ultradiscrete Painlevé equations, which are ultradiscrete limits of the discrete Painlevé equations. In the following, we will present a brief explanation of the content of each section.

In Sect. 2, we focus on the Painlevé equations. The Painlevé equations have special solutions expressed in terms of the special functions for particular values of the parameters. As famous examples of special solutions, rational solution

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and hypergeometric solution are presented. The Painlevé equations have Bäcklund transformations, which generate an infinite number of special solutions starting from one special solution. It is also known that the Bäcklund transformations form an affine Weyl group. In this part, we study the special solutions and the affine Weyl group symmetries of the Painlevé equations using the P_{IV} equation as an example.

In Sect. 3, as an example we derive a discrete Painlevé equation from the Bäcklund transformation s of the P_{IV} equation of Sect. 2. In fact many of the first examples of discrete Painlevé equations were found this way [1, 13], until the classification of Sakai in 2001 [46]. We give a brief overview of this classification, noting that it comprises of three lists of—additive, multiplicative and elliptic—difference equations. One important aspect of the discrete Painlevé equations highlighted here is their formulations as birational realizations of the affine Weyl groups. We give two discrete Painlevé equations associated with the extended affine Weyl group of type A_2 $\widetilde{W}(A_2^{(1)})$, an additive difference equation: d-P_{II}, and a multiplicative difference equation: q-P_{IV}. Many interesting properties of the discrete Painlevé equations are reminiscent of those of the Painlevé equations. As an example, we derive the hypergeometric type special solutions for the q-P_{IV}equation. The section concludes with an overview on the hypergeometric type special solutions for the elliptic and multiplicative difference Painlevé equations of Sakai's list.

In Sect. 4, we focus on the so-called ultradiscrete limits of the discrete Painlevé equations, and the relations between theses ultradiscrete equations. In 1996, Tokihiro and his collaborators invented the limiting procedure called ultradiscretization [52], by which various "integrable" cellular automata have been obtained. These cellular automata are called the ultradiscrete equations and are defined over the max-plus semifield. In this part, after introducing the technique of ultradiscretization through examples, we present several ultradiscrete analogues of the discrete Painlevé equations: i.e., second nonlinear difference equations over the max-plus semifield. For example one of the ultradiscrete Painlevé II equations has the form

$$X_{n+1} + X_{n-1} - X_n = a + \max[0, n - X_n] - \max[0, n + X_n] \,,$$

where n is the independent variable and a is a parameter. Many of the properties in previous parts including the degeneration diagrams remain true even in this simplified setting. Ultradiscrete analogues of special solutions described by piecewise linear functions are also presented.

2 Painlevé Equations

The first part by N. Nakazono focuses on the Painlevé equations, which are integrable nonlinear ordinary differential equations of the second order. It is well known that the Painlevé equations have many interesting properties: special solutions, affine Weyl group symmetries, Hamiltonian structures, isomonodromy problems (Lax pairs), and so on. Here we study the special solutions and affine

Weyl group symmetries using the Painlevé IV equation as an example. This section is written based on [23, 32].

2.1 Introduction

A singularity that depends upon the initial conditions of the equation is referred to as a *movable singularity*. For example, the differential equation

$$\frac{\mathrm{d}w(t)}{\mathrm{d}t} = -w(t)^2 , \quad w(t) \neq 0 \tag{1}$$

can be exactly solved, and its solution is given by

$$w(t) = \frac{1}{t-c} , \tag{2}$$

where c is an integral constant. The solution has a singularity at a point $t = c$. Since c is determined by the initial condition at $t = t_0$, that is,

$$c = t_0 - \frac{1}{w(t_0)} , \tag{3}$$

this singularity is a movable singularity. A differential equation is said to have the *Painlevé property* if its solutions do not have movable singularities other than poles. For example, the Eq. (1) has the Painlevé property. With the Painlevé property, Painlevé et al. classified all the rational ordinary differential equations of second order of the form

$$y'' = R(t, y, y') , \tag{4}$$

where

$$y = y(t) , \quad y' = \frac{\mathrm{d}y}{\mathrm{d}\,t} , \quad y'' = \frac{\mathrm{d}^2 y}{\mathrm{d}\,t^2} . \tag{5}$$

As a result, they showed that except for the differential equations which can be integrated algebraically or transformed into linear equations or into the differential equations solvable by elliptic functions, any differential equation of the form (4) with the Painlevé property is reduced to one of the following equations (the *Painlevé equations*) [2, 3, 42]:

$\mathrm{P_I}$: $y'' = 6y^2 + t$

$\mathrm{P_{II}}$: $y'' = 2y^3 + ty + \alpha$

$$\mathrm{P_{III}} : y'' = \frac{(y')^2}{y} - \frac{y'}{t} + \frac{\alpha y^2 + \beta}{t} + \gamma y^3 + \frac{\delta}{y}$$

$$\mathrm{P_{IV}} : y'' = \frac{(y')^2}{2y} + \frac{3y^3}{2} + 4ty^2 + 2(t^2 - \alpha)y + \frac{\beta}{y}$$

$$\mathrm{P_V} : y'' = \left(\frac{1}{2y} + \frac{1}{y-1}\right)(y')^2 - \frac{y'}{t} + \frac{(y-1)^2}{t^2}\left(\alpha y + \frac{\beta}{y}\right) + \frac{\gamma y}{t} + \frac{\delta y(y+1)}{y-1}$$

$$\mathrm{P_{VI}} : y'' = \frac{1}{2}\left(\frac{1}{y} + \frac{1}{y-1} + \frac{1}{y-t}\right)(y')^2 - \left(\frac{1}{t} + \frac{1}{t-1} + \frac{1}{y-t}\right)y' + \frac{y(y-1)(y-t)}{t^2(t-1)^2}\left(\alpha + \frac{\beta t}{y^2} + \frac{\gamma(t-1)}{(y-1)^2} + \frac{\delta t(t-1)}{(y-t)^2}\right)$$

Here, α, β, γ and δ are complex parameters. Starting from $\mathrm{P_{VI}}$ we can, through appropriate limiting processes, obtain the other Painlevé equations as the following diagram of degenerations:

$$\begin{array}{ccccc} \mathrm{P_{VI}} & \longrightarrow & \mathrm{P_V} & \longrightarrow & \mathrm{P_{III}} \\ (4) & & (3) & & (2) \\ & & \downarrow & & \downarrow \\ & & \mathrm{P_{IV}} & \longrightarrow & \mathrm{P_{II}} \quad \longrightarrow \quad \mathrm{P_I} \\ & & (2) & & (1) \qquad\quad (0) \end{array}$$

We note that the numbers inside the parentheses indicate the number of essential parameters of the equations.

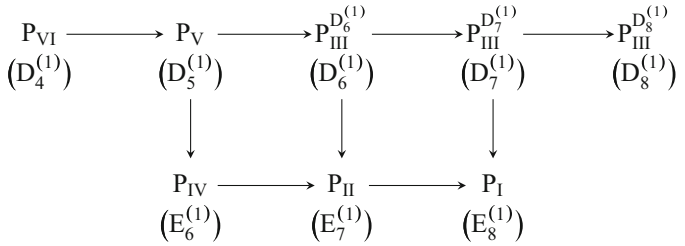
In [33, 35–38], Okamoto introduced the notion of *space of initial conditions* for the Painlevé equations. The space of initial conditions is a rational surface constructed by resolving the singularities of the equation by blowing-up at each singular point. The space of initial conditions is characterized by the root systems, and its type is called by the type of the corresponding root system. In view of the space of initial conditions, $\mathrm{P_{III}}$ can be divided into three types: $\mathrm{D}_6^{(1)}$-, $\mathrm{D}_7^{(1)}$- and $\mathrm{D}_8^{(1)}$-type by the values of parameters as follows:

$$\mathrm{P_{III}}^{\mathrm{D}_6^{(1)}} : \quad \gamma\delta \neq 0$$

$$\mathrm{P_{III}}^{\mathrm{D}_7^{(1)}} : \quad \gamma = 0\,,\ \alpha\delta \neq 0 \quad (\text{or } \delta = 0, \beta\gamma \neq 0)$$

$$\mathrm{P_{III}}^{\mathrm{D}_8^{(1)}} : \quad \alpha\beta \neq 0\,,\ \gamma = 0\,,\ \delta = 0\,.$$

Therefore, it is quite natural to classify the Painlevé equations into eight types and to consider the following diagram of degenerations:



We note that the symbols inside the parentheses indicate the types of the space of initial conditions.

Exercise 2.1 Find movable singularities of the following differential equation:

$$\frac{\mathrm{d}w(t)}{\mathrm{d}t} = -\frac{w(t)^2}{t} \,. \tag{6}$$

2.2 Special Solutions

Painlevé et al. had a motivation to find a new class of special functions defined by nonlinear differential equations. In this sense, the solutions of the Painlevé equations are called the *Painlevé transcendents*. With the exception of special cases it is known that the solutions of the Painlevé equations are really transcendental. On the other hand, we are also interested in the special cases. We call such solutions *special solutions*. Famous examples of special solutions, *rational solution* and *hypergeometric solution* are well known. Note that the rational solution is a solution expressed in terms of a rational function of the independent variable t,while the hypergeometric solution is a solution expressed in terms of the hypergeometric function.

In this section, we consider the rational and hypergeometric solutions of $\mathrm{P_{IV}}$:

$$y'' = \frac{(y')^2}{2y} + \frac{3y^3}{2} + 4ty^2 + 2(t^2 - \alpha)y + \frac{\beta}{y} \,. \tag{7}$$

2.2.1 Rational Solutions

We construct the rational solutions of $\mathrm{P_{IV}}$ of the form

$$y = \frac{c_1 t + c_2}{c_3 t + c_4} \,, \tag{8}$$

where c_i, $i = 1, 2, 3, 4$, are constants such that $c_1 c_4 \neq c_2 c_3$.

Substituting (8) in P_{IV}, we obtain the following equation:

$$A_0 - 4A_1 t - 2A_2 t^2 - 4A_3 t^3 + A_4 t^4 - 8c_1c_3(c_1^2 + c_1c_4 + c_2c_3)t^5 - 4c_1^2c_3^2t^6 = 0, \quad (9)$$

where

$$A_0 = -c_1^2c_4^2 - 2c_1c_2c_3c_4 - 3c_2^4 + 3c_2^2c_3^2 + 4\alpha c_2^2c_4^2 - 2\beta c_4^4 , \quad (10)$$

$$A_1 = c_1^2c_3c_4 + 3c_1c_2^3 - c_1c_2c_3^2 - 2\alpha c_1c_2c_4^2 + 2c_2^3c_4 - 2\alpha c_2^2c_3c_4 + 2\beta c_3c_4^3 , \quad (11)$$

$$A_2 = 9c_1^2c_2^2 - 2\alpha c_1^2c_4^2 + 12c_1c_2^2c_4 - 8\alpha c_1c_2c_3c_4 + 4c_2^3c_3 - 2\alpha c_2^2c_3^2 + 2c_2^2c_4^2 + 6\beta c_3^2c_4^2 , \quad (12)$$

$$A_3 = 3c_1^3c_2 + 6c_1^2c_2c_4 - 2\alpha c_1^2c_3c_4 + 6c_1c_2^2c_3 - 2\alpha c_1c_2c_3^2 + 2c_1c_2c_4^2 + 2c_2^2c_3c_4 + 2\beta c_3^3c_4 , \quad (13)$$

$$A_4 = -3c_1^4 - 8c_1^3c_4 - 24c_1^2c_2c_3 + 4\alpha c_1^2c_3^2 - 4c_1^2c_4^2 - 16c_1c_2c_3c_4 - 4c_2^2c_3^2 - 2\beta c_3^4 . \quad (14)$$

From the coefficient of t^6, we obtain

$$c_1 = 0 \quad \text{or} \quad c_3 = 0 . \quad (15)$$

Let us here choose the case

$$c_3 = 0 . \quad (16)$$

Then, (9) becomes

$$3c_2^4 - 4\alpha c_2^2c_4^2 + 2\beta c_4^4 + c_1^2c_4^2 + 4c_2(3c_1c_2^2 - 2\alpha c_1c_4^2 + 2c_2^2c_4)t + 2(9c_1^2c_2^2 - 2\alpha c_1^2c_4^2 + 12c_1c_2^2c_4 + 2c_2^2c_4^2)t^2 + 4c_1c_2(3c_1^2 + 6c_1c_4 + 2c_4^2)t^3 + c_1^2(c_1 + 2c_4)(3c_1 + 2c_4)t^4 = 0 . \quad (17)$$

From the coefficient of t^4, we obtain

$$c_1 + 2c_4 = 0 \quad \text{or} \quad 3c_1 + 2c_4 = 0 . \quad (18)$$

Let us consider the case of

$$3c_1 + 2c_4 = 0 . \quad (19)$$

This gives the following conditions:

$$c_2 = 0\,, \quad \alpha = 0\,, \quad \beta = -\tfrac{2}{9}\,. \tag{20}$$

Therefore, we finally obtain the rational solution

$$y = -\frac{2t}{3}\,, \tag{21}$$

when parameters take the following special values:

$$\alpha = 0, \quad \beta = -\frac{2}{9}. \tag{22}$$

Exercise 2.2 Find the other rational solutions in the form of (8).

2.2.2 Hypergeometric Solutions

In this section, we construct a hypergeometric solution which can be obtained through the Riccati equation. Let

$$\beta = -2(\alpha+1)^2\,. \tag{23}$$

Then, $\mathrm{P_{IV}}$ can be reduced to the following first-order differential equation:

$$y' = y(2t+y) - 2(\alpha+1)\,. \tag{24}$$

This equation is known as the Riccati equation. It is well known that the Riccati equation can be solved by a hypergeometric function. In fact, letting

$$y = -\frac{G'}{G}\,, \tag{25}$$

the Riccati equation (24) can be reduced to the following linear differential equation:

$$G'' = 2tG' + 2(\alpha+1)G\,. \tag{26}$$

This equation is known as Hermite's differential equation whose solution is called the Weber function.

Remark 2.3 For

$$\alpha = -n-1\,, \tag{27}$$

where $n \in \mathbb{Z}_{\geq 0}$, (26) can be solved by using the Hermite polynomial:

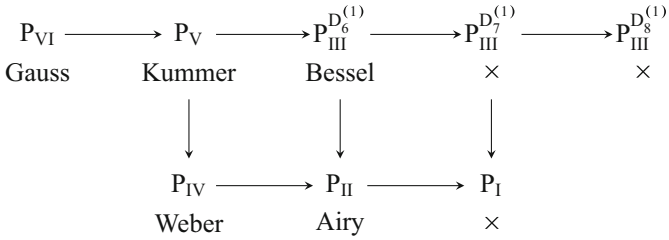
$$G = H_n(t)\,, \tag{28}$$

where

$$H_n(t) = (-1)^n \mathrm{e}^{t^2/2} \frac{\mathrm{d}^n}{\mathrm{d}t^n} (\mathrm{e}^{-t^2/2}) \ . \tag{29}$$

This gives the rational solutions of $\mathrm{P_{IV}}$. In this sense, the hypergeometric solutions contain some rational solutions.

Remark 2.4 It is well known that the coalescence cascades of hypergeometric functions, from the Gauss's hypergeometric function to the Airy function, correspond to the diagram of degenerations of the Painlevé equations, from $\mathrm{P_{VI}}$ to $\mathrm{P_{II}}$, in the sense of the hypergeometric solutions [12]:



Note that $\mathrm{P_{III}^{D_7^{(1)}}}$, $\mathrm{P_{III}^{D_8^{(1)}}}$ and $\mathrm{P_I}$ do not have hypergeometric solutions. In this sense, solutions of the Painlevé equations can be regarded as nonlinear analogues of the hypergeometric functions.

Exercise 2.5 Confirm that the Riccati equation (24) satisfies $\mathrm{P_{IV}}$ (7) under the condition (23).

2.3 Bäcklund Transformations

In this section, we consider the Bäcklund transformations which leave the form of the Painlevé equation invariant but change the parameters. Here we present two of the important properties of the Bäcklund transformations: (1) generating an infinite number of solutions starting from one solution, and (2) forming an affine Weyl group, using $\mathrm{P_{IV}}$ as an example.

2.3.1 A Bäcklund Transformation

For later convenience, we use parameters α_1 and α_2 defined by

$$\alpha = 1 - \alpha_1 - 2\alpha_2 \ , \quad \beta = -2\alpha_1^2 \ . \tag{30}$$

Then, $\mathrm{P_{IV}}$ is rewritten as follows:

$$y'' = \frac{(y')^2}{2y} + \frac{3y^3}{2} + 4ty^2 + 2(t^2 - 1 + \alpha_1 + 2\alpha_2)y - \frac{2\alpha_1^2}{y} . \tag{31}$$

Let us define the variable $\bar{y}$ by

$$\bar{y} = -2t - y + \frac{(2t+y)y - y' - 2\alpha_1}{2y} + \frac{4y(1-\alpha_1-\alpha_2)}{(2t+y)y - y' - 2\alpha_1} . \tag{32}$$

Then, $\bar{y}$ also satisfies $\mathrm{P_{IV}}$:

$$\bar{y}'' = \frac{(\bar{y}')^2}{2\bar{y}} + \frac{3\bar{y}^3}{2} + 4t\bar{y}^2 + 2(t^2 - 2 + \alpha_1 + 2\alpha_2)\bar{y} - \frac{2(\alpha_1 - 1)^2}{\bar{y}} . \tag{33}$$

Therefore, the transformation T_1 defined by

$$T_1 \colon (y, \alpha_1, \alpha_2) \mapsto (\bar{y}, \alpha_1 - 1, \alpha_2) , \tag{34}$$

is a Bäcklund transformation of $\mathrm{P_{IV}}$.

Remark 2.6 We can redefine a Bäcklund transformation to be an operator on the variables which commute with the operation of differentiation.

Remark 2.7 Compositions of Bäcklund transformations are also Bäcklund transformations.

Exercise 2.8 Confirm that $\bar{y}$ satisfies (33) if y is a solution of (31).

Exercise 2.9 Confirm that T_1 commutes with $\mathrm{d}/\mathrm{d}t$.

2.3.2 Higher Solutions

In this section, we construct other special solutions of $\mathrm{P_{IV}}$ by using the special solutions given in Sect. 2.2 and the Bäcklund transformation T_1 given in Sect. 2.3.1.

Substituting the rational solution (21) with the conditions for the parameter (22) or, equivalently,

$$3\alpha_1 = 3\alpha_2 = 1 , \tag{35}$$

into (32), we obtain the following rational solution of (33):

$$\bar{y} = \frac{1}{t} - \frac{2t}{3} . \tag{36}$$

In other words, by applying the Bäcklund transformation T_1 to the known rational solution (21), we obtain the following new rational solution of (31):

$$y = \frac{1}{t} - \frac{2t}{3} , \tag{37}$$

when

$$3\alpha_1 = -2 , \quad 3\alpha_2 = 1 . \tag{38}$$

In a similar manner, from the hypergeometric solution (25) with the condition of the parameter (23), or equivalently,

$$\alpha_1 + \alpha_2 = 1 , \tag{39}$$

we obtain the following new hypergeometric solution:

$$y = \frac{\alpha_1 G}{G'} + \frac{G'}{G} - \frac{G''}{2G'} - t , \tag{40}$$

when

$$\alpha_1 + \alpha_2 = 0 . \tag{41}$$

Repeating this procedures, we can obtain an infinite number of rational solutions (see [18]) when

$$3\alpha_1 = 1 - 3n , \quad 3\alpha_2 = 1 , \tag{42}$$

where $n \in \mathbb{Z}_{\geq 0}$, and an infinite number of hypergeometric solutions (see [27]) when

$$\alpha_1 + \alpha_2 = 1 - n , \tag{43}$$

where $n \in \mathbb{Z}_{\geq 0}$.

Remark 2.10 The special solutions which can be directly obtained from equations such as (21) and (25) are called seed solutions, while the solutions which can be obtained from these seed solutions using Bäcklund transformation such as (37) and (40) are called the higher solutions.

Remark 2.11 In general, higher solutions can be expressed by the ratio of determinants whose entries are the seed solutions (for further details see Remark 6.1 of [23] and references therein). The structure of the determinant is one of the most important properties of the Painlevé equations, since it shows the connections between the Painlevé equations and various areas, such as the theory of orthogonal polynomials, that of two-dimensional quantum gravity, that of random matrices, and so on.

Exercise 2.12 Confirm that (37) with (38) and (40) with (41) are solutions of (31).

2.3.3 Affine Weyl Group Symmetry

In this section, we show that the Bäcklund transformations of a Painlevé equation form an affine Weyl group.

Let us consider the following system of the differential equations:

$$f_0' = f_0(f_1 - f_2) + \alpha_0 \,, \quad f_1' = f_1(f_2 - f_0) + \alpha_1 \,, \quad f_2' = f_2(f_0 - f_1) + \alpha_2 \,, \tag{44}$$

where

$$f_i = f_i(s) \ (i = 0, 1, 2) \,, \quad ' = \frac{\mathrm{d}}{\mathrm{d}s} \,. \tag{45}$$

Here, f_i and α_i satisfy

$$\alpha_0 + \alpha_1 + \alpha_2 = 1 \,, \quad f_0 + f_1 + f_2 = s \,. \tag{46}$$

This system is equivalent to (31) and is called the symmetric form of $\mathrm{P_{IV}}$. Indeed, we can obtain (31) from the system (44) as follows. From the system (44) and the relation (46), we obtain

$$f_1' = f_1(f_1 + 2f_2 - s) + \alpha_1 \,, \tag{47}$$

$$f_1'' = f_1'(f_1 + 2f_2 - s) + f_1(f_1' + 2f_2' - 1) \,, \tag{48}$$

$$f_2' = -f_2(2f_1 + f_2 - s) + \alpha_2 \,. \tag{49}$$

Eliminating f_2 and f_2' from these three equations and applying the change of variables

$$f_1(s) = -\frac{y(t)}{\sqrt{2}} \,, \quad s = \sqrt{2}t \,, \tag{50}$$

we obtain the Eq. (31).

We introduce the transformations $\{s_0, s_1, s_2, \pi\}$ by the following actions:

$$s_i(\alpha_j) = \alpha_j - \alpha_i a_{ij} \,, \quad s_i(f_j) = f_j + \frac{\alpha_i}{f_i} u_{ij} \,, \quad \pi(\alpha_i) = \alpha_{i+1} \,, \quad \pi(f_i) = f_{i+1} \,, \tag{51}$$

where $i, j \in \mathbb{Z}/3\mathbb{Z}$. Here, $A = (a_{ij})_{i,j=0}^{2}$ is given as the following symmetric 3×3 matrix:

$$A = \begin{pmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{pmatrix} \,, \tag{52}$$

which is the Cartan matrix of type $\mathrm{A}_2^{(1)}$. The matrix $U = (u_{ij})_{i,j=0}^2$ is given by the following the skew-symmetric matrix:

$$U = \begin{pmatrix} 0 & 1 & -1 \\ -1 & 0 & 1 \\ 1 & -1 & 0 \end{pmatrix} . \tag{53}$$

These transformations are Bäcklund transformations of $\mathrm{P_{IV}}$. The transformations $\{s_0, s_1, s_2, \pi\}$ satisfy the following relations

$$s_i^2 = (s_i s_{i+1})^3 = 1 , \tag{54a}$$

$$\pi^3 = 1 , \quad \pi s_i = s_{i+1}\pi , \tag{54b}$$

where $i \in \mathbb{Z}/3\mathbb{Z}$. The relations (54a) are the fundamental relations of the affine Weyl group of type $\mathrm{A}_2^{(1)}$. Therefore, these transformations generate the extended affine Weyl group of type $\mathrm{A}_2^{(1)}$: $\widetilde{\mathrm{W}}\big(\mathrm{A}_2^{(1)}\big) = \langle s_0, s_1, s_2, \pi \rangle$. Thus $\mathrm{P_{IV}}$ is said to have the affine Weyl group symmetry of type $\mathrm{A}_2^{(1)}$.

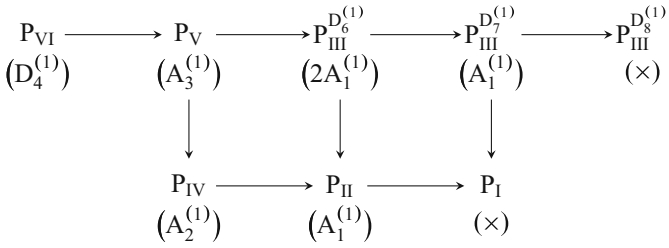
Remark 2.13 The transformation T_1 defined by (34) is an element of $\widetilde{\mathrm{W}}\big(\mathrm{A}_2^{(1)}\big)$. Indeed, it is given by the composition of the generators of $\widetilde{\mathrm{W}}\big(\mathrm{A}_2^{(1)}\big)$ as follows:

$$T_1 = \pi s_2 s_1 . \tag{55}$$

Moreover, we can easily construct the inverse mapping of T_1 by the following:

$$T_1{}^{-1} = s_1 s_2 \pi^2 . \tag{56}$$

Other Painlevé equations except for $\mathrm{P_I}$ and $\mathrm{P}_{\mathrm{III}}^{\mathrm{D}_8^{(1)}}$ also have the affine Weyl group symmetries [33, 35–38]:



Inside the parentheses, we have presented the types of the extended affine Weyl groups.

Exercise 2.14 Confirm that the transformations $\{s_0, s_1, s_2, \pi\}$ are Bäcklund transformations of $\mathrm{P_{IV}}$.

Exercise 2.15 Confirm that the fundamental relations (54) hold under the actions (51).

3 Discrete Painlevé Equations

This section by Y. Shi looks at the discrete analogue of the Painlevé equations. Many remarkable properties of the continuous Painlevé equations remain true in the discrete setting. With an emphasis on the affine Weyl symmetries of the equations, we explore some of these properties such as Bäcklund transformations and special solutions. Material covered in this section is based on those of [23, 32], where extensions and generalizations of this material can be found for the interested reader.

3.1 A Brief Introduction with an Example

Discrete Painlevé equations were initially recognized as difference equations arising from Bäcklund transformations Bäcklund transformations of the continuous Painlevé equations [1, 13]. Many familiar features of the continuous Painlevé equations also exist for the discrete Painlevé equations. For example, just as the Painlevé equations can be seen as nonautonomous generalizations of the elliptic equations, discrete Painlevé equations have been derived [7] by de-autonomizing the QRT maps (integrable second order maps known as the discrete analogues of elliptic functions [43]). More examples of discrete Painlevé equations have been derived as reductions of discrete analogues of integrable PDEs [8, 16, 30, 31]; and by a discrete analogue of the isomonodromy approach [14]. In 2001, Sakai gave the classification for the discrete Painlevé equations [46] via a geometric approach inspired by Okamoto's work on the space of initial conditions for the Painlevé equations [34].

Before going into the details of discrete Painlevé equations, we continue on with the discussion of the Bäcklund transformations of the fourth Painlevé equation (P_{IV}) from the last section and explain how a purely discrete Painlevé equation can be derived through the symmetry of the Bäcklund transformations of a continuous Painlevé equation.

3.2 A Discrete Painlevé Equation Arising from the Bäcklund Transformations of the P_{IV} Equation

In Sect. 2.3.1 we have seen that if y is a solution of the P_{IV} equation

$$y'' = \frac{(y')^2}{2y} + \frac{3y^3}{2} + 4ty^2 + 2(t^2 - 1 + \alpha_1 + 2\alpha_2)y - \frac{2\alpha_1^2}{y} \tag{57}$$

here $' = \mathrm{d}/\mathrm{d}t$. Then the function $\bar{y}$, related to y by the Bäcklund transformation,

$$\bar{y} = -2t - y + \frac{(2t+y)y - y' - 2\alpha_1}{2y} + \frac{4y(1-\alpha_1-\alpha_2)}{(2t+y)y - y' - 2\alpha_1} \tag{58}$$

is also a solution of (57) with the corresponding parameters $\bar{\alpha}_1 = \alpha_1 - 1$ and $\bar{\alpha}_2 = \alpha_2$. This transformation is denoted by

$$T_1 \colon (y, \alpha_1, \alpha_2) \mapsto (\bar{y}, \alpha_1 - 1, \alpha_2) \ . \tag{59}$$

Moreover in Sect. 2.3.3, after a change of variables the $\mathrm{P_{IV}}$ equation was recast into a more symmetric form

$$f_0' = f_0(f_1 - f_2) + \alpha_0 \ , \quad f_1' = f_1(f_2 - f_0) + \alpha_1 \ , \quad f_2' = f_2(f_0 - f_1) + \alpha_2 \ , \tag{60}$$

here $' = \mathrm{d}/\mathrm{d}s$ and

$$\alpha_0 + \alpha_1 + \alpha_2 = 1 \ , \quad f_0 + f_1 + f_2 = s \ . \tag{61}$$

Exercise 3.1 Verify that the simplest special (seed) rational solution of the $\mathrm{P_{IV}}$ equation given by (21) and (22) in terms of the symmetric variables and parameters is given by

$$(\alpha_0, \alpha_1, \alpha_2; f_0, f_1, f_2) = \left(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}; \frac{s}{3}, \frac{s}{3}, \frac{s}{3}\right) . \tag{62}$$

In this symmetric parametrization, the $\mathrm{P_{IV}}$ equation can be described as a birational realization of $\widetilde{\mathrm{W}}\big(\mathrm{A}_2^{(1)}\big) = \langle s_0, s_1, s_2, \pi \rangle$, with the generators satisfying the defining relations given in (54a).

Birational transformations associated with the generators s_0, s_1, s_2, π given by (51)–(53) are summarized in Table 1.

The Bäcklund transformation (59), corresponds to a translational element of the group $\widetilde{\mathrm{W}}\big(\mathrm{A}_2^{(1)}\big)$, can now be expressed in terms of a composition of transformations associated to the generators: $T_1 = \pi s_2 s_1$.

Table 1 The $\mathrm{P_{IV}}$ equation as birational realization of $\widetilde{\mathrm{W}}\big(\mathrm{A}_2^{(1)}\big)$

	α_0	α_1	α_2	f_0	f_1	f_2
s_0	$-\alpha_0$	$\alpha_1 + \alpha_0$	$\alpha_2 + \alpha_0$	f_0	$f_1 + \dfrac{\alpha_0}{f_0}$	$f_2 - \dfrac{\alpha_0}{f_0}$
s_1	$\alpha_0 + \alpha_1$	$-\alpha_1$	$\alpha_2 + \alpha_1$	$f_0 - \dfrac{\alpha_1}{f_1}$	f_1	$f_2 + \dfrac{\alpha_1}{f_1}$
s_2	$\alpha_0 + \alpha_2$	$\alpha_1 + \alpha_2$	$-\alpha_2$	$f_0 + \dfrac{\alpha_2}{f_2}$	$f_1 - \dfrac{\alpha_2}{f_2}$	f_2
π	α_1	α_2	α_0	f_1	f_2	f_0

Transformations associated with the elements of $\widetilde{\mathrm{W}}\big(\mathrm{A}_2^{(1)}\big)$ on the $\mathrm{P_{IV}}$ equation (60), that is their effects on the symmetric variables f_0, f_1, f_2 and parameters $\alpha_0, \alpha_1, \alpha_2$ can be nicely visualized using the geometric realization of the Weyl groups in Euclidean space. We now give a brief introduction on the Weyl group and this geometric interpretation using the $\widetilde{\mathrm{W}}\big(\mathrm{A}_2^{(1)}\big)$ case as an example. We follow closely the terminology and notation of Humphreys [11].

3.2.1 Weyl Group

Let $A_2^{(1)} = (A_{ij})_{0\le i,j\le 2}$ be an extended Cartan matrix of type A_2,

$$(A_{ij})_{0\le i,j\le 2} = \begin{pmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{pmatrix}. \tag{63}$$

Let $V^{(1)}$ be a 3-dimensional real vector space spanned by

$$\Delta^{(1)} = \{\alpha_0, \alpha_1, \alpha_2\} \quad \text{and let } \delta = \alpha_0 + \alpha_1 + \alpha_2 \ , \tag{64}$$

then we see that $\{\alpha_1, \alpha_2, \delta\}$ is also a basis of $V^{(1)}$. Let $V^{(1)*}$ be a 3-dimensional real vector space spanned by $\{h_1, h_2, h_\delta\}$ and define a bilinear pairing $\langle\ ,\ \rangle\colon V^{(1)} \times V^{(1)*} \to \mathbb{R}$ by

$$\langle \alpha_i, h_j\rangle = \delta_{ij} \ , \quad \langle \alpha_i, h_\delta\rangle = \langle \delta, h_j\rangle = 0 \text{ for } 1 \le i,j \le 2 \ , \quad \text{and} \quad \langle \delta, h_\delta\rangle = 1 \ . \tag{65}$$

Vectors α_1, α_2 are called the simple roots, $\Delta^{(1)}$ the set of simple affine roots, δ the null root and h_1, h_2 the fundamental weights, and finally $P = \mathbb{Z}\{h_1, h_2\}$ is the weight lattice. Define the set of simple coroots ${\Delta^{(1)}}^\vee = \{\alpha_0^\vee, \alpha_1^\vee, \alpha_2^\vee\}$ in $V^{(1)*}$ by

$$\alpha_i^\vee = \sum_{j=1}^{2} A_{ij} h_j \quad \text{and} \quad \alpha_0^\vee = -h_1 - h_2 \ , \tag{66}$$

we see that $\alpha_0^\vee + \alpha_1^\vee + \alpha_2^\vee = 0$ and it can be easily checked that

$$\langle \alpha_i, \alpha_j^\vee\rangle = A_{ij} \tag{67}$$

for all $i, j \in \{0, 1, 2\}$. For each $i \in \{0, 1, 2\}$ define a linear transformation s_i on $V^{(1)}$ by

$$s_i\alpha_j = \alpha_j - \langle \alpha_j, \alpha_i^\vee\rangle \alpha_i = \alpha_j - A_{ji}\alpha_i \ , \tag{68}$$

and on $V^{(1)*}$ we have

$$s_i.\alpha_j^\vee = \alpha_j^\vee - A_{ij}\alpha_i^\vee \ . \tag{69}$$

The affine Weyl group of type A_2 is the group $W\big(A_2^{(1)}\big) = \langle s_0, s_1, s_2\rangle$, with the generators satisfying

$$s_j^2 = 1\ , \quad (s_j s_{j+1})^3 = 1 \quad (j \in \mathbb{Z}/3\mathbb{Z})\ . \tag{70}$$

The affine root system is given by $\Phi^{(1)} = W(A_2^{(1)}).\Delta^{(1)} = \{\alpha + k\delta \mid \alpha \in \Phi, k \in \mathbb{Z}\}$, where $\Phi = W(A_2).\{\alpha_1, \alpha_2\}$ is the finite root system and $W(A_2) = \langle s_1, s_2\rangle$ the finite Weyl group of A_2 type. The affine Weyl group can be further extended by a Dynkin diagram automorphism π to the *extended* affine Weyl group $\widetilde{W}(A_2^{(1)}) = \langle s_0, s_1, s_2, \pi\rangle$, with the additional relation to (70):

$$\pi^3 = 1\ , \quad \pi s_j = s_{j+1}\pi\ . \tag{71}$$

The group $\widetilde{W}(A_2^{(1)})$ decomposes into the semidirect product of translations on the weight lattice P and the finite Weyl group acting on the weight lattice:

$$\widetilde{W}(A_2^{(1)}) = \langle t_{h_1}, t_{h_2}\rangle \rtimes W(A) = T_P \rtimes W(A_2)\ , \tag{72}$$

where $t_{h_i} \in \widetilde{W}(A_2^{(1)})$ $(i = 1, 2)$ are the translational elements associated to the two fundamental weights.

Let $\mu \in V$, so that $\langle \delta, \mu^\vee\rangle = 0$ and $\langle \mu, \mu^\vee\rangle \neq 0$. The translational element associated to μ in $\widetilde{W}(A_2^{(1)})$ is given in terms of a composition of reflections

$$t_\mu = s_{\delta-\mu} s_\mu\ , \tag{73}$$

and

$$w t_\mu w^{-1} = t_{w.\mu}\ , \quad w \in \widetilde{W}(A_2^{(1)})\ . \tag{74}$$

The action of t_μ on the simple affine roots α_i for $i \in \{0, 1, 2\}$ is given by

$$t_\mu.\alpha_i = \alpha_i - \langle \alpha_i, \mu^\vee\rangle\delta = \alpha_i - \mu_i\delta\ , \tag{75}$$

where we have let $\langle \alpha_i, \mu^\vee\rangle = \mu_i$, that is t_μ shifts α_i by $-\mu_i$ multiples of δ.

The translational motions by the affine Weyl group can be understood by considering the transformations on a hyperplane in $V^{(1)*}$. Define a hyperplane H in $V^{(1)*}$ by,

$$H = \{\, h \in V^{(1)*} \mid \langle \delta, h\rangle = 1\}\ . \tag{76}$$

Then generators $s_{\alpha-k\delta}$ associated with the affine roots $\alpha - k\delta \in \Phi^{(1)}$ act on $h \in H$ by the formula

$$s_{\alpha-k\delta}.h = h - (\langle \alpha, h\rangle - k)\alpha^\vee\ , \tag{77}$$

where $\alpha^\vee \in \Phi^\vee$, $k \in \mathbb{N}$. The generator $s_{\alpha-k\delta}$ act by reflection about the plane $H_{\alpha-k\delta}$ given by

$$H_{\alpha-k\delta} = \{\, h \in H \mid \langle \alpha, h \rangle = k \} \,, \quad \text{note that } H_{\alpha-k\delta} = H_{-\alpha+k\delta} \,. \tag{78}$$

Observe that $s_{\alpha-k\delta}$ given in (77) are reflections about planes that do not pass through the origin for $k \neq 0$, that is, they are *affine transformations* on H.

Exercise 3.2 Verify that the action of t_μ on H is given by

$$t_\mu . h = h + \mu^\vee \,. \tag{79}$$

using (69), (73) and (77).

Remark 3.3 We will see later that it is the translations by weights on the weight lattice P that give rise to the Bäcklund transformations and "time evolution" of the discrete Painlevé equations.

Recall, the Bäcklund transformation T_1 of the $\mathrm{P_{IV}}$ equation is given by

$$T_1 = t_{h_1} = \pi s_2 s_1 \,. \tag{80}$$

This is the translational element associated to the fundamental weight h_1. Its linear action on the simple affine roots is given by:

$$t_{h_1} \colon (\alpha_0, \alpha_1, \alpha_2) \mapsto (\alpha_0 + \delta, \alpha_1 - \delta, \alpha_2) \,, \tag{81}$$

and as translational motion in the affine hyperplane H is:

$$t_{h_1} . h = h + h_1 \,. \tag{82}$$

Exercise 3.4 Verify (81) using formula (75).

Exercise 3.5 Using (74) and (80), show that the translation by fundamental weight h_2 is given by

$$t_{h_2} = \pi^{-1} s_1 s_2 \,. \tag{83}$$

3.2.2 The Parameter Space of the $\mathrm{P_{IV}}$ Equation

Now we can interpret the $\mathrm{P_{IV}}$ equation (60), in particular its birational formulation given in Table 1 using the objects of $\widetilde{\mathrm{W}}(\mathrm{A}_2^{(1)})$ which we have just discussed. First, let us look at the actions of the generators on the parameters $\alpha_0, \alpha_1, \alpha_2$. Recall that, the parameters satisfy the condition $\alpha_0 + \alpha_1 + \alpha_2 = 1$. This condition is represented geometrically as the triangular lattice in Fig. 1. This triangular lattice, namely the

A_2 lattice, is associated to the infinite Weyl group $\widetilde{W}(A_2^{(1)}) = \langle s_0, s_1, s_2, \pi \rangle$ as follows. The fundamental triangular region F of the lattice is bounded by the reflection hyperplanes associated with three reflection generators s_0, s_1, s_2; whereas the Dynkin diagram automorphism π acts by anti-clockwise rotation of $2\pi/3$ centered at the center of F. The fundamental region F can be mapped to any triangles on the lattice by compositions of these transformations.

Exercise 3.6 Pick a general point inside F, $p = (\alpha_0, \alpha_1, \alpha_2)$ and verify geometrically the transformations associated to s_0, s_1, s_2 given in Table 1.

The special solutions of the P_{IV} equation discussed in Sect. 2.2, correspond to the special values of the symmetric parameters, are associated to the special points on this lattice, can be easily read off. For example, the seed rational special solution in Sect. 2.2.1 given by (62) can be located as the center of F, where $\alpha_0 = \alpha_1 = \alpha_2 = \frac{1}{3}$. The seed hypergeometric special solutions of Sect. 2.2.2 given by (25) and (26) for the parameter value $\alpha_1 + \alpha_2 = 1$ or equivalently $\alpha_0 = 0$ is represented as a line in the A_2 lattice of Fig. 1. The chain of special solutions of rational and hypergeometric type generated by the Bäcklund transformation T_1 discussed in Sect. 2.3 are the center of F and the line $\alpha_0 = 0$, shifted one step to the left by T_1, respectively.

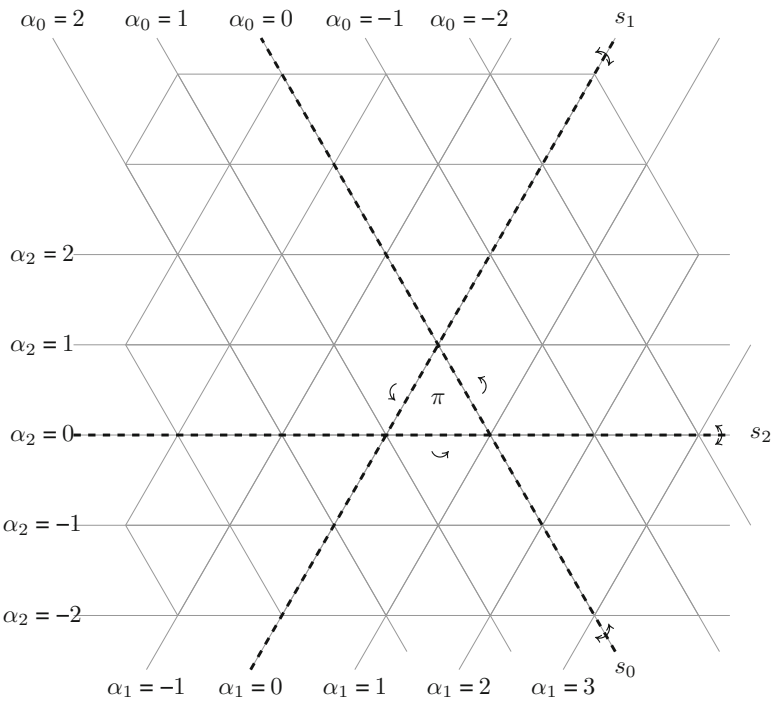


Fig. 1 The parameter space of P_{IV}

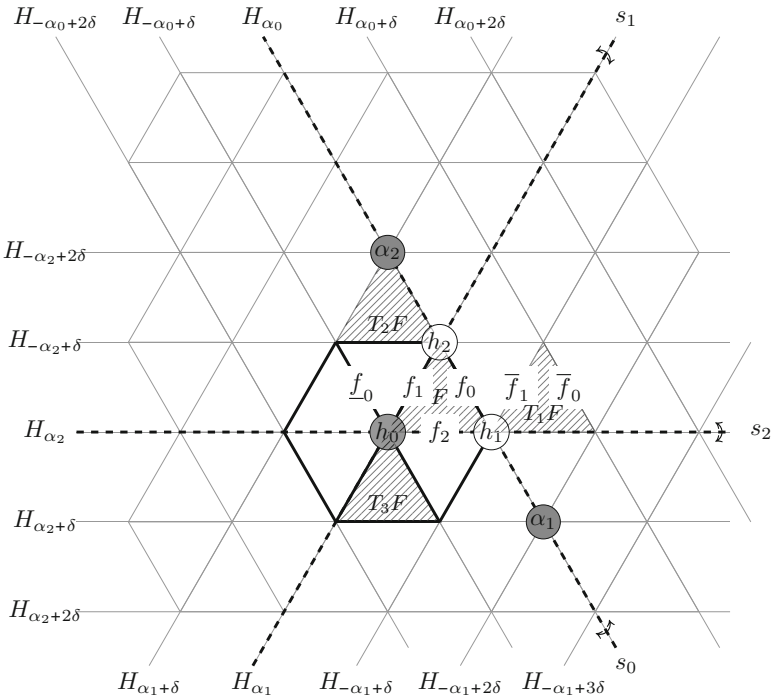


Fig. 2 The A_2 lattice with the f-variables. The *black vertices* are the coroots and *white vertices* are the weights. The (f_0, f_1, f_2) variables are defined on the three edges of the fundamental region F, that is, as ratios of the weights. Translation in the T_1 direction is denoted by $\overline{\ }$ and translation in the opposite direction of T_1 is denoted by $\underline{\ }$. The translated fundamental region F by T_1, T_2, T_3 are also indicated on the lattice

Exercise 3.7 Locate the special rational et hypergeometrical solutions of the P_{IV} equation given by (37) and (40), respectively, on the triangular lattice in Fig. 1.

3.2.3 An Additive Difference Painlevé Equation

To understand the actions of the generators on the (f_0, f_1, f_2) variables given in Table 1 we use the A_2 weight lattice P, associating the (f_0, f_1, f_2) variables with the three edges of the fundamental region F (see Fig. 2). Then transformations on the f-variables are induced from the actions of $\widetilde{W}(A_2^{(1)})$ on the weights (vertices of the lattice). In this representation, the parameters the P_{IV} equation $\alpha_0, \alpha_1, \alpha_2$, associated with the simple affine roots of A_2 type, can be read off from the index of the reflection planes $H_{\pm\alpha_i+k\delta}$ for $i \in \{0, 1, 2\}$.

For example, the fundamental region F bounded by the three reflection planes $H_{\alpha_0}, H_{\alpha_1}$ and H_{α_2}, is associated with the parameter values: $\alpha_0, \alpha_1, \alpha_2$. The translated fundamental region $T_1.F$ is bounded by the hyperplanes $H_{\alpha_0+\delta}, H_{-\alpha_1+\delta}, H_{\alpha_2}$, which

are associated with the parameter values: $\alpha_0+1, \alpha_1-1, \alpha_2$. Notice that the direction of T_1 is opposite to that on the parameter lattice in Fig. 1. This is because the parameters are associated with roots in $V^{(1)}$, whereas the f-variables are associated with weights in the dual space $V^{(1)*}$.

The birational formulation the symmetric form of the $\mathrm{P_{IV}}$ equation (60) given in Table 1, that is the transformations associated to the actions of the generators, satisfy the defining relations (70) and (71). We say that (60) has $\widetilde{\mathrm{W}}(\mathrm{A}_2^{(1)})$ symmetry.

Now using the formula for $T_1 = \pi s_2 s_1$ and the transformations given in Table 1 we have

$$T_1(f_1) = t - f_0 - f_1 - \frac{\alpha_0}{f_0}\ , \quad T_1^{-1}(f_0) = t - f_0 - f_1 + \frac{\alpha_1}{f_1}\ , \tag{84}$$

and

$$T_1(\alpha_0) = \alpha_0 + 1\ , \quad T_1(\alpha_1) = \alpha_1 - 1\ , \quad T_1(\alpha_2) = \alpha_2\ . \tag{85}$$

Exercise 3.8 Verify (84)–(85).

Let $x_n = T_1^n(f_1)$, $y_n = T_1^n(f_0)$. Apply T_1 n times to system (84) and rearrange, we obtain

$$x_{n+1} + x_n = t - y_n - \frac{\alpha_0 + n}{y_n}\ , \quad y_{n-1} + y_n = t - x_n + \frac{\alpha_1 - n}{x_n}\ . \tag{86}$$

Equation (86) was first found in [44], and its continuum limit shown to be the second Painlevé equation [5], hence it is denoted as d-$\mathrm{P_{II}}$.

Now define $\pi T_i = T_{i+1}\pi$, $(i = 1, 2, 3)$, then we have:

$$T_1 = \pi s_2 s_1 = t_{h_1}\ , \quad T_2 = \pi s_0 s_2 = t_{h_2 - h_1}\ , \quad T_3 = \pi s_1 s_0 = t_{-h_2}\ , \tag{87}$$

that is, they correspond to the translations by: h_1, $h_2 - h_1$ and $-h_2$, respectively, and it can be easily checked that they satisfy the relation

$$T_1 T_2 T_3 = 1\ . \tag{88}$$

Exercise 3.9 Identify the directions of translation by T_1, T_2, T_3 in Fig. 2 and verify that condition (88) is indeed satisfied. Follow the previous procedure and now let $x_n = T_2^n(f_1), y_n = T_2^n(f_0)$. Obtain the additive difference for this case and compare with system (86).

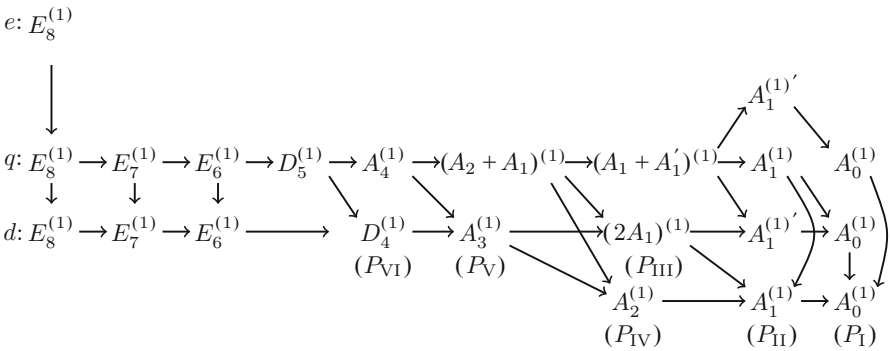


Fig. 3 Sakai's classification by symmetry [46]. The symmetry associated with the continuous P_{IV} equation discussed in Sect. 3.2.3 is of type $A_2^{(1)}$

3.3 Classification and Some Properties of the Discrete Painlevé Equations

Sakai's classification (summarized in Fig. 3) contains three types of difference equations: additive, multiplicative and elliptic. The symmetries of some of the additive type equations are also the discrete symmetries of the continuous Painlevé equations (indicated in the bracket below).We have shown in the last section for the case of the d-P_{II} with $A_2^{(1)}$ symmetry share the same symmetry group with that of the P_{IV} equation.

3.3.1 Additive Difference

Just as we have seen in (86), the independent variable n change by discrete step $n \to n+1$ while the dependent variable $f(n)$ iterates by: $f(n) \to f(n+1)$. This is consistent with how one takes the continuous limit for an additive type difference equation. Let the continuous independent variable be $t = n\epsilon$, then in the limit of $\epsilon \to 0$, we have the usual definition of derivative of a function $f(t)$.

$$\lim_{\epsilon\to 0} \frac{f((n+1)\epsilon) - f(n\epsilon)}{\epsilon} = \lim_{\epsilon\to 0} \frac{f(t+\epsilon) - f(t}{\epsilon} = \frac{\mathrm{d}f(t)}{\mathrm{d}t} .$$

3.3.2 Multiplicative Difference

Let $t = q^n$, we see that as $n \to n+1$, $t \to qt$. That is, the independent variable changes by multiples of $q \in \mathbb{C}$ and the dependent variable iterates by $f(t) \to f(qt)$. Hence multiplicative type difference equations are also sometimes referred to as

q-type equations. The continuous limit of the q-difference is obtained by letting $q \to 1$, and we have the usual definition for the derivative in q-Calculus,

$$\lim_{q\to 1} \frac{f(q^{n+1}) - f(q^n)}{q^n(q-1)} = \frac{\mathrm{d}f(t)}{\mathrm{d}t}.$$

3.3.3 Elliptic Difference

The parameter and independent variables of the elliptic difference type equations enter through the argument of the elliptic functions, for example in terms of the Weierstrass $\wp$ function: $\wp(a) \to \wp(a+b)$. Iterations are computed using addition formulae of elliptic functions.

In what follows, using an example from Sakai's q-list of equations we discuss some further relations and properties which the discrete equations share with their continuous counter-parts. Such as admitting special solutions for particular values of the parameters; possessing Bäcklund transformations that give rise to affine Weyl groups, and can be used to generate chains of special solutions.

3.4 A q-Discrete Analogue of the Fourth Painlevé Equation

A q-discrete analogue of the $\mathrm{P_{IV}}$ equation (60), which we call the q-$\mathrm{P_{IV}}$ equation is given by

$$\begin{aligned}
\bar{f}_0 &= a_0 a_1 f_1 \frac{1 + a_2 f_2 + a_2 a_0 f_2 f_0}{1 + a_0 f_0 + a_0 a_1 f_0 f_1}, \\
\bar{f}_1 &= a_1 a_2 f_2 \frac{1 + a_0 f_0 + a_0 a_1 f_0 f_1}{1 + a_1 f_1 + a_1 a_2 f_1 f_2}, \\
\bar{f}_2 &= a_2 a_0 f_0 \frac{1 + a_1 f_1 + a_1 a_2 f_1 f_2}{1 + a_2 f_2 + a_2 a_0 f_2 f_0},
\end{aligned} \tag{89}$$

where $\bar{}$ stands for the multiplicative difference iteration, that is, c the independent variable iterates by $\bar{c} = qc$; whereas the dependent variables change by $\bar{f}_i(c) = f_i(qc)$; finally a_0, a_1, a_2 are the parameters of the equation. Moreover, we have the conditions $a_0 a_1 a_2 = q$ and $f_0 f_1 f_2 = qc^2$ on the parameters and the variables, so system (89) is really a second-order nonlinear q-difference equation. It belongs to Sakai's q-list and is of $(\mathrm{A_2} + \mathrm{A_1})^{(1)}$ type.

Exercise 3.10 Verify that in the limit $\epsilon \to 0$, the substitution $a_i = \mathrm{e}^{-\epsilon^2 \alpha_i/2}, f_i = -\mathrm{e}^{-\epsilon \psi_i}$ takes (89) to the symmetric $\mathrm{P_{IV}}$ equation (60) for the ψ_i variables, with parameters α_i for $i = 0, 1, 2$.

Table 2 The q-$\mathrm{P_{IV}}$ equation as birational realization of $\widetilde{\mathrm{W}}(\mathrm{A}_2^{(1)})$

	a_0	a_1	a_2	f_0	f_1	f_2
s_0	a_0^{-1}	a_1a_0	a_2a_0	f_0	$f_1\dfrac{a_0+f_0}{1+a_0f_0}$	$f_2\dfrac{1+a_0f_0}{a_0+f_0}$
s_1	a_0a_1	a_1^{-1}	a_2a_1	$f_0\dfrac{1+a_1f_1}{a_1+f_1}$	f_1	$f_2\dfrac{1+a_1f_1}{a_1+f_1}$
s_2	a_0a_2	a_1a_2	a_2^{-1}	$f_0\dfrac{1+a_2f_2}{a_2+f_2}$	$f_1\dfrac{1+a_2f_2}{a_2+f_2}$	f_2
π	a_1	a_2	a_0	f_1	f_2	f_0

The Bäcklund transformations of (89) form $\widetilde{\mathrm{W}}(\mathrm{A}_2^{(1)}) = \langle s_0, s_1, s_2, \pi\rangle$ group symmetry. The transformations associated to the generators on f_i and a_i are summarized in Table 2, they were first given in [19].

Notice the similarity between the transformations on the parameters a_i of q-$\mathrm{P_{IV}}$ equation (89) and on that of the parameters α_i of the $\mathrm{P_{IV}}$ equation (60) given in Table 1. Here, the parameters a_i are related to the affine simple roots of $\widetilde{\mathrm{W}}(\mathrm{A}_2^{(1)})$: α_i by relation $a_i = q^{\alpha_i}$ for $i = 0, 1, 2$. The transformations given in Table 2 satisfy the defining relations (70) and (71) of $\widetilde{\mathrm{W}}(\mathrm{A}_2^{(1)})$. That is, the Bäcklund transformations of $\mathrm{P_{IV}}$ equation (89) form $\widetilde{\mathrm{W}}(\mathrm{A}_2^{(1)})$ group symmetry.

Recall that the translational element associated to the fundamental weight h_1 is $T_1 = t_{h_1} = \pi s_2 s_1$, in particular, we have

$$T_1(a_0) = qa_0\,, \quad T_1(a_1) = q^{-1}a_1\,, \quad T_1(a_2) = a_2\,, \tag{90}$$

$$T_1(f_1) = \frac{qc^2}{f_1f_0}\frac{1+a_0f_0}{a_0+f_0}\,, \quad T_1(f_0) = \frac{qc^2}{f_0T_1(f_1)}\frac{1+a_0a_2T_1(f_1)}{a_0a_2+T_1(f_1)}\,. \tag{91}$$

Exercise 3.11 Verify (90)–(91) by direct computation.

Remark 3.12 We have seen from the discussion above that the Bäcklund transformations of a discrete equation (89) give rise to another multiplicative difference equation (91), where a_0 now has the role of the independent variable, that is $T_1(a_0) = qa_0$, whereas a_0a_2 and c are parameters of (91). Equation (89) can then be interpreted as a Bäcklund transformation of (91), and vice versa. This comes from the fact that time evolution of an equation and its Bäcklund transformations are both discrete iterations. This property of the discrete Painlevé equations does not have a counter-part in the Painlevé equations, where time evolution is differential.

3.4.1 Special Solutions of q-Painlevé Equations

Now we take a look at the hypergeometric type special solutions of the q-Painlevé equations, but first we give a summary on the q-hypergeometric functions, where

we have followed the conventions on the notations of the q-special functions in [4]. The general q-hypergeometric function (also referred to as the *basic hypergeometric function*) is defined by:

$$
\begin{aligned}
&{}_m\phi_n(a_1,\ldots,a_m;b_1,\ldots,b_n;q,z) \\
&\qquad = \sum_{k\geq 0} \frac{(a_1;q)_k \cdots (a_m;q)_k}{(b_1;q)_k \cdots (b_n;q)_k (q;q)_k} \left[(-1)^k q^{\binom{n}{2}}\right]^{1+n-m} z^k
\end{aligned} \tag{92}
$$

where $(a;q)_n = (1-a)(1-aq)\cdots(1-aq^{n-1})$, $|q| < 1$. For $m = 2, n = 1, a_1 = a$, $a_2 = b$ and $b_1 = c$, we have

$$
{}_2\phi_1(a,b;c;q,z) = \sum_{k\geq 0} \frac{(a;q)_k (b;q)_k}{(c;q)_k (q;q)_k} z^k \,, \tag{93}
$$

it is the q-discrete analogue of Gauss's hypergeometric function. Equation (93) solves the q-discrete analogue of Gauss's hypergeometric equation

$$
\left(abz - \frac{c}{q}\right)\sigma^2\phi - \left(a+b)z - \left(1+\frac{c}{q}\right)\right)\sigma\phi + (z-1)\phi = 0 \,, \tag{94}
$$

where $\sigma y(x) = \sigma y = y(qx)$.

Exercise 3.13 Show that the q-hypergeometric series (93) becomes the hypergeometric series

$$
{}_2F_1(\alpha,\beta;\gamma;z) = \sum_{n\geq 0} \frac{(\alpha)_n (\beta)_n}{(\gamma)_n n!} z^n
$$

in the limit $q \to 1$, where $(\alpha)_n = \alpha(\alpha+1)\cdots(\alpha+n-1)$.

Remark 3.14 Letting $a = q^\alpha$, $b = q^\beta$, $c = q^\gamma$, the above can be easily shown using the fact that $(1-q^k)/(1-q) \to k$, as $q \to 1$.

3.5 *q-Hypergeometric Type Special Solutions of q-*$\mathrm{P_{IV}}$

Recall that in section Sect. 3.2.2 on the special solutions of the $\mathrm{P_{IV}}$ equation (60), a hypergeometric type special solution is associated with a line in the parameter space given by $\alpha_0 = 0$ for example (see Fig. 1). Similarly, the q-$\mathrm{P_{IV}}$ equation (89) admits a hypergeometric type special solution when the parameter takes the value $a_2 = q^{\alpha_2} = q^0 = 1$. In this case $f_2 = -1$ and the q-$\mathrm{P_{IV}}$ equation reduces to a q-Riccati equation [19], that is a first-order nonlinear difference equation:

$$\bar{f}_1 = -\frac{q}{a_0}\frac{(1-q^2c^2)f_1 - a_0^2c^2}{f_1} \,. \tag{95}$$

In the same way that the Riccati equation (24) can be linearised by a Cole–Hopf type transformation (25), the q-Riccati equation (95) can be linearized by a discrete analogue of the Cole–Hopf type transformation:

$$f_1 = -\frac{q}{a_0}\frac{\overline{G}}{G} \,. \tag{96}$$

Then (95) implies a second-order linear q-difference equation for the variable G,

$$\overline{\overline{G}} = (1-q^2c^2)\overline{G} + a_0^2c^2G \,, \tag{97}$$

which is the q-Hermite–Weber equation: ${}_1\phi_1(a_0^2/q^2;0;q^2,q^2c^2)$ in the notation of q-hypergeometric function (92). In a further specialization $a_0 = q$, solutions of (97) are q-Hermite polynomials.

All of the discrete Painlevé equations in the degeneration diagram (Fig. 3) of Sakai's classification (except for the three types in the last column on the right) admit hypergeometric series special solutions. The simplest (seed) special hypergeometric solutions for each symmetry types in the classification have been obtained via a geometric approach [20–22]. Geometry gives the specialization of parameters for when discrete Painlevé equations reduce to a discrete Riccati type equation. The discrete Riccati equation is then linearized to a second-order linear discrete equation with which a hypergeometric series is identified. Corresponding to the degeneration diagram we have the following elliptic and multiplicative type hypergeometric special solutions,

$$\begin{array}{ccccccccccc}
\mathrm{E}_8^{(1)} & & & & & & & & & & \\
({}_{12}V_{11}) & & & & & & & & & & \\
\downarrow & & & & & & & & & & \\
\mathrm{E}_8^{(1)} & \longrightarrow & \mathrm{E}_7^{(1)} & \longrightarrow & \mathrm{E}_6^{(1)} & \longrightarrow & \mathrm{D}_5^{(1)} & \longrightarrow & \mathrm{A}_4^{(1)} & \longrightarrow & (\mathrm{A}_2+\mathrm{A}_1)^{(1)} \longrightarrow (\mathrm{A}_2+\mathrm{A}_1)^{(1)} \\
({}_{10}W_9) & & ({}_8W_7) & & ({}_3\phi_2) & & ({}_2\phi_1) & & ({}_1\phi_1) & & ({}_1\phi_1(a;0;q,z)) \quad ({}_1\phi_1(0;-q;q,z))
\end{array} \tag{98}$$

The symbol ${}_sV_t$ denotes the terminating very-well-posed elliptic hypergeometric series; ${}_tW_s$ is the very-well-posed q-hypergeometric series. When the q-hypergeometric series terminates for particular values of the parameters it leads to the following corresponding q-orthogonal polynomials [25] summarised in Table 3. There exist also another type of hypergeometric special solutions for the symmetric discrete Painlevé equations, which are discussed in [17].

Table 3 q-hypergeometric series and their corresponding q-orthogonal polynomials in the terminating case

Balanced ${}_{10}W_9$	Ismail Masson Rahman
${}_8W_7$	Askey Wilson
Balanced ${}_3\phi_2$	Big q-Jacobi
${}_2\phi_1$	Little q-Jacobi
${}_1\phi_1$	q-Laguerre
${}_1\phi_1(a;0;q,z)$	Stieltjes Wigert

4 Ultradiscrete Painlevé Equations

Section 4 by M. Kanki focuses on the so-called *ultradiscrete* limits of the discrete Painlevé equations, and on the properties regarding theses ultradiscrete equations. Various types of "integrable" cellular automata have been obtained through *ultradiscretization*. These cellular automata are called ultradiscrete equations and are defined over the max-plus semifield $(\mathbb{R}, +, \max)$. In this section, after introducing the technique of ultradiscretization through examples, we present several ultradiscrete analogues of the discrete Painlevé equations: i.e., second order nonlinear difference equations over the max-plus semifield. For example one of the ultradiscrete Painlevé II equations has the form

$$X_{n+1} - X_n + X_{n-1} = a + \max[0, n - X_n] - \max[0, n + X_n] \,,$$

where n is the independent variable and a is a parameter. It will be introduced in later sections as $\mathrm{udP}_{\mathrm{II\text{-}2}}$ from the paper of Ramani and others [45].

4.1 Introduction

In Sect. 3 by Y. Shi, we introduced discrete versions of the Painlevé equations; how they have been discovered, how to classify these equations, and so on. In this section we will try to further "simplify" those equations by a method called *ultradiscretization*. In 1996, T. Tokihiro et al. invented a limiting procedure called ultradiscretization [52]. The procedure was used to correlate the discrete KdV equation with a cellular automaton of Takahashi–Satsuma [47, 49]. It is a powerful tool to discretize the dependent variables of discrete dynamical systems, by which various "integrable" cellular automata and their solitary wave solutions have been obtained. These cellular automata are called the ultradiscrete equations and are defined over the max-plus semifield.

In this section, after introducing the technique of ultradiscretization through an example of the ultradiscrete KdV equation and its cellular automaton interpretation, we present several ultradiscrete analogues of the discrete Painlevé equations (ud-Painlevé equations) [6, 19, 45]. The ud-Painlevé equations are second-order nonlinear difference equations over the max-plus semifield. Many of the properties

in previous sections remain true even in this simplified setting. For example, the ud-Painlevé equations have coalescence cascaded, which is in parallel to those for continuous and discrete Painlevé equations. A τ-function form, which is an analogue of the bilinear equation in a discrete setting, is introduced for the ud-Painlevé equation, and its piecewise linear special solution is presented following the paper by Takahashi et al. [50].

Lastly we remark on several applications. One of the weak points of ultradiscretization is that it is not usually applicable to equations with minus signs. Later, the method of "ultradiscretization with parity variables" was constructed, which widens the application of ultradiscretization to equations with arbitrary signs [28]. We will also discuss the relation of our topics to other closely related areas such as tropical geometry and integrability detection of ultradiscrete equations.

4.2 Ultradiscretization

In the case of discrete equations (or difference equations), independent variables take only discrete values (usually integer values: e.g., sub/superscripts $t, n \in \mathbb{Z}$), however dependent variables can take continuous values in $\mathbb{R}$ (or in $\mathbb{C}$). In the ultradiscrete equations, both the independent and dependent variables take only discrete values. In this section, we briefly review the *ultradiscretization* procedure and the ultradiscrete equations. Originally, Tokihiro and others had considered the name "nonanalytic limit" for this method, and later the fashionable name ultradiscretization was given by B. Grammaticos.

The process of ultradiscretization is done by discretizing the dependent variables of a discrete equation by the following limiting procedure:

$$\lim_{\epsilon \to +0} \epsilon \log(\cdot) \ .$$

For example, if we have a dependent variable u in the discrete equation, we first introduce a parameter $\epsilon > 0$, and the new dependent variable U by

$$u = \exp(U/\epsilon) \ .$$

Then, by taking the limit $\lim_{\epsilon \to +0} \epsilon \log(\cdot)$, on both sides of the equation for u, we obtain the equation for U. It is trivial that $\epsilon \log(u)$ goes to U in this setting. One minor but important restriction is that the original variable u should have a *positive* value so that we can take a ultradiscrete limit.

Let us introduce two basic properties of ultradiscrete limit (ud-limit):

(i) *A multiplication $a \cdot b$ becomes an addition $A + B$, when we take the ud-limit by $a = \exp(A/\epsilon)$ and $b = \exp(B/\epsilon)$.*
(ii) *In the same setting as in* (i), *an addition $a + b$ becomes maximization* $\max[A, B]$.

Proof of (i)

$$\lim_{\epsilon \to +0} \epsilon \log(a \cdot b) = \lim_{\epsilon \to +0} \epsilon \log\left(\mathrm{e}^{(A+B)/\epsilon}\right) = A + B \,. \qquad \square$$

Proof of (ii)

$$\lim_{\epsilon \to +0} \epsilon \log(a + b) = \lim_{\epsilon \to +0} \epsilon \log\left(\mathrm{e}^{A/\epsilon} + \mathrm{e}^{B/\epsilon}\right) = \max[A, B] \,. \qquad \square$$

Exercise 4.1 Confirm the last equality to obtain $\max[A, B]$.

4.3 Ultradiscrete KdV Equation

Korteweg–de Vries equation (KdV equation) [26] is the following partial differential equation for the dependent variable $u(x, t)$:

$$\frac{\partial u}{\partial t} + 6u\frac{\partial u}{\partial x} + \frac{\partial^3 u}{\partial x^3} = 0 \,.$$

The KdV equation has soliton solutions [54] and an infinite number of conserved quantities. One of the integrable full discretized versions (i.e., both of the independent variables t and x are discretized) of the KdV equation is as follows [10]:

$$(1 + \delta)\sigma_{n+1}^{t+1}\sigma_n^{t-1} = \delta\sigma_{n+1}^{t-1}\sigma_n^{t+1} + \sigma_n^t\sigma_{n+1}^t \,, \tag{99}$$

where n, t are independent variables, $\sigma_n^t = \sigma(n, t)$ is the dependent variable, and δ is a parameter. It is worth noting that Eq. (99) can be derived by a reduction from the famous Hirota–Miwa equation [9] (which is also called the discrete KP equation). The Hirota–Miwa equation is derived through the Miwa transformation from the KP hierarchy.

We shall show an ultradiscrete version of (99). Let us introduce a new parameter ϵ by

$$\delta = \mathrm{e}^{-1/\epsilon} \,.$$

Next we define a new dependent variable $\rho_n^t(\epsilon)$ by

$$\sigma_n^t(\epsilon) = \exp\left(\frac{\rho_n^t(\epsilon)}{\epsilon}\right) ,$$

which will be a variable of the ultradiscrete KdV equation. By taking the logarithms of both sides of (99), we have

$$\rho_{n+1}^{t+1} + \rho_n^{t-1} + \epsilon \log\left(1 + \mathrm{e}^{-1/\epsilon}\right) = \epsilon \log\left\{ \exp\left(\frac{\rho_{n+1}^{t-1} + \rho_n^{t+1} - 1}{\epsilon} \right) + \exp\left(\frac{\rho_n^t + \rho_{n+1}^t}{\epsilon} \right) \right\} . \tag{100}$$

If we suppose that $\rho_n^t(\epsilon)$ continuously depends on ϵ, and that

$$\lim_{\epsilon \to +0} \rho_n^t(\epsilon) := \rho_n^t$$

exists for every $n, t \in \mathbb{Z}$, then we have from (100) that

$$\rho_{n+1}^{t+1} + \rho_n^{t-1} = \max[\rho_{n+1}^{t-1} + \rho_n^{t+1} - 1, \rho_n^t + \rho_{n+1}^t] . \tag{101}$$

Equation (101) is called the ultradiscrete KdV equation, which is closely related to the cellular automaton of Takahashi–Satsuma [47, 49]. The cellular automaton of Takahashi–Satsuma is now called the *Box and Ball system* (BBS). The BBS consists of a one-dimensional array of boxes with balls in some of the boxes. We suppose that there are an infinite number of boxes, and there are only a finite number of balls, and count the location of the box from a certain point ($n = 0$) to the right. The dependent variable u_n^t of the BBS denotes the number of balls in the nth box at the time step t. A ball of BBS moves from one box to another according to the following rules (see Fig. 4).

The number of balls in the nth box at time step t is the dependent variable u_n^t. To obtain the state at time $t + 1$ from the state at time t, we sweep from the left to the right and move the balls as follows:

1. We move the ball at the most left-hand side (ball "1") to the nearest empty box to the right of the ball "1."
2. We move the second ball from the left (ball "2") of the initial state at time t, to the nearest empty box to the right, excluding the one used in 1.
3. We repeat this movement until every ball is moved exactly once.

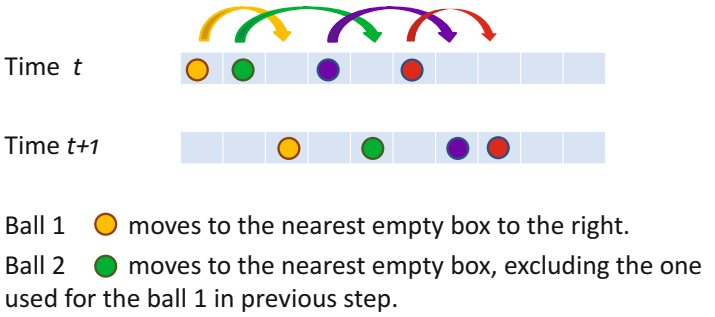


Fig. 4 Evolution rule of the box and ball system (a cellular automaton related to the ultradiscrete KdV equation)

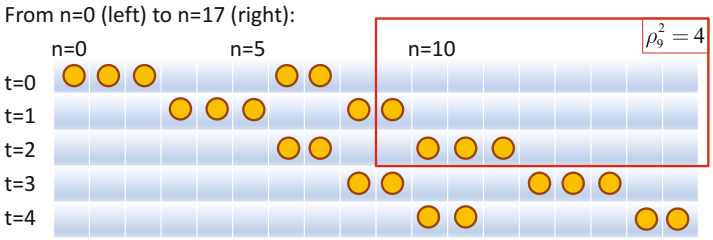


Fig. 5 A soliton solution of the box and ball system (BBS). An array of $m(>0)$ balls moves to the right with a speed m. The array is an analogue of the soliton solution of the (continuous) KdV equation, and is called the solitons of the BBS

In this paper, let us suppose that the capacity of each box is one: i.e., we only consider $u_n^t = 0$ and $u_n^t = 1$. Then the rules from 1 to 3 can be written down as the evolution equation:

$$u_n^{t+1} = \min\left[1 - u_n^t, \sum_{k=-\infty}^{n-1} (u_k^t - u_k^{t+1})\right],$$

where we have assumed that the total number of balls in the system is finite. The relation of u_n^t with the variable ρ_n^t of the ultradiscrete KdV equation (101) is as follows:

$$\rho_n^t = \sum_{s=-\infty}^{t} \sum_{m=n}^{\infty} u_m^s \,, \tag{102}$$

where the summation is essentially finite. When we describe (102) in Fig. 5 of the time evolution of the BBS, the number of balls in the rectangle in the upper-right corner from the cell at (n, t) is equal to the value of ρ_n^t. For example, we have $\rho_8^0 = 0$, $\rho_8^1 = 2$, $\rho_8^2 = 5$, $\rho_9^0 = 0$, $\rho_9^1 = 1$, $\rho_9^2 = 4$, and so on. We can easily reassure that the Eq. (101) is satisfied for $n = 8$, $t = 1$:

$$\rho_9^2 + \rho_8^0 = \max[\rho_9^0 + \rho_8^2 - 1, \rho_8^1 + \rho_9^1] \,.$$

Exercise 4.2 Pick up several ρ_n^ts in Fig. 5, and confirm that (101) is satisfied, by counting the number of balls in the upper-right corner above (n, t).

Note that (101) is a piecewise-linear equation. The ultradiscretization is a process to construct a piecewise-linear equation from a fully discrete one. Piecewise-linear equations can be interpreted as evolution rules for cellular automata, and are useful not only in the theory of integrable systems but also in the modeling of phenomena in physics and engineering. For further study, we pick up [48, 53] on generalizations of the BBS: e.g., the capacity of the box can be larger than one, and [24] on integrable nature such as their conserved quantities.

4.4 Ultradiscrete Painlevé Equations (ud-Ps)

We will apply ud-limits to the discrete Painlevé equations. We mainly review the paper *The ultimate discretization of the Painlevé equations* by Ramani et al. [45]. In the paper [45], the ultradiscrete versions of the discrete Painlevé equations are systematically constructed.

Before starting, let us note that ud-limit of the Riccati equation

$$x_{n+1} = \frac{\alpha x_n + \beta}{\gamma x_n + \delta}$$

becomes just a linear equation as explained in [45]. (Since the Riccati equation is a linearizable equation, this result is not strange.) We need more complex structures (in particular we need more than first order recurrences) for the discrete equations to yield nonlinear ultradiscrete equations. Therefore we will study second order difference equations whose typical nonautonomous examples are discrete Painlevé equations.

As one of the simplest examples, let us introduce one of ultradiscrete Painlevé I equations (udP$_\mathrm{I}$). We use the following form of the discrete Painlevé I equation:

$$x_{n+1}x_{n-1} = \frac{\lambda^n}{x_n} + \frac{1}{x_n^2}\,, \tag{103}$$

where λ is a positive constant. Equation (103) is of the multiplicative type, and is often called the q-discrete Painlevé I equation since the nonautonomous term q^n was originally used instead of λ^n here. In this section we only use multiplicative types, not additive types. Let us suppose that $x_n > 0$ for every n, and introduce ϵ by $\lambda = \mathrm{e}^{1/\epsilon}$ and a new dependent variable X_n by

$$x_n = \exp\left(\frac{X_n}{\epsilon}\right).$$

Then (103) is equivalent to

$$\exp\left(\frac{X_{n+1} + X_{n-1}}{\epsilon}\right) = \exp\left(\frac{n - X_n}{\epsilon}\right) + \exp\left(\frac{-2X_n}{\epsilon}\right). \tag{104}$$

By taking the ud-limit of both sides of (104), we obtain

$$X_{n+1} + X_{n-1} = \max[n - X_n, -2X_n]\,,$$

and thus

$$X_{n+1} + X_{n-1} + 2X_n = \max[X_n + n, 0]\,. \tag{105}$$

Equation (105) is one form of the ultradiscrete Painlevé I equation (udP$_{\rm I}$). Note that we often use the symbol $(A)_+ := \max[A, 0]$ for simplicity. The identity $A + (-A)_+ = (A)_+$ is often useful in the deformations of equations. Then udP$_{\rm I}$ becomes

$$X_{n+1} + X_{n-1} + 2X_n = (X_n + n)_+ \,. \qquad (\text{udP}_{\text{I}-1})$$

The form of ultradiscrete Painlevé I equation is not unique. Another form of the ultradiscrete Painlevé I equation is

$$X_{n+1} + X_{n-1} = (X_n + n)_+ \,, \qquad (\text{udP}_{\text{I-3}}) \quad (106)$$

which is obtained by taking the ultradiscrete limit of another version of the discrete Painlevé I equation:

$$x_{n+1}x_{n-1} = \lambda^n x_n + 1 \,.$$

We can obtain one form of the ultradiscrete Painlevé II equations from a discrete analogue of the Painlevé II equation:

$$x_{n+1}x_{n-1} = \frac{\alpha(x_n + \lambda^n)}{1 + \lambda^n x_n} \,, \qquad (107)$$

where α is a nonzero parameter. By taking the ultradiscrete limit of (107) as $\lambda = \mathrm{e}^{1/\epsilon}$ and $\alpha = \mathrm{e}^{a/\epsilon}$, we obtain

$$X_{n+1} + X_{n-1} - X_n = a + (n - X_n)_+ - (n + X_n)_+ \,, \qquad (\text{udP}_{\text{II-2}}) \quad (108)$$

where a is a constant. Equation (108) is one of the two ultradiscrete Painlevé II equations introduced in [45]. Another form is

$$X_{n+1} + X_{n-1} = a + (n - X_n)_+ - (n + X_n)_+ \,, \qquad (\text{udP}_{\text{II-1}}) \quad (109)$$

which comes from the ultradiscrete limit of another discretization of the Painlevé II equation

$$x_{n+1}x_{n-1} = \frac{(x_n + \lambda^n)}{x_n(1 + \alpha\lambda^n x_n)} \,. \qquad (110)$$

We list other ultradiscrete equations only with brief explanation. Here is the ultradiscrete Painlevé III equation (udP$_{\rm III}$):

$$\begin{aligned} X_{n+1} + X_{n-1} - 2X_n = {} & (n + a - X_n)_+ + (n - a - X_n)_+ \\ & -(X_n + b + n)_+ - (X_n - b + n)_+ . \quad (\text{udP}_{\text{III}}) \end{aligned} \qquad (111)$$

The following coupled system is the ultradiscrete Painlevé V equation ($\mathrm{udP_V}$):

$$\begin{cases} X_{n+1} + X_n = (Y_n)_+ \\ Y_n + Y_{n-1} = (X_n - a)_+ + (X_n + a)_+ + (X_n - b)_+ + (X_n + b)_+ \\ \qquad\qquad -(X_n + c + n)_+ - (X_n - c + n)_+ \end{cases} . \tag{112}$$

Other ultradiscrete Painlevé equations ($\mathrm{udP_{I\text{-}2}}$, $\mathrm{udP_{IV\text{-}1}}$, $\mathrm{udP_{IV\text{-}2}}$, $\mathrm{udP_{VI}}$) can be found in [45]. In [19], the authors have obtained another form of the ultradiscrete Painlevé IV equation from the symmetric form of the (q-)discrete Painlevé IV equation.

4.5 Degeneration Diagram of Ud-Painlevé Equations

We explain one of the main properties of the ultradiscrete Painlevé equations: degeneration diagram (coalescence cascades). The ultradiscrete Painlevé equations have the following cascades in Fig. 6, which is quite similar to those for continuous and discrete Painlevé equations. Here, the arrow $P \to Q$ indicates that the equation Q is derived from P by introducing a large parameter Ω in the parameters of ultradiscrete Painlevé equations and by taking a limit $\Omega \to +\infty$. This limiting process can be seen as a ultradiscrete 'degeneration,' by which the number of discontinuities of the piecewise linear equation is decreased one by one at each limit. As we can see in the work by Joshi and Lafortune [15], a discontinuity of an ultradiscrete piecewise linear equation can be interpreted as an analogue of a singularity of discrete (and continuous) mappings.

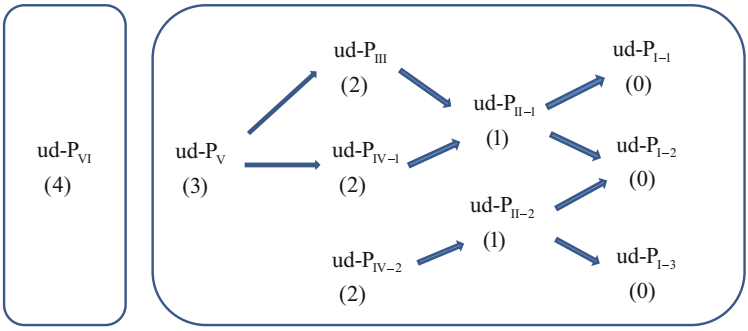


Fig. 6 Coalescence cascades of ultradiscrete Painlevé equations. Under each equation, we have added the number of essential parameters, that always coincides with the case of continuous equation

As an example we show how to obtain udP$_{\text{I-3}}$ (106) from udP$_{\text{II-2}}$ (108). Let us take

$$a = -\Omega\ , \quad n = -\Omega - m\ , \quad X_n = \tfrac{1}{2}(Z_m - m) - \Omega\ ,$$

in (108). Then we have

$$\begin{aligned}&\left\{\tfrac{1}{2}(Z_{m-1} - m + 1) - \Omega\right\} + \left\{\tfrac{1}{2}(Z_{m+1} - m - 1) - \Omega\right\} + \left\{-\tfrac{1}{2}(Z_m - m) + \Omega\right\}\\ &= -\Omega + (-\Omega - m - \tfrac{1}{2}(Z_m - m) + \Omega)_+ - (-\Omega - m + \tfrac{1}{2}(Z_m - m) - \Omega)_+\ ,\end{aligned}$$

and thus

$$\begin{aligned}\tfrac{1}{2}(Z_{m+1} + Z_{m-1}) = \tfrac{1}{2}(Z_m + m) + \max\left[-\tfrac{1}{2}(Z_m + m), 0\right]\\ - \max\left[-2\Omega + \tfrac{1}{2}Z_m - \tfrac{3}{2}m, 0\right]\ .\end{aligned} \tag{113}$$

When we take the limit $\Omega \to +\infty$ in the last term of (113), we have

$$\max[-2\Omega + \tfrac{1}{2}Z_m - \tfrac{3}{2}m, 0] \to 0\ .$$

Therefore the large parameter limit of (113) is

$$Z_{m+1} + Z_{m-1} = Z_m + m + (-Z_m - m)_+ = (Z_m + m)_+\ ,$$

which is nothing but the ultradiscrete Painlevé I equation (106).

Exercise 4.3 Check other degenerations. For example, introduce a large parameter Ω in ud-Painlevé V as $X_n = \Omega + (Z_m - m)/2$ (and also suitably transform parameters a and b), to derive ud-Painlevé III as a coalescence limit.

It is worth noting that the number of parameters in the ultradiscrete Painlevé X equation is always equal to the number of essential parameters in the (continuous) Painlevé X equation (X $= 1, 2, 3, 4, 5, 6$). Therefore it is natural to conjecture that, a mechanism similar to that for continuous Painlevé equations which has been reviewed by Nakazono in Sect. 2, should apply to the coalescence cascades (Fig. 6): e.g., affine Weyl groups, the space of initial conditions, and so on. However, the complete classifications of the ultradiscrete Painlevé equations is not done, and we do not have enough knowledge on the underlying structures of the ultradiscrete systems. For example, it is not clear how to define singular points of ultradiscrete equations. For example, a criterion for integrability of ultradiscrete equations is proposed in [15] and further developed in view of the tropical geometry in [40]. The work can be considered as a tropical counterpart of an integrability criterion for discrete equations called "the singularity confinement test" [7]. However, the notion of the space of initial conditions does not seem to be well-defined for ultradiscrete systems. In the continuous and discrete cases, symmetries of the evolution of the

equations appear as affine Weyl groups, whose complements are the symmetry groups of the space of initial conditions. We can formulate symmetries for ud-Painlevé equations in terms of affine Weyl groups. For example, in [41], the authors study tropical representations of affine Weyl groups—a representation of the group without subtractions has an ultradiscrete limit—so that elements of the groups describe the evolution of many of the ud-Painlevé equations in [45] and [19].

4.6 Special Solutions to the Ud-Painlevé Equations

In [50], rational solutions of the two types of ultradiscrete Painlevé II equations and those of the ultradiscrete Painlevé III equation are presented. The results are in perfect parallel to the continuous and discrete cases. As in the case of discrete equations, we have ultradiscrete analogues of the bilinear equation. For example, in the case of ultradiscrete Painlevé II equation (109), by conducting the transformation

$$X_n = \tau_{n-1} - \tau_{n-2} \ ,$$

we obtain a "bilinear" form

$$\tau_n + \max[\tau_{n-2}, \tau_{n-1} + n] = \tau_{n-3} + \max[\tau_{n-1}, \tau_{n-2} + n] + a \ . \tag{114}$$

In the ultradiscrete world, $\times$ changes to $+$, and $+$ changes to 'max,' therefore, (114) is indeed analogous to a bilinear equation in the "discrete world." For the simplicity of the following computations, let us slightly transform (114) and use

$$\tau_n + \max[\tau_{n-2}, \tau_{n-1} + n - a] = \tau_{n-3} + \max[\tau_{n-1}, \tau_{n-2} + n] \ , \tag{115}$$

as one form of bilinear udP$_{\rm II}$ equations. We can construct a special solution

$$\tau_n = \sum_{j=0}^{m-1} \max[0, n - 3j] \ , \tag{116}$$

for $a = 4m$ with $m \in \mathbb{Z}_{\geq 0}$. The same τ_n can be expressed in another form:

$$\tau_n = \max_{0 \leq j \leq m} [jn - \tfrac{3}{2} j(j-1)] \ , \tag{117}$$

whose graph is easier to understand: τ_n is a weakly monotonously increasing piecewise linear function increasing its slope at $n = 3j$ $(j = 0, 1, \ldots, m-1)$.

Exercise 4.4 Prove that expressions (116) and (117) give the same τ_n, and that they are solutions to (115).

The form (116) can be seen as the ultradiscrete analog of the Casorati determinant special solutions for discrete equations, and the form (117) can be seen as an expansion of the "determinant."

4.7 Ultradiscrete Limit with Sign Variables

One of the weak points of ultradiscretization is that we require the original equations to possess only plus signs (in other words, free of minus signs). In order to overcome this difficulty, the generalization of the ultradiscrete limit is introduced. The method is called "the ultradiscrete limit with sign (or parity) variables", and it enables us to ultradiscretize directly equations with arbitrary signs [28]. Let u be a dependent variable of a discrete equation. If $u \neq 0$, we introduce a parity variable ω by $\omega = u/|u|$, and the amplitude variable U by $U = \epsilon \log|u|$, where ϵ is a positive small parameter. By introducing the parity function $s(\omega)$, by

$$s(\omega) = \begin{cases} 1, & \omega = +1 \\ 0, & \omega = -1, \end{cases}$$

we can rewrite the variable u as

$$u = \{s(\omega) - s(-\omega)\}\mathrm{e}^{U/\epsilon} .$$

An ultradiscrete analogue of $s(\omega)$ is defined as

$$S(\omega) = \begin{cases} 0, & \omega = +1 \\ -\infty, & \omega = -1, \end{cases}$$

Therefore the ultradiscretization of u is defined regardless of its sign as

$$\lim_{\epsilon \to +0} \epsilon \log\bigl(s(\omega)\mathrm{e}^{U/\epsilon}\bigr) = S(\omega) + U .$$

Mimura et al. have constructed the ultradiscrete analogue of the q-Airy function. The ultradiscrete q-Airy function that they have constructed is one of the special solutions of the ultradiscrete Painlevé II equation [28]. They are also intensively studying special solutions of other ultradiscrete Painlevé equations by using the ultradiscrete limit with parity variables. Takemura and Tsutsui have constructed the ultradiscrete analogue of the q-discrete Painlevé VI equation [51].

4.8 Answers to the Exercises in Sect. 4

Here are hints and answers to the exercises.

4.8.1 Solution to Exercise 4.1

We prove the case of $A > B$. It is not hard to see that

$$\epsilon \log(\mathrm{e}^{A/\epsilon} + \mathrm{e}^{B/\epsilon}) = A + \epsilon \log(1 + \mathrm{e}^{(B-A)/\epsilon}) \to A \quad (\epsilon \to +0) \, .$$

4.8.2 Solution to Exercise 4.3

Let us introduce a new variable m and a parameter α as

$$a = \Omega + \alpha, \; b = \Omega - \alpha, \; n = m - \Omega, \; X_n = \Omega + \tfrac{1}{2}(Z_m - m)$$

The coupled form (112) of udP$_{\mathrm{V}}$ can be written down in one equation as

$$X_{n+1} + 2X_n + X_{n-1} = (Y_n)_+ + (Y_{n-1})_+,$$

where we can substitute the second equation of (112) in the right-hand side. Since $X_n \to \infty$ when $\Omega \to \infty$, we have $Y_n > 0$ for $\Omega > 0$ that is large enough. Thus the term $()_+$ is omitted, and the equation udP$_{\mathrm{V}}$ should be

$$\begin{aligned} &X_{n+1} + 2X_n + X_{n-1} \\ &\qquad = Y_n + Y_{n-1} \\ &\qquad = (X_n - \Omega - \alpha)_+ + (X_n + \Omega + \alpha)_+ + (X_n - \Omega + \alpha)_+ \\ &\qquad\quad + (X_n + \Omega - \alpha)_+ - (X_n + c + m - \Omega)_+ - (X_n - c + m - \Omega)_+ . \end{aligned}$$

Substituting Z_m in the right hand side, and taking the limit $\Omega \to \infty$, we have

$$\begin{aligned} &Z_{m+1} + Z_{m-1} - 2m \\ &= (Z_m - m + 2\alpha)_+ + (Z_m - m - 2\alpha)_+ - (Z_m + m + 2c)_+ - (Z_m + m - 2c)_+ \, . \end{aligned} \tag{118}$$

Since we have

$$(Z_m - m \pm 2\alpha)_+ = (m \mp 2\alpha - Z_m)_+ - m \pm 2\alpha + Z_m \, ,$$

(118) becomes

$$Z_{m+1} - 2Z_m + Z_{m-1} = (m + 2\alpha - Z_m)_+ + (m - 2\alpha - Z_m)_+ \\ - (Z_m + m + 2c)_+ - (Z_m + m - 2c)_+ ,$$

which is nothing but the udP$_{\mathrm{III}}$ equation (111), where the parameters are $b \to 2c$, $a \to 2\alpha$.

4.8.3 Solution to Exercise 4.4

First it is easy to prove that τ_n in (117) is equal to

$$\tau_n = \begin{cases} 0 & (n \le 0) \\ jn - \frac{3}{2}j(j-1) & (3(j-1) \le n \le 3j)\ (j = 1, 2, \ldots, m-1) \\ mn - \frac{3}{2}m(m-1) & (3(m-1) \le n). \end{cases}$$

Since we have $\sum_{j=0}^{k-1}(n - 3j) = kn - \frac{3}{2}k(k-1)$ for a nonnegative integer k, we can prove that (116) is in fact equivalent to (117). Next we prove that (117) is a solution to (115). For a fixed $j \in \{0, 1, \ldots, m-1\}$, it is enough to confirm that (115) is satisfied for τ_n of three cases $n = 3(j-1)$, $n = 3(j-1)+1$ and $n = 3(j-1)+2$. For example, when $n = 3(j-1)$ we can obtain by direct computation that

$$\tau_{n-3} = \tfrac{3}{2}(j-1)(j-2) , \qquad \tau_{n-2} = \tfrac{1}{2}(j-1)(3j-4) , \\ \tau_{n-1} = \tfrac{1}{2}(j-1)(3j-2) , \qquad \tau_n = \tfrac{3}{2}j(j-1) .$$

Therefore (115) is equivalent to

$$\tau_n + \tau_{n-2} = \tau_{n-3} + \tau_{n-2} + n ,$$

which is identically satisfied. The remaining cases of $n = 3(j-1)+1$ and $n = 3(j-1)+2$ can be proved in the same manner.

4.9 *Conclusion of Sect. 4*

In Sect. 4, we have introduced ultradiscrete analogues of the discrete Painlevé equations. After introducing the technique of ultradiscretization through the cellular automaton of box and balls (BBS), we have presented several ultradiscrete analogues of the q-discrete Painlevé equations: i.e., second-order nonlinear difference equations over the max-plus semifield. Many of the properties in previous sections

have been shown to remain true even in this simplified setting, including the degeneration diagram and the special solutions. We have omitted many of the interesting properties of the ultradiscrete Painlevé equations. For further reading, we pick up [41] for the relation with tropical curves, [29, 39] for the special solutions other than those introduced in [50].

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References

1. A.S. Fokas, B. Grammaticos, A. Ramani, From continuous to discrete Painlevé equations. J. Math. Anal. Appl. **180**(2), 342–360 (1993)
2. R. Fuchs, Sur quelques équations différentielles linéaires du second ordre. C. R. Acad. Sci. Paris **141**(1), 555–558 (1905)
3. B. Gambier, Sur les équations différentielles du second ordre et du premier degré dont l'intégrale générale est àă points critiques fixes. Acta Math. **33**(1), 1–55 (1910)
4. G. Gasper, M. Rahman, *Basic Hypergeometric Series*, vol. 35. Encyclopedia of Mathematics and Its Applications (Cambridge University Press, Cambridge, 1990)
5. B. Grammaticos, Y. Ohta, A. Ramani, H. Sakai, Degeneration through coalescence of the q-Painlevé VI equation. J. Phys. A **31**(15), 3545–3558 (1998)
6. B. Grammaticos, Y. Ohta, A. Ramani, D. Takahashi, K.M. Tamizhmani, Cellular automata and ultra-discrete Painlevé equations. Phys. Lett. A **226**(1–2), 53–58 (1997)
7. B. Grammaticos, A. Ramani, V. Papageorgiou, Do integrable mappings have the Painlevé property? Phys. Rev. Lett. **67**(14), 1825–1828 (1991)
8. B. Grammaticos, A. Ramani, J. Satsuma, R. Willox, A. Carstea, Reductions of integrable lattices. J. Nonlinear Math. Phys. **12**(Suppl. 1), 363–371 (2005)
9. R. Hirota, Discrete analogue of a generalized Toda equation. J. Phys. Soc. Jpn. **50**(11), 3785–3791 (1981)
10. R. Hirota, S. Tsujimoto, T. Imai, Difference scheme of soliton equations. Sūrikaisekikenkyūsho Kōkyūroku **822**, 144–152 (1993)
11. J.E. Humphreys, *Reflection Groups and Coxeter Groups*. Cambridge Studies in Advanced Mathematics, vol. 29 (Cambridge University Press, Cambridge, 1990)
12. K. Iwasaki, H. Kimura, S. Shimomura, M. Yoshida, *From Gauss to Painlevé*, vol. E16. Aspects of Mathematics (Friedrich Vieweg & Sohn, Braunschweig, 1991)
13. M. Jimbo, T. Miwa, Monodromy preserving deformation of linear ordinary differential equations with rational coefficients. II. Phys. D **2**(3), 407–448 (1981)
14. M. Jimbo, H. Sakai, A q-analog of the sixth Painlevé equation. Lett. Math. Phys. **38**(2), 145–154 (1996)
15. N. Joshi, S. Lafortune, How to detect integrability in cellular automata. J. Phys. A **38**(28), L499–L504 (2005)
16. N. Joshi, N. Nakazono, Y. Shi, Reflection groups and discrete integrable systems. J. Intell. Syst. **1**(1), xyw006 (2016)
17. K. Kajiwara, N. Nakazono, Hypergeometric solutions to the symmetric q-Painlevé equations. Int. Math. Res. Not. **2015**(4), 1101–1140 (2015)
18. K. Kajiwara, Y. Ohta, Determinant structure of the rational solutions for the Painlevé IV equation. J. Phys. A **31**(10), 2431–2446 (1998)
19. K. Kajiwara, M. Noumi, Y. Yamada, A study on the fourth q-Painlevé equation. J. Phys. A **34**(41), 8563–8581 (2001)

20. K. Kajiwara, T. Masuda, M. Noumi, Y. Ohta, Y. Yamada, ${}_{10}E_9$ solution to the elliptic Painlevé equation. J. Phys. A **36**, L263–L272 (2003)
21. K. Kajiwara, T. Masuda, Noumi, M., Ohta, Y., Yamada, Y.: Hypergeometric solutions to the q-Painlevé equations. Int. Math. Res. Not. **2004**(47), 2497–2521 (2004)
22. K. Kajiwara, T. Masuda, M. Noumi, Y. Ohta, Y. Yamada, Construction of hypergeometric solutions to the q-Painlevé equations. Int. Math. Res. Not. **2005**(24), 1441–1463 (2005)
23. K. Kajiwara, M. Noumi, Yamada, Y.: Geometric aspects of Painlevé equations. J. Phys. A **50**(7), 073001, 164 (2017)
24. M. Kanki, J. Mada, T. Tokihiro, Conserved quantities and generalized solutions of the ultradiscrete KdV equation. J. Phys. A **44**(14), 145202, 13 (2011)
25. R. Koekoek, R.F. Swarttouw, The Askey-scheme of hypergeometric orthogonal polynomials and its q-analogue. Online notes (1998)
26. D.J. Korteweg, G. de Vries, On the change of form of long waves advancing in a rectangular canal, and on a new type of long stationary waves. Philos. Mag. (5) **39**(240), 422–443 (1895)
27. T. Masuda, Classical transcendental solutions of the Painlevé equations and their degeneration. Tohoku Math. J. (2) **56**(4), 467–490 (2004)
28. N. Mimura, S. Isojima, M. Murata, J. Satsuma, Singularity confinement test for ultradiscrete equations with parity variables. J. Phys. A **42**(31), 315206, 7 (2009)
29. M. Murata, Exact solutions with two parameters for an ultradiscrete Painlevé equation of type $A_6^{(1)}$. SIGMA Symmetry Integrability Geom. Methods Appl. **7**, 15 pp. (2011). Paper 059
30. F.W. Nijhoff, V.G. Papageorgiou, Similarity reductions of integrable lattices and discrete analogues of the Painlevé II equation. Phys. Lett. A **153**(6), 337–344 (1991)
31. F.W. Nijhoff, A. Ramani, B. Grammaticos, Y. Ohta, On discrete Painlevé equations associated with the lattice KdV systems and the Painlevé VI equation. Stud. Appl. Math. **106**(3), 261–314 (2001)
32. M. Noumi, *Painlevé Equations Through Symmetry*, vol. 223. Translations of Mathematical Monograph (American Mathematical Society, Providence, RI, 2004)
33. Y. Ohyama, H. Kawamuko, H. Sakai, K. Okamoto, Studies on the Painlevé equations. V. Third Painlevé equations of special type $P_{iii}(D_7)$ and $P_{iii}(D_8)$. J. Math. Sci. Univ. Tokyo **13**(2), 145–204 (2006)
34. K. Okamoto, Sur les feuilletages associés aux équations du second ordre àă points critiques fixes de P. Painlevé. Jpn. J. Math. (N.S.) **5**(1), 1–79 (1979)
35. K. Okamoto, Studies on the Painlevé equations. III. Second and fourth Painlevé equations, P_{ii} and P_{iv}. Math. Ann. **275**(2), 221–255 (1986)
36. K. Okamoto, Studies on the Painlevé equations. I. Sixth Painlevé equation P_{vi}. Ann. Mat. Pura Appl. (4) **146**, 337–381 (1987)
37. K. Okamoto, Studies on the Painlevé equations. II. Fifth Painlevé equation P_v. Jpn. J. Math. (N.S.) **13**(1), 47–76 (1987)
38. K. Okamoto, Studies on the Painlevé equations. IV. Third Painlevé equation P_{iii}. Funkcial. Ekvac. **30**(2–3), 305–332 (1987)
39. C.M. Ormerod, Hypergeometric solutions to an ultradiscrete Painlevé equation. J. Nonlinear Math. Phys. **17**(1), 87–102 (2010)
40. C.M. Ormerod, Tropical geometric interpretation of ultradiscrete singularity confinement. J. Phys. A **46**(30), 305204, 15 (2013)
41. C.M. Ormerod, Y. Yamada, From polygons to ultradiscrete Painlevé equations. SIGMA Symmetry Integrability Geom. Methods Appl. **11**, 36 pp. (2015). Paper 056
42. P. Painlevé, Sur les équations différentielles du second ordre et d'ordre supérieur dont l'intégrale générale est uniforme. Acta Math. **25**(1), 1–85 (1902)
43. G.R.W. Quispel, J.A.G. Roberts, C.J. Thompson, Integrable mappings and soliton equations. Phys. Lett. A **126**(7), 419–421 (1988)
44. A. Ramani, B. Grammaticos, J. Hietarinta, Discrete versions of the Painlevé equations. Phys. Rev. Lett. **67**(14), 1829–1832 (1991)

45. A. Ramani, D. Takahashi, B. Grammaticos, Y. Ohta, The ultimate discretisation of the Painlevé equations. Phys. D **114**(3–4), 185–196 (1998)
46. H. Sakai, Rational surfaces associated with affine root systems and geometry of the Painlevé equations. Commun. Math. Phys. **220**(1), 165–229 (2001)
47. D. Takahashi, On some soliton systems defined by using boxes and balls, in *International Symposium on Nonlinear Theory and its Applications* (*NOLTA* '93), pp. 555–558 (1993)
48. D. Takahashi, J. Matsukidaira, Box and ball system with a carrier and ultradiscrete modified KdV equation. J. Phys. A **30**(21), L733–L739 (1997)
49. D. Takahashi, J. Satsuma, A soliton cellular automaton. J. Phys. Soc. Japan **59**(10), 3514–3519 (1990)
50. D. Takahashi, T. Tokihiro, B. Grammaticos, Y. Ohta, A. Ramani, Constructing solutions to the ultradiscrete Painlevé equations. J. Phys. A **30**(22), 7953–7966 (1997)
51. K. Takemura, T. Tsutsui, Ultradiscrete Painlevé VI with parity variables. SIGMA Symmetry Integrability Geom. Methods Appl. **9**, 12 pp. (2013). Paper 070
52. T. Tokihiro, D. Takahashi, J. Matsukidaira, J. Satsuma, From soliton equations to integrable cellular automata through a limiting procedure. Phys. Rev. Lett. **76**, 3247–3250 (1996)
53. T. Tokihiro, D. Takahashi, J. Matsukidaira, Box and ball system as a realization of ultradiscrete nonautonomous KP equation. J. Phys. A **33**(3), 607–619 (2000)
54. N.J. Zabusky, M.D. Kruskal, Interaction of solitons in a collisionless plasma and the recurrence of initial states. Phys. Rev. Lett. **15**, 240–243 (1965)

Elliptic Hypergeometric Functions

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Abstract These lecture notes discuss some of the basics of elliptic hypergeometric functions. These are fairly recent generalizations of ordinary hypergeometric functions. In this chapter we first discuss both ordinary hypergeometric functions and elliptic functions, as you need to know both to define elliptic hypergeometric series. We subsequently discuss some of the important properties these series satisfy, in particular we consider the biorthogonal functions found by Spiridonov and Zhedanov, both with respect to discrete and continuous measure. In doing so we naturally encounter the most important evaluation and transformation formulas for elliptic hypergeometric series, and for the associated elliptic beta integral.

1 Introduction

While the theory of ordinary and basic hypergeometric functions goes back to the time of Euler and Gauß, the study of elliptic hypergeometric functions only started in the late 1990s, after the publication of a paper [2] by Frenkel and Turaev. As a testament to the usefulness of hypergeometric functions, and specifically also elliptic hypergeometric functions, Frenkel and Turaev introduced the elliptic hypergeometric functions when studying solutions to the Yang-Baxter equation. Since then, elliptic hypergeometric functions have appeared in many other applications. To get an impression of their applications you can browse the list of papers on elliptic hypergeometric functions on the website of Rosengren (see the note at the top of the bibliography).

Given the name, it might come as no surprise that to understand elliptic hypergeometric series and integrals it is important to understand both ordinary hypergeometric functions and elliptic functions. The theory of elliptic hypergeometric functions is really a reflection of the theory for ordinary hypergeometric functions, but usually twisted in a slightly more complicated way. One of the questions one should often ask is "I know hypergeometric functions satisfy this property,

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does it have an elliptic hypergeometric analogue?" and the other way around "What is the ordinary/basic hypergeometric version of this elliptic hypergeometric result?" On the other hand the basic building blocks for elliptic hypergeometric series are elliptic functions, so it is important to know the basic properties of elliptic functions as well.

This explains the order of these notes: First we briefly discuss the basics of (basic) hypergeometric series, then the basics of elliptic functions, before we consider the elliptic hypergeometric functions themselves. We then continue by showcasing a few of the most important identities satisfied by elliptic hypergeometric functions. In particular we will be focused on the generalizations of the classical orthogonal polynomials (Legendre, Jacobi, Wilson, etc.) to the elliptic level.

2 Hypergeometric Series

A general reference for ordinary hypergeometric functions is [1].

Definition 2.1 A hypergeometric series is a series $\sum d_n$ for which the quotient of two subsequent terms $r(n) = d_{n+1}/d_n$ is a rational function of n.

The name hypergeometric originates from the geometric series $\sum_{k=0}^{\infty} x^k = 1/(1-x)$, which is a special case of hypergeometric series where the quotient $r(n)$ is a constant function. Other examples of hypergeometric series are $\mathrm{e}^x = \sum_{n=0}^{\infty} x^n/(n!)$ and the binomial $(1+x)^n = \sum_{k=0}^{n} \binom{n}{k} x^k$.

Notice that any rational function can be factored

$$r(n) = \frac{(n+a_1)(n+a_2)\cdots(n+a_r)}{(n+b_1)(n+b_2)\cdots(n+b_s)}z.$$

Thus the zeros are at $n = -a_j$ and the poles at $n = -b_j$. This means that

$$d_n = d_0 \prod_{k=0}^{n-1} r(k) = d_0 \frac{(a_1, a_2, \ldots, a_r)_n}{(b_1, b_2, \ldots, b_s)_n} z^n$$

where we use the notation

Definition 2.2 The pochhammer symbol $(a)_n$ is defined for $n \in \mathbb{Z}_{\geq 0}$ as

$$(a)_n = \prod_{k=0}^{n-1} (a+k) \ .$$

Note that this implies that $(a)_0 = 1$. We use an abbreviations for products of these pochhammer symbols:

$$(a_1, a_2, \ldots, a_r)_n = (a_1)_n (a_2)_n \cdots (a_r)_n$$

Considering this general expression for the terms of a hypergeometric series we introduce the notation

Definition 2.3 The hypergeometric series are defined as

$$ {}_rF_s\left[\begin{matrix}a_1,\dots,a_r\\ b_1,\dots,b_s\end{matrix};z\right]=\sum_{n=0}^{\infty}\frac{(a_1,\dots,a_r)_n}{(1,b_1,\dots,b_s)_n}z^n\,. $$

Notice the 1 which is always added as a numerator parameter. First of all $(1)_n = n!$, so it indeed appears in the series we gave before. Indeed we have

$$ \mathrm{e}^x={}_0F_0\left[\begin{matrix}-\\ -\end{matrix};x\right],\quad (1+x)^n={}_1F_0\left[\begin{matrix}-n\\ -\end{matrix};-x\right]. $$

Thus it often saves us some writing. But more importantly it means that the summand $d_n = 0$ for $n < 0$ (in generic cases), so the starting point of our series is an inherent boundary. If you really do not want the 1 as a b-parameter, you can add it as an a-parameter, after which the $(1)_n$ in the numerator cancels to the $(1)_n$ in the denominator, so the geometric series is written as $1/(1-x) = {}_1F_0(1;-;x)$.

For positive integer n the series for $(1+x)^n$ only contains a finite number of nonzero terms. Such a series is called a *terminating* hypergeometric series. You can easily spot them in the ${}_rF_s$ notation, as one of the numerator arguments must be a negative integer.

To consider a series as an analytic function, we need to consider whether it converges. Since hypergeometric series are defined by a pretty property for the quotient of two subsequent terms, the ratio test can be easily applied. Indeed we have to consider the limit $\lim_{n\to\infty} r(n)$. Any rational function has a limit at infinity, and this gives the following result for the convergence of hypergeometric series:

Theorem 2.4 *The series* ${}_rF_s(a_1,\dots,a_r;b_1,\dots,b_s;z)$ *converges if one of the following holds*

- *It is terminating*
- *If* $r \le s$
- *If* $r = s+1$ *and* $|z| < 1$

and it diverges if one of the following holds

- *It is nonterminating and* $r > s+1$
- *It is nonterminating and* $r = s+1$ *and* $|z| > 1$.

Hypergeometric series are intricately linked to the Gamma function.

Definition 2.5 The Gamma function is defined as the unique meromorphic function which equals

$$ \Gamma(z)=\int_0^{\infty} t^{z-1}\mathrm{e}^{-t}\,\mathrm{d}t $$

for $\Re(z) > 0$.

Note that $\Gamma(z+1) = z\Gamma(z)$ (by integration by parts), so we can easily extend the domain of the function to $\mathbb{C} \setminus \mathbb{Z}_{\leq 0}$ once we have defined it for $\Re(z) > 0$. This difference equation also ensures that Γ has simple poles at $\mathbb{Z}_{\leq 0}$, as it would imply for example that for $\Re(z) > -1$ we have $\Gamma(z) = (1/z)\int_{t=0}^{\infty} t^z \mathrm{e}^{-t}\,\mathrm{d}t$, which is an analytic function times $1/z$. The first relation to hypergeometric series comes from the fact that

$$(a)_n = \frac{\Gamma(a+n)}{\Gamma(a)}$$

which only uses the difference equation for the Gamma function. Thus hypergeometric series can be written as

$${}_rF_s\left[\begin{matrix} a_1, \ldots, a_r \\ b_1, \ldots b_s \end{matrix}; z\right] = \frac{\Gamma(1, b_1, \ldots, b_s)}{\Gamma(a_1, \ldots, a_r)} \sum_{n=0}^{\infty} \frac{\Gamma(a_1+n, \ldots, a_r+n, 1)}{\Gamma(1+n, b_1+n, \ldots, b_s+1)} z^n$$

using the same abbreviation for products of Gamma functions as we introduced before for pochhammer symbols. The second relation to hypergeometric series comes from integrals. Consider the integral (over a complex contour)

$$\int_{-i\infty}^{i\infty} \frac{\Gamma(a+s, b+s, -s)}{\Gamma(c+s)} (-z)^s \frac{\mathrm{d}s}{2\pi \mathrm{i}}$$

where the integration contour separates the poles of $\Gamma(a+s)$ and $\Gamma(b+s)$ from those of $\Gamma(-s)$. (Notice that $1/\Gamma(z)$ is an entire function). The contour, and the poles are pictured in Fig. 1.

The $(-z)^s$ is defined using a branch cut at the negative real axis (for $-z$, so not for the integration variable s). Shifting the contour to the right we encounter all the

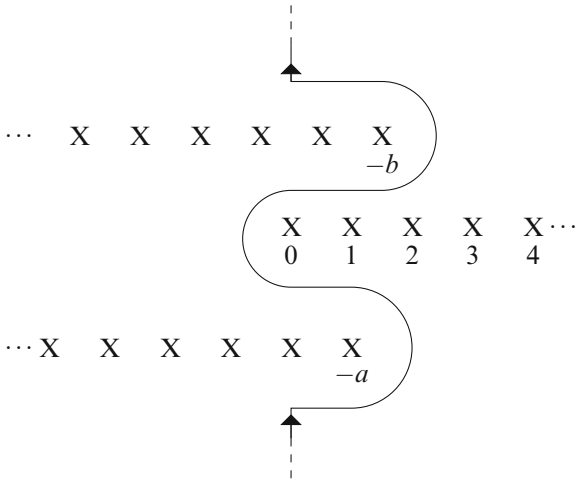


Fig. 1 The contour for the Barnes' integral weaves between the poles of the integrand

poles of $\Gamma(-s)$. If we move the contour over those poles, the limit of the resulting integral goes to zero (use Stirling's formula to prove this). Thus the result of the original integral is the infinite series of residues we have to pick up. That is

$$\begin{aligned}
&\int_{-i\infty}^{i\infty} \frac{\Gamma(a+s,b+s,-s)}{\Gamma(c+s)}(-z)^s \frac{\mathrm{d}s}{2\pi \mathrm{i}} \\
&= \sum_{n=0}^{\infty} \operatorname{Res}\left(\frac{\Gamma(a+s,b+s,-s)}{\Gamma(c+s)}(-z)^s, s=n\right) \\
&= \operatorname{Res}\left(\frac{\Gamma(a+s,b+s,-s)}{\Gamma(c+s)}(-z)^s, s=0\right) \sum_{n=0}^{\infty} \frac{\operatorname{Res}\left(\frac{\Gamma(a+s,b+s,-s)}{\Gamma(c+s)}(-z)^s, s=n\right)}{\operatorname{Res}\left(\frac{\Gamma(a+s,b+s,-s)}{\Gamma(c+s)}(-z)^s, s=0\right)} \\
&= \frac{\Gamma(a,b)}{\Gamma(c)} \sum_{n=0}^{\infty} \frac{(a,b)_n}{(c,-n)_n}(-z)^n = \frac{\Gamma(a,b)}{\Gamma(c)} \sum_{n=0}^{\infty} \frac{(a,b)_n}{(c,1)_n} z^n
\end{aligned}$$

which is the hypergeometric series ${}_2F_1$. Thus integrals involving Gamma functions are related to hypergeometric series by the picking up of residues. And a third relation is that a hypergeometric series can sometimes be evaluated, that is, written without an infinite sum in terms of simple functions, using Gamma functions. For example the famous evaluation (for convergent series)

$$ {}_2F_1\left[\begin{matrix} a,b \\ c \end{matrix}; 1\right] = \frac{\Gamma(c,c-a-b)}{\Gamma(c-b,c-a)} \,. \tag{1}$$

Exercise 2.6 Use Stirling's formula to show that the Gauß hypergeometric series ${}_2F_1(a,b;c;1)$ converges for $\Re(c-a-b) > 0$. When does a hypergeometric series ${}_{r+1}F_r$ evaluated at $z=1$ converge?

Exercise 2.7 Fill in the details of the derivation that

$$\int_{-i\infty}^{i\infty} \frac{\Gamma(a+s,b+s,-s)}{\Gamma(c+s)}(-z)^s \frac{\mathrm{d}s}{2\pi \mathrm{i}} = \frac{\Gamma(a,b)}{\Gamma(c)} {}_2F_1\left[\begin{matrix} a,b \\ c \end{matrix}; 1\right].$$

That is, show that (when the series converges) the integrand converges to zero as $\Re(s) \to \infty$.

3 Basic Hypergeometric Series

A generalization of the hypergeometric series are the basic hypergeometric, or q-hypergeometric series. The basic reference on this topic is [3].

Definition 3.1 A basic hypergeometric series is a series $\sum d_n$ for which the quotient of two subsequent terms $r(n) = d_{n+1}/d_n$ is a rational function of q^n.

We will assume from now on that $|q| < 1$. Notice that this means that $r(n)$ is periodic with period $2\pi \mathrm{i}/\log(q)$. Many results from ordinary hypergeometric series generalize. There exists a q-Gamma function which generalizes the ordinary Gamma function, but it is actually often more convenient to work with the q-pochhammer symbols:

Definition 3.2 The q-pochhammer symbols are defined for $n \in \mathbb{N} \cup \{\infty\}$ as

$$(a;q)_n = \prod_{k=0}^{n-1}(1-aq^k) ,$$

For $n = \infty$ we often omit the subscript;

Notice that the infinite product $(a;q) = (a;q)_\infty$ converges for $|q| < 1$. If the rational function is factored as

$$r(n) = \frac{(1-a_1q^n)\cdots(1-a_rq^n)}{(1-b_1q^n)\cdots(1-b_sq^n)}z$$

then we can express the terms in the series using the q-pochhammer symbols as

$$d_n = d_0 \frac{(a_1,\ldots,a_r;q)_n}{(b_1,\ldots,b_s;q)_n} z^n .$$

Notice that $\lim_{n\to\infty} r(n) = z$, so the q-hypergeometric series converge for $|z| < 1$.

We want to keep this discussion brief, so we will end with mentioning that the limit $q \to 1$ returns us to the theory of ordinary hypergeometric series, as

$$\lim_{q\to 1} \frac{(q^a;q)_n}{(1-q)^n} = \prod_{k=0}^{n-1} \lim_{q\to 1} \frac{1-q^{a+k}}{1-q} = \prod_{k=0}^{n-1}(a+k) = (a)_n .$$

4 Elliptic Functions

As for information about elliptic functions, I like the by now ancient *Modern Analysis* [12]. We just need a few basic results.

Definition 4.1 An elliptic function is a meromorphic function $f\colon \mathbb{C} \to \mathbb{C}$ which is periodic in two directions. That is, there are $\omega_1, \omega_2 \in \mathbb{C} \setminus \{0\}$ with $\omega_2/\omega_1 \notin \mathbb{R}$ such that $f(z+\omega_i) = f(z)$ for $i = 1, 2$.

We will often write elliptic functions as functions of $x = q^z$ instead of as functions of z. One of the two periods is then equal to $2\pi\mathrm{i}/\log(q)$. If we write the other period as $\log(p)/\log(q)$, we see that $f(x) = f(q^z) = f(q^{z+\log(p)/\log(q)}) = f(px)$. Thus we say a function is p-elliptic if it is invariant under multiplying the argument by a factor p. In this section we will not use this notation yet, but we will once we get to elliptic hypergeometric series.

It can be convenient to consider the group $\omega_1\mathbb{Z} + \omega_2\mathbb{Z}$ (under addition) which acts on $\mathbb{C}$. A fundamental domain of this action is the parallelogram with vertices 0, ω_1, $\omega_1 + \omega_2$ and ω_2.

It should be realized that the condition of ellipticity is a rather strict condition. For example

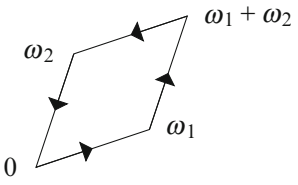
Theorem 4.2 *An analytic, elliptic function is constant.*

Proof Let f be an analytic, elliptic function. On the closure of the fundamental domain f is a continuous function on a compact domain, hence it is bounded. But as it takes all its values on this fundamental domain, f is bounded on $\mathbb{C}$. Liouville's theorem now shows that f must be constant. □

Moreover it can have only as many zeros as poles

Theorem 4.3 *If f is an elliptic function, which is not constant zero, then it has as many poles as zeros counted with multiplicity.*

Proof Assume no poles/zeros are located on the boundary of the fundamental domain D. If there are, you should shift the fundamental domain so that this is the case (which is possible since there are at most countably many poles/zeros). Then consider the integral $\int_{\partial D} f'(z)/f(z)\,\mathrm{d}z/(2\pi\mathrm{i})$ which gives the difference between the number of poles and the number of zeros. The contour consists of four parts: let's call the line from 0 to ω_1 the bottom, the line from ω_1 to $\omega_1 + \omega_2$ the right side, the line from $\omega_1 + \omega_2$ to ω_2 the top, and the line from ω_2 back to 0 the left side. This is consistent with the following picture (note that if the orientation of the contour is different the argument remains the same)



This integral now evaluates to zero, as the part of the integral over the left edge of the fundamental domain equals the part of the integral over the right edge with opposite orientation. (One shift by a period does not change the integrand). Thus the left and right edge cancel each other. Likewise for the top and bottom edge. □

And you can even prove

Theorem 4.4 *If an elliptic function f has poles in a fundamental domain at $p_1, \ldots, p_k$ and zeros at $z_1, \ldots, z_k$ (multiple poles/zeros listed multiple times) then $\sum_{n=1}^{k} p_n = \sum_{n=1}^{k} z_n \bmod \omega_1\mathbb{Z} + \omega_2\mathbb{Z}$.*

Proof Consider the contour integral $\int_{\partial D} zf'(z)/f(z)\,\mathrm{d}z/(2\pi\mathrm{i}z)$, with the contour as before. Now the integral of the bottom edge plus the integral of the top edge equals the integral $-\omega_2 \int f'(z)/f(z)\,\mathrm{d}z/(2\pi\mathrm{i})$ along the bottom edge 0 to ω_1. However since $f(\omega_1)$ and $f(0)$ are identical, the difference $\log(f)(\omega_1) - \log(f)(0)$ must be a multiple of $2\pi\mathrm{i}$. Thus the sum of the integrals over the bottom edge and the top edge is an integer multiple of ω_2. Likewise the sum of the integrals over the left and right edges equals an integer multiple of ω_1. □

Together the last two theorems imply that no elliptic function with just a single pole/zero in a fundamental domain exists. This fact can often be used to prove identities for elliptic functions:

> If you can show an elliptic function has at most one pole in a fundamental domain, it must be constant!

5 Elliptic Hypergeometric Series

Elliptic hypergeometric series first appeared in [2], in which Frenkel and Turaev were considering solutions to the Yang–Baxter equation. In the second edition of [3] a chapter was added about elliptic hypergeometric series, which gives a nice overview, but for some aspects it was written a bit prematurely as the theory was at the time in big development. A nice introduction, a little more expansive than this one, can be found in the recent lecture notes [7] by Rosengren.

The definition of elliptic hypergeometric series should not come as a surprise anymore:

Definition 5.1 An elliptic hypergeometric series is a series $\sum d_n$ for which the quotient of two subsequent terms $r(n) = d_{n+1}/d_n$ is an elliptic function of n.

We would like to proceed as before by factoring the quotient $r(n)$ in elementary building blocks for elliptic functions, but we can't do that using elliptic functions. Indeed nonconstant elliptic functions must always have both multiple zeros and multiple poles, so they won't function well as bricks in our construction. Therefore we consider the theta functions

Definition 5.2 We define the theta functions as

$$\theta(x;p) = (x, p/x; p)_\infty = \prod_{k=0}^{\infty}(1 - p^k x)(1 - p^{k+1}/x)\ .$$

The associated theta pochhammer symbols are given by

$$\theta(x;p;q)_n = \theta(x;p)_n = \prod_{k=0}^{n-1} \theta(xq^k;p)$$

(where we often suppress the q-dependence).

These theta functions are a different way of writing the Jacobi theta function. The product formula is related to the Jacobi theta function using the famous Jacobi triple product formula:

$$(x, q/x, q; q)_\infty = \sum_{k=-\infty}^{\infty} q^{k(k-1)/2}(-x)^k \ .$$

Now observe that these theta functions have a simple behavior if you multiply x by p:

$$\theta(px;p) = \theta(1/x;p) = (1/x, px; p) = \frac{(1-1/x)}{1-x}(p/x, x; p) = -\frac{1}{x}\theta(x;p) \ .$$

So if we now write

$$r(n) = \frac{\theta(a_1q^n, \ldots, a_rq^n; p)}{\theta(b_1q^n, \ldots, b_rq^n; p)}z$$

we have a function which has one period $2\pi i/\log(q)$ and a second period $\log(p)/\log(q)$ if the balancing condition $\prod_{k=1}^{r} a_k = \prod_{r=1}^{r} b_k$ holds (and observe that we have to take as many numerator terms as denominator terms). Note that $\theta(aq^n;p)$ is an entire function of n and in a fundamental domain of $2\pi \mathrm{i}/\log(q)\mathbb{Z} + \log(p)/\log(q)\mathbb{Z}$ it has a single zero. Thus these theta functions allow us to write elliptic functions with given zeros and poles as a simple product. Like the ${}_rF_s$ notation we now define

Definition 5.3 If the balancing condition $a_1a_2\cdots a_r = qb_1b_2\cdots b_{r-1}$ holds then we define

$${}_rE_{r-1}\left[\begin{matrix} a_1, \ldots, a_r \\ b_1, \ldots, b_{r-1} \end{matrix}; z\right] = \sum_{k=0}^{\infty} \frac{\theta(a_1, \ldots, a_r; p)_k}{\theta(q, b_1, \ldots, b_{r-1}; p)_k} z^k \ .$$

Let us consider the convergence of this series. The ratio test does not work as the limit as the argument of an elliptic function goes to infinity does not exist. While you can have convergent elliptic hypergeometric nonterminating series, in practice everybody only works with terminating series. That is series with a $\theta(q^{-n};q)_k$ in the numerator, which becomes 0 for $k > n$.

It turns out that most results, and the only series we will encounter throughout these lecture notes, are so-called very well-poised series, which are a special case:

Definition 5.4 Assuming r is even and the balancing condition

$$b_1 b_2 \cdots b_{r-6} = a^{r/2-3} q^{r/2+n-4}$$

holds, the terminating very-well-poised series is given by

$$\begin{aligned} {}_rV_{r-1}(a; b_1, \ldots, b_{r-6}, q^{-n}; q, p) \\ &= {}_rE_{r-1}\left[\begin{matrix} a, \pm q\sqrt{a}, \pm q\sqrt{ap}, b_1, \ldots, b_{r-6}, q^{-n} \\ \pm\sqrt{a}, \pm\sqrt{ap}, aq/b_1, \ldots, aq/b_{r-6}, aq^{n+1} \end{matrix}; q\right] \\ &= \sum_{k=0}^{n} \frac{\theta(aq^{2k}; p)}{\theta(a; p)} \frac{\theta(a, b_1, \ldots, b_{r-6}, q^{-n}; p)_k}{\theta(q, aq/b_1, \ldots, aq/b_{r-6}, aq^{n+1}; p)_k} q^k \,. \end{aligned}$$

Proof of equivalence of two expressions above Here we use

$$\begin{aligned} \theta(x; p)_{2k} &= \prod_{r=0}^{2k-1} (xq^r, pq^{-r}/x; p) = \prod_{r=0}^{2k-1} \prod_{s=0}^{\infty} (1 - xq^r p^s)(1 - p^{s+1} q^{-r}/x) \\ &= \prod_{r=0}^{2k-1} \prod_{s=0}^{\infty} (1 - \sqrt{x} q^{r/2} p^{s/2})(1 + \sqrt{x} q^{r/2} p^{s/2}) \\ &\qquad \times (1 - p^{(s+1)/2} q^{-r/2}/\sqrt{x})(1 + p^{(s+1)/2} q^{-r/2}/\sqrt{x}) \\ &= \prod_{r=0}^{2k-1} (\pm\sqrt{x} q^{r/2}, \pm\sqrt{px} q^{r/2}, \pm q^{-r/2}\sqrt{p/x}, \pm pq^{-r/2}/\sqrt{x}; p) \\ &= \prod_{r=0}^{2k-1} \theta(\pm\sqrt{x} q^{r/2}, \pm\sqrt{px} q^{r/2}; p) \\ &= \theta(\pm\sqrt{x}, \pm\sqrt{qx}, \pm\sqrt{px}, \pm\sqrt{pqx}; p)_k \end{aligned}$$

which implies

$$\begin{aligned} \frac{\theta(aq^{2k}; p)}{\theta(a; p)} = \frac{\theta(aq; p)_{2k}}{\theta(a; p)_{2k}} &= \frac{\theta(\pm\sqrt{aq}, \pm q\sqrt{a}, \pm\sqrt{pqa}, \pm q\sqrt{pa}; p)_k}{\theta(\pm\sqrt{a}, \pm\sqrt{aq}, \pm\sqrt{ap}, \pm\sqrt{apq}; p)_k} \\ &= \frac{\theta(\pm q\sqrt{a}, \pm q\sqrt{ap}; p)_k}{\theta(\pm\sqrt{a}, \pm\sqrt{ap}; p)_k} \,. \end{aligned}$$

□

It should be noted that for ordinary and basic hypergeometric series we have

$$\frac{a+2k}{a} = \frac{(a/2+1)_k}{(a/2)_k} , \quad \frac{1-aq^{2k}}{1-a} = \frac{(\pm q\sqrt{a};q)_k}{(\pm\sqrt{a};q)_k}$$

thus we only need 1 or 2 parameters for this first factor instead of 4. So a very well-poised ${}_{10}V_9$ corresponds to the basic hypergeometric very-well poised ${}_8W_7$, and the ordinary hypergeometric very-well poised ${}_7F_6$.

As far as I know, all identities for elliptic hypergeometric series (and integrals) are based on a single identity:

Theorem 5.5 *For $w,x,y,z \in \mathbb{C} \setminus \{0\}$ we have*

$$\frac{1}{y}\theta(wx^{\pm 1}, yz^{\pm 1}; p) + \frac{1}{z}\theta(wy^{\pm 1}, zx^{\pm 1}; p) + \frac{1}{x}\theta(wz^{\pm 1}, xy^{\pm 1}; p) = 0 .$$

Proof One of the most common techniques for proving identities involving theta functions is to use the argument that elliptic functions with more zeros than poles are constant zero. Let us consider what happens if we change $w \to pw$. Then the first term becomes

$$\begin{aligned}\frac{1}{y}\theta(pwx^{\pm 1}, yz^{\pm 1}; p) &= \frac{1}{y}\theta(wx^{\pm 1}, yz^{\pm 1}; p)\Big(-\frac{1}{wx}\Big)\Big(-\frac{x}{w}\Big) \\ &= \frac{1}{y}\theta(wx^{\pm 1}, yz^{\pm 1}; p)\frac{1}{w^2} .\end{aligned}$$

By symmetry the other two terms are also multiplied by $1/w^2$ upon setting $w \to pw$. So we do not have an elliptic function (it could not really be because it is analytic and has zeros). However if we divide by the first term the left-hand side does become an elliptic function in w, which is even (invariant under $w \to 1/w$)

$$f(w) = 1 + \frac{y}{z}\frac{\theta(wy^{\pm 1}, zx^{\pm 1}; p)}{\theta(wx^{\pm 1}, yz^{\pm 1}; p)} + \frac{y}{x}\frac{\theta(wz^{\pm 1}, xy^{\pm 1}; p)}{\theta(wx^{\pm 1}, yz^{\pm 1}; p)} .$$

In a fundamental domain, this function has at most a (simple) pole at $w = x$ and $w = x^{-1}$. If we set $w = z$ we obtain that the function vanishes:

$$f(z) = 1 + \frac{y}{z}\frac{\theta(zy^{\pm 1}, zx^{\pm 1}; p)}{\theta(zx^{\pm 1}, yz^{\pm 1}; p)} + 0 = 1 + \frac{y}{z}\frac{\theta(z/y; p)}{\theta(y/z; p)} = 0 ,$$

using the identity $\theta(1/x; p) = -(1/x)\theta(x; p)$. Likewise there are zeros at $w = y^{\pm 1}$ and $w = z^{-1}$. As a nonconstant elliptic function with at most two poles can have at most two zeros the function $f(w)$ must therefore be constant zero. □

As a generalization of the ordinary Gamma function, there is an elliptic Gamma function [9] which satisfies the simple difference equation

$$\Gamma_{\mathrm{e}}(qx) = \theta(x; p)\Gamma_{\mathrm{e}}(x) ,$$

ensuring that

$$\theta(x;p)_k = \frac{\Gamma_{\mathrm{e}}(xq^k)}{\Gamma_{\mathrm{e}}(x)} .$$

This is a reflection of the difference relation $\Gamma(z+1) = z\Gamma(z)$ and $(a)_k = \Gamma(a+k)/\Gamma(a)$ for the ordinary Gamma function.

Definition 5.6 The elliptic Gamma function is defined as

$$\Gamma_{\mathrm{e}}(x) = \Gamma_{\mathrm{e}}(x;p,q) = \prod_{r,s\geq 0} \frac{1-p^{r+1}q^{s+1}/x}{1-p^rq^sx} .$$

Notice that the elliptic Gamma function is symmetric under $p \leftrightarrow q$. In a specific way you can consider it to be the simplest function satisfying the difference equations $\Gamma_{\mathrm{e}}(qx) = \theta(x;p)\Gamma_{\mathrm{e}}(x)$ and $\Gamma_{\mathrm{e}}(px) = \theta(x;q)\Gamma_{\mathrm{e}}(x)$. Where the ordinary Gamma function has poles at the negative integers, the elliptic Gamma function has (generically simple) poles at $x = p^{\mathbb{Z}_{\leq 0}}q^{\mathbb{Z}_{\leq 0}}$; as any function must if it is to satisfy the two difference equations. Just to be explicit: the elliptic Gamma function is itself not an elliptic function, however it can be used to simply express elliptic hypergeometric series.

Exercise 5.7 Prove the following basic relations for theta functions:

(a) $\theta(px;p) = \theta(1/x;p)$
(b) $\theta(p^nx;p) = (-1/x)^np^{-\binom{n}{2}}\theta(x;p)$

Exercise 5.8 Prove the following basic relations for the elliptic Gamma function:

(a) Reflection identity: $\Gamma_{\mathrm{e}}(x,pq/x) = 1$
(b) Limit: $\lim_{p\to 0}\Gamma_{\mathrm{e}}(x;p,q) = 1/(z;q)_\infty$
(c) Quadratic transformation: $\Gamma_{\mathrm{e}}(x^2;p,q) = \Gamma_{\mathrm{e}}(\pm x;\sqrt{p},\sqrt{q})$
(d) Quadratic transformation: $\Gamma_{\mathrm{e}}(x;p,q) = \Gamma_{\mathrm{e}}(x,qx;p,q^2)$

Exercise 5.9 Calculate the residue

$$\mathrm{Res}\left(\frac{1}{z}\Gamma_{\mathrm{e}}(az);z=1/a\right) = \frac{1}{(p;p)(q;q)} .$$

Exercise 5.10 Show that an ${}_rV_{r-1}$ is a p-elliptic function of its arguments, as long as the balancing condition $b_1b_2\cdots b_{r-6} = a^{r/2-3}q^{r/2+n-4}$ remains satisfied. Thus for example

$${}_rV_{r-1}(a;b_1,\ldots,b_{r-6},q^{-n};q,p) = {}_rV_{r-1}(a;pb_1,b_2/p,b_3,\ldots,b_{r-6},q^{-n};q,p) .$$

6 6*j*-Symbols and Spiridonov–Zhedanov Biorthogonal Functions

This section introduces the biorthogonal functions of Spiridonov and Zhedanov [11].

The Askey scheme and q-Askey scheme [4] contain many families of orthogonal polynomials. We will not reprint them here, because the schemes take up a lot of space. Basically they contain all classical families of orthogonal polynomials[1]. The (q)-Askey scheme can even be generalized to include pairs of families of biorthogonal rational functions. That is: we consider two families of rational functions $\mathcal{F} = \{f_0, f_1, \dots\}$ and $\mathcal{G} = \{g_0, g_1, \dots\}$ and a bilinear form such that $\langle f_n, g_m \rangle = \delta_{nm}\mu_n$. Generalizing in this way you can make the schemes a few times larger. On the elliptic level the scheme for pairs of families of biorthogonal functions becomes very simple: There is just one family.

However, everything in the (q-)Askey scheme is a limit of this family. To be completely honest this is not completely fair, as there are biorthogonal functions with respect to a continuous measure, and specializing the product of two parameters to q^{-N} you obtain biorthogonality with respect to a finite point measure (for a finite set of functions). This difference is similar to the relation of Wilson to Racah polynomials. So in a way you might consider there to be two pairs of families of biorthogonal functions. In this section we will focus on the discrete biorthogonality on a measure with finite support, while in Sect. 8 we consider the continuous measure. In Exercise 8.6 you can verify the relation between these two measures yourselves.

I feel that Rosengren's [8] elementary derivation of the biorthogonality using 6*j*-symbols is a nice exposition, so I will follow that here. We first introduce the functions

$$h_k(x;a) = \theta(a\xi, a\xi^{-1}; p)_k \,, \quad \xi + \xi^{-1} = x \,.$$

which are entire functions of x for $a \neq 0$. Then we can consider (for given N, a and b) the set of functions

$$\mathcal{B} = \{h_k(x;a)h_{N-k}(x;b) \mid 0 \leq k \leq N\} \,.$$

Then these $N+1$ functions are all of the form $f(x) = \prod_{j=1}^{N} \theta(a_j\xi, a_j\xi^{-1}; p)$. That is, writing $\xi = \mathrm{e}^{2\pi \mathrm{i} z}$ and $F(z) = f(\mathrm{e}^{2\pi \mathrm{i} z} + \mathrm{e}^{-2\pi \mathrm{i} z})$, we have even theta functions of degree $2N$ with characteristic 0, which means these functions satisfy: $f(-z) = f(z)$, $f(z+1) = f(z)$ and $f(z+\tau) = \mathrm{e}^{-2\pi \mathrm{i} N(2z+\tau)} f(z)$ where $p = \mathrm{e}^{2\pi \mathrm{i} \tau}$. These functions

[1] You might ask: What is classical? There are many different definitions based on properties such a classical family should have, which result in different families being called classical or not. As far as I know any definition includes only families from the (q)-Askey scheme, but some are more restrictive. I just use the definition "Everything in the (q-)Askey scheme is classical."

form a space of degree $N+1$. It turns out that if

$$p^m a/b \notin \{q^k \mid 1-N \leq k \leq N-1\}\,, \quad p^m ab \notin \{q^k \mid 0 \leq k \leq N-1\}$$

the functions in $\mathcal{B}$ form a basis of this space. But if we replace the parameters a and b by c and d, we obtain another basis for this same space. As such there is a basis transformation

$$h_k(x;a)h_{N-k}(x;b) = \sum_{l=0}^{N} R_k^l(a,b,c,d;N;q,p)h_l(x;c)h_{N-l}(x;d)\,.$$

Let us calculate these coefficients R_k^l. First we prove a binomial theorem

Theorem 6.1 *We have*

$$h_N(x;a) = \sum_{k=0}^{N} C_k^N(a,b,c)h_k(x;b)h_{N-k}(x;c)$$

with

$$C_k^N = q^{k(k-N)}\frac{\theta(q;p)_N\theta(a/c,q^{N-k}ac;p)_k\theta(a/b,abq^k;p)_{N-k}}{\theta(bc;p)_N\theta(q,(b/c)q^{k-N};p)_k\theta(q,(c/b)q^{-k};p)_{N-k}}\,.$$

Compare this theorem to $(x+y)^N = \sum_{k=0}^{N}\binom{N}{k}x^k y^{N-k}$.

Proof We will prove this using recurrence relations for the binomial coefficients, so let us see what happens if we increase N by one: First of all

$$h_{N+1}(x;a) = h_N(x;a)\theta(a\xi q^N, a\xi^{-1}q^N;p)\,.$$

To get a nice expression on the right-hand side we have to somehow write

$$h_k(x;b)h_{N-k}(x;c)\theta(a\xi q^N, a\xi^{-1}q^N;p) \\ = c_1 h_k(x;b)h_{N-k+1}(x;c) + c_2 h_{k+1}(x;b)h_{N-k}(x;c)\,,$$

that is

$$\theta(a\xi q^N, a\xi^{-1}q^N;p) = c_1\theta(c\xi q^{N-k}, c\xi^{-1}q^{N-k};p) + c_2\theta(b\xi q^k, b\xi^{-1}q^k;p)\,.$$

Now we need to find an identity between three terms involving theta functions, so we hope we can apply Theorem 5.5. We have got three terms of the form $\theta(s\xi^{\pm 1};p)$ for $s = aq^N$, $s = cq^{N-k}$ and $s = bq^k$, so we know what the parameters in Theorem 5.5 should be. Taking $w = \xi$, $x = aq^N$, $y = bq^k$ and $z = cq^{N-k}$ the identity from the theorem becomes

$$\frac{1}{bq^k}\theta(\xi aq^N,\xi a^{-1}q^{-N},bcq^N,\frac{b}{c}q^{2k-N};p)$$
$$+\frac{1}{cq^{N-k}}\theta\left(\xi bq^k,\xi b^{-1}q^{-k},acq^{2N-k},\frac{c}{a}q^{-k};p\right)$$
$$+\frac{1}{aq^N}\theta\left(\xi cq^{N-k},\xi c^{-1}q^{k-N},abq^{N+k},\frac{a}{b}q^{N-k};p\right)=0\,.$$

Using $\theta(1/x;p)=-(1/x)\theta(x;p)$ we can clean this up to

$$\theta\left(a\xi q^N,a\xi^{-1}q^N,bcq^N,\frac{b}{c}q^{2k-N};p\right)$$
$$+\frac{aq^k}{c}\theta\left(b\xi q^k,b\xi^{-1}q^k,acq^{2N-k},\frac{c}{a}q^{-k};p\right)$$
$$+\frac{b}{cq^{N-2k}}\theta\left(c\xi q^{N-k},c\xi^{-1}q^{N-k},abq^{N+k},\frac{a}{b}q^{N-k};p\right)=0$$

and then find

$$\theta(a\xi q^N,a\xi^{-1}q^{-N};p)=\frac{\theta(acq^{2N-k},(a/c)q^k;p)}{\theta(bcq^N,(b/c)q^{2k-N};p)}\theta(b\xi q^k,b\xi^{-1}q^k;p)$$
$$+\frac{\theta(abq^{N+k},(a/b)q^{N-k};p)}{\theta(bcq^N,(c/b)q^{N-2k};p)}\theta(c\xi q^{N-k},c\xi^{-1}q^{N-k};p)\,.$$

Therefore we find the recurrence relation

$$C_k^{N+1}=\frac{\theta(acq^{2N+1-k},(a/c)q^{k-1};p)}{\theta(bcq^N,(b/c)q^{2k-N-2};p)}C_{k-1}^N+\frac{\theta(abq^{N+k},(a/b)q^{N-k};p)}{\theta(bcq^N,(c/b)q^{N-2k};p)}C_k^N\,.$$

With the initial conditions $C_0^0=1$ and $C_{-1}^N=C_{N+1}^N=0$ the coefficients are determined uniquely. Indeed we can now prove the formula for C_k^N by induction. Note first that $1/\theta(q;p)_{-1}=\theta(qq^{-1};p)=0$, so indeed the expression satisfies the initial conditions $C_{-1}^N=C_{N+1}^N=0$. Next we use induction and using Theorem 5.5 once more in a tedious calculation find that our formula for C_k^N is correct. □

Now we can determine the coefficients R_k^l explicitly by twice applying this binomial theorem:

Theorem 6.2 *We have*

$$R_k^l(a,b,c,d;N;q,p) = q^{l(l-N)}\frac{\theta(q;p)_N}{\theta(q;p)_l\theta(q;p)_{N-l}} \times \frac{\theta(ac^{\pm 1};p)_k\theta\left(bdq^{N-l},\frac{b}{d};p\right)_l\theta\left(\frac{b}{c},bc;p\right)_{N-k}\theta\left(\frac{b}{c};p\right)_{N-l}}{\theta\left(\frac{c}{d}q^{l-N};p\right)_l\theta\left(\frac{d}{c}q^{-l};p\right)_{N-l}\theta\left(cd,\frac{b}{c};p\right)_N\theta(bc;p)_l} \times {}_{12}V_{11}\left(\frac{c}{b}q^{-N};q^{-k},q^{-l},\frac{a}{b}q^{k-N},\frac{c}{d}q^{l-N},cd,\frac{1}{ab}q^{1-N},\frac{qc}{b}\right).$$

Proof Indeed we have

$$\begin{aligned} &h_k(x;a)h_{N-k}(x;b) \\ &\quad= \sum_{j=0}^{k} C_j^k(a,c,bq^{N-k})h_j(x;c)h_{N-j}(x;b) \\ &\quad= \sum_{j=0}^{k}\sum_{m=0}^{N-j} C_j^k(a,c,bq^{N-k})C_m^{N-j}(b,cq^j,d)h_{j+m}(x;c)h_{N-j-m}(x;d) \\ &\quad= \sum_{l=0}^{N}\sum_{j=0}^{\min(k,l)} C_j^k(a,c,bq^{N-k})C_{l-j}^{N-j}(b,cq^j,d)h_l(x;c)h_{N-l}(x;d)\,. \end{aligned}$$

Thus we obtain

$$R_k^l(a,b,c,d;N;q,p) = \sum_{j=0}^{\min(k,l)} C_j^k(a,c,bq^{N-k})C_{l-j}^{N-j}(b,cq^j,d)$$

which is exactly the series from the statement of the theorem. □

Note that we can find several different expressions by using a different proof. So this gives transformation formulas for the ${}_{12}V_{11}$.

Having proved that these elliptic hypergeometric series form the coefficients in a base transformation, we can derive some properties. First of all

Theorem 6.3 (Biorthogonality) *We have*

$$\sum_{l=0}^{N} R_n^l(a,b,c,d;N;q,p)R_l^m(c,d,a,b;N;q,p) = \delta_{nm}\,.$$

You can view this theorem as $\langle R^{\cdot}_n, R^m_{\cdot}\rangle = \delta_{nm}$, where $\cdot$ denotes the parameter, and the bilinear form has support on the set of integers $\{0, 1, \ldots, N\}$.

Proof Perform the basis transformation first from the basis $h_k(x;a)h_{N-k}(x;b)$ to the basis $h_l(x;c)h_{N-l}(x;d)$ and then back again. This gives

$$\begin{aligned}
&h_k(x;a)h_{N-k}(x;b)\\
&=\sum_{l=0}^{N} R^l_k(a,b,c,d;N;q,p)h_l(x;c)h_{N-l}(x;d)\\
&=\sum_{l=0}^{N}\sum_{j=0}^{N} R^l_k(a,b,c,d;N;q,p)R^j_l(c,d,a,b;N;q,p)h_j(x;a)h_{N-j}(x;b)\\
&=\sum_{j=0}^{N}\sum_{l=0}^{N} R^l_k(a,b,c,d;N;q,p)R^j_l(c,d,a,b;N;q,p)h_j(x;a)h_{N-j}(x;b)\ .
\end{aligned}$$

Then we see that the final series only has a nonzero term for the $j = k$ case, and the corresponding coefficient must be 1. □

If we consider the special case of the biorthogonality where $n = m = 0$, the series in the functions R^l_n and R^m_l both contain just a single term, and thus the resulting identity becomes an evaluation of a single sum. This summation is the original Frenkel–Turaev summation formula [2]

Theorem 6.4 *We have*

$${}_{10}V_9\left(a;b_1,b_2,b_3,\frac{q^{n+1}a}{b_1b_2b_3},q^{-n}\right)=\frac{\theta\left(\frac{aq}{b_1b_2},\frac{aq}{b_1b_3},\frac{aq}{b_2b_3},aq;p\right)_n}{\theta\left(\frac{aq}{b_1},\frac{aq}{b_2},\frac{aq}{b_3},\frac{aq}{b_1b_2b_3};p\right)_n}\ .$$

Proof For $n = m = 0$ the result simplifies to

$$\begin{aligned}
1&=\sum_{k=0}^{N} R^k_0(a,b,c,d;N;q,p)R^0_k(c,d,a,b;N;q,p)\\
&=\frac{\theta(q,bc;p)_N}{\theta(cd,b/a,ab;p)_N}\\
&\quad\times\sum_{k=0}^{N} q^{k(k-N)}\frac{\theta(bdq^{N-k},b/d,ca^{\pm1};p)_k\theta(b/c,da^{\pm1};p)_{N-k}}{\theta(q,(c/d)q^{k-N},bc;p)_k\theta(q,(d/c)q^{-k};p)_{N-k}}\ .
\end{aligned}$$

Next we use the elementary identities

$$\theta(xq^{-k};p)_k = \theta(pq/x;p)_k \qquad \theta(x;p)_{N-k} = \frac{\theta(x;p)_N}{\theta(pq^{1-N}/x;p)_k}$$

$$\theta(xq^{k};p)_k = \frac{\theta(x;p)_{2k}}{\theta(x;p)_k} \qquad \theta(xq^{-k};p)_{N-k} = \frac{\theta(x;p)_N\theta(pq/x;p)_k}{\theta(pq^{1-N}/x;p)_{2k}}$$

$$\theta(px;p)_k = \left(-\frac{1}{x}\right)^k q^{-\binom{k}{2}}\theta(x;p)_k$$

to obtain

$$\begin{aligned} 1 &= \frac{\theta(bc^{\pm 1}, da^{\pm 1};p)_n}{\theta(dc^{\pm 1}, ba^{\pm 1};p)_N} \\ &\quad \times \sum_{k=0}^{N} \frac{\theta((c/d)q^{1-N};p)_{2k}}{\theta((c/d)q^{-N};p)_{2k}} \frac{\theta(q^{1-N}/(bd), b/d, ca^{\pm 1}, (c/d)q^{-N}, q^{-N};p)_k}{\theta(q, bc, qc/d, q^{1-N}c/b, q^{1-N}(1/d)a^{\pm 1};p)_k} q^k \\ &= \frac{\theta(bc^{\pm 1}, da^{\pm 1};p)_n}{\theta(dc^{\pm 1}, ba^{\pm 1};p)_N} {}_{10}V_9\left(\frac{c}{d}q^{-N}; \frac{q^{1-N}}{bd}, \frac{b}{d}, ca^{\pm 1}, q^{-N}\right). \end{aligned}$$

Renaming the parameters gives the desired result. □

Exercise 6.5 Prove the addition formula

$$R_n^m(a,b,e,f;N;q) = \sum_{k=0}^{N} R_n^k(a,b,c,d;N;q) R_k^m(c,d,e,f;N;q) .$$

Exercise 6.6 The two functions which are biorthogonal are quite similar. Find a relation

$$R_k^l(a,b,c,d;N;q,p) = \text{Prefactor}\, R_l^k(?;N;q,p) .$$

You can do this by choosing a new set of parameters such that the arguments in the ${}_{12}V_{11}$ on both sides are equal.

7 Elliptic Beta Integral

In contrast to the ordinary and basic hypergeometric theory, we do not want to consider nonterminating elliptic hypergeometric series. Thus to find a proper generalization of nonterminating identities we consider integrals. The elliptic beta integral was proven by Spiridonov [10]. Taking the proper limit $p \to 0$ and then $q \to 1$ you can reduce it to the classical beta integral (proper means that we let the parameters behave in a certain way as $p \to 0$ and $q \to 1$), but many other famous integrals and nonterminating series of hypergeometric type are possible limits as well. For example the identity (1) is also a limit.

Theorem 7.1 *For parameters satisfying the balancing condition* $\prod_{r=1}^{6} t_r = pq$ *we have*

$$\frac{(p;p)(q;q)}{2}\int_{\mathcal{C}} \frac{\prod_{r=1}^{6}\Gamma_{\mathrm{e}}(t_r z^{\pm 1})}{\Gamma_{\mathrm{e}}(z^{\pm 2})}\frac{\mathrm{d}z}{2\pi \mathrm{i}z} = \prod_{\substack{r,s=1\\ r<s}}^{6}\Gamma_{\mathrm{e}}(t_r t_s)\ .$$

Here the contour $\mathcal{C}$ *is a deformation of the unit circle traversed in positive direction which contains the poles at* $z = t_r p^{\mathbb{Z}_{\geq 0}} q^{\mathbb{Z}_{\geq 0}}$ *and excludes the poles at* $z = t_r^{-1} p^{\mathbb{Z}_{\leq 0}} q^{\mathbb{Z}_{\leq 0}}$. *In particular for* $|t_r| < 1$ *you can take the unit circle itself.*

There are several different proofs, but I prefer the one below. The bilinear form returns later as the form with respect to which we obtain biorthogonal functions.

Proof Let us define the bilinear form

$$\langle f, g\rangle_{t_1,\dots,t_6} = \frac{(p;p)(q;q)}{2\prod_{\substack{r,s=1\\ r<s}}^{6}\Gamma_{\mathrm{e}}(t_r t_s)}\int_{\mathcal{C}} f(z)g(z)\frac{\prod_{r=1}^{6}\Gamma_{\mathrm{e}}(t_r z^{\pm 1})}{\Gamma_{\mathrm{e}}(z^{\pm 2})}\frac{\mathrm{d}z}{2\pi \mathrm{i}z}\ . \tag{2}$$

Here we want $f(z)$ and $g(z)$ to be even (that is, $z \to z^{-1}$-symmetric) meromorphic functions such that $f(z)\Gamma_{\mathrm{e}}(t_6 z^{\pm 1})/\Gamma_{\mathrm{e}}(q^{-m} t_6 z^{\pm 1})$ is an analytic function (which restricts the poles of f) and likewise $g(z)\Gamma_{\mathrm{e}}(t_5 z^{\pm 1})/\Gamma_{\mathrm{e}}(q^{-l} t_5 z^{\pm 1})$ is analytic. The contour then has to be adjusted to consider the poles of $\Gamma_{\mathrm{e}}(q^{-m} t_6 z^{\pm 1})$ and $\Gamma_{\mathrm{e}}(q^{-l} t_5 z^{\pm 1})$.

Let us also consider the difference operator

$$(D(u_1,u_2,u_3)f)(z) = \sum_{\sigma=\pm 1}\frac{\theta(u_1 z^{\sigma}, u_2 z^{\sigma}, u_3 z^{\sigma}, u_1 u_2 u_3 z^{-\sigma};p)}{\theta(u_1u_2, u_1u_3, u_2u_3, z^{2\sigma};p)} f(q^{\sigma/2}z)\ . \tag{3}$$

First observe that D maps even functions to even functions, and a direct calculation shows that p-elliptic functions are mapped to p-elliptic functions. Then the result of the application of the difference operator to the constant function 1 is an even p-elliptic function with poles at most when $\theta(z^{\pm 2};p) = 0$. But this means it must be a constant function. Plugging in the value $z = u_1$ the term with $\sigma = -1$ vanishes and we obtain

$$(D(u_1,u_2,u_3)1)(z) = \frac{\theta(u_1^2, u_2u_1, u_3u_1, u_2u_3;p)}{\theta(u_1u_2, u_1u_3, u_2u_3, u_1^2;p)} = 1\ .$$

This identity can also be viewed as a form of the fundamental theta-function identity from Theorem 5.5. Moreover we can calculate that

$$\begin{aligned}&\langle D(t_1,t_2,t_6)f, g\rangle_{t_1,\dots,t_6}\\ &\qquad = \langle f, D(q^{-1/2}t_3, q^{-1/2}t_4, q^{-1/2}t_5)g\rangle_{q^{1/2}t_1, q^{1/2}t_2, q^{-1/2}t_3, q^{-1/2}t_4, q^{-1/2}t_5, q^{1/2}t_6}\end{aligned}$$

where we apply the difference equation $\theta(z;p)\Gamma_e(z) = \Gamma_e(qz)$ several times, split the sum in its two constituent parts and shift the integration variable $z \to zq^{-1/2\sigma}$ and then recombine. Notice that we do not have to worry about the contour in the shift, as we have defined the contour as separating several different poles and that definition just shifts the contour along with z. We also have to use the balancing condition $\prod_{r=1}^{6} t_r = pq$ to equate $\theta(q^{1/2}t_1t_2t_6z^\sigma;p) = \theta(t_3t_4t_5/(q^{3/2}z^\sigma);p)$.

Specializing this to $f = g = 1$ we obtain for the constant term

$$\langle 1,1\rangle_{t_1,\ldots,t_6} = \langle 1,1\rangle_{q^{1/2}t_1,q^{1/2}t_2,q^{-1/2}t_3,q^{-1/2}t_4,q^{-1/2}t_5,q^{1/2}t_6}\ .$$

In particular we can shift three parameters by some half-integer power of q upwards, and three others downwards. Applying this twice we obtain

$$\langle 1,1\rangle_{t_1,\ldots,t_6} = \langle 1,1\rangle_{qt_1,t_2,t_3,t_4,t_5,q^{-1}t_6}\ .$$

Thus if we consider the constant term as a function of t_1 up to t_5 (with t_6 determined by the balancing condition), it is invariant under multiplying one of the parameters by an integer power of q. Due to $p \leftrightarrow q$ symmetry it is also invariant under multiplication by integer powers of p.

Since the constant term is a meromorphic function of the parameters, and since for generic values of p and q the set $p^{\mathbb{Z}}q^{\mathbb{Z}}$ has an accumulation point (other than 0 or infinity), we can conclude that the constant term is a constant function. It remains to see what the constant is.

Therefore we want to evaluate it at a single point. For $t_1t_2 = 1$ there is no contour of the desired shape as the pole at $z = t_1$ should be included, whereas the pole at $z = 1/t_2$ should be excluded (and in this specialization they are at the same point). The same holds for the poles at $z = t_2$ and $z = 1/t_1$. This problem can be resolved by shifting the contour first over the poles at $z = t_1$ and $z = 1/t_1$, picking up the associated residues, and then specializing to $t_1t_2 = 1$ (which is then perfectly possible). Due to symmetry the residue at $z = t_1$ is minus the residue at $z = 1/t_1$ (and we have to add the one at $z = t_1$ and subtract the one at $z = 1/t_1$) so this gives a factor 2. The prefactor of the remaining integral contains the factor $1/\Gamma_e(t_1t_2) = 0$ at $t_1t_2 = 1$, so the remaining integral vanishes. The result of the constant is thus equal to twice the residue at $z = t_1$ evaluated at $t_1t_2 = 1$. Thus we find

$$\begin{aligned}
&\langle 1,1\rangle_{t_1,\ldots,t_6} \\
&\quad = 2\,\mathrm{Res}\left(\frac{(p;p)(q;q)}{2\prod_{\substack{r,s=1\\r<s}}^{6}\Gamma_e(t_rt_s)}\frac{\prod_{r=1}^{6}\Gamma_e(t_rz^{\pm1})}{\Gamma_e(z^{\pm2})}\frac{1}{z}, z=t_1\right)\Bigg|_{t_1t_2=1} \\
&\quad = \frac{(p;p)(q;q)}{\prod_{\substack{r,s=1\\r<s}}^{6}\Gamma_e(t_rt_s)}\frac{\prod_{r=2}^{6}\Gamma(t_1^2,t_rt_1^{\pm1})}{\Gamma(t_1^{\pm2})}\,\mathrm{Res}\left(\frac{\Gamma_e(t_1/z)}{z}, z=t_1\right)\Bigg|_{t_1t_2=1} \\
&\quad = \frac{\prod_{r=2}^{6}\Gamma(t_r/t_1)}{\prod_{\substack{r,s=2\\r<s}}^{6}\Gamma_e(t_rt_s)\Gamma(t_1^{-2})}\Bigg|_{t_1t_2=1} = \frac{1}{\prod_{\substack{r,s=3\\r<s}}^{6}\Gamma_e(t_rt_s)}\Bigg|_{t_1t_2=1} = 1
\end{aligned}$$

where in the last step we use that $\Gamma_e(x) = \Gamma_e(pq/x)$ and that $t_3t_4 = pq/t_1t_2t_5t_6 = pq/t_5t_6$ (and similar). □

To make the connection from integral to elliptic hypergeometric series we again can use the technique of picking up residues (as we did for ordinary hypergeometric series). In order to specialize the elliptic beta integral to $t_1t_2 = q^{-n}$ we have to change the contour by moving it over the poles at $z^{\pm 1} = t_1q^k$ for $0 \le k \le n$ and their inverses. After picking up these residues we can make the specialization. Due to the prefactor $1/\Gamma_e(t_1t_2)$ of the integral, the remaining integral is multiplied by zero. Thus we are left with a sum of residues: $\sum_{k=0}^{n} \mathrm{Res}(\cdot, z = t_1q^k)$. This will be a terminating elliptic hypergeometric series. In fact, in this way we will recover the original Frenkel–Turaev summation formula (Theorem 6.4).

A series obtained in this way will be an elliptic hypergeometric series for any integral $\int \Delta(z)\,\mathrm{d}z/(2\pi \mathrm{i}z)$ for which the integrand satisfies

$$\frac{\Delta(qz)}{\Delta(z)} = \frac{\Delta(pqz)}{\Delta(pz)}\,. \tag{4}$$

In particular we will only consider integrals which satisfy this condition. For the elliptic beta integral it can be checked directly by using the difference equations of the elliptic Gamma function and some elementary identities of the theta function.

Transformations for more complicated integrals can now be easily derived. For an elliptic beta integral with 8 parameters (satisfying a balancing condition) the symmetries can be obtained by iterating the identity below.

Theorem 7.2 *For parameters $\prod_{r=1}^{8} t_r = (pq)^2$ define the integral*

$$I(t_1,\dots,t_8;p,q) = \frac{(p;p)(q;q)}{2}\int_{\mathcal{C}} \frac{\prod_{r=1}^{8}\Gamma_e(t_rz^{\pm 1})}{\Gamma_e(z^{\pm 2})}\frac{\mathrm{d}z}{2\pi \mathrm{i}z}$$

where the contour circles the origin in positive direction separating the poles of $\Gamma_e(t_rz)$ from those of $\Gamma_e(t_r/z)$. If $|t_r| < 1$ then we can take the unit circle. Then we have

$$I(t_1,\dots,t_8;p,q) = \prod_{\substack{r,s=1\\ r<s}}^{4}\Gamma_e(t_rt_s)\prod_{\substack{r,s=5\\ r<s}}^{8}\Gamma_e(t_rt_s)I\left(\frac{t_1}{\sigma},\dots,\frac{t_4}{\sigma},t_5\sigma,\dots,t_8\sigma;p,q\right)$$

where $\sigma^2 = t_1t_2t_3t_4/(pq) = pq/(t_5t_6t_7t_8)$.

Proof The equation is obtained by evaluating in two different orders the double integral

$$\iint_{\mathcal{C}\times\mathcal{C}} \frac{\Gamma_e(\sigma z^{\pm 1}w^{\pm 1})\prod_{r=1}^{4}\Gamma_e((t_r/\sigma)z^{\pm 1})\prod_{r=5}^{8}\Gamma_e(t_rw^{\pm 1})}{\Gamma_e(z^{\pm 2},w^{\pm 2})}\frac{\mathrm{d}z}{2\pi \mathrm{i}z}\frac{\mathrm{d}w}{2\pi \mathrm{i}w}\,.$$

□

If you turn this integral into a series by specializing two parameters to (for example) $t_1t_8 = q^{-N}$ you obtain a ${}_{12}V_{11}$ series on both sides of the equation. As this can be done for both sides of the integral transformation at once, you can derive transformation formulas for the ${}_{12}V_{11}$ in this way.

Exercise 7.3 Show that an elliptic beta integral

$$\int_{\mathcal{C}} \frac{\prod_{r=1}^{2m+4} \Gamma_{\mathrm{e}}(t_r z^{\pm 1})}{\Gamma_{\mathrm{e}}(z^{\pm 2})} \frac{\mathrm{d}z}{2\pi \mathrm{i}z}$$

satisfies (4) if and only if $\left(\prod_{r=1}^{2m+4} t_r\right)^2 = (pq)^{2m}$.

Exercise 7.4 Show that the beta integral

$$\frac{(p;p)(q;q)}{2\prod_{1\leq r<s\leq 2m+4} \Gamma_{\mathrm{e}}(t_r t_s)} \int_{\mathcal{C}} \frac{\prod_{r=1}^{2m+4} \Gamma_{\mathrm{e}}(t_r z^{\pm 1})}{\Gamma_{\mathrm{e}}(z^{\pm 2})} \frac{dz}{2\pi i z}, \quad \prod_{r=1}^{2m} t_r = (pq)^m$$

evaluates at $t_1t_2 = q^{-n}$ to the series

$$\text{prefactor}\, {}_{2m+8}V_{2m+7}\left(t_1^2; t_1t_3, \ldots, t_1t_{2m+3}, \frac{q^{n+m}t_1}{t_3\cdots t_{2m+3}}, q^{-n}\right).$$

Also determine the prefactor explicitly. **Hint:** Move the integration contour over an appropriate sequence of poles and pick up the associated residues.

Exercise 7.5 Obtain Frenkel–Turaev's summation formula for a ${}_{10}V_9$ as a special case of the elliptic beta integral evaluation.

Exercise 7.6 (a) Assume the balancing condition $a^3q^{n+2} = b_1b_2b_3b_4b_5b_6$ holds. Obtain the transformation formula

$$\begin{aligned}
&{}_{12}V_{11}(a; b_1, b_2, b_3, b_4, b_5, b_6, q^{-n}; p, q) \\
&= \frac{\theta\left(aq, \frac{a}{b_4b_5}, \frac{aq}{b_4b_6}, \frac{aq}{b_5b_6}; p\right)_n}{\theta\left(\frac{aq}{b_4}, \frac{aq}{b_5}, \frac{aq}{b_6}, \frac{aq}{b_4b_5b_6}; p\right)_n} \\
&\quad \times {}_{12}V_{11}\left(\frac{a^2q}{b_1b_2b_3}; \frac{aq}{b_2b_3}, \frac{aq}{b_1b_3}, \frac{aq}{b_1b_2}, b_4, b_5, b_6, q^{-n}; p, q\right)
\end{aligned}$$

as a special case of Theorem 7.2. Alternatively you can derive this directly copying the proof of the transformation for the integrals, using a double sum and Frenkel–Turaev's summation formula.

(b) Iterate the above formula to obtain

$$
\begin{aligned}
&{}_{12}V_{11}(a;b_1,b_2,b_3,b_4,b_5,b_6,q^{-n};p,q)\\
&=\frac{\theta\left(aq,\frac{b_2}{p},\frac{aq}{b_1b_3},\frac{aq}{b_1b_4},\frac{aq}{b_1b_5},\frac{aq}{b_1b_6};p\right)}{\theta\left(\frac{aq}{b_1},\frac{b_2}{pb_1},\frac{aq}{b_3},\frac{aq}{b_4},\frac{aq}{b_5},\frac{aq}{b_6};p\right)}\\
&\quad\times{}_{12}V_{11}\left(\frac{b_1}{q^nb_2};b_1,\frac{b_1}{aq^n},\frac{aq}{b_2b_3},\frac{aq}{b_2b_4},\frac{aq}{b_2b_5},\frac{aq}{b_2b_6},q^{-n}\right).
\end{aligned}
$$

(c) Can you find more transformations satisfied by the ${}_{12}V_{11}$ by iterating the transformation from part (a)? (You should be able to find two more, one of which is the inversion of summation transformation which sends the summation index $k\to n-k$.)

8 Continuous Biorthogonality

This section discusses a slightly more general pair of families of biorthogonal functions than we did before. The difference between what we did before is similar to the difference between Wilson polynomials and Racah polynomials, in that a specialization of parameters in the Wilson polynomials gives the Racah polynomials, such that you obtain only a finite set of orthogonal polynomials (which then are orthogonal to a discrete measure). The discussion here follows the work of Eric Rains [5, 6], who actually generalized the theory to multivariate biorthogonality (such as how Koornwinder polynomials generalize Askey–Wilson polynomials). In these notes we restrict ourselves to the univariate case though; which makes some formulas more explicit.

The relevant functions are defined as

Definition 8.1 Suppose $t_1t_2t_3t_4u_1u_2=pq$ then we define

$$
\begin{aligned}
&R_n(z;t_1:t_2,t_3,t_4;u_1,u_2)\\
&\qquad={}_{12}V_{11}\left(\frac{t_1}{u_1};\frac{pq^n}{u_1u_2},q^{-n},t_1z^{\pm1},\frac{q}{u_1t_2},\frac{q}{u_1t_3},\frac{q}{u_1t_4};p,q\right).
\end{aligned}
$$

Recall the bilinear form introduced to prove the elliptic beta integral (2). These functions are biorthogonal with respect to this form. To be precise we have

Theorem 8.2 *We have*

$$\langle R_n(\,\cdot\,;t_1:t_2,t_3,t_4;u_1,u_2),R_m(\,\cdot\,;t_1:t_2,t_3,t_4;u_2,u_1)\rangle_{t_1,t_2,t_3,t_4,u_1,u_2}$$
$$=\delta_{n,m}\frac{\theta\left(\frac{p}{u_1u_2};p\right)_{2n}\theta\left(q,t_2t_3,t_2t_4,t_3t_4,\frac{qt_1}{u_1},\frac{pqt_1}{u_2};p\right)_n}{\theta\left(\frac{pq}{u_1u_2};p\right)_{2n}\theta\left(\frac{p}{u_1u_2},t_1t_2,t_1t_3,t_1t_4,\frac{p}{t_1u_2},\frac{1}{t_1u_1};p\right)_n}q^{-n}\,.$$

Observe that u_1 and u_2 are interchanged in the second function; hence we have biorthogonality and not plain orthogonality. After specializing $t_1t_2=q^{-N}$ this biorthogonality reduce to the biorthogonality from Theorem 6.3 (see Exercise 8.6). The proof of this biorthogonality follows at the end of these notes.

The biorthogonal functions are self-dual

Theorem 8.3 *We have*

$$R_n(t_1q^k;t_1:t_2,t_3,t_4;u_1,u_2)=R_k(\hat{t}_1q^n;\hat{t}_1;\hat{t}_2,\hat{t}_3,\hat{t}_4;\hat{u}_1,\hat{u}_2)$$

for dual parameters

$$\hat{t}_1=\sqrt{\frac{t_1t_2t_3t_4}{pq}}\,,\quad \hat{t}_1\hat{t}_r=t_1t_r\ (r=2,3,4)\,,\quad \frac{\hat{t}_1}{\hat{u}_r}=\frac{t_1}{u_r}\ (r=1,2)\,.$$

Proof This can be seen by directly plugging the values in the definition. □

The biorthogonal functions are "eigenfunctions" of the difference operator from (3) (with "eigenvalue" 1).

Theorem 8.4 *We have*

$$D(u_1,t_1,t_2)R_n(\,\cdot\,;q^{1/2}t_1:q^{1/2}t_2,q^{-1/2}t_3,q^{-1/2}t_4;q^{1/2}u_1,q^{-1/2}u_1)$$
$$=R_n(\,\cdot\,;t_1:t_2,t_3,t_4;u_1,u_2)\,.$$

Proof You can apply the difference operator to the individual terms on the left-hand side and equate the results term by term. The required theta function identity is (what else) Theorem 5.5. □

On the level of elliptic hypergeometric series the previous result is an example of a contiguous relation. It relates three series whose parameters are almost equal, they differ only by some (integer) powers of q. There is an identity between any three ${}_{12}V_{11}$'s whose parameters differ by some integer powers of q, though making it explicit is often quite a lot of work.[2]

[2]One might observe that the name "contiguous relation" is somewhat of a misnomer. It is not so much that the relation itself is contiguous (which means "next to") but that it relates functions

A less trivial result is the fact that the biorthogonal functions are symmetric under permutations of t_1, t_2, t_3 and t_4 (up to a factor independent of z). From the definition as a series you can only read off the permutation symmetry of t_2, t_3, and t_4. Indeed we have

Theorem 8.5 *We have*

$$R_n(z; t_2 : t_1, t_3, t_4; u_1, u_2) = \frac{R_n(z; t_1 : t_2, t_3, t_4; u_1, u_2)}{R_n(t_2; t_1 : t_2, t_3, t_4; u_1, u_2)}$$

and

$$R_n(t_2; t_1 : t_2, t_3, t_4; u_1, u_2) = \frac{\theta(t_2t_3, t_2t_4, p/(u_2t_2), qt_1/u_1; p)_n}{\theta(qt_2/u_1, t_1t_3, t_1t_4, p/(t_1u_2); p)_n} .$$

Proof The evaluation of $R_n(t_2; t_1 : t_2, t_3, t_4; u_1, u_2)$ is Frenkel–Turaev's summation formula, Theorem 6.4. We can apply it after cancelling identical parameters from the numerator and the denominator of the elliptic hypergeometric series.

The $t_1 \leftrightarrow t_2$ symmetry of the biorthogonal functions is given by a transformation formula for ${}_{12}V_{11}$'s. This formula can be derived as a discrete version of the transformation for elliptic beta integrals from Theorem 7.2 by setting the product of two parameters equal to q^{-n}, see Exercise 7.6. □

Given the symmetry above and the difference operators, we find that the R_n are "eigenfunctions" of $D(u_1, t_2, t_3)$ (etc.) with "generically different eigenvalues" for different n (as we will see shortly). Since the D's are "self-adjoint," we would expect that biorthogonality now follows directly. Unfortunately the fact that the parameters change after applying the difference operators/taking the adjoint means that the standard proof does not apply anymore. Thus we have to resort to a slightly different proof.

Proof of biorthogonality Using the symmetry of the biorthogonal functions, and the effect of the difference operator $D(u_1, t_1, t_2)$ we find that

$$\begin{aligned} &D(u_1, t_3, t_4)R_n(\,\cdot\,; q^{-1/2}t_1 : q^{-1/2}t_2, q^{1/2}t_3, q^{1/2}t_4; q^{1/2}u_1, q^{-1/2}u_2) \\ &\qquad = \frac{\theta(t_1t_2q^{n-1}, q^nt_3t_4, u_2t_1, t_1/u_1; p)}{\theta(t_1t_2/q, t_3t_4, u_2t_1q^{-n}, (t_1/u_1)q^n; p)} R_n(\,\cdot\,; t_1 : t_2, t_3, t_4; u_1, u_2) . \end{aligned}$$

at parameter values which are contiguous. A better term which is sometimes used, would be "contiguity relation." However in these notes I prefer to use the terminology of the standard work [1].

Thus we obtain as result of repeated difference operators

$$D(u_1,t_1,t_2)D(q^{1/2}u_1,q^{-1/2}t_3,q^{-1/2}t_4)R_n(\,\cdot\,;t_1:t_2,t_3,t_4;qu_1,u_2/q)$$
$$=\frac{\theta(t_1t_2q^n,q^{n-1}t_3t_4,u_2t_1,t_1/u_1;p)}{\theta(t_1t_2,t_3t_4/q,u_2t_1q^{-n},(t_1/u_1)q^n;p)}R_n(\,\cdot\,;t_1:t_2,t_3,t_4;u_1,u_2)$$

and likewise

$$D(u_1,t_1,t_3)D(q^{1/2}u_1,q^{-1/2}t_2,q^{-1/2}t_4)R_n(\,\cdot\,;t_1:t_2,t_3,t_4;qu_1,u_2/q)$$
$$=\frac{\theta\left(t_1t_3q^n,q^{n-1}t_2t_4,u_2t_1,t_1/u_1;p\right)}{\theta\left(t_1t_3,\frac{t_2t_4}{q},u_2t_1q^{-n},(t_1/u_1)q^n;p\right)}R_n(\,\cdot\,;t_1:t_2,t_3,t_4;u_1,u_2)\,.$$

Now notice that we have two different (second order) difference operators, which map the same old R_n to the same new R_n with a different factor. In particular we find

$$D(u_1,t_1,t_2)D(q^{1/2}u_1,q^{-1/2}t_3,q^{-1/2}t_4)R_n(\,\cdot\,;t_1:t_2,t_3,t_4;qu_1,u_2/q)$$
$$=\frac{\theta(t_1t_2q^n,q^{n-1}t_3t_4,t_1t_3,t_2t_4/q;p)}{\theta(t_1t_2,t_3t_4/q,t_1t_3q^n,q^{n-1}t_2t_4;p)}$$
$$\times D(u_1,t_1,t_3)D(q^{1/2}u_1,q^{-1/2}t_2,q^{-1/2}t_4)R_n(\,\cdot\,;t_1:t_2,t_3,t_4;qu_1,u_2/q)\,.$$

Now we observe that these generalized eigenvalues are different for different choices of n (for generic values of the t_r). Let us write

$$L_1=D(u_1,t_1,t_2)D(q^{1/2}u_1,q^{-1/2}t_3,q^{-1/2}t_4)\,,$$
$$L_2=D(u_1,t_1,t_3)D(q^{1/2}u_1,q^{-1/2}t_2,q^{-1/2}t_4)\,,$$
$$L_1^*=D(u_2/q,t_1,t_2)D(q^{-1/2}u_2,q^{-1/2}t_3,q^{-1/2}t_4)\,,$$
$$L_2^*=D(u_2/q,t_1,t_3)D(q^{-1/2}u_2,q^{-1/2}t_2,q^{-1/2}t_3)\,,$$

and then re-express the difference equations as

$$L_iR_n(\,\cdot\,;t_1:t_2,t_3,t_4;qu_1,u_2/q)$$
$$=\lambda_{i,n}(t_1,t_2,t_3,t_4,u_1,u_2)R_n(\,\cdot\,;t_1:t_2,t_3,t_4;u_1,u_2)\,.$$

Note that L_1^* is the same as L_1 with $u_1\leftrightarrow u_2/q$, so we also have difference equations

$$L_i^*R_n(\,\cdot\,;t_1:t_2,t_3,t_4;u_2,u_1)$$
$$=\lambda_{i,n}^*(t_1,t_2,t_3,t_4,u_1,u_2)R_n(\,\cdot\,;t_1:t_2,t_3,t_4;u_2/q,qu_1)\,.$$

Now we can calculate

$$\begin{aligned}
&\langle R_n(\,\cdot\,;t_1:t_2,t_3,t_4;u_1,u_2),R_m(\,\cdot\,;t_1:t_2,t_3,t_4;u_2,u_1)\rangle_{t_r,u_r}\\
&\quad=\frac{1}{\lambda_{1,n}}\langle L_1R_n(\,\cdot\,;t_1:t_2,t_3,t_4;qu_1,u_2/q),R_m(\,\cdot\,;t_1:t_2,t_3,t_4;u_2,u_1)\rangle_{t_r,u_r}\\
&\quad=\frac{1}{\lambda_{1,n}}\langle R_n(\,\cdot\,;t_1:t_2,t_3,t_4;qu_1,u_2/q),L_1^*R_m(\,\cdot\,;t_1:t_2,t_3,t_4;u_2,u_1)\rangle_{t_r,qu_1,u_2/q}\\
&\quad=\frac{\lambda_{1,m}^*}{\lambda_{1,n}}\langle R_n(\,\cdot\,;t_1:t_2,t_3,t_4;qu_1,u_2/q),R_m(\,\cdot\,;t_1:t_2,t_3,t_4;u_2/q,qu_1)\rangle_{t_r,qu_1,u_2/q}\\
&\quad=\frac{\lambda_{2,n}\lambda_{1,m}^*}{\lambda_{1,n}\lambda_{2,m}^*}\langle R_n(\,\cdot\,;t_1:t_2,t_3,t_4;u_1,u_2),R_m(\,\cdot\,;t_1:t_2,t_3,t_4;u_2,u_1)\rangle_{t_r,u_r}\ .
\end{aligned}$$

Thus we see that the bilinear form vanishes unless the prefactor equals 1. However we have

$$\begin{aligned}
&\frac{\lambda_{2,n}\lambda_{1,m}^*}{\lambda_{1,n}\lambda_{2,m}^*}\\
&\quad=\frac{\theta\left(t_1t_2,\frac{t_3t_4}{q},u_2t_1q^{-n},\frac{t_1}{u_1}q^n;p\right)}{\theta\left(t_1t_2q^n,q^{n-1}t_3t_4,u_2t_1,\frac{t_1}{u_1};p\right)}\frac{\theta\left(t_1t_3q^n,q^{n-1}t_2t_4,u_2t_1,\frac{t_1}{u_1};p\right)}{\theta\left(t_1t_3,\frac{t_2t_4}{q},u_2t_1q^{-n},\frac{t_1}{u_1}q^n;p\right)}\\
&\qquad\times\frac{\theta\left(t_1t_2q^m,q^{m-1}t_3t_4,qu_1t_1,\frac{qt_1}{u_2};p\right)}{\theta\left(t_1t_2,\frac{t_3t_4}{q},qu_1t_1q^{-m},\frac{qt_1}{u_2}q^m;p\right)}\frac{\theta\left(t_1t_3,\frac{t_2t_4}{q},qu_1t_1q^{-m},\frac{qt_1}{u_2}q^m;p\right)}{\theta\left(t_1t_3q^m,q^{m-1}t_2t_4,qu_1t_1,\frac{qt_1}{u_2};p\right)}\\
&\quad=\frac{\theta(t_1t_2q^m,q^{m-1}t_3t_4,t_1t_3q^n,q^{n-1}t_2t_4;p)}{\theta(t_1t_2q^n,q^{n-1}t_3t_4,t_1t_3q^m,q^{m-1}t_2t_4;p)}\ .
\end{aligned}$$

And thus the prefactor is generically not equal to 1 (except when $n=m$). □

We will not prove the squared norm formula for the biorthogonal functions under the continuous measure. There are several proofs in the quoted literature. The proof in [6] proceeds by induction using a raising operator, and you can explore this in the exercises. This raising operator also gives rise to a Rodriguez-type formula for the biorthogonal functions: If you define

$$\begin{aligned}
&D_+(u_1:u_2:u_3,u_4,u_5)f(z)\\
&\qquad=\frac{\theta(pqu_2/u_1;p)}{\theta(u_2u_3,u_2u_4,u_2u_5,u_2u_6;p)}\sum_{\sigma=\pm1}\frac{\prod_{r=2}^6\theta(u_rz^\sigma;p)}{\theta(pqz^\sigma/u_1,z^{2\sigma};p)}f(q^{\sigma/2}z)
\end{aligned}$$

where

$$u_6 = \frac{p^2 q}{u_1 u_2 u_3 u_4 u_5} ,$$

then the following identity holds:

$$D_+(u_1 : t_1 : t_2, t_3, t_4) R_n(\,\cdot\,; q^{1/2} t_1 : q^{1/2} t_2, q^{1/2} t_3, q^{1/2} t_4; q^{-1/2} u_1, q^{-3/2} u_2) = R_{n+1}(\,\cdot\,; t_1 : t_2, t_3, t_4; u_1, u_2) \qquad (5)$$

Indeed you can now write R_n as the result of applying n difference operators consecutively on the constant function 1, which is a Rodriguez-type formula.

Exercise 8.6 (a) Specialize the biorthogonal functions of this section at $t_1 t_2 = q^{-N}$ and $z = t_1 q^k$. Now show that there is a change of parameters which turns the resulting functions into the biorthogonal functions of Sect. 6. That is, you want an identity

$$R_l(t_1 q^k; t_1 : 1/(t_1 q^N), t_3, t_4; u_1, u_2) = \text{prefactor}\, R_l^k(a, b, c, d; N) ,$$

where $t_r = t_r(a, b, c, d, N)$ and $u_r = u_r(a, b, c, d, N)$.

(b) Check that interchanging u_1 and u_2 corresponds to changing $R_l^k(a, b, c, d; N)$ to $R_k^l(c, d, a, b; N)$.

You can now check that the biorthogonality for the R_k^l of Sect. 6 is indeed a special case of the biorthogonality of the R_l from this section. Note that in the special case $t_1 t_2 = q^{-N}$ there is no proper contour for the integral defining the biorthogonality. In order to make sense of the integral, you have to move the contour over the poles at $z = t_1, t_1 q, \ldots, t_1 q^N$ before taking this specialization, thus creating discrete point masses in the measure at these values.

In the final exercises you can explore difference equations satisfied by the biorthogonal functions.

Exercise 8.7 In this exercise you will derive the elliptic hypergeometric equation: the second order difference equation satisfied by the biorthogonal functions generalizing the Askey–Wilson difference equation.

(a) Show that

$$\begin{aligned} &{}_{12}V_{11}(a; b_1, b_2, b_3, b_4, b_5, b_6, q^{-n}; p, q) \\ &= \frac{\theta\left(b_2, \frac{b_2}{a}, \frac{b_1}{b_3 q}, \frac{b_1 b_3}{aq}; p\right)}{\theta\left(\frac{b_1}{q}, \frac{b_1}{aq}, \frac{b_2}{b_3}, \frac{b_2 b_3}{a}; p\right)} {}_{12}V_{11}(a; b_1/q, b_2 q, b_3, b_4, b_5, b_6, q^{-n}; p, q) \\ &\qquad + (b_2 \leftrightarrow b_3) \end{aligned}$$

by considering this identity term by term. The notation means that we have a second term on the right-hand side, identical to the first term except with b_2 and b_3 interchanged.

(b) Use the transformation formula from Exercise 7.6(a) on all three terms of the above transformation to obtain other contiguous relations, in particular the relation

$$
\begin{aligned}
&{}_{12}V_{11}(a;b_1,b_2,b_3,b_4,b_5,b_6,q^{-n};p,q)\\
&\quad=\frac{\theta\left(\frac{a}{b_1},\frac{b_2}{aq^{n+1}},\frac{b_3}{b_1q};p\right)}{\theta\left(\frac{b_1}{aq^n},\frac{aq}{b_2},\frac{b_3}{b_2};p\right)}\prod_{r=4}^{6}\frac{\theta\left(\frac{aq}{b_2b_r};p\right)}{\theta\left(\frac{a}{b_1b_r};p\right)}\\
&\qquad\qquad\times{}_{12}V_{11}(a;b_1q,b_2/q,b_3,b_4,b_5,b_6,q^{-n};p,q)\\
&\qquad\qquad\qquad+(b_2\leftrightarrow b_3)
\end{aligned}
$$

(c) Combine the contiguous relations above to obtain a relation

$$
\begin{aligned}
&\left(\frac{\theta\left(\frac{q}{b_1},\frac{b_1}{aq^{n+1}},\frac{b_1q}{b_2},\frac{b_2}{b_3},\frac{b_2b_3}{a},\frac{aq}{b_1b_4},\frac{aq}{b_1b_5},\frac{aq}{b_1b_6};p\right)}{\theta\left(\frac{b_2}{b_1},\frac{b_3q}{b_1};p\right)}\right.\\
&+\frac{\theta\left(\frac{q}{b_2},\frac{b_2}{aq^{n+1}},\frac{b_2q}{b_1},\frac{b_1}{b_3},\frac{b_1b_3}{a},\frac{aq}{b_2b_4},\frac{aq}{b_2b_5},\frac{aq}{b_2b_6};p\right)}{\theta\left(\frac{b_1}{b_2},\frac{b_3q}{b_2};p\right)}\\
&\left.+\frac{\theta\left(\frac{b_1q}{b_2},\frac{b_2q}{b_1},\frac{b_1b_2}{aq},\frac{1}{b_3},\frac{b_3}{aq^n},\frac{a}{b_3b_4},\frac{a}{b_3b_5},\frac{a}{b_3b_6};p\right)}{\theta\left(\frac{b_1}{qb_3},\frac{b_2}{qb_3};p\right)}\right)\\
&\qquad\times{}_{12}V_{11}(a;b_1,b_2,b_3,b_4,b_5,b_6,q^{-n};p,q)\\
&\quad=\frac{\theta\left(b_1,\frac{b_1}{a},\frac{b_2}{aq^{n+1}},\frac{b_2q}{b_1};p\right)}{\theta\left(\frac{aq}{b_2},\frac{b_1}{b_2};p\right)}\prod_{r=3}^{6}\theta\left(\frac{aq}{b_2b_r};p\right)\\
&\qquad\times{}_{12}V_{11}(a;b_1q,b_2/q,b_3,b_4,b_5,b_6,q^{-n};p,q)\\
&\qquad\qquad+(b_1\leftrightarrow b_2)
\end{aligned}
$$

Hint: You need to use either one of the two relations above twice. Recall that the ${}_{12}V_{11}$ is permutation symmetric in its 6 b_r-parameters to obtain different versions of the same contiguous relation.

The coefficient on the left-hand side is of course unique, but can be written in many ways as the sum of three products of theta functions. For example the left-hand side of this equation is symmetric under interchanging b_3 and b_4, which is not apparent from its explicit expression. It might well be that you found a different expression. If you want to show equality between any pair of these different expressions you need to use Theorem 5.5.

(d) Derive a difference equation of the form

$$A(z)R_n(qz) + B(z)R_n(z/q) = C(z)R_n(z)$$

using the above contiguous relation.

Exercise 8.8 In this exercise you will prove the Rodriguez-type formula for the biorthogonal functions.

(a) Prove the following difference equation by equating both sides termwise. You have to shift the summation index of one of the two series on the right-hand side first.

$$\begin{aligned}
&{}_{12}V_{11}(a;b_1,b_2,b_3,b_4,b_5,b_6,q^{-n-1};p,q)\\
&\qquad = {}_{12}V_{11}(a;b_1/q,b_2,b_3,b_4,b_5,b_6,q^{-n};p,q)\\
&-\frac{\theta\left(aq,aq^2,\dfrac{b_1}{aq^{n+2}},b_1q^n;p\right)}{\theta\left(aq^{n+1},aq^{n+2},\dfrac{aq}{b_1},\dfrac{b_1}{aq^2};p\right)}\prod_{r=2}^{6}\frac{\theta(b_r;p)}{\theta(aq/b_r;p)}\\
&\qquad\times {}_{12}V_{11}(aq^2;b_1,b_2q,b_3q,b_4q,b_5q,b_6q,q^{-n};p,q)
\end{aligned}$$

(b) Now apply the symmetry of the ${}_{12}V_{11}$ of Exercise 7.6(b) to all three sides of the previous equation to derive the relation

$$\begin{aligned}
&{}_{12}V_{11}(a;b_1,b_2,b_3,b_4,b_5,b_6,q^{-n-1};p,q)\\
&=\frac{\theta\left(aq,\dfrac{b_1b_3}{aq^{n+1}},b_2,\dfrac{aq}{b_3b_4},\dfrac{aq}{b_3b_5},\dfrac{aq}{b_3b_6};p\right)}{\theta\left(\dfrac{b_1}{aq^{n+1}},\dfrac{b_2}{b_3},\dfrac{aq}{b_3},\dfrac{aq}{b_4},\dfrac{aq}{b_5},\dfrac{aq}{b_6};p\right)}\\
&\times {}_{12}V_{11}(aq;b_1q,b_2q,b_3,b_4,b_5,b_6,q^{-n};p,q)\\
&\qquad\qquad + (b_2 \leftrightarrow b_3).
\end{aligned}$$

(c) Use this relation to prove (5).

Exercise 8.9 In this final exercise you will prove the squared norm formula for the biorthogonal functions. Define the difference operator

$$(D_-(u_0)f)(z) = \sum_{\sigma=\pm 1} \frac{\theta\left(u_0 z^\sigma, u_0 q z^\sigma, \frac{p}{u_0} z^\sigma, \frac{1}{u_0 q} z^\sigma; p\right)}{\theta(z^{2\sigma})} f(q^{\sigma/2} z)$$

(a) Show that D_- is "adjoint" to the D_+ operator in the sense that

$$\langle D_+(u_1 : t_1 : t_2, t_3, t_4) f(z), g(z)\rangle_{t_r, u_r} = \langle f(z), D_-(q^{-3/2} u_2) g(z)\rangle_{q^{1/2} t_r, q^{-1/2} u_1, q^{-3/2} u_2} .$$

(b) Show that the following relation holds term-by-term

$$\begin{aligned} &{}_{12}V_{11}(a; b_1, \ldots, b_6, q^{1-n}; p, q) \\ &= \frac{\theta\left(b_1, \frac{b_1}{a}, \frac{aq^n}{b_2}, q^n b_2; p\right)}{\theta\left(q^n, aq^n, \frac{b_1}{b_2}, \frac{b_1 b_2}{a}; p\right)} {}_{12}V_{11}(a; b_1 q, b_2, b_3, b_4, b_5, b_6, q^{-n}; p, q) \\ &\qquad + (b_1 \leftrightarrow b_2) . \end{aligned}$$

(c) Apply symmetries of the ${}_{12}V_{11}$ to all terms in the above relation to derive

$$\begin{aligned} &{}_{12}V_{11}(a; b_1, \ldots, b_6, q^{1-n}; p, q) \\ &= \frac{\theta\left(\frac{b_3}{a}, \frac{b_1 b_3}{aq^{n+1}}, \frac{aq^n}{b_2}, \frac{b_1 b_2}{aq}, \frac{a}{b_4}, \frac{a}{b_5}, \frac{a}{b_6}; p\right)}{\theta\left(a, q^n, \frac{b_1}{q}, \frac{b_3}{b_2}, \frac{a}{b_4 b_5}, \frac{a}{b_4 b_6}, \frac{a}{b_5 b_6}; p\right)} \\ &\quad \times {}_{12}V_{11}\left(\frac{a}{q}; \frac{b_1}{q}, \frac{b_2}{q}, b_3, b_4, b_5, b_6, q^{-n}\right) \\ &\qquad + (b_2 \leftrightarrow b_3). \end{aligned}$$

(d) Use the above relation to show that

$$\begin{aligned} &D_-(q^{-3/2} u_2) R_n(\,\cdot\,; t_1 : t_2, t_3, t_4; u_1, u_2) \\ &\qquad = \lambda_n R_{n-1}(\,\cdot\,; q^{1/2} t_1 : q^{1/2} t_2, q^{1/2} t_3, q^{1/2} t_4; q^{-1/2} u_1, q^{-3/2} u_2) \end{aligned}$$

for some coefficients λ_n.

(e) Using induction, prove the quadratic norm formula $\langle R_n, R_n \rangle = \cdots$ from Theorem 8.2.

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References

1. G.E. Andrews, R. Askey, R. Roy, *Special Functions*. Encyclopedia of Mathematics and its Applications, vol. 71 (Cambridge University Press, Cambridge, 1999)
2. I.B. Frenkel, V.G. Turaev, Elliptic solutions of the Yang–Baxter equation and modular hypergeometric functions. in *The Arnold–Gelfand Mathematical Seminars*, ed. by V.I. Arnold, I.M. Gelfand, V.S. Retakh, M. Smirnov (Birkhäuser Boston, Boston, MA, 1997), pp. 171–204
3. G. Gasper, M. Rahman, *Basic Hypergeometric Series*, 2nd edn. Encyclopedia of Mathematics and its Applications, vol. 96 (Cambridge University Press, Cambridge, 2004)
4. R. Koekoek, P.A. Lesky, R.F. Swarttouw, *Hypergeometric Orthogonal Polynomials and Their q-Analogues*. Springer Monographs in Mathematics (Springer, Berlin, 2010)
5. E.M. Rains, BC_n-symmetric Abelian functions. Duke Math. J. **135**(1), 99–180 (2006)
6. E.M. Rains, Transformations of elliptic hypergeometric integrals. Ann. Math. (2) **171**(1), 169–243 (2010)
7. H. Rosengren, Bibilography of Elliptic Hypergeometric Functions. www.math.chalmers.se/~hjalmar/bibliography.html
8. H. Rosengren, An elementary approach to 6*j*-symbols (classical, quantum, rational, trigonometric, and elliptic). Ramanujan J. **13**(1–3), 131–166 (2007)
9. S.N.M. Ruijsenaars, First order analytic difference equations and integrable quantum systems. J. Math. Phys. **38**(2), 1069–1146 (1997)
10. V.P. Spiridonov, An elliptic beta integral, in *New Trends in Difference Equations*, ed. by S. Elaydi, J. López Fenner, G. Ladas, M. Pinto (Taylor & Francis, London, 2002), pp. 273–282
11. V.P. Spiridonov, A. Zhedanov, Spectral transformation chains and some new biorthogonal rational functions. Commun. Math. Phys. **210**(1), 49–83 (2000)
12. E.T. Whittaker, G.N. Watson, *A Course of Modern Analysis*, 4th edn. (Cambridge University Press, Cambridge, 1962)

Integrability of Difference Equations Through Algebraic Entropy and Generalized Symmetries

Giorgio Gubbiotti

Abstract Given an equation arising from some application or theoretical consideration one of the first questions one might ask is: What is its behavior? It is integrable? In these lectures we will introduce two different ways for establishing (and in some sense also defining) integrability for difference equations: Algebraic Entropy and Generalized Symmetries. Algebraic Entropy deals with the degrees of growth of the solution of any kind of discrete equation (ordinary, partial or even differential-difference) and usually provides a quick test to establish if an equation is or not integrable. The approach based on Generalized Symmetries also provides tools for investigating integrable equations and to find particular solutions by symmetry reductions. The main focus of the lectures will be on the computational tools that allow us to calculate Generalized Symmetries and extract the value of the Algebraic Entropy from a finite number of iterations of the map.

1 Introduction: The Meaning of Integrability

The topic of these notes will be discrete equations of different kinds and their integrability properties. We will consider *ordinary difference equations*, i.e., relations of the form

$$u_{n+k} = f_n(u_{n+k-1}, \dots, u_{n+k'}) \ , \quad k', k, n \in \mathbb{Z} \ , \ k' < k \tag{1}$$

where the unknown function u_n is a function of the discrete integer variable $n \in \mathbb{Z}$. We will also discuss *differential-difference equations*, i.e., equations where the unknown is a function $u_n(t)$ of two variables, one continuous $t \in \mathbb{R}$ and one discrete $n \in \mathbb{Z}$. Typical examples of such equations are the so-called Volterra-like equations:

$$u_n' = f_n(u_{n+1}, u_n, u_{n-1}), \quad n \in \mathbb{Z}, \tag{2}$$

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or Toda-like equations:

$$u_n'' = f_n(u_n', u_{n+1}, u_n, u_{n-1}) \ , \quad n \in \mathbb{Z}, \tag{3}$$

where by a prime we indicate the derivative with respect to t. Finally we will deal with *two-dimensional partial difference equations* defined on a square lattice for an unknown function $u_{n,m}$ with $(n, m) \in \mathbb{Z}^2$, i.e., relations of the form:

$$Q(u_{n,m}, u_{n+1,m}, u_{n,m+1}, u_{n+1,m+1}) = 0 \ , \quad (n, m) \in \mathbb{Z}^2. \tag{4}$$

If the function Q is a multiaffine irreducible polynomial of its arguments we say that (4) is a *quad-equation*. This will be the kind of two-dimensional partial difference equation we will consider mostly.

We wish to study the *integrability* of these equations. The notion of integrability comes from Classical Mechanics and roughly means the existence of a "sufficiently" high number of *first integrals*. Indeed given a Hamiltonian system with Hamiltonian $H = H(p, q)$ with N degrees of freedom we say that this system is integrable if there exists N integrals of motions, i.e., N functions H_i $i = 1, \ldots, N$ which Poisson-commutes with the Hamiltonian:

$$\{H_i, H\} = 0 \ . \tag{5}$$

The Hamiltonian, which commutes with itself, is included in the list as $H_1 = H$. These first integrals must be well-defined functions on the phase space and *in involution*:

$$\{H_i, H_j\} = 0 \ , \quad i, j \in \{1, \ldots, N\} \tag{6}$$

and finally they should be functionally independent:

$$\operatorname{rank} \frac{\partial(H_1, \ldots, H_n)}{\partial(p_1, \ldots, p_n, q_1, \ldots, q_n)} = N. \tag{7}$$

Indeed the knowledge of these kinds of integrals gives the knowledge of the remaining $N - 1$ integrals and this is the content of the famous *Liouville theorem* [89, 129]. When more than N independent integrals exists, we say that the system is *superintegrable* [37, 110]. Note that in this case the additional integrals will not be in involution with the previous ones. Integrability in Classical Mechanics means that the motion is constrained on a subspace of the full phase space. With some additional assumptions on the geometric structure of the first integral it is possible to prove that the motion is quasi-periodic on some tori in the phase space [9, 10].

In the infinite-dimensional case, i.e., for partial differential equations, the notion of integrability has been studied and developed in the second half of the twentieth century. In this case one should be able to find *infinitely many conservation laws*.

These infinitely many conservations laws can be obtained, for example, from the so-called *Lax pair* [75], that is an overdetermined *linear* problem whose compatibility is ensured if and only if the nonlinear equation is satisfied. A bona fide Lax pair can be used to produce the required conservations laws, with the associated generalized symmetries (see Sect. 3.2). The form of the Lax pair will be different depending on the kind of equation we are considering. It is worthwhile noting that Lax pairs can be used also in Classical Mechanics [33] and that there exist examples of Lax pairs which are not bona fide [19, 22, 82, 85, 91, 92, 113, 114], the so-called *fake Lax pairs*. These fake Lax pairs cannot provide nor the infinite sequence of first integrals, nor the generalized symmetries, so they are useless in proving integrability.

In general we can say that integrability is a property affecting the regularity of the motion. In the case of discrete equations given an initial condition we can compute the whole set of solutions with machine precision. The question of regularity can seem futile, but in fact what we want is to understand the behavior of the given equation without having to compute a full sequence of iterates!

As a final remark on terminology it is worthwhile noting that the concept of integrability and the concept of solvability are very different. This can be easily explained with an example, the famous logistic map:

$$u_{n+1} = 4u_n(1 - u_n). \tag{8}$$

The solution of this equation is given by [115]:

$$u_n = \sin^2(c_0 2^{n-1}), \tag{9}$$

where c_0 is an arbitrary constant linked with the initial condition via $u_0 = \sin^2(c_0/2)$. Equation (9) is very sensitive to the initial condition, which is the intuitive definition of chaos. Indeed computing the derivative with respect to the initial condition we have:

$$\frac{\mathrm{d}u_n}{\mathrm{d}c_0} = 2^n \sin(c_0 2^{n-1}) \cos(c_0 2^{n-1}). \tag{10}$$

Thus we can see that the error grows exponentially with n, which is one of the indicators of "chaos."

If by integrability we mean the existence of a Lax pair then the proof of the integrability of an equation is a highly nontrivial task and there is no general algorithm to do so. So in these notes we will provide the methods of *Algebraic Entropy* and *Generalized Symmetries* which can be used to detect integrability without the need of proving (or disproving) the existence of a Lax pair.

2 Algebraic Entropy

In this section we will focus on the integrability detector called Algebraic Entropy. In Sect. 2.1 we will expand the intuitive idea given in the example of the logistic map. Then we will introduce the precise definition of Algebraic Entropy for difference equations, differential equations and quad equations. We will address the problem from the theoretical point of view discussing mainly the setting and then derive the main properties of Algebraic Entropy and we will discuss briefly the geometric setting of the Algebraic Entropy. In Sect. 2.2 we will discuss the computational tools that allow us to extract the value of the Algebraic Entropy from finite sequence. In Sect. 2.3 we will provide some relevant examples.

2.1 Definition and Basic Properties

As we saw in the example of the logistic equation (8) the notion of chaos is related with the exponential growth of the solution with respect to the initial condition. Equation (8) possesses an explicit solution therefore it is easy to understand a posteriori its properties. Let us now consider the general logistic map with an arbitrary parameter $r \in \mathbb{R}$:

$$u_{n+1} = ru_n(1 - u_n). \tag{11}$$

We wish to understand how this equation evolves, therefore we fix an initial condition u_0 and we compute the iterates:

$$u_1 = -ru_0^2 + ru_0 \,, \tag{12a}$$

$$u_2 = -r^3u_0^4 + 2r^3u_0^3 - (r^3 + r^2)u_0^2 + r^2u_0 \,, \tag{12b}$$

$$u_3 = -r^7u_0^8 + 4r^7u_0^7 - (6r^7 - 2r^6)u_0^6 + (4r^7 + 6r^6)u_0^5 + \text{l.o.t.}, \tag{12c}$$

$$u_4 = -r^{15}u_0^{16} + 8r^{15}u_0^{15} - (28r^{15} + 4r^{14})u_0^{14} + \text{l.o.t}, \tag{12d}$$

where by l.o.t. we mean terms with lower powers in u_0. Then it is clear that there is a regularity in how the degree of the polynomial u_n in u_0, d_n, grows. Indeed one can guess that $d_n = 2^n$ and check this guess for successive iterations. This is a clear indication that our system is chaotic as it was in the solvable case $r = 4$. This should be no surprise since the generic r case is even more general!

This simple example shows how examining the iterates of a recurrence relation can be a good way to extract information about integrability even if we cannot solve the equation explicitly. However in more complicated examples it is usually impossible to calculate explicitly these iterates by hand or even with any state-of-the-art formal calculus software, simply because the expressions one should manipulate are rational fractions of increasing degree of the various initial conditions. The complexity and size of the calculation make it impossible to calculate the iterates.

It was nevertheless observed that "integrable" maps are not as complex as generic ones. This was done primarily experimentally, by an accumulation of examples, and later by the elaboration of the concept of *Algebraic Entropy* for difference equations [14, 28, 31, 111, 122]. In [121, 124] the method was developed in the case of quad equations and then used as a classifying tool [61]. Finally in [27] the same concept was introduced for differential-difference equation and later [123] to the very similar case of differential-delay equations. In our review we will mainly follow [45].

The basic idea, given a rational map, which can be an ordinary difference equation, a differential-difference equation or even a partial difference equation, is to examine the growth of the degree of its iterates as we did for (11), and extract a canonical quantity, which is an index of complexity of the map. This will be the algebraic entropy (or its avatar the dynamical degree).

For theoretical purposes it is usual to consider maps in a projective space rather than in the affine one. One then transforms its recurrence relation into a polynomial map in the homogeneous coordinates of the proper projective space over some closed field[1]:

$$x_i \mapsto \varphi_i(x_k), \tag{13}$$

with $x_i, x_k \in \mathcal{IN}$ where $\mathcal{IN}$ is the space of the initial conditions. The recurrence is then obtained by iterating the polynomial map φ_i. It is usual to ask that the map φ_i be *birational*, i.e., it possesses an inverse which is again a rational map. This fact is of crucial theoretical importance, as it will be explained at the end of this section. The space of the initial condition depends on which type of recurrence relation we are considering. Let us enumerate the various cases.

1. If we are dealing with a $k-k'$ order difference equation in the form (1) the initial conditions will be just the starting $(k-k')$-tuple:

$$\mathcal{IN} = \{u_{k'}, u_{k'+1}, \dots, u_{k-2}, u_{k-1}\}. \tag{14}$$

   To obtain the map we just need to pass to homogeneous coordinates in (1) and in (14). Note that the logistic map we considered above (11) is a polynomial map, but it is not birational, since its inverse is algebraic.
2. If we are dealing with a differential-difference equation of the discrete $(k-k')$h order and of the pth continuous order, the space of initial conditions is infinite dimensional. Indeed, in the case the order of the equation is $k-k'$, we need the initial value of $(k-k')$-tuple as a function of the parameter t, but also the value of *all its derivatives*:

$$\mathcal{IN} = \{u^{(j)}_{k'}(t), u^{(j)}_{k'+1}(t), \dots, u^{(j)}_{k-2}(t), u^{(j)}_{k-1}(t)\}_{j\in\mathbb{N}_0}, \tag{15}$$

[1] The reader can think this field to be the complex one $\mathbb{C}$, but we will see in Sect. 2.2 that in practice finite fields can be useful.

where by $u_i^{(j)}(t)$ we mean the j-derivative of $u_i(t)$ with respect to t. We need all the derivatives of $u_i(t)$ and not just the first p because at every iteration the order of the equation is raised by p. To obtain the map one just need to pass to homogeneous coordinates in the equation and in (15).

For both kinds of equations we are in the position to define the concept of Algebraic Entropy. Indeed if we factor out any common polynomial factors we can say that the degree with respect to the initial conditions is well defined, in a given system of coordinates, although it is not invariant with respect to changes of coordinates. We can therefore form the sequence of degrees of the iterates of the map φ and call it $d_k = \deg \varphi^k$:

$$\underbrace{1, \ldots, 1}_{k-k'}, d_1, d_2, d_3, d_4, d_5, \ldots, d_k, \ldots . \tag{16}$$

The degree of the birational projective map φ has to be understood as the *maximum of the total polynomial degree in the initial conditions* $\mathcal{IN}$ of the entries of φ. The same definition in the affine case just translates to the *maximum of the degree of the numerator and of the denominator* of the kth iterate in terms of the affine initial conditions. Degrees in the projective and in the affine setting can be different, but the global behaviour will be the same due to the properties of homogenization and de-homogenization. Then the entropy of such a sequence is defined to be:

$$\eta = \lim_{k\to\infty} \frac{1}{k} \log d_k. \tag{17}$$

Such limit exists since from the elementary property of any pair of birational maps φ and ψ:

$$\deg(\psi \circ \varphi) \leq \deg \psi \deg \varphi. \tag{18}$$

Furthermore the inequality (18) proves that there is an upper bound for the Algebraic Entropy:

$$\eta \leq \deg \varphi. \tag{19}$$

We see then that if $\eta = 0$ we must have

$$d_k \sim k^\nu \ , \quad \text{with } \nu \in \mathbb{N}_0 \ , \text{as } k \to \infty. \tag{20}$$

We will then have the following classification of equations according to their Algebraic Entropy [61]:

Linear growth: The equation is linearizable.
Polynomial growth: The equation is integrable.
Exponential growth: The equation is chaotic.

Furthermore it is easy to see that the Algebraic Entropy is a *birational invariant of such maps*. Indeed if we suppose that we have two *birationally equivalent maps* φ and ψ then there exists a birational map χ such that:

$$\psi = \chi^{-1} \circ \varphi \circ \chi \tag{21}$$

implying:

$$\deg \psi^k \leq K \deg \varphi^k, \tag{22}$$

where $K \in \mathbb{N}$ is a constant depending on the degree of the map χ. Since we can obtain an analogous equation as $\varphi = \chi \circ \psi \circ \chi^{-1}$ we conclude that $\eta_\psi = \eta_\varphi$.

To clarify the theory we presented we now give three very simple examples of calculation of the Algebraic Entropy of difference equations.[2]

Example 2.1 (Hénon Map) In this example we consider the so called Hénon map of the plane [56]. It relates the iterates of a two component vector (x_n, y_n) via the recurrence[3]:

$$x_{n+1} = 1 - \alpha x_n^2 + y_n \ , \tag{23a}$$

$$y_{n+1} = \beta x_n. \tag{23b}$$

It easy to see that it can be written as a second-order difference equation:

$$u_{n+1} = 1 - \alpha u_n^2 + \beta u_{n-1} \tag{24}$$

Computing the degrees of the iterates we get:

$$1, 1, 2, 4, 8, 16, 32, 64, 128, 256, 512 \ldots \tag{25}$$

The Hénon map is of degree 2. It is easy to see that the sequence it is not only bounded by 2^k, but it saturates its bound. The sequence is exactly fitted by 2^k and its entropy will be $\log 2$.

The trajectory of this map as system (23) in the plane are displayed in Fig. 1, which clearly shows the "chaoticity" of the system.

Example 2.2 (Nonsaturating exponential difference equation) Consider the second-order nonlinear difference equation:

$$u_{n+1} = \alpha u_n u_{n-1} + \beta u_n + \gamma u_{n-1}, \tag{26}$$

[2] We will consider the degrees always computed in the affine setting.

[3] In the original work we have the particular choice of parameters $\alpha = 1.4$ and $\beta = 0.3$

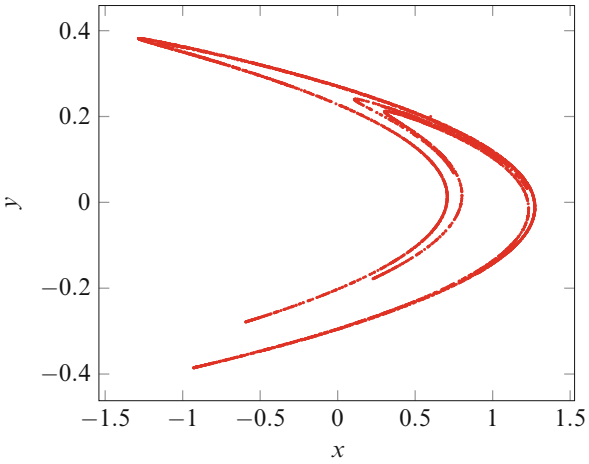

Fig. 1 The Hénon map in the plane (x, y) with $a = 1.4$ and $b = 0.3$ and the initial conditions $(x_0, y_0) = (0.6, 0.2)$

where α, β and γ are real constants. Computing the degrees of the iterates we get:

$$1, 1, 2, 3, 5, 8, 13, 21, 34, 55, 89, 144, 233, 377 \ldots \tag{27}$$

Also this map is of degree 2, but now its growth is different. We see that from the second iterate there is a drop in the degree, so $d_k < 2^k$ asymptotically. The reader may recognize in this sequence the Fibonacci sequence. The Fibonacci sequence is known to solve the second-order linear difference equation:

$$d_{k+1} = d_k + d_{k-1}. \tag{28}$$

This means that we have asymptotically:

$$d_k \sim \left(\frac{1+\sqrt{5}}{2}\right)^k \tag{29}$$

and the algebraic entropy of the recurrence relation (26) will be:

$$\eta = \log\left(\frac{1+\sqrt{5}}{2}\right), \tag{30}$$

i.e., the logarithm of the Golden Ratio.

Example 2.3 (Hirota–Kimura–Yahagi equation) Consider the nonlinear second-order difference equation:

$$u_{n+1}u_{n-1} = u_n^2 + \beta^2. \tag{31}$$

This equation possess the first integral [62]:

$$K(u_n, u_{n-1}) = \frac{2u_n u_{n-1}}{u_n^2 + u_{n-1}^2 + \beta^2}, \tag{32}$$

i.e.,

$$K(u_{n+1}, u_n) - K(u_n, u_{n-1}) = 0, \tag{33}$$

along the solutions of (31). First integrals are a constraint to the motion of a system, so in this case we expect a great drop in the degrees. Indeed we have:

$$1, 1, 2, 4, 6, 8, 10, 12, 14, 16, 18, 20, 22, 24, 26, 28 \ldots \tag{34}$$

The degrees appear to grow *linearly*: $d_k = 2k$ and the discrepancy from the saturation starts from the third iterate.

Now we introduce the concept of Algebraic Entropy for quad equations which was introduced in [121]. We will follow mainly the exposition presented in [124] with some generalizations which were given in [50].

In the case of quad equations the situation is more complicated than in the case of one-dimensional equations. First of all in the one-dimensional case one has to worry only about the evolution in two opposite directions (this was the meaning of the birationality condition). In the two-dimensional case we have to worry about four possible directions of evolution corresponding to the four ways we can solve the quad equation. In general, initial conditions can be given along straight lines in the four directions. However usually it is preferred to give initial conditions on *staircase* configurations. The evolution from any staircase-like arrangement of initial values is possible in the quadrilateral lattice. This in principle does not rules out configurations in which are present hook-like configurations (see (4) in Fig. 2). This kinds of configuration will require compatibility conditions on the initial data, since they give more than one way to calculate the same value for the dependent variable which is not ensured to be the equal. The staircases need to go from $(n = -\infty, m = -\infty)$ to $(n = \infty, m = \infty)$, or from $(n = -\infty, m = +\infty)$ to $(n = \infty, m = -\infty)$ because the space of initial conditions is infinite. We will restrict ourselves to regular diagonals which are staircases with steps of *constant* horizontal length, and *constant* vertical height. Figure 2 shows four diagonals. The ones labeled (1) and (2) are regular. The one labeled (3) would be acceptable, but we will not consider such diagonals. Line (4) is excluded since it may lead to incompatibilities.

Given a line of initial conditions, it is possible to calculate the values $u_{n,m}$ all over the two-dimensional lattice. We have a well defined evolution, since we restrict ourselves to regular diagonals. Moreover, and this is a crucial point, *if we want to evaluate the transformation formula for a finite number of iterations, we only need a diagonal of initial conditions with finite extent*.

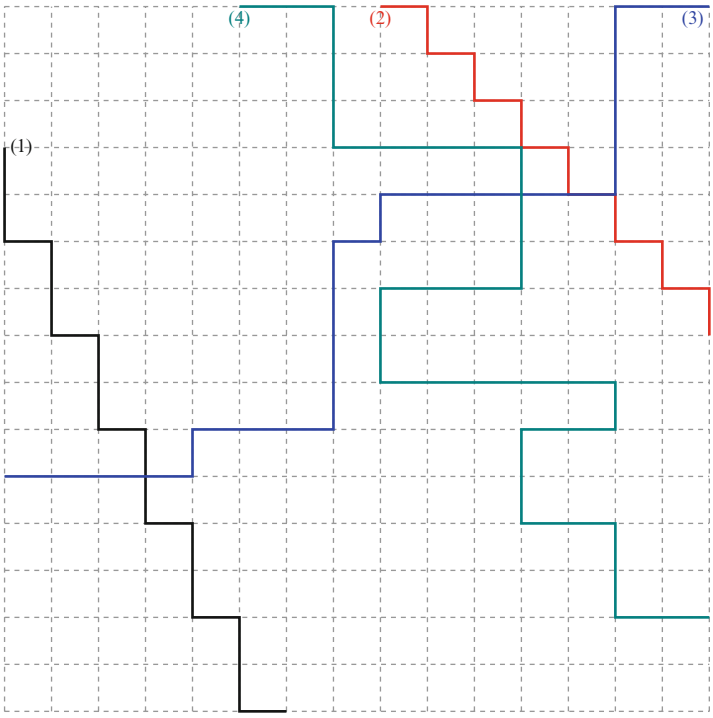

Fig. 2 Regular and nonregular staircases

For any positive integer N, and each pair of relative integers $[\lambda_1, \lambda_2]$, we denote by $\Delta^{(N)}_{[\lambda_1,\lambda_2]}$, a regular diagonal consisting of N steps, each having horizontal size $l_1 = |\lambda_1|$, height $l_2 = |\lambda_2|$, and going in the direction of positive (resp. negative) n_k, if $\lambda_k > 0$ (resp. $\lambda_k < 0$), for $k = 1, 2$. See Fig. 3.

Suppose we fix the initial conditions on $\Delta^{(N)}_{[\lambda_1,\lambda_2]}$. We may calculate u over a rectangle of size $(Nl_1 + 1) \times (Nl_2 + 1)$. The diagonal cuts the rectangle in two halves. One of them uses all initial values, and we will calculate the evolution only on that part. See Fig. 4.

We are now in a position to calculate "iterates" of the evolution. Choose some restricted diagonal $\Delta^{(N)}_{[\lambda_1,\lambda_2]}$. The total number of initial points is $q = N(l_1 + l_2) + 1$. For such restricted initial data, the natural space where the evolution acts is the projective space $\mathbb{P}^q$ of dimension q. We may calculate the iterates and fill Fig. 4, considering the q initial values as inhomogeneous coordinates of $\mathbb{P}^q$. Evaluating the degrees of the successive iterates, we will produce double sequences of degrees $d^{(l)}_k$. The simplest possible choice is to apply this construction to the restricted diagonals $\Delta^{(N)}_{[\pm1,\pm1]}$, which we will denote $\Delta^{(N)}_{++}$, $\Delta^{(N)}_{+-}$, $\Delta^{(N)}_{-+}$ and $\Delta^{(N)}_{--}$. We will call them fundamental diagonals (the upper index (N) is omitted for infinite lines). The four principal diagonals are showed in Fig. 5.

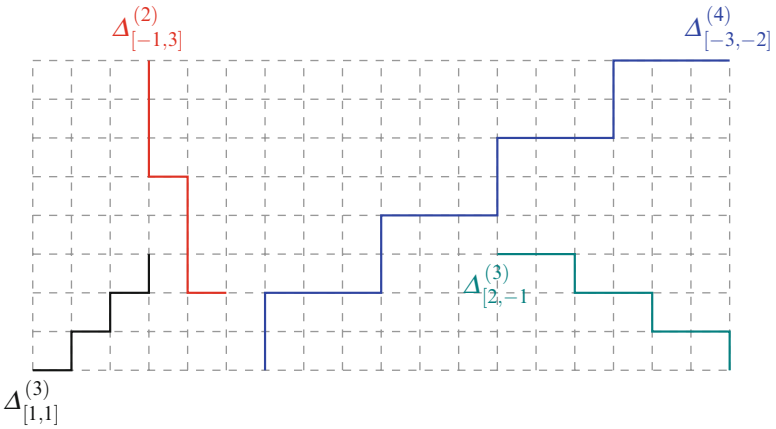

Fig. 3 Various kinds of restricted initial conditions

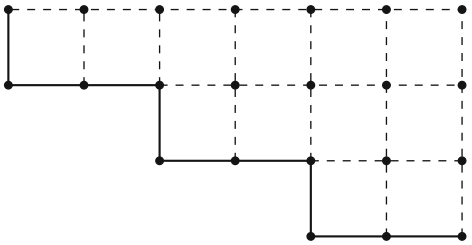

Fig. 4 The range for the initial conditions $\Delta^{(3)}_{[-2,1]}$

The pattern of degrees is then of the form

$$\begin{array}{ccccccc} 1 & d_1^{(N-1)} & d_2^{(N-2)} & \dots & d_{N-1}^{(2)} & d_n^{(1)} \\ 1 & 1 & d_1^{(N-2)} & d_2^{(3)} & \dots & d_{N-1}^{(1)} \\ & 1 & 1 & d_1^{(3)} & d_2^{(2)} & \dots \\ & & 1 & 1 & d_1^{(2)} & d_2^{(1)} \\ & & & 1 & 1 & d_1^{(1)} \\ & & & & 1 & 1 \end{array} \tag{35}$$

To each choice of indices $[\pm 1, \pm 1]$ we associate a sequence of degrees $d^{(l)}_{k,\pm\pm}$.

We shall call the sequence

$$1, d^{(1)}_{1,\pm\pm}, d^{(1)}_{2,\pm\pm}, d^{(1)}_{3,\pm\pm}, d^{(1)}_{4,\pm\pm}, \dots \tag{36}$$

the *principal sequence* of growth. A sequence as

$$1, d^{(l)}_{1,\pm\pm}, d^{(l)}_{2,\pm\pm}, d^{(l)}_{3,\pm\pm}, d^{(l)}_{4,\pm\pm}, \dots \tag{37}$$

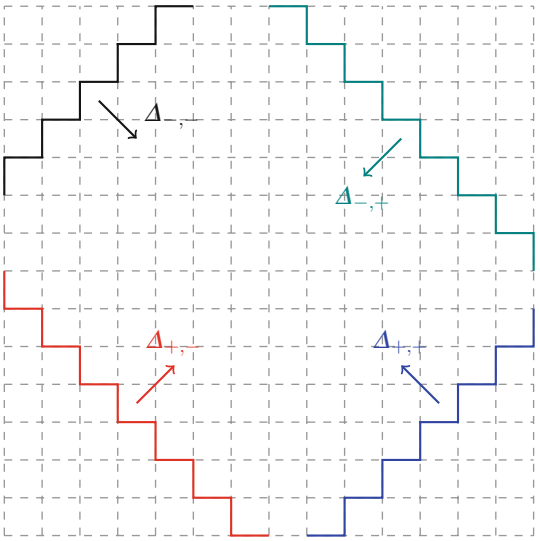

Fig. 5 The four principal diagonals

with $l = 2$ will be a *secondary sequence* of growth, for $l = 3$ a *third*, and so on. The fundamental entropies of the lattice equation are given by:

$$\eta^{(i)}_{\pm\pm} = \lim_{k\to\infty} \frac{1}{k} \log d^{(i)}_{k,\pm,\pm}. \tag{38}$$

The existence of this limit can be proved in an analogous way as for one dimensional systems. We note that a priori the degrees along the diagonals of a quad equation do not need to be equal, however in most cases they are.[4] In the cases in which the degrees along the diagonals are not equal it is important to isolate repeating patterns in (35). For the moment the only known examples of such behavior are the trapezoidal H_4 equations and the H_6 equations which are nonautonomous two-dimensional lattice equations with two-periodic coefficients [16]. They possess a principal and a secondary sequence reflecting the periodicity of the coefficients. At the moment quad equations exhibiting more complicated behavior are not known. An explicit example is discussed in Sect. 2.3 following the paper where this "extended notion" of growth of degrees for quad equations was introduced [50]. Equations with higher periodicity, as those introduced in [42], may have different behavior, but they are still unstudied from the point of view of Algebraic Entropy.

One may wonder about the origin of the drop of the degree. It is actually geometrically very simple, and comes from the singularity structure. We will discuss this problem in the case of difference equations, since the other cases are essentially the same, but they are less intuitive. We recall that to a difference equation (1) of

[4] In the original definition in [124] those degrees are supposed equal.

order $n = k - k'$ we can associate a map projective map $\varphi\colon \mathbb{P}^n \to \mathbb{P}^n$. A point of homogeneous coordinates $[x] = [x_0, x_1, \ldots, x_n]$ is *singular* if all the homogeneous coordinates of the image by φ vanish. The set of these points is thus given by $n + 1$ homogeneous equations. This set has co-dimension at least 2: it will be points in $\mathbb{P}^2$, complex curves and points in $\mathbb{P}^3$, and so on. One important point is that, as soon as the map is nonlinear, and this is the case we will be interested in, there are always singular points. The vanishing of all homogeneous coordinates means that there is no image point in $\mathbb{P}^n$. The mere vanishing of a few, but not all coordinates, means that the image "goes to infinity", but this is harmless, contrary to what happens in affine space. This is what projective space has been invented for: to cope with points at infinity, which are not to be forgotten when one consider algebraic varieties and rational maps. Moreover, using projective space over closed fields simplifies a lot the counting of intersection points by Bezout theorem. The maps we consider are almost invertible. They are diffeomorphisms on a Zariski open set, i.e., they are invertible everywhere except on an algebraic variety. We can find this set as follows: suppose the map φ and its inverse $\psi = \varphi^{-1}$ are written in terms of homogeneous coordinates. The composed maps $\varphi \circ \psi$ and respectively $\psi \circ \varphi$ are then just multiplication of all coordinates by some polynomial κ_φ and respectively κ_ψ:

$$\varphi \circ \psi([x]) = \kappa_\varphi([x])\,\mathrm{Id}([x])\ , \quad \psi \circ \varphi([x]) = \kappa_\psi([x])\,\mathrm{Id}([x])\ . \tag{39}$$

The map φ is clearly not invertible on the image of the variety of equation $\kappa_\varphi([x])$. What may happen is that further action of φ on these points leads to images in the singular set of φ. This means that $\kappa_\varphi([x])$ (or a piece of it if it is decomposable) has to factorize from all the components of the iterated map. This is the origin of the drop of the degree! This is the link between singularity (in the projective sense) and the degree sequence. A graphical explanation of this procedure is illustrated schematically in Fig. 6.

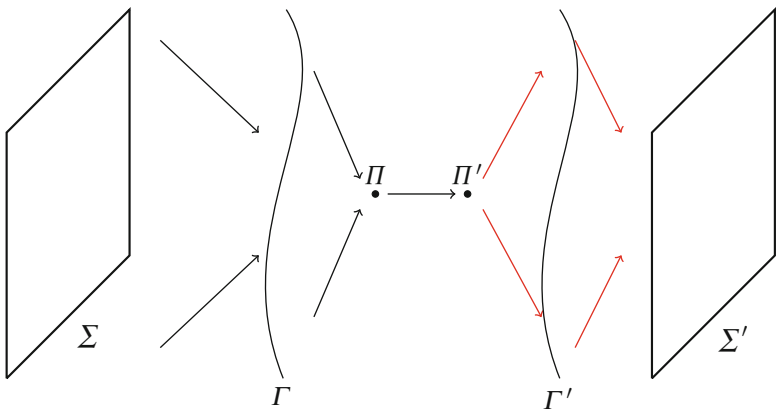

Fig. 6 A possible blow-down blow-up scheme in $\mathbb{P}^3$

This is the link with the famous method of *singularity confinement* [43, 66, 108]. If for all components of the variety $\kappa_\varphi([x]) = 0$ one encounters singular points of φ in such a way that some finite order iterate of φ (once the common factors are trimmed) define nonambiguously a proper image in $\mathbb{P}^n$, we have "singularity confinement."

The relationship of the notion of Algebraic Entropy with the structure of the singularities of maps and lattice equations have been used also as a computational tool. Examples of such approach are given in [29, 112, 119] and more recently in [126] where it was also proved that for equation of order higher than the second not all the singularities play the same rôle.

2.2 Computational Tools

Now that we have introduced the definition of Algebraic Entropy and discussed the origin of the dropping of the degrees, it is time to turn to the computational tools which help us to calculate it.

First of all it is clear from our first example with the logistic map that the complexity of the calculations grow more the more iterates we compute. A good way to reduce the computational complexity of the problem is to consider a particular set of initial condition given by *straight lines* in the appropriate projective space $\mathbb{P}^q$. This corresponds to the following choice of inhomogeneous coordinates:

$$u_i = \frac{\alpha_i t + \beta_i}{\alpha_0 t + \beta_0}\,, \quad u_i \in \mathcal{IN}. \tag{40}$$

In the case differential-difference equation we will assume that the parameter t is the same which describes the "time" evolution of the problem.

A useful simplification consists in using only integer numbers in the computations. Since we want to avoid accidental cancellation the best way is to consider only *prime numbers*. This means that we must choose the α_i, β_i and the eventual parameters appearing in the equation as prime numbers. A final simplification which can speed up the calculations is to consider the factorization of the iterates on a finite field $\mathbb{K}_p$, with p prime. This is particularly useful since otherwise we are dealing with factorization over the integer domain and the most common algorithms for factorization over the integer domain actually at first compute factorization over finite fields [127].

With these rules we should be able to avoid eventual accidental cancellations and therefore to have a bona fide sequence of degrees. Since the result is experimental it is still better to do it more than once to be sure of the result. In [46] a `python` implementation of these ideas is given in the case of lattice equation. The prime number p is chosen adaptively as the next prime after the square plus one of the biggest prime in α_i, β_i and the equation parameters.

Now let us assume that we have computed our iterations and we are given the finite sequence:

$$d_0, d_1, \ldots, d_n. \tag{41}$$

To obtain information about the asymptotic behavior of such a sequence (41) we calculate its generating function [74], i.e., a function $g = g(s)$ such that its Taylor series coincides with the elements of the obtained series. In looking for such functions it is important to try to *use the minimum number of d_k possible*. It is reasonable to suppose that such a generating function is rational even if it is known that it is not always the case [55]. Such generating functions can therefore be calculated by using Padé approximants [12, 107].

The *Padé approximant* is a way of representing a function as a rational function, i.e., as the ratio of two polynomials. Indeed let us assume to know a function $f = f(s)$ analytic in some domain $D \subset \mathbb{C}$ containing $s = 0$.[5] Therefore the function f can be represented as *power series* centered at $s = 0$:

$$f(s) = \sum_{k=0}^{\infty} d_k s^k. \tag{42}$$

To find the Padé approximant of order $[L : M]$ for the function f means to find a rational function:

$$[L : M](s) = \frac{P^{[L:M]}(s)}{Q^{[L:M]}(s)} = \frac{a_0 + a_1 s + \cdots + a_L s^L}{1 + b_1 s + \cdots + b_M s^M}, \tag{43}$$

such that its Taylor series centered at $s = 0$ coincides with (42) as much as possible (here $P^{[L:M]}(s)$ and $Q^{[L:M]}(s)$ are assumed to be polynomials). Notice that the choice of $b_0 = 1$ into the denominator [i.e., in the polynomial $Q^{[L:M]}(s)$] is purely conventional, since the ratio of the two polynomial $P^{[L:M]}(s)$ and $Q^{[L:M]}(s)$ is defined up to a common factor. A Padé approximant of order $[L : M]$ has a priori $L + 1$ independent coefficients in the numerator and M independent coefficients in denominator, making $L + M + 1$ coefficients at all. This means that given a full Taylor series as in (42) and a Padé approximant of order $[L : M]$ we will have a precision of order s^{L+M+1}:

$$f(s) = [L : M](s) + \mathrm{O}\big(s^{L+M+1}\big). \tag{44}$$

In the same way as a polynomial is its own Taylor series a rational function is its own Padé approximant for the right choice of L and M. This is why the best approach in the search for rational generating functions is the use of Padé approximants: by computing a sufficiently high number of terms if my generating function is rational

[5] This is always possible to be done up to a translation.

I will eventually find it. Without going into the details of such beautiful theory we note that the simplest way to compute the Padé approximant of order $[L:M]$ (43) is from Linear Algebra and one only needs to compute two determinants:

$$Q^{[L:M]}(s) = \begin{vmatrix} d_{L-M+1} & d_{L-M+2} & \dots & d_L & d_{L+1} \\ d_{L-M+2} & d_{L-M+3} & \dots & d_{L+1} & d_{L+2} \\ \vdots & \vdots & & \vdots & \vdots \\ d_{L-1} & d_L & \dots & d_{L+M-2} & d_{L+M-1} \\ d_L & d_{L+1} & \dots & d_{L+M-1} & d_{L+M} \\ s^M & s^{M-1} & \dots & s & 1 \end{vmatrix}, \tag{45a}$$

$$P^{[L:M]}(z) = \begin{vmatrix} d_{L-M+1} & d_{L-M+2} & \dots & d_{L+1} \\ d_{L-M+2} & d_{L-M+3} & \dots & d_{L+2} \\ \vdots & \vdots & & \vdots \\ d_{L-1} & d_L & \dots & d_{L+M-1} \\ d_L & d_{L+1} & \dots & d_{L+M} \\ \sum_{k=0}^{L-M} d_k s^{M+k} & \sum_{k=0}^{L-M+1} d_k s^{M+k-1} & \dots & \sum_{k=0}^{L} d_k s^k \end{vmatrix}, \tag{45b}$$

and then the Padé approximant of order $[L:M]$ is given by [65]:

$$[L:M](s) = \frac{P^{[L:M]}(s)}{Q^{[L:M]}(s)}. \tag{46}$$

That is all we need from the theory of Padé approximants to calculate generating functions. The interested reader can consult the above references for a more complete exposition.

Suppose now we have obtained a generating function using a subset of elements of (41). Such a generating function is a *predictive tool*, since we can confront the next terms in (41) with the successive terms of the Taylor expansion of the generating function. If they agree we are almost surely on the right way. This is the reason why it is important to find the generating function with the minimum number of d_k possible. If we used all the terms in the sequence (41) then we need to compute more iterates in order to have a predictive result. Notice that since the sequence (41) is a series of degrees, i.e., of positive integers, if the Taylor series of the generating functions give rise to rational numbers it can be immediately discarded as a non-bona fide generated function. A reasonable strategy for finding rational generating functions with Padé approximants is to use Padé approximants of equal order $[j:j]$ which, as stated above, need $2j+1$ point to be determined. Let us remark, that a rational generating function satisfies a finite order linear recurrence relation [30].

Once we have a generating function we need to calculate the asymptotic behavior of the coefficients of its Taylor series. To do this we will use the *inverse $\mathcal{Z}$-transform* [26, 30, 67] method. Indeed let $f(\tau)$ be a function expressible in Laurent series of only *negative powers* of its argument:

$$f(\tau) = \sum_{k=0}^{\infty} d_k \tau^{-k}. \tag{47}$$

The inverse $\mathcal{Z}$-transform of f is the defined to be [67]:

$$\mathcal{Z}^{-1}[f(\tau)]_k = \frac{1}{2\pi \mathrm{i}} \int_C f(\tau)\tau^{k-1}\,\mathrm{d}\tau\ , \quad k \in \mathbb{N} \tag{48}$$

where C is a simple closed path outside of which $f(\tau)$ is analytic. If f is rational function, C can be taken as a circle of radius R enclosing all the singularities of $f(\tau)$ in the complex τ plane. By the residue theorem [23, 130], this implies, as the rational functions have only a finite numbers of poles $\tau_j \in \mathbb{C}, j \in \{1, \ldots, P\}$:

$$\mathcal{Z}^{-1}[f(\tau)] = \sum_{j=1}^{P} \operatorname*{Res}_{\tau=\tau_j} \{f(\tau)\tau^{k-1}\}. \tag{49}$$

Indeed given the generating function g which is expressed as the Taylor series

$$g(s) = \sum_{k=0}^{\infty} d_k s^k, \tag{50}$$

i.e., a series of *positive powers* of s, we have by the definition (48):

$$d_k = \mathcal{Z}^{-1}[g(\tau^{-1})]_k. \tag{51}$$

Since we suppose our generating function to be rational, $g(\tau^{-1})$ is again a rational function and we can easily compute it using the residue approach (49).

Formula (49) will be valid asymptotically, and for rational $f(\tau)$ we can estimate for which k it will be valid. Assume that $f(\tau) = \widehat{P}(\tau)/\widehat{Q}(\tau)$ with $\widehat{P}, \widehat{Q} \in \mathbb{C}[\tau]$, i.e., polynomials in τ. Indeed if $\tau = 0$ is a root of $\widehat{Q}$ of order k_0 we must distinguish the cases when $k > k_0 + 1$ and $k \leq k_0 + 1$. For $k \leq k_0 + 1$ we will have a pole in $\tau = 0$ of order $k_0 + 1 - k$. So the general formula (49) will be valid only for $n > k_0 + 1$. In the case of rational generating functions $g(s) = P(s)/Q(s)$, with $P, Q \in \mathbb{C}[s]$ we will introduce a spurious $\tau = 0$ singularity in $g(\tau^{-1})$ if we will have $\deg P \geq \deg Q$.

From the generating function we can get the Algebraic Entropy, defined by (17). Recalling that notion of radius of convergence R of a power series [130]:

$$R^{-1} = \lim_{k\to\infty} |d_k|^{1/n} \tag{52}$$

and the continuity of the logarithm function we have from (17) that the Algebraic Entropy can be always given by the logarithm of the inverse of the smallest root of the denominator of g:

$$\eta = \min_{\{s\in\mathbb{C}|Q(s)=0\}} \log|s|^{-1}. \tag{53}$$

To conclude this section we examine the growths of Examples 2.1, 2.2 and 2.3 using the generating functions in order to have a more rigorous proof of their growth.

Example 2.4 (Growth of the Hénon Map) The first and very trivial example is to consider the growth of the Hénon map (23) [or (24)] as given by (25). We see that computing the Padé approximant with the first three points, i.e., $[1:1](s)$ we obtain:

$$[1:1](s) = \frac{1-s}{1-2s}. \tag{54}$$

This first Padé approximant is already predictive since

$$[1:1](s) = 1 + s + 2s^2 + 4s^3 + 8s^4 + 16s^5 + 32s^5 + \mathrm{O}(s^6). \tag{55}$$

So we can conclude $g(s) = [1:1](s)$. This obviously gives the growth as $d_k = 2^{k-1}$ for every $k \geq 1$.[6] The only pole of $g(s)$ is then $s_0 = 1/2$ which according to (53) yields $\eta = \log 2$.

Example 2.5 (Growth of the Map (26)) We see that in this case the Padé approximant $[1:1](s)$ gives exactly the same result as (54), therefore it does not describe the series. The next one $[2:2](s)$ instead gives:

$$[2:2](s) = \frac{1}{1-s-s^2}, \tag{56}$$

which is predictive. We conclude that in this case $g(s) = [2:2](s)$. This gives the growth:

$$d_k = \frac{5+3\sqrt{5}}{10}\left(\frac{1+\sqrt{5}}{2}\right)^k + \frac{5-3\sqrt{5}}{10}\left(\frac{1-\sqrt{5}}{2}\right)^k, \tag{57}$$

which, as we said before, has the asymptotic behavior (29). The poles of (56) are then:

$$s_\pm = \frac{-1\pm\sqrt{5}}{2} \tag{58}$$

and as $|s_+| > |s_-|$ the algebraic entropy is given by (30).

[6] We note that in terms of the iterations the first 1 in (25) have to be interpreted as d_{-1}, but this is just matter of notation.

Example 2.6 (Growth of the Hirota–Kimura–Yahagi Equation) We now consider the very slow growth of (31) given by (34). Again the $[1:1](s)$ is the same as in (54) and therefore does not describes (34) as well as $[2;2](s)$. On the other hand $[3:3](s)$ gives:

$$[3:3](s) = \frac{s^3 + s^2 - s + 1}{(1-s)^2} \tag{59}$$

and again this approximant is predictive. So we conclude that $g(s) = [3:3](s)$ and that $d_k = 2k-2$. Since the only pole lays on the unit circle we have that the entropy is zero.

2.3 Examples

In this section we will discuss four examples, one for recurrence relations one for a differential-difference equation and finally two for quad equations.

Example 2.7 (Solvable Chaos [44]) We consider an instructive example taken from [44] to see what happens if one considers *transcendental* transformations in place of birational ones. Our starting point is a trivial linear second-order recurrence relation:

$$\omega_{n+1} + \omega_{n-1} = \kappa\omega_n \ , \quad k \in \mathbb{N} \ . \tag{60}$$

This linear map has obviously constant degree of growth $d_L = 1$. We can obtain from it a nonlinear equation if we apply the transcendental transformation:

$$u_n = \tan \omega_n. \tag{61}$$

Under such transformation we have:

$$\frac{u_{n+1} + u_{n-1}}{1 - u_{n+1}u_{n-1}} = \tan[\kappa \arctan(u_n)], \tag{62}$$

where the right-hand side is in fact a rational function of u_n depending on the value of $\kappa \in \mathbb{N}$. We shall consider the cases $\kappa = 1, 2, 3$.

Case $\kappa = 1$: In this case (62) becomes the trivial equation:

$$\frac{u_{n+1} + u_{n-1}}{1 - u_{n+1}u_{n-1}} = u_n. \tag{63}$$

It is almost immediate to see that if we compute u_{n+2} and substitute u_{n+1} from (63) into it we find $u_{n+2} = -u_{n-1}$: *the equation is periodic of period* 3. Its degree of growth is then trivially:

$$1, 1, 2, 1, 1, 2, 1, 1, 2, \ldots \ . \tag{64}$$

Its generating function is given by:

$$g_{k=1}(s) = \frac{2s^2 + s + 1}{(1 - s^3)}\ , \tag{65}$$

and the entropy is clearly zero.

Case $\kappa = 2$: In this case (62) becomes:

$$\frac{u_{n+1} + u_{n-1}}{1 - u_{n+1}u_{n-1}} = \frac{2u_n}{1 - u_n^2}. \tag{66}$$

This case has growth of degrees:

$$1, 1, 3, 5, 7, 9, 11, 13, 15, 17, 19, \ldots \tag{67}$$

with generating function:

$$g_{k=2}(s) = \frac{2s - s + 1}{(1 - s)^2}, \tag{68}$$

with clear zero entropy and growth of degrees $d_k = 2k - 1$ for $k > 1$. In fact this equation possess a first integral:

$$\frac{u_{n-1} - u_n}{1 - u_{n-1}u_n} = c, \tag{69}$$

which is a discrete Riccati equation. This discrete Riccati equation can be linearized through the Möbius transformation:

$$u_n = -\mathrm{i} - \frac{\mathrm{i}}{v_n}. \tag{70}$$

to

$$(\mathrm{i} - c)v_n - (\mathrm{i} + c)v_{n-1} = c. \tag{71}$$

So up to now the transcendental transformation has preserved somehow the linearity of the equation.

Case $\kappa = 3$: In this case (62) becomes more interesting:

$$\frac{u_{n+1} + u_{n-1}}{1 - u_{n+1}u_{n-1}} = \frac{3u_n - u_n^3}{1 - 3u_n^2}. \tag{72}$$

The degrees of its iterates are:

$$1, 1, 4, 11, 29, 76, 199, 521, 1364, 3571, \ldots \tag{73}$$

exhibiting a clearly chaotic behavior. The generating function for the sequence (73) is given by:

$$g_{k=3}(s) = \frac{2s^2 - 2s + 1}{s^2 - 3s + 1}. \tag{74}$$

The Algebraic Entropy is then given by:

$$\eta = \log\left(\frac{3+\sqrt{5}}{2}\right), \tag{75}$$

while the degrees asymptotically grow as:

$$d_k = \frac{1+\sqrt{5}}{2}\left(\frac{3+\sqrt{5}}{2}\right)^k + \frac{1-\sqrt{5}}{2}\left(\frac{3-\sqrt{5}}{2}\right)^k. \tag{76}$$

Therefore (72) is both chaotic and solvable! Using a transcendental transformation we have linearized a chaotic equation.

In Fig. 7 we confront the trajectories of the cases $\kappa = 2$ and $\kappa = 3$. We see the equations as maps in the (x, y)-plane by making the identification $(x_n, y_n) = (u_n, u_{n-1})$. The reader can easily see the difference between the regular structure of the case $\kappa = 2$ for different initial values and the complicated structure of the case $\kappa = 3$.

This example shows that if we consider more general transformations than the birational ones then Algebraic Entropy can't be used as an indicator of integrability.

Example 2.8 (The YdKN equation [133, 134]*)* Consider the class of differential-difference equations:

$$u_n' = \frac{A(u_n)u_{n+1}u_{n-1} + B(u_n)(u_{n+1} + u_{n-1}) + C(u_n)}{u_{n+1} - u_{n-1}}, \tag{77}$$

where A, B and C are second-order polynomials in u_n:

$$A(u_n) = c_1 u_n^2 + c_2 u_n + c_3\ , \tag{78a}$$

$$B(u_n) = c_4 u_n^2 + c_5 u_n + c_6\ , \tag{78b}$$

$$C(u_n) = c_7 u_n^2 + c_8 u_n + c_9, \tag{78c}$$

depending on nine arbitrary parameters. This equation for generic values of the parameters is not integrable. In fact it has the following growth of degrees:

$$1, 1, 3, 7, 17, 41, 99, 239, 577, \ldots. \tag{79}$$

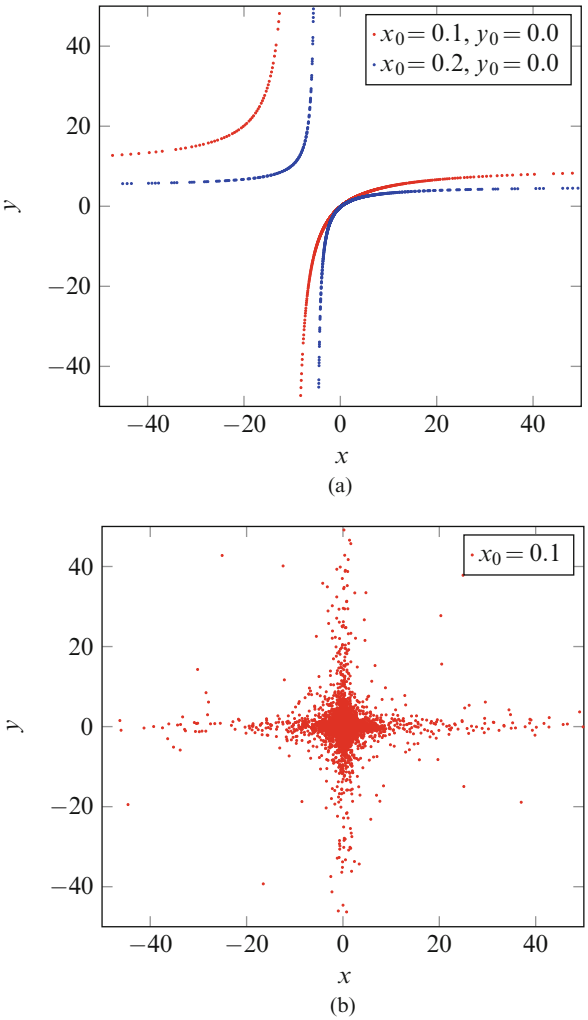

Fig. 7 Trajectories for the maps (62) for $\kappa = 2$ and $\kappa = 3$ with the identification $(x_n, y_n) = (u_n, u_{n-1})$. (**a**) $\kappa = 2$ (66). (**b**) $\kappa = 3$ (72)

This sequence has generating function:

$$g^{\text{gen}}(s) = \frac{s-1}{s^2 + 2s - 1}, \tag{80}$$

and then we have:

$$d_k^{\text{gen}} = \frac{(1+\sqrt{2})^{k+1}}{2} + \frac{(1-\sqrt{2})^{k+1}}{2} \tag{81}$$

and, as expected, the entropy is nonzero:

$$\eta^{\text{gen}} = \log(1+\sqrt{2}). \tag{82}$$

In [133] it was proved using the Generalized Symmetry approach[7] that for the particular combination of coefficients given by:

$$\begin{gathered} c_1 = a\,, \quad c_2 = 2b\,, \quad c_3 = c\,, \quad c_4 = b\,, \quad c_5 = d\,, \\ c_6 = e\,, \quad c_7 = c\,, \quad c_8 = 2e\,, \quad c_9 = f, \end{gathered} \tag{83}$$

the equation satisfies the necessary conditions of integrability.[8] As it was proved that the continuum limit [84, 133] of (78) with (83) is the Krichever–Novikov equation [73] the resulting equation was called the Yamilov discretization of the Krichever–Novikov equation (shortly YdKN equation). Integrability of such an equation was established in [5] through the Master Symmetries approach. If we compute the growth of degrees with the particular choice given by (83) we obtain:

$$1, 1, 3, 7, 13, 21, 31, 43, 57, 73, \ldots \tag{84}$$

with generating function:

$$g^{\text{int}}(s) = \frac{3s^2 - 2s + 1}{(1-s)^3}. \tag{85}$$

This generating function gives the quadratic growth $d_k^{\text{int}} = k^2 - k + 1$ and the entropy is clearly zero.

Considering the sequences (79) and (84) we see that the first drop of the degrees happens at the second iteration. To understand this degree dropping we consider the particular case $a = c = d = e = f = 0$ and $b = 1$. Computing the iterates without the assumptions made in Sect. 2.2 we have:

$$u_1 = -\frac{u_0' u_{-1} + u_0^2 u_{-1}}{-u_0' + 2u_0 u_{-1} + u_0^2}\,, \tag{86a}$$

$$u_2 = \frac{\begin{gathered}(3u_0'^2 u_{-1}^2 + 4u_0'^2 u_{-1} u_0 - 2u_0 2u_{-1}^2 u_0 \\ - 2u_0^2 u_{-1} u_0 2 + u_0'^2 u_{-1}' - u_0^4 u_{-1}' + u_0^4 u_{-1}^2) u_0\end{gathered}}{\begin{gathered}(u_0'^2 u_{-1}^2 + 2u_0'^2 u_{-1} u_0 - 2u_0'' u_{-1}^2 u_0 + 2u_0^5 u_{-1} \\ - 2u_0^2 u_{-1} u_0'' + u_0'^2 u_{-1}' - u_0^4 u_{-1}' + 3u_0^4 u_{-1}^2)\end{gathered}}\,, \tag{86b}$$

[7] In fact was solved the more general problem of finding the integrable cases inside the whole Volterra-like differential-difference equations (2).

[8] Only 6 independent coefficients are left.

$$u_3 = \frac{(u_0^2 - u_0')(u_0^2 + u_0') \cdot (\text{degree 13 polynomial})}{(u_0^2 - u_0')(u_0^2 + u_0') \cdot (\text{degree 13 polynomial})} , \tag{86c}$$

and we see that there is a cancellation of a factor of order 4! Therefore with respect to the general case we have a drop of degrees $13 = 17 - 4$.

Example 2.9 (The Q_V equation [125]*)* We will now see our first example of quad equations. We will show the integrability of the so called Q_V in the same way as it was done in the paper where the equation was introduced [125].

Our starting point is the three forms of the Q_4 equation. The Q_4 equation is obtained by the *Consistency Around the Cube* (CAC). This equation was first found in [1] and then its form has been improved in [95] and in [58]. It was shown to be the most general case of CAC in a series of papers [3, 6, 7].

Its different avatars are respectively:

- Adler's form:

$$\begin{aligned}
&k_0 u_{n,m}u_{n+1,m}u_{n,m+1}u_{n+1,m+1} \\
&- k_1(u_{n,m}u_{n+1,m}u_{n,m+1} + u_{n+1,m}u_{n,m+1}u_{n+1,m+1} \\
&+ u_{n,m}u_{n,m+1}u_{n+1,m+1} + u_{n,m}u_{n+1,m}u_{n+1,m+1}) \\
&+ k_2(u_{n,m}u_{n+1,m+1} + u_{n+1,m}u_{n,m+1}) \\
&- k_3(u_{n,m}u_{n+1,m} + u_{n,m+1}u_{n+1,m+1}) \\
&- k_4(u_{n,m}u_{n,m+1} + u_{n+1,m}u_{n+1,m+1}) \\
&+ k_5(u_{n,m} + u_{n+1,m} + u_{n,m+1} + u_{n+1,m+1}) + k_6 = 0
\end{aligned} \tag{87}$$

with

$$\begin{aligned}
k_0 = \alpha + \beta , \quad k_1 = \alpha\nu + \beta\mu , \quad k_2 = \alpha\nu^2 + \beta\mu^2 , \\
k_3 = \frac{\alpha\beta(\alpha+\beta)}{2(\nu-\mu)} - \alpha\nu^2 + \beta\left(2\mu^2 - \frac{g_2}{4}\right) , \\
k_4 = \frac{\alpha\beta(\alpha+\beta)}{2(\mu-\nu)} - \beta\mu^2 + \alpha\left(2\nu^2 - \frac{g_2}{4}\right), \\
k_5 = \frac{g_3}{2}k_0 + \frac{g_2}{4}k_1 , \quad k_6 = \frac{g_2^2}{r}16k_0 + g_3k_1,
\end{aligned} \tag{88}$$

where

$$\alpha^2 = r(\mu) , \quad \beta^2 = r(\nu) , \quad r(z) = 4z^3 - g_2 z - g_3 \tag{89}$$

- Nijhoff's form:

$$\begin{aligned} &A\big((u_{n,m}-b)(u_{n,m+1}-b)-d\big)\big((u_{n+1,m}-b)(u_{n+1,m+1}-bt)-d\big)\\ &+B\big((u_{n,m}-a)(u_{n+1,m}-a)-e\big)\big((u_{n,m+1}-a)(u_{n+1,m+1}-a)-e\big)=f \end{aligned} \tag{90}$$

  where the points $(a,A),(b,B),(c,C)=(b,B)-(a,A)$ are on the curve $Z^2=r(z)$ with $r(z)$ as in (89) and

$$d=(a-b)(c-b)\ ,\quad e=(b-a)(c-a)\ ,\quad f=ABC(a-b). \tag{91}$$

- Hietarinta's form:

$$\begin{aligned} &\operatorname{sn}(\alpha)\operatorname{sn}(\beta)\operatorname{sn}(\alpha+\beta)(k^2u_{n,m}u_{n+1,m}u_{n,m+1}u_{n+1,m+1}+1)\\ &\quad+\operatorname{sn}(\alpha+\beta)(u_{n,m}u_{n+1,m+1}+u_{n+1,m}u_{n,m+1})\\ &\quad-\operatorname{sn}(\alpha)(u_{n,m}u_{n+1,m}+u_{n,m+1}u_{n+1,m+1})\\ &\quad-\operatorname{sn}(\beta)(u_{n,m}u_{n,m+1}+u_{n+1,m}u_{n+1,m+1})=0\ . \end{aligned} \tag{92}$$

All three forms are parametrized through elliptic functions.

The most general form of quad equation having the same symmetry as Q_4, namely the *Klein symmetry*:

$$\begin{aligned} &Q(u_{n+1,m},u_{n,m},u_{n+1,m+1},u_{n,m+1})\\ &\qquad=\tau Q(u_{n,m},u_{n+1,m},u_{n,m+1},u_{n+1,m+1}),\\ &Q(u_{n,m+1},u_{n+1,m+1},u_{n,m},u_{n,m+1})\\ &\qquad=\tau' Q(u_{n,m},u_{n+1,m},u_{n,m+1},u_{n+1,m+1}), \end{aligned} \tag{93}$$

where $\tau,\tau'\in\{1,-1\}$ is given by:

$$\begin{aligned} &a_1u_{n,m}u_{n+1,m}u_{n,m+1}u_{n+1,m+1}\\ &+a_2(u_{n,m}u_{n,m+1}u_{n+1,m+1}+u_{n+1,m}u_{n,m+1}u_{n+1,m+1}\\ &\quad+u_{n,m}u_{n+1,m}u_{n+1,m+1}+u_{n,m}u_{n+1,m}u_{n,m+1})\\ &+a_3(u_{n,m}u_{n+1,m}+u_{n,m+1}u_{n+1,m+1})\\ &+a_4(u_{n,m}u_{n+1,m+1}+u_{n+1,m}u_{n,m+1})\\ &+a_5(u_{n+1,m}u_{n+1,m+1}+u_{n,m}u_{n,m+1})\\ &+a_6(u_{n,m}+u_{n+1,m}+u_{n,m+1}+u_{n+1,m+1})+a_7=0. \end{aligned} \tag{94}$$

We calculate the degrees of growth of the Q_4 equation. To keep things simple we evaluate for some choices of parameter one of the three forms of the Q_4 equation [(87), (90), (92)]. Following Sect. 2.2 we wish to find some integer values for the coefficients $\{a_1, \ldots, a_7\}$ satisfying the given conditions. For example, choosing $r(z) = 4z^3 - 32z + 4$ and the points $(a, A) = (0, 2)$, $(c, C) = (3, 4)$, $(b, B) = (a, A) \oplus (c, C) = (-26/9, 2/27)$,[9] we get the sequence:

$$1, 3, 7, 13, 21, 31, 43, 57, 73, 91, 111, \ldots \tag{95}$$

corresponding to the generating function

$$g(s) = \frac{1 + s^2}{(1 - s)^3}, \tag{96}$$

which corresponds to a *quadratic growth*:

$$d_l = l^2 + l + 1. \tag{97}$$

However we may also take (94) *without any constraint on the coefficients* $\{a_1, \ldots, a_7\}$. *With arbitrary values of the parameters, we get the same quadratic growth as with constrained values*:

$$1, 3, 7, 13, 21, 31, 43, 57, 73, 91, 111, \ldots. \tag{98}$$

This indicates *integrability of the unconstrained form*, with seven free homogeneous parameters (intersection of hyperplanes in the space of multilinear relations). This is the so-called Q_V equation.

To analyze the origin of the entropy vanishing, one has to examine the factorization process, which explains the degree drop. To this end consider the most generic quad equation with no Klein symmetries at all:

$$\begin{aligned}
&c_1 u_{n,m} u_{n+1,m} u_{n,m+1} u_{n+1,m+1} + c_2 u_{n,m} u_{n,m+1} u_{n+1,m+1} \\
&+ c_3 u_{n+1,m} u_{n,m+1} u_{n+1,m+1} + c_4 u_{n,m} u_{n+1,m} u_{n+1,m+1} \\
&+ c_5 u_{n,m} u_{n+1,m} u_{n,m+1} + c_6 u_{n,m} u_{n+1,m} + c_7 u_{n,m+1} u_{n+1,m+1} \\
&+ c_8 u_{n,m} u_{n+1,m+1} + c_9 u_{n+1,m} u_{n,m+1} \\
&+ c_{10} u_{n+1,m} u_{n+1,m+1} + c_{11} u_{n,m} u_{n,m+1} \\
&+ c_{12} u_{n,m} + c_{13} u_{n+1,m} + c_{14} u_{n,m+1} + c_{15} u_{n+1,m+1} + c_{16} = 0.
\end{aligned} \tag{99}$$

[9] Here $\oplus$ denotes the sum in the sense of elliptic curves.

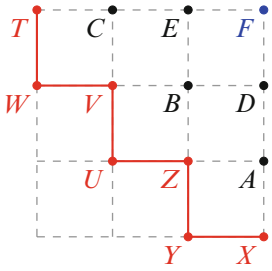

Fig. 8 Initial conditions for the Q_{V} equation

It depends on 16 homogeneous parameters c_i, $i = 1, \ldots, 16$. Its sequence of degrees is given by:

$$1, 3, 7, 17, 41, 99, 239, 577, \ldots \tag{100}$$

fitted by:

$$g(s) = -\frac{s+1}{s^2 + 2s - 1} \tag{101}$$

giving nonzero entropy $\eta = \log(1 + \sqrt{2})$.

We see that in (95) there is a factorization at the third iterations and we want to see its origin. Suppose we are given the initial data as in Fig. 8 then making the computations we see that:

$$F = \frac{H(Z, V) \cdot (\text{degree 13 polynomial})}{H(Z, V) \cdot (\text{degree 13 polynomial})} \tag{102}$$

The factor $H(Z, V)$ is a biquadratic (elliptic) curve given for general values of n and m by:

$$H(u_{n+1,m}, u_{n,m+1}) = \frac{\partial Q}{\partial u_{n,m}, u_{n+1,m+1}} - \frac{\partial Q}{\partial u_{n,m}} \frac{\partial Q}{\partial u_{n+1,m+1}} \tag{103}$$

where Q is given by the right-hand side of (94). We see than that with respect to the general case we have a drop of degrees $13 = 17 - 4$. It is worth noting that the biquadratic (103) was a key element in the proof of the classification in [6], however to have the factorization we do not need to introduce the elliptic function relation.

We conclude this example by noting that in [48] the Q_{V} equation was generalized to a new nonautonomous equation. It was proved that the only multilinear quad equations with 2-periodic coefficients, i.e., $p_i = p_{i,0} + p_{i,1}(-1)^n + p_{i,2}(-1)^M + p_{i,3}(-1)^{n+m}$, which possess the *nonautonomous Klein symmetries*:

$$\begin{aligned} &Q(u_{n+1,m}, u_{n,m}, u_{n+1,m+1}, u_{n,m+1}; (-1)^n, (-1)^m) \\ &\qquad = \tau Q(u_{n,m}, u_{n+1,m}, u_{n,m+1}, u_{n+1,m+1}; -(-1)^n, (-1)^m), \\ &Q(u_{n,m+1}, u_{n+1,m+1}, u_{n,m}, u_{n+1,m}; (-1)^n, (-1)^m) \\ &\qquad = \tau' Q(u_{n,m}, u_{n+1,m}, u_{n,m+1}, u_{n+1,m+1}; (-1)^n, -(-1)^m), \end{aligned} \tag{104}$$

is given by:

$$\begin{aligned} &a_1 u_{n,m}u_{n+1,m}u_{n,m+1}u_{n+1,m+1} \\ &+ [a_{2,0} - (-1)^n a_{2,1} - (-1)^M a_{2,2} + (-1)^{n+m} a_{2,3}]u_{n,m}u_{n,m+1}u_{n+1,m+1} \\ &+ [a_{2,0} + (-1)^n a_{2,1} - (-1)^M a_{2,2} - (-1)^{n+m} a_{2,3}]u_{n+1,m}u_{n,m+1}u_{n+1,m+1} \\ &+ [a_{2,0} + (-1)^n a_{2,1} + (-1)^M a_{2,2} + (-1)^{n+m} a_{2,3}]u_{n,m}u_{n+1,m}u_{n+1,m+1} \\ &+ [a_{2,0} - (-1)^n a_{2,1} + (-1)^M a_{2,2} - (-1)^{n+m} a_{2,3}]u_{n,m}u_{n+1,m}u_{n,m+1} \\ &+ [a_{3,0} - (-1)^M a_{3,2}]u_{n,m}u_{n+1,m} + [a_{3,0} + (-1)^M a_{3,2}]u_{n,m+1}u_{n+1,m+1} \\ &+ [a_{4,0} - (-1)^{n+m} a_{4,3}]u_{n,m}u_{n+1,m+1} + [a_{4,0} + (-1)^{n+m} a_{4,3}]u_{n+1,m}u_{n,m+1} \\ &+ [a_{5,0} - (-1)^n a_{5,1}]u_{n+1,m}u_{n+1,m+1} + [a_{5,0} + (-1)^n a_{5,1}]u_{n,m}u_{n,m+1} \\ &+ [a_{6,0} + (-1)^n a_{6,1} - (-1)^M a_{6,2} - (-1)^{n+m} a_{6,3}]u_{n,m} \\ &+ [a_{6,0} - (-1)^n a_{6,1} - (-1)^M a_{6,2} + (-1)^{n+m} a_{6,3}]u_{n+1,m} \\ &+ [a_{6,0} + (-1)^n a_{6,1} + (-1)^M a_{6,2} + (-1)^{n+m} a_{6,3}]u_{n,m+1} \\ &+ [a_{6,0} - (-1)^n a_{6,1} + (-1)^M a_{6,2} - (-1)^{n+m} a_{6,3}]u_{n+1,m+1} + a_7 = 0. \end{aligned} \tag{105}$$

This equation depends on 16 *arbitrary homogeneous parameters* and upon the substitution $a_{2,1} = a_{2,2} = a_{2,3} = a_{3,2} = a_{4,3} = a_{5,1} = a_{6,1} = a_{6,2} = a_{6,3} = 0$ (105) it reduces to the Q_{V} equation (94). Therefore this equation is called *the nonautonomous Q_{V} equation*. Again in [48] it was found that this equation possesses the same degree of growth as the original Q_{V} equation (94), this suggests that this is a *nonautonomous integrable generalization of the Q_{V} equation*.

Example 2.10 (The ${}_tH_2^{\varepsilon}$ Equation) As a last example we consider a nonautonomous equation coming from the classification of general quad equations possessing the CAC property introduced by Boll [16–18]. The ${}_tH_2^{\varepsilon}$ is:

$$
\begin{aligned}
{}_tH_2 : &(u_{n,m} - u_{n+1,m})(u_{n,m+1} - u_{n+1,m+1}) \\
&+ \alpha_2(u_{n,m} + u_{n+1,m} + u_{n,m+1} + u_{n+1,m+1}) \\
&+ \frac{\varepsilon\alpha_2}{2}(2F_M^{(+)}u_{n,m+1} + 2\alpha_3 + \alpha_2)(2F_M^{(+)}u_{n+1,m+1} + 2\alpha_3 + \alpha_2) \\
&+ \frac{\varepsilon\alpha_2}{2}(2F_M^{(-)}u_{n,m} + 2\alpha_3 + \alpha_2)(2F_M^{(-)}u_{n+1,m} + 2\alpha_3 + \alpha_2) \\
&+ (\alpha_3 + \alpha_2)^2 - \alpha_3^2 - 2\varepsilon\alpha_2\alpha_3(\alpha_3 + \alpha_2) = 0,
\end{aligned} \tag{106}
$$

where:

$$
F_m^{(\pm)} = \frac{1 \pm (-1)^m}{2}. \tag{107}
$$

This equation shows two sequences of growth [50], a principal and a secondary one. Furthermore it is not isotropic: its growth in different directions is different. Indeed the growth in the directions $\Delta_{-,+}$ and $\Delta_{+,+}$ is given by the following sequences:

$$
\begin{aligned}
&\text{principal} \quad 1, 2, 4, 6, 11, 10, 19, 14, 27, 18, 35, 22, 43, \ldots, \\
&\text{secondary} \quad 1, 2, 4, 7, 8, 15, 12, 23, 16, 31, 20, 39, 24, \ldots.
\end{aligned} \tag{108}
$$

To these sequences correspond the generating functions:

$$
\begin{aligned}
g^{\mathrm{p}}_{\pm,+}(s) &= \frac{s^6 + 4s^4 + 2s^3 + 2s^2 + 2s + 1}{(s-1)^2(s+1)^2}, \\
g^{\mathrm{s}}_{\pm,+}(s) &= \frac{3s^5 + s^4 + 3s^3 + 2s^2 + 2s + 1}{(s-1)^2(s+1)^2}.
\end{aligned} \tag{109}
$$

The two sequences (108) are very peculiar, since they are not monotonically increasing, but exhibit very large oscillations. Moreover the asymptotic behavior which can be extrapolated from the generating functions is *linear*:

$$
\begin{aligned}
d^{\mathrm{p}}_{l,\pm,+} &= (-1)^l(l - \tfrac{5}{2}) + 3l - \tfrac{5}{2}, \\
d^{\mathrm{s}}_{l,\pm,+} &= (-1)^{l+1}(l - \tfrac{5}{2}) + 3l - \tfrac{5}{2}.
\end{aligned} \tag{110}
$$

Both these two patterns of growth satisfy the fourth order recurrence relation:

$$
d_{l+1} - 2d_{l-1} + d_{l-3} = 0, \tag{111}
$$

which gives rise to these highly oscillatory terms.

The growth in the directions $\Delta_{+,-}$ and $\Delta_{-,-}$ is given by the following sequences:

$$
\begin{aligned}
&\text{principal} \quad 1,\ 2,\ 4,\ 7,\ 11,\ 15,\ 19,\ 23,\ 27,\ 31,\ 35,\ 39,\ 43, \ldots, \\
&\text{secondary} \quad 1,\ 2,\ 4,\ 6,\ 8,\ 10,\ 12,\ 14,\ 16,\ 18,\ 20,\ 22,\ 24, \ldots.
\end{aligned} \tag{112}
$$

We have the following generating functions:

$$g^{\mathrm{p}}_{\pm,-}(s) = \frac{s^4 + s^3 + s^2 + 1}{(s-1)^2}\,, \qquad g^{\mathrm{s}}_{\pm,-}(s) = \frac{s^2 + 1}{(s-1)^2} \tag{113}$$

and again the growth is *linear*:

$$d^{\mathrm{p}}_{l,\pm,-} = 4l - 5\,, \quad d^{\mathrm{s}}_{l,\pm,-} = 2l. \tag{114}$$

Since the growth is linear in every direction we can infer that the equation should be linearizable. This was conjectured in [50] and then proved by using the concept of Darboux integrability for lattice equations [2] in [47, 53].

3 Generalized Symmetries

In this second part of these notes we will introduce another definition of integrability based on the existence of Generalized Symmetries. Mainly we will develop computational methods for finding generalized symmetries. In Sect. 3.1 we will discuss the relationship of the Generalized Symmetries with integrability properties. To do so we will treat the well known example of the Korteweg–de Vries equation. In Sect. 3.2 we will consider the case of differential-difference equations. In Sect. 3.3 we will construct three point generalized symmetries for quad equations. In Sect. 3.4 we will discuss a direct methods to find hierarchies of symmetries through the so-called Master Symmetries. In Sect. 3.5 we will conclude these notes with some specially selected examples of nonautonomous equations.

3.1 Generalized Symmetries and Integrability

At the time of the Franco-Prussian war in 1870 the Norwegian mathematician Sophus Lie considered the question of the invariance of differential equations with respect to continuous infinitesimal transformation, i.e., transformations which can be seen as continuous deformations of the identity. In the successive 30 years Lie developed a theory which includes all the implications of such invariance. The *summa* of the work of Sophus Lie on the subject is contained in [88].

Lie's works on differential equations had a brief moment of success, but soon they were forgotten. They were subsequently rediscovered around the middle of the twentieth century by Russian mathematicians under the leadership of Ovsiannikov [104, 105]. On the other hand Lie's work on continuous groups was a powerful

tool in the development of Quantum Mechanics where they were used to show unexpected results about the spectra [128]. However the "physicists" theory of Lie groups turns out to be completely separated from the application of continuous groups to differential equations in such a way that it was possible that somebody knew much of one and completely ignore the other.

The original idea of Sophus Lie was to unify the methods of solution for differential equations uncovering the underlying geometrical structure in the same spirit as it was done by Évariste Galois for algebraic equations. Lie's theory of infinitesimal point transformation is linear, but one is able to reconstruct the full group of transformation by solving some differential equations.

In his work Lie [86] considered infinitesimal transformations depending also on the first derivatives of the dependent variables, the so-called contact transformations [8, 63]. Later Bäcklund considered finite transformations depending on finitely many derivatives of the dependent variables adding some closure relations in order to preserve the geometrical structure of the transformations [11]. The first to recognize the possibility of considering also transformations depending on higher order derivatives *without additional conditions* was Emmy Noether in her fundamental paper [97]. The mathematical objects Noether considered was what now we call *Generalized Symmetries*.

In modern times due to their algorithmic nature generalized symmetry have been used both as tools for the study of given systems [8, 34, 40, 63, 68, 71, 72, 101, 103] and as a tool to classify integrable equations. The symmetry approach to integrability has mainly been developed by a group of researchers belonging to the scientific school of A.B. Shabat. It has been developed in the continuum case [5, 54, 93, 94, 116–118], in the differential-difference case [78, 133, 134] and more recently also in the completely discrete case [79, 80].

Let us start discussing the relation between integrability and generalized symmetries in the case of partial differential equations. Let us assume we are given a partial differential equation (PDE) of order k in *evolutionary form* for an unknown function $u = u(x, t)$:

$$u_t = f(u, u_1, \dots, u_k) \,, \tag{115}$$

where $u_t = \partial u/\partial t$ and $u_j = \partial^j u/\partial x^j$ for any $j > 0$.

A generalized symmetry of order m for (115) is an equation of the form:

$$u_\tau = g(u, u_1, u_2, \dots, u_m) \tag{116}$$

compatible with (115). Here τ plays the role of the group parameter and of course we are assuming $u = u(x, t, \tau)$. The compatibility condition between (115) and (116) implies the following PDE for the functions f and g:

$$\frac{\partial^2 u}{\partial t \partial \tau} - \frac{\partial^2 u}{\partial \tau \partial t} = D_t g - D_\tau f = 0, \tag{117}$$

where D_t, D_τ are the operators of total differentiation corresponding to (115)–(116), defined, together with the operator of total x-derivative D, by

$$D = \frac{\partial}{\partial x} + \sum_{i\geq 0} u_{i+1}\frac{\partial}{\partial u_i}\,, \quad D_t = \frac{\partial}{\partial t} + \sum_{i\geq 0} D^i f \frac{\partial}{\partial u_i}\,, \quad D_\tau = \frac{\partial}{\partial \tau} + \sum_{i\geq 0} D^i g \frac{\partial}{\partial u_i}. \tag{118}$$

When (117) is satisfied we say that (116) is *a generalized symmetry of order m* for (115).

We will now see in a concrete example how from the integrability properties is possible to obtain an infinite sequence of generalized symmetries of the form (116). Let us consider the well-known Korteweg–de Vries equation (KdV equation) [70]:

$$u_t = 6uu_1 + u_3. \tag{119}$$

It is known [75] that the KdV equation (119) possess the following linear representation:

$$L_t = [L, M], \tag{120}$$

where L and M are differential operators given by:

$$L = -\partial_{xx} + u\,, \tag{121a}$$

$$M = 4\partial_{xxx} - 6u\partial_x - 3\partial_x(u). \tag{121b}$$

and by $[\ ,\ ]$ we mean the commutator of two differential operators. We look for a chain of differential operators M_j which correspond to different equations associated with the same L:

$$L_{t_j} = [L, M_j], \tag{122}$$

Since $L_t = u_t$ is a scalar operator one must have $[L, M] = V$ with V scalar operator. If there exists another equation associated to L then there must exists another $\tilde{M}$ such that $[L, \widetilde{M}] = \widetilde{V}$ where $\widetilde{V}$ is another scalar operator.

Now one can relate M and $\widetilde{M}$. Noting that the equation $u_t = u_x$ can be written in the form (122) with $M_j = \partial_x$ we see that the operators M_j are characterized by the power of the operator ∂_x and that the relation between one and the other is of order two, as the order of the operator L. We can therefore make the general assumption:

$$\widetilde{M} = LM + F\partial_x + G, \tag{123}$$

where F and G are scalar operators. Imposing the condition (123) we find that:

$$\widetilde{V} = \mathcal{L}V + u_x, \tag{124}$$

where:

$$\mathcal{L}V = -\frac{1}{4}V_{xx} + uV - \frac{1}{2}u_x \int_x^\infty V(y)\,\mathrm{d}y. \tag{125}$$

This yields an infinite family of equations for any entire function $F(z)$,

$$u_t = F(\mathcal{L})u_x. \tag{126}$$

Equations (126) are associated to the same L operator and, by solving the Spectral Problem associated to it [21], they are shown to be commuting with the original KdV equation (119). In particular for $F(\mathcal{L}) = \mathcal{L}^n$ we find a whole hierarchy of generalized symmetries for the KdV equation (119). The operator (125) is called the *recursion operator* for the KdV equation (119).

In general any evolution equation possessing a recursion operator has an infinite hierarchy of equations and if they commute they are generalized symmetries, and, then, in an appropriate sense, an evolution equation is integrable. We therefore propose a symmetry based definition of integrability: *An evolution equation is called integrable if it possesses nonconstant generalized symmetries of any order m* [102]. Note that this definition a priori does not distinguish between C-integrable and S-integrable equations. Indeed both C-integrable and S-integrable equations possess the property of having recursion operators like (125), but C-integrable equations are *linearizable* [20]. The most famous C-integrable equation, the Burgers equation, also possesses a recursion operator. The difference between C-integrable and S-integrable equations is in the fact that the S-integrable equations possess infinitely many conservation laws of any order whereas the C-integrable ones only up to the order of the equation itself.

3.2 Generalized Symmetries for Differential-Difference Equations

In this section we look for generalized symmetries of Volterra-like equations:

$$\dot{u}_n = f(u_{n+1}, u_n, u_{n-1}) \equiv f_n\ , \quad \frac{\partial f_n}{\partial u_{n+1}} \neq 0\ , \ \frac{\partial f_n}{\partial u_{n-1}} \neq 0, \tag{127}$$

for the unknown function $u_n = u_n(t)$.[10] We assume that $f = f(z_1, z_2, z_3)$, an arbitrary function of three variable, is independent of $n \in \mathbb{Z}$.

[10] In this section and in the following we use the dot notation for derivatives.

Generalized symmetries of (127) will be equations of the form

$$\begin{aligned} u_{n,\tau} &= g(u_{n+m}, u_{n+m-1}, \dots u_{n+m'+1}, u_{n+m'}) \equiv g_n \ , \\ &\frac{\partial g_n}{\partial u_{n+m}} \frac{\partial g_n}{\partial u_{n+m'}} \neq 0, \end{aligned} \tag{128}$$

where $u_n = u_n(t, \tau)$. By the index τ, the group parameter, we denote its τ-derivative, and $m \geq m'$ are two finite fixed integers.

The symmetry is defined by a function of many variables:

$$g = g(z_1, z_2, z_3, \dots z_{1+m-m'}), \tag{129}$$

called the *characteristic of the symmetry* which depends on (127). We will call (128) a *local* generalized symmetry of (127) if in the right-hand side it does not contain integrals or summations. Moreover, we choose this symmetry to have no explicit dependence on the discrete spatial variable n and on the variable t of (127).

Lie point symmetries of (127) are of the form:

$$u_{n,\tau} = a(t)\dot{u}_n + b_n(t, u_n) \tag{130}$$

and are a sub-case of the generalized symmetries. We will be interested in symmetries (128) with $m > 1$ and $m' < -1$ which are not Lie point symmetries, more precisely, with $m = -m' > 1$.

A *generalized symmetry* of (127) is an equation of the form (128) *compatible* with (127), i.e., such that they have a common set of solutions. Before giving a precise definition of generalized symmetries, we derive and discuss the conditions necessary for their existence. If $u_n(t, \tau)$ is a common solution of (127)–(128), we have

$$\frac{\partial^2 u_n}{\partial t \partial \tau} - \frac{\partial^2 u_n}{\partial \tau \partial t} = D_t g_n - D_\tau f_n = 0, \tag{131}$$

where D_t, D_τ are differentiation operators corresponding to (127)–(128):

$$D_t g_n = \sum_{j=m'}^{m} \frac{\partial g_n}{\partial u_{n+j}} f_{n+j} \ , \quad D_\tau f_n = \sum_{j=-1}^{1} \frac{\partial f_n}{\partial u_{n+j}} g_{n+j}. \tag{132}$$

By f_{n+j}, g_{n+j} we mean

$$\begin{aligned} f_{n+j} &= f(u_{n+j+1}, u_{n+j}, u_{n+j-1}), \\ g_{n+j} &= g(u_{n+j+m}, u_{n+j+m-1}, \dots u_{n+j+m'}). \end{aligned} \tag{133}$$

From (131)–(132) we obtain the following *compatibility condition*:

$$D_t g_n = \frac{\partial f_n}{\partial u_{n+1}} g_{n+1} + \frac{\partial f_n}{\partial u_n} g_n + \frac{\partial f_n}{\partial u_{n-1}} g_{n-1} \tag{134}$$

which is satisfied for any common solution of (127)–(128) and, given f_n, is an equation for the function g_n.

In the generalized symmetry method, we assume that (134) must be identically satisfied for all values of the variables:

$$u_0, u_1, u_{-1}, u_2, u_{-2}, \dots, \tag{135}$$

which are considered as *independent*, and for all $n \in \mathbb{Z}$.

To clarify this point, let us consider a simple, but important, difference equation:

$$\varphi_{n+1} - \varphi_n = 0\,. \tag{136}$$

We are looking for solutions of (136), such that φ_n is a function defined on a finite number of independent variables:

$$\varphi_n = \varphi(u_{n+k}, u_{n+k-1}, \dots u_{n+k'})\,, \quad k \geq k', \tag{137}$$

where

$$\frac{\partial \varphi_n}{\partial u_{n+k}} \neq 0\,, \quad \frac{\partial \varphi_n}{\partial u_{n+k'}} \neq 0. \tag{138}$$

Solving (134) we often get relations of the form (136) to be satisfied identically for all values of the variables (135).

Assuming that there exists a nonconstant solution φ_n of (136) we can differentiate (136) with respect to $u_{n+k'}$ and we get $\partial\varphi_n/\partial u_{n+k'} = 0$ identically. This contradicts (138), and the relation (136) implies that φ_n must be a constant function. Introducing the standard shift operator T, such that for any integer power j we have:

$$T^j \varphi_n = \varphi_{n+j} = \varphi(u_{n+j+k}, u_{n+j+k-1}, \dots u_{n+j+k'})\,, \tag{139}$$

we can rewrite (136) as $(T - \mathrm{Id})\varphi_n = 0$ and thus we get

$$\ker(T - \mathrm{Id}) = \mathbb{C}\,. \tag{140}$$

Equation (128) is called a *generalized symmetry* of (127) if the compatibility condition (134) is identically satisfied for all values of the independent variables (135). The numbers m and m' are called respectively *the left order* (or *the order*) and *the right order* of the generalized symmetry (128). For any generalized symmetry (128), the integers m and m' are fixed and define essentially different cases.

The definition of generalized symmetry is constructive. For any given (127) and any given orders m and m', with $m \geq m'$, one is able either to find a generalized symmetry (128) or to prove that it does not exist. In fact it can be proved [135] that for S-integrable equations we have $m = -m'$, and for this reason the left order m is usually just called the *order* of the generalized symmetry. C-integrable equations can have $m \neq -m'$ and they can still have infinite symmetries. An example is given by the semidiscrete Burgers equation [81]:

$$\dot{u}_n = u_n(u_{n+1} - u_n). \tag{141}$$

We now see a complete example of calculation of generalized symmetries for Volterra-like equations (127). We will see that it will be necessary to make an extensive use of the property (140) and of the fact that in the compatibility condition not all the function appearing will depend on the same variables.

Example 3.1 (The modified volterra equation) Let us consider the following Volterra-like equation:

$$\dot{u}_n = (c^2 - u_n^2)(u_{n+1} - u_{n-1}). \tag{142}$$

This equation is known in literature as the *modified Volterra equation*. We wish to compute the lowest order Generalized Symmetries of (142), i.e., the instances of (128) with $m = 2$ and $m' = -2$:

$$u_{n,\tau} = g_n(u_{n-2}, u_{n-1}, u_n, u_{n+1}, u_{n+2}). \tag{143}$$

In this case the compatibility condition (131) is given by:

$$\begin{aligned} &\frac{\partial g_n}{\partial u_{n-2}} f_{n-2} + \frac{\partial g_n}{\partial u_{n-1}} f_{n-1} + \frac{\partial g_n}{\partial u_n} f_n + \frac{\partial g_n}{\partial u_{n+1}} f_{n+1} + \frac{\partial g_n}{\partial u_{n+2}} f_{n+2} \\ &\qquad = \frac{\partial f_n}{\partial u_{n-1}} g_{n-1} + \frac{\partial f_n}{\partial u_n} g_n + \frac{\partial f_n}{\partial u_{n+1}} g_{n+1} \,. \end{aligned} \tag{144}$$

We note that the g_{n+1}, f_{n+2} and g_{n-1}, f_{n-2} depend on u_{n+3} and u_{n-3} respectively, whereas the other functions do not depend on these variables. Therefore our first step is to isolate the dependence on these variable. We start by differentiating with respect to u_{n+3}:

$$(c^2 - u_n^2)\frac{\partial g_{n+1}}{\partial u_{n+3}} - (c^2 - u_{n+2}^2)\frac{\partial g_n}{\partial u_{n+2}} = 0. \tag{145}$$

Diving by $(c^2 - u_n^2)(c^2 - u_{n+1}^2)(c^2 - u_{n+2}^2)$ we have:

$$\frac{1}{(c^2 - u_{n+1}^2)(c^2 - u_{n+2}^2)} \frac{\partial g_{n+1}}{\partial u_{n+3}} - \frac{1}{(c^2 - u_n^2)(c^2 - u_{n+1}^2)} \frac{\partial g_n}{\partial u_{n+2}} = 0 \,. \tag{146}$$

This is a total difference:

$$(T-\mathrm{Id})\left(\frac{1}{(c^2-u_n^2)(c^2-u_{n+1}^2)}\frac{\partial g_n}{\partial u_{n+2}}\right)=0\,, \tag{147}$$

which using (140) yields:

$$\frac{1}{(c^2-u_n^2)(c^2-u_{n+1}^2)}\frac{\partial g_n}{\partial u_{n+2}}=k_1 \tag{148}$$

i.e.:

$$g_n=k_1(c^2-u_n^2)(c^2-u_{n+1}^2)u_{n+2}+h_n \tag{149}$$

where $h_n=h_n(u_{n+1},u_n,u_{n-1},u_{n-2})$. Substituting (149) into (144) and differentiating with respect to u_{n-3} we get:

$$(c^2-u_{n-2}^2)\frac{\partial h_n}{\partial u_{n-2}}-(c^2-u_n^2)\frac{\partial h_{n-1}}{\partial u_{n-3}}=0\,. \tag{150}$$

As above we can write this expression as a total difference:

$$(T-\mathrm{Id})\left(\frac{1}{(c^2-u_{n-1}^2)(c^2-u_{n-2}^2)}\frac{\partial h_{n-1}}{\partial u_{n-3}}\right)=0, \tag{151}$$

which yields:

$$h_n=k_2(c^2-u_n^2)(c^2-u_{n-1}^2)u_{n-2}+l_n \tag{152}$$

where $l_n=l_n(u_{n+1},u_n,u_{n-1})$.

We have exhausted the higher order terms. We pass then to the lower order ones, i.e., u_{n+2} and u_{n-2}. First of all we substitute (152) into (149) and differentiate (144) with respect to u_{n+2}:

$$\begin{aligned}&(c^2-u_n^2)\frac{\partial l_{n+1}}{\partial u_{n+2}}-(c^2-u_{n+1}^2)\frac{\partial l_n}{\partial u_{n+1}}\\&\quad+2k_1(c^2-u_{n+1}^2)(c^2-u_n^2)(u_{n+2}-u_n)u_{n+1}=0.\end{aligned} \tag{153}$$

This can be written as:

$$(T-\mathrm{Id})\left(\frac{1}{(c^2-u_n^2)}\frac{\partial l_n}{\partial u_{n+1}}+2k_1(u_{n+1}u_n)\right)=0\,, \tag{154}$$

whose solution is given by:

$$l_n=(c^2-u_n^2)(k_3u_{n+1}-k_1u_nu_{n+1}^2)+m_n\,, \tag{155}$$

where $m_n = m_n(u_n, u_{n-1})$. Substituting (155) into (152) and (149) and differentiating (144) with respect to u_{n-2} we obtain:

$$(c^2 - u_{n-1}^2)\frac{\partial m_n}{\partial u_{n-1}} - (c^2 - u_n^2)\frac{\partial m_{n-1}}{\partial u_{n-2}} + 2k_2(c^2 - u_n^2)(c^2 - u_{n-1}^2)(u_n - u_{n-2})u_{n-1} = 0. \tag{156}$$

This implies:

$$(T - \mathrm{Id})\left(\frac{1}{(c^2 - u_{n-1}^2)}\frac{\partial m_{n-1}}{\partial u_{n-2}} + 2k_2(u_{n-1}u_{n-2})\right) = 0\ , \tag{157}$$

whose solution is given by:

$$m_n = (c^2 - u_n^2)\left(k_4 u_{n-1} - k_2 u_n u_{n-1}^2\right) + q_n\ , \tag{158}$$

with $q_n = q_n(u_n)$.

At this point from (158), (155), (152) and (149) we have the following form for the symmetry:

$$g_n = (c^2 - u_n^2)\{k_1[(c^2 - u_{n+1}^2)u_{n+2} - u_n u_{n+1}^2] + k_2[(c^2 - u_{n-1}^2)u_{n-2} - u_n u_{n-1}^2] + k_3 u_{n+1} + k_4 u_{n-1}\} + q_n \tag{159}$$

which we can substitute into the determining equation (144). The result is too long to be displayed, but if we differentiate three times with respect to u_{n+1} we have:

$$(c^2 - u_n^2)\left(6(k_1 + k_2)u_n^2 + \frac{\partial^3 q_{n+1}}{\partial u_{n+1}^3}\right) = 0\ . \tag{160}$$

Since $q_{n+1} = q(u_{n+1})$ this implies $k_2 = -k_1$ and

$$q_n = k_5 u_n^2 + k_6 u_n + k_7\ . \tag{161}$$

We just need to determine the relation between the constants k_i, $i \neq 2$. Returning to (144) we can take the coefficients with respect to u_n:

$$(k_3 + k_4)(u_{n+1}^2 - u_{n-1}^2) = 0\ , \tag{162a}$$

$$[(u_{n-1} + u_{n+1})k_5 + 2k_6](u_{n-1} - u_{n+1}) = 0\ , \tag{162b}$$

$$\{[(k_3 + k_4)(u_{n-1} + u_{n+1}) + 2k_5]c^2 + 2k_7\}(u_{n-1} - u_{n+1}) = 0\ , \tag{162c}$$

$$c^2(u_{n+1}^2 - u_{n-1}^2)k_5 = 0\ . \tag{162d}$$

Regardless of the value of the constant c, (162) is solved by $k_4 = -k_3$ and $k_5 = k_6 = k_7 = 0$. The generalized symmetry generator is then given by:

$$g_n = k_1[(c^2 - u_{n+1}^2)u_{n+2} - (u_{n+1}^2 - u_{n-1}^2)u_n - (c^2 - u_{n-1}^2)u_{n-2}](c^2 - u_n^2) + k_3(c^2 - u_n^2)(u_{n+1} - u_{n-1}) \ . \tag{163}$$

The symmetry with $k_1 = 0$ and $k_3 = 1$ is the modified Volterra equation itself (142) therefore the only true second-order symmetry is given by:

$$g_n = [(c^2 - u_{n+1}^2)u_{n+2} - (u_{n+1}^2 - u_{n-1}^2)u_n - (c^2 - u_{n-1}^2)u_{n-2}](c^2 - u_n^2) \ . \tag{164}$$

Any generalized symmetry (128) is a nonlinear difference-differential equation which has common solutions $u_n(t, \tau)$ with (127). As in the case of Lie point symmetries [15, 87, 102, 106], for generalized symmetries we can perform a *symmetry reduction* [77] by considering stationary solutions of the Eq. (128):

$$\frac{\partial u_n}{\partial \tau} = 0 \implies g(u_{n+m}, u_{n+m-1}, \dots u_{n+m'}) = 0 \ , \tag{165}$$

which is a fully discrete equation. This is the analog of the reduced ordinary differential equation we obtain in the case of partial differential equations in two variables. If we solve this equation we obtain a function $u_n(t)$ which depends on arbitrary functions of t. These arbitrary functions can be obtained by introducing $u_n(t)$ into (127). In such a way we can construct particular solutions of (127) such as, for example, soliton solutions.

We now see an example of how to perform symmetry reductions.

Example 3.2 (Symmetry solution of the volterra equation) Let us consider the Volterra equation:

$$\dot{u}_n = u_n(u_{n+1} - u_{n-1}) \ . \tag{166}$$

The reader may verify that this equation possess the following generalized symmetry (128) with $m = 2$ and $m' = -2$:

$$\frac{\partial u_n}{\partial \tau} = u_n u_{n+1}(u_{n+2} + u_{n+1} + u_n) - u_n u_{n-1}(u_n + u_{n-1} + u_{n-2}) \ . \tag{167}$$

The stationary solutions of (167) are the functions $u_n = u_n(t)$ such that:

$$u_{n+1}(u_{n+2} + u_{n+1} + u_n) - u_{n-1}(u_n + u_{n-1} + u_{n-2}) = 0 \ . \tag{168}$$

It can be seen by direct inspection that such equation can be written as a double shift:

$$(T^2 - \mathrm{Id})[u_{n-1}(u_n + u_{n-1} + u_{n-2})] = 0 \ . \tag{169}$$

This means that u_n will solve the second-order ordinary difference equation:

$$u_n + u_{n-1} + u_{n-2} = \frac{K_1(-1)^n + K_2}{u_{n-1}} \,. \tag{170}$$

This equation is known as the discrete Painlevé I equation (dPI equation), a well-known integrable equation [108]. Due to the nature of the dPI equation we cannot, in general, write an explicit solution in terms of elementary functions, but for some particular values of the parameters K_1 and K_2 we can find the symmetry reduction of the Volterra equation (166).

For example if $K_1 = K_2 = 0$ (170) becomes *linear* and the solution is:

$$u_n = U_0 \cos\left(\frac{2\pi n}{3}\right) + U_1 \sin\left(\frac{2\pi n}{3}\right) \tag{171}$$

where $U_i = U_i(t)$. Introducing (171) into (166) we obtain the following system of coupled ordinary differential equations:

$$\frac{\mathrm{d}U_0}{\mathrm{d}t} = \sqrt{3} U_0 U_1 \,, \tag{172a}$$

$$\frac{\mathrm{d}U_1}{\mathrm{d}t} = \frac{\sqrt{3}}{2}(U_0^2 - U_1^2) \,. \tag{172b}$$

From (172a) we can solve with respect to U_1 and substitute into (172b) to obtain a single second-order equation:

$$\frac{\mathrm{d}^2 U_0}{\mathrm{d}t^2} = \frac{1}{2U_0}\left(\frac{\mathrm{d}U_0}{\mathrm{d}t}\right)^2 + \frac{3}{2}U_0^3 \,. \tag{173}$$

This equation can be solved by quadratures in terms of elliptic integrals:

$$\pm \int^{U_0} \frac{\mathrm{d}v}{\sqrt{Cv + v^4}} = t - t_0 \,, \tag{174}$$

where C and t_0 are constants of integrations. This gives a symmetry solution of the Volterra equation corresponding to the five point generalized symmetry (167) with $K_1 = K_2 = 0$.

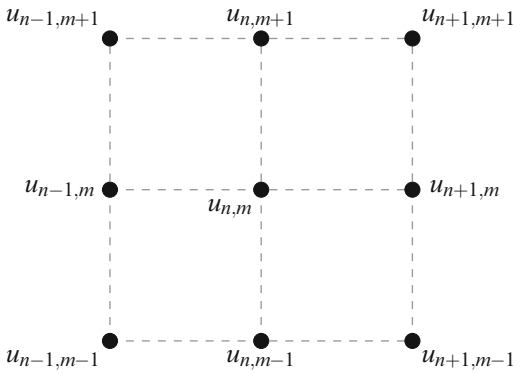

Fig. 9 The extended square lattice with nine points

3.3 Three-Point Generalized Symmetries for Quad Equation

In this section we discuss the construction of the simplest generalized symmetries for quad equations (4).[11] The exposition is mainly based on [41, 79, 80]. The simplest Generalized Symmetries for a quad equation in the form (4) are those depending on nine points defined on a square of vertices $u_{n-1,m-1}, u_{n-1,m+1}, u_{n+1,m+1}$ and $u_{n+1,m-1}$ as depicted in Fig. 9. A priori the symmetry generator can depend on all these points, however by taking into account the difference equation (4), we can express the extremal points $u_{n-1,m-1}, u_{n-1,m+1}, u_{n+1,m+1}$ and $u_{n+1,m-1}$ in terms of the remaining five points $u_{n-1,m}, u_{n+1,m}, u_{n,m}, u_{n,m-1}$ and $u_{n,m+1}$. In general this means that we are taking as independent variables those lying on the coordinate axes, i.e., $u_{n+j,m}$ and $u_{n,m+k}$ with $j, k \in \mathbb{Z}$. This choice of independent variable is acceptable, since these points do not lie on squares. In this way the most general nine points generalized symmetry generator is represented by the infinitesimal symmetry generator

$$\widehat{X} = g(u_{n-1,m}, u_{n+1,m}, u_{n,m}, u_{n,m-1}, u_{n,m+1})\partial_{u_{n,m}} \ . \tag{175}$$

As in the case of the differential-difference equation the function g is called the *characteristic of the symmetry*. We note that this is not the only possible choice for the independent variables. Another viable choice of independent variables is given by an appropriate restriction of an infinite staircase, e.g., to consider the points $u_{n+1,m-1}, u_{n,m-1}, u_{n,m}, u_{n-1,m}$ and $u_{n-1,m+1}$. This was the choice we made in the case of the Algebraic Entropy, but for the calculation of symmetries the choice of the independent variables on the axes is more convenient.

Now we need to prolong the operator (175) in order to apply it on the quad equation (4) and construct the determining equations. This prolongation is naturally

[11] This kind of reasoning in fact can hold for every kind of partial difference equations on the square which are solvable with respect to all its variables.

given by:

$$\begin{aligned}\mathrm{pr}\widehat{X} = {} & g(u_{n-1,m}, u_{n+1,m}, u_{n,m}, u_{n,m-1}, u_{n,m+1})\partial_{u_{n,m}} \\ & + g(u_{n,m}, u_{n+2,m}, u_{n+1,m}, u_{n+1,m-1}, u_{n+1,m+1})\partial_{u_{n+1,m}} \\ & + g(u_{n-1,m+1}, u_{n+1,m+1}, u_{n,m+1}, u_{n,m-1+1}, u_{n,m+2})\partial_{u_{n,m+1}} \\ & + g(u_{n,m+1}, u_{n+2,m+1}, u_{n+1,m+1}, u_{n+1,m}, u_{n+1,m+2})\partial_{u_{n+1,m+1}} \,. \end{aligned} \tag{176}$$

Applying the prolonged vector field to (4), we get:

$$g\frac{\partial Q}{\partial u_{n,m}} + [T_n g]\frac{\partial Q}{\partial u_{n+1,m}} + [T_m g]\frac{\partial Q}{\partial u_{n,m+1}} + [T_n T_m g]\frac{\partial Q}{\partial u_{n+1,m+1}} = 0 \,, \tag{177}$$

where $T_n f_{n,m} = f_{n+1,m}$ and $T_m f_{n,m} = f_{n,m+1}$. A priori (177) contains $u_{n+i,m+j}$ with $i = -1, 0, 1, 2, j = -1, 0, 1, 2$.

The invariance condition requires that (177) be satisfied on the solutions of (4). To be consistent with our choice of independent variables, which now include also $u_{n,m+2}$ and $u_{n+2,m}$, we must use (4) and its shifted consequences to express:

- $u_{n+2,m+1} = u_{n+2,m+1}(u_{n+2,m}, u_{n+1,m+1}, u_{n+1,m})$,
- $u_{n+1,m+1} = u_{n+1,m+1}(u_{n+1,m}, u_{n,m+1}, u_{n,m})$,
- $u_{n-1,m+1} = u_{n-1,m+1}(u_{n-1,m}, u_{n,m+1}, u_{n,m})$,

Doing so we reduce the determining equation (177) to an equation, written just in terms of independent variables, which thus must be identically satisfied. Differentiating (177) with respect to $u_{n,m+2}$ and to $u_{n+2,m}$, we get

$$\frac{\partial^2 T_n T_m g}{\partial u_{n+2,m+1}\partial u_{n+1,m+2}} = T_n T_m \frac{\partial^2 g}{\partial u_{n+1,m}\partial u_{n,m+1}} = 0 \,. \tag{178}$$

Consequently the symmetry coefficient g is the sum of *two simpler functions*,

$$g = g_0(u_{n-1,m}, u_{n+1,m}, u_{n,m}, u_{n,m-1}) + g_1(u_{n-1,m}, u_{n,m}, u_{n,m-1}, u_{n,m+1}) \,. \tag{179}$$

Introducing this result into the determining equation (177) and differentiating it with respect to $u_{n,m+2}$ and to $u_{n-1,m}$, we have that g_1 reduces to $g_1 = g_{10}(u_{n-1,m}, u_{n,m}, u_{n,m-1}) + g_{11}(u_{n,m}, u_{n,m-1}, u_{n,m+1})$. In a similar way, if we differentiate the resulting determining equation with respect to $u_{n+2,m}$ and to $u_{n,m-1}$, we have that g_0 reduces to $g_0 = g_{00}(u_{n-1,m}, u_{n,m}, u_{n,m-1}) + g_{01}(u_{n-1,m}, u_{n+1,m}, u_{n,m})$. Combining these results and taking into account the property symmetrical to (178), i.e., $\partial^2 g/(\partial u_{n-1,m}\partial u_{n,m-1}) = 0$, we obtain the following form for g:

$$g = g_0(u_{n,m-1}, u_{n,m}, u_{n,m+1}) + g_1(u_{n-1,m}, u_{n,m}, u_{n+1,m}) \,. \tag{180}$$

So, *the infinitesimal symmetry coefficient is the sum of functions that either involve shifts only in n with m fixed or only in m with n fixed* [79, 109].

Let us consider the subcase when the symmetry generator is given by

$$\frac{\mathrm{d}u_{n,m}}{\mathrm{d}\varepsilon} = g_1(u_{n-1,m}, u_{n,m}, u_{n+1,m}) \ . \tag{181}$$

This is a differential-difference equation depending parametrically on m. Setting $u_{n,m} = u_n$ and $u_{n,m+1} = \tilde{u}_n$, a different solution, the compatible partial difference equation (4) turns out to be an ordinary difference equation for a new solution $\tilde{u}_n$ of (181):

$$Q(u_n, u_{n+1}, \tilde{u}_n, \tilde{u}_{n+1}) = 0, \tag{182}$$

i.e., a Bäcklund transformation [83] for (181). A similar result is obtained in the case of g_0. This result was first presented in [109]. We note that the same splitting will also appear for higher order symmetries of this class of equations [41].

To find the specific form of g_1 we have to differentiate the determining equation (177) with respect to the independent variables and get some *further necessary conditions* on its shape. Let us discuss the case in which the symmetry is given in terms of shifts in the n direction, since the m direction shift case can be treated analogously[12]:

$$X = g\,(u_{n+1,m}, u_{n,m}, u_{n-1,m})\,\partial_{u_{n,m}} \ . \tag{183}$$

We don't impose restrictions on the dependence of g on the lattice variables, so in principle $g = g_{n,m}$.

To obtain g we have to solve the *functional equation* (177). The best way to so is to use some consequences of (177) and convert them into a system of *linear partial differential equations*, which we can solve. This will impose restrictions on the form of g and will allow us to solve the functional equation (177). Using the assumption that Q is multilinear we can express $u_{n+1,m+1}$ as:

$$u_{n+1,m+1} = f(u_{n+1,m}, u_{n,m}, u_{n,m+1}) \ , \tag{184}$$

therefore the determining equation takes the form:

$$T_n T_m g = T_n g \frac{\partial f}{\partial u_{n+1,m}} + T_m g \frac{\partial f}{\partial u_{n,m+1}} + g \frac{\partial f}{\partial u_{n,m}}. \tag{185}$$

[12] In fact the more convenient way for treating the symmetries in the m direction is to consider the transformation $n \leftrightarrow m$ and make the computations in the new n direction. Performing again the same transformation in the obtained symmetry will yield the result.

Let us start to differentiate (185) with g given by (183) with respect to $u_{n+2,m}$ which is the higher order shift:

$$T_n T_m \frac{\partial g}{\partial u_{n+1,m}} T_n \frac{\partial f}{\partial u_{n+1,m}} = \frac{\partial f}{\partial u_{n+1,m}} T_n \frac{\partial g}{\partial u_{n+1,m}} . \tag{186}$$

Define:

$$z = \log \frac{\partial g}{\partial u_{n+1,m}} \tag{187}$$

then we can rewrite (186) in the form of a conservation law:

$$T_m z = z + (T_n^{-1} - \mathrm{Id}) \log \frac{\partial f}{\partial u_{n+1,m}}. \tag{188}$$

Furthermore we also have another representation for (185) which will be useful in deriving another relation similar to (188), but with respect to $u_{n-1,m}$. Indeed apply T_n^{-1} to (185) then solving for $T_n^{-1} T_M g$ we obtain the equivalent representation:

$$\begin{aligned} T_n^{-1} T_m g = & -T_n^{-1} \left(\frac{\partial f}{\partial u_{n,m}} \Big/ \frac{\partial f}{\partial u_{n,m+1}} \right) T_n^{-1} g \\ & + T_n^{-1} \left(1 \Big/ \frac{\partial f}{\partial u_{n,m+1}} \right) T_M g - T_n^{-1} \left(\frac{\partial f}{\partial u_{n+1,m}} \Big/ \frac{\partial f}{\partial u_{n,m+1}} \right) g . \end{aligned} \tag{189}$$

Differentiating this equation with respect to $u_{n-2,m}$ we obtain:

$$\begin{aligned} & T_n^{-1} T_m \frac{\partial g}{\partial u_{n-1,m}} \frac{\partial u_{n-2,m+1}}{\partial u_{n-2,m}} \\ & \qquad = -T_n^{-1} \left(\frac{\partial f}{\partial u_{n,m}} \Big/ \frac{\partial f}{\partial u_{n,m+1}} \right) T_n^{-1} \frac{\partial g}{\partial u_{n-1,m}} . \end{aligned} \tag{190}$$

From the implicit function theorem we get:

$$\frac{\partial u_{n-2,m+1}}{\partial u_{n-2,m}} = T_n^{-1} \frac{\partial u_{n-1,m+1}}{\partial u_{n-1,m}} = -T_n^{-2} \left(\frac{\partial f}{\partial u_{n,m}} \Big/ \frac{\partial f}{\partial u_{n,m+1}} \right) . \tag{191}$$

So introducing

$$v = \log \frac{\partial g}{\partial u_{n-1,m}} \tag{192}$$

we obtain from (190):

$$T_m v = v + (T_n - \mathrm{Id}) \log \left(\frac{\partial f}{\partial u_{n,m}} \Big/ \frac{\partial f}{\partial u_{n,m+1}} \right) . \tag{193}$$

Equations (188), (193) are still functional equations, but we can derive from them a system of first-order PDEs. Indeed let s be a function such that $s = s(u_{n+1,m}, u_{n,m}, u_{n-1,m})$. Then the function $T_M s = s(u_{n+1,m+1}, u_{n,m+1}, u_{n-1,m+1})$ can be annihilated applying the differential operator:

$$Y_{-1} = \frac{\partial}{\partial u_{n,m}} - \frac{\partial f/\partial u_{n,m}}{\partial f/\partial u_{n,m+1}} \frac{\partial}{\partial u_{n+1,m}} - T_n^{-1}\left(\frac{\partial f/\partial u_{n+1,m}}{\partial f/\partial u_{n,m}}\right)\frac{\partial}{\partial u_{n-1,m}} . \tag{194}$$

On the other hand the function $T_M^{-1} s = s\,(u_{n+1,m-1}, u_{n,m-1}, u_{n-1,m-1})$ is annihilated by the operator:

$$Y_1 = \frac{\partial}{\partial u_{n,m}} - T_m^{-1}\frac{\partial f}{\partial u_{n,m+1}} \frac{\partial}{\partial u_{n+1,m}} - T_n^{-1}T_m^{-1}\left(\frac{\partial f}{\partial u_{n,m+1}}\right)^{-1}\frac{\partial}{\partial u_{n-1,m}} . \tag{195}$$

Therefore we can apply the operator Y_{-1} as given by (194)–(188) and this will give us the linear PDE:

$$Y_{-1} z = -Y_{-1}(T_n^{-1} - \mathrm{Id}) \log \frac{\partial f}{\partial u_{n+1,m}} . \tag{196}$$

Analogously by applying T_M^{-1} to (188) we can write

$$T_m^{-1} z = z - T_m^{-1}(T_n^{-1} - \mathrm{Id}) \log \frac{\partial f}{\partial u_{n+1,m}} , \tag{197}$$

which applying Y_1 gives us the linear PDE:

$$Y_1 z = Y_1 T_M^{-1}(T_n^{-1} - \mathrm{Id}) \log \frac{\partial f}{\partial u_{n+1,m}} . \tag{198}$$

Since we have that z must be independent from $u_{n,m\pm1}$, whereas the coefficients in (196), (198) may depend on it, we may write down a final system for the function z as:

$$Y_1 z = Y_1 T_m^{-1}(T_n^{-1} - \mathrm{Id}) \log \frac{\partial f}{\partial u_{n+1,m}} , \tag{199a}$$

$$Y_{-1} z = -Y_{-1}(T_n^{-1} - \mathrm{Id}) \log \frac{\partial f}{\partial u_{n+1,m}} , \tag{199b}$$

$$\frac{\partial z}{\partial u_{n,m+1}} = \frac{\partial z}{\partial u_{n,m-1}} = 0 . \tag{199c}$$

In general the system (199) can be not closed, however it is possible to add an equation using Lie brackets:

$$[Y_1, Y_{-1}] z = -[Y_1 Y_{-1} T_m^{-1} - Y_{-1} Y_1](T_n^{-1} - \mathrm{Id}) \log \frac{\partial f}{\partial u_{n+1,m}} . \tag{200}$$

Applying the same line of reasoning we deduce a system of equations also for v:

$$Y_1 v = Y_1 T_m^{-1}(T_n - \mathrm{Id}) \log\left(\frac{\partial f}{\partial u_{n,m}} \Big/ \frac{\partial f}{\partial u_{n,m+1}}\right), \tag{201a}$$

$$Y_{-1} v = -Y_{-1}(T_n - \mathrm{Id}) \log\left(\frac{\partial f}{\partial u_{n,m}} \Big/ \frac{\partial f}{\partial u_{n,m+1}}\right), \tag{201b}$$

$$\frac{\partial v}{\partial u_{n,m+1}} = \frac{\partial v}{\partial u_{n,m-1}} = 0\,. \tag{201c}$$

As before if the system is not closed we may add the Lie bracket condition:

$$[Y_1, Y_{-1}]z = -[Y_1 Y_{-1} T_m^{-1} - Y_{-1} Y_1](T_n^{-1} - \mathrm{Id}) \log\left(\frac{\partial f}{\partial u_{n,m}} \Big/ \frac{\partial f}{\partial u_{n,m+1}}\right), \tag{202}$$

Once we have solved the systems (199) and (201) [eventually with the aid of the auxiliary equations (200), (202)] we insert the values for z and v we found into (188) and (193). This step can be used to fix the dependency on the explicit functions of the lattice variables n, m. We can then solve the potential-like equation:

$$\frac{\partial g}{\partial u_{n+1,m}} = \mathrm{e}^z, \quad \frac{\partial g}{\partial u_{n-1,m}} = \mathrm{e}^v\,. \tag{203}$$

Therefore if the compatibility condition

$$\frac{\partial \mathrm{e}^z}{\partial u_{n-1,m}} = \frac{\partial \mathrm{e}^v}{\partial u_{n+1,m}}\,. \tag{204}$$

is satisfied we can write:

$$g = \int \mathrm{e}^z \,\mathrm{d}u_{n+1,m} + g^{(1)}(u_{n,m})\,. \tag{205}$$

It only remains to determine the function $g^{(1)}(u_{n,m})$. This can be easily done by plugging g as defined by (205) into the determining equations (185). This determining equation will still be a functional equation, but the only implicit dependence will be only in $g^{(1)}\big(f(u_{n+1,m}, u_{n,m}, u_{n,m+1})\big)$ and can be annihilated by applying the operator

$$S = \frac{\partial}{\partial u_{n,m}} - \frac{\partial f/\partial u_{n,m}}{\partial f/\partial u_{n+1,m}} \frac{\partial}{\partial u_{n+1,m}}\,. \tag{206}$$

Differentiating in an appropriate way the resulting equation we can determine $g^{(1)}(u_{n,m})$ and check its functional form by plugging it back into (185).

To conclude this discussion we present two examples of calculations of generalized symmetries.

Example 3.3 (The dKdV Equation) Consider the so-called discrete Korteweg–de Vries equation (dKdV):

$$(u_{n,m} - u_{n+1,m+1})(u_{n,m+1} - u_{n+1,m}) - \alpha_1 + \alpha_2 \ . \tag{207}$$

We will compute its autonomous three-point symmetries in the n direction using the method we outlined above. These symmetries were presented in many papers, see [109] and references therein.

We first have to find the function $z = \log \partial g / \partial u_{n+1,m}$. Using the definition we can write down (199a) with f given by solving (207):

$$\begin{aligned}(u_{n,m-1}^2 - 2u_{n,m-1}u_{n+1,m} + u_{n+1,m}^2)\frac{\partial z}{\partial u_{n+1,m}} + (\alpha_1 - \alpha_2)\frac{\partial z}{\partial u_{n,m}} \\ + (u_{n-1,m} - u_{n,m-1})^2 \frac{\partial z}{\partial u_{n-1,m}} = 2(2u_{n,m-1} - u_{n+1,m} - u_{n-1,m}) \ .\end{aligned} \tag{208}$$

By taking the coefficients of $u_{n,m-1}$ we get:

$$\begin{aligned}(\alpha_1 - \alpha_2)\frac{\partial z}{\partial u_{n,m}} + \frac{\partial z}{\partial u_{n-1,m}} u_{n-1,m}^2 + \frac{\partial z}{\partial u_{n+1,m}} u_{n+1,m}^2 \\ = -2(u_{n+1,m} + 2u_{n-1,m}) \ , \\ \frac{\partial z}{\partial u_{n+1,m}} u_{n+1,m} + \frac{\partial z}{\partial u_{n-1,m}} u_{n-1,m} = -2 \ , \\ \frac{\partial z}{\partial u_{n-1,m}} + \frac{\partial z}{\partial u_{n+1,m}} = 0 \ .\end{aligned} \tag{209}$$

This equation can be easily solved to give the form of z:

$$z = \log C^1 (u_{n+1,m} - u_{n-1,m})^{-2} \ , \tag{210}$$

being C^1 a constant.

We do the same computations for v and we see that v has to solve exactly the same equations as z, therefore we conclude that:

$$v = \log C^2 (u_{n+1,m} - u_{n-1,m})^{-2} \ , \tag{211}$$

where C^2 is a new constant of integration. Using the compatibility condition (204) we obtain that $C^2 = -C^1$ and integrating (203) we have:

$$g = \frac{C^1}{u_{n-1,m} - u_{n+1,m}} + g^{(1)}(u_{n,m}) \ . \tag{212}$$

Inserting this form of g into the determining equations (185) and applying the operator S (206) we obtain the following equation:

$$u_{n,m+1}\frac{\mathrm{d}g^{(1)}}{\mathrm{d}u_{n,m+1}}(u_{n+1,m}) - u_{n,m+1}\frac{\mathrm{d}g^{(1)}}{\mathrm{d}u_{n,m}}(u_{n,m}) + 2g^{(1)}(u_{n+1,m})$$
$$- u_{n+1,m}\frac{\mathrm{d}g^{(1)}}{\mathrm{d}u_{n+1,m}}(u_{n+1,m}) + u_{n+1,m}\frac{\mathrm{d}g^{(1)}}{\mathrm{d}u_{n,m}}(u_{n,m}) - 2g^{(1)}(u_{n,m+1}) = 0\,. \tag{213}$$

Differentiating it with respect to $u_{n,m}$ we obtain $\mathrm{d}^2g^{(1)}(u_{n,m})/\mathrm{d}u_{n,m}^2 = 0$ which implies $g^{(1)} = C^3u_{n,m} + C^4$. Substituting this result in (213) we obtain the restriction $C^3 = 0$.

In conclusion we have found:

$$g = \frac{C^1}{u_{n-1,m} - u_{n+1,m}} + C^4\,, \tag{214}$$

which satisfies identically the determining equations (185). This shows that (214) is the most general three-point symmetry in the n direction. Note that whereas the coefficient of C^1 is a genuine generalized symmetry, the coefficient of C^4 is in fact a *point symmetry*. Since the dKdV equation (207) is invariant under the exchange of variables $n \leftrightarrow m$ we have the symmetry in the m direction:

$$\tilde{g} = \frac{\widetilde{C}^1}{u_{n,m-1} - u_{n,m+1}}\,. \tag{215}$$

Therefore (214), (215) represent the most general autonomous five point symmetries of the dKdV equation (207).

It is worth to note that the differential-difference equation defined by the (214) and (215) i.e:

$$\frac{\mathrm{d}u_k}{\mathrm{d}t} = \frac{1}{u_{k+1} - u_{k-1}}\,, \quad k \in \mathbb{Z}\,, \tag{216}$$

is a spatial discretization of the KdV equation [76, 96].

We will return to the symmetry (214) in Example 3.5 concerning *symmetry reduction*.

Example 3.4 (An autonomous equation with non-autonomous symmetries [41]*)* Let us consider the quad equation:

$$u_{n+1,m+1}u_{n,m}(u_{n+1,m} - 1)(u_{n,m+1} + 1) + (u_{n+1,m} + 1)(u_{n,m+1} - 1) = 0\,. \tag{217}$$

It was proved in [80] that (217) does not admit any autonomous three point generalized symmetry, but it was conjectured there that it might have a nonautonomous symmetry. This conjecture was proved in [41] and we will shall give here such proof.

We first have to construct the function $z = \log \partial g/\partial u_{n+1,m}$. Using this definition we can write down (199) with f obtained from (217) as:

$$\frac{u_{n-1,m}^2 - 1}{2u_{n,m}} \frac{\partial z}{\partial u_{n-1,m}} + \frac{\partial z}{\partial u_{n,m}} + \frac{2u_{n+1,m}}{u_{n,m}^2 - 1} \frac{\partial z}{\partial u_{n+1,m}} = \frac{u_{n,m}^2 - 2u_{n,m} - 1}{u_{n,m}(u_{n,m}^2 - 1)} , \tag{218a}$$

$$\frac{2u_{n-1,m}}{u_{n,m}^2 - 1} \frac{\partial z}{\partial u_{n-1,m}} - \frac{\partial z}{\partial u_{n,m}} + \frac{u_{n+1,m}^2 - 1}{2u_{n,m}} \frac{\partial z}{\partial u_{n+1,m}} = \frac{u_{n,m}^2 u_{n+1,m} + 2u_{n,m}^2 - u_{n+1,m}}{u_{n,m}(1 - u_{n,m}^2)} . \tag{218b}$$

Since there is no dependence on $u_{n,m\pm1}$ we can omit the equations concerning these variables. The system (218) is not closed. To close this system one has to add the equation for the Lie bracket (200). Solving the obtained system of three equations with respect to the partial derivatives of z we have:

$$\begin{aligned} &\frac{\partial z}{\partial u_{n-1,m}} = 0 , \quad \frac{\partial z}{\partial u_{n+1,m}} = -\frac{2(u_{n,m} + 1)}{u_{n+1,m}(u_{n,m} + 1) + 1 - u_{n,m}} , \\ &\frac{\partial z}{\partial u_{n,m}} = -\frac{2(u_{n+1,m} - 1)}{u_{n+1,m}(u_{n,m} + 1) + 1 - u_{n,m}} + \frac{1}{u_{n,m}} \\ &\qquad + \frac{1}{u_{n,m} + 1} + \frac{1}{u_{n,m} - 1} . \end{aligned} \tag{219}$$

These three equations form an overdetermined system of equations for z which is consistent because it is closed. Hence its general solution z is easily found. It contains arbitrary function $C_{n,m}^1$ depending on both discrete variables:

$$z = \log \frac{C_{n,m}^1 u_{n,m}(u_{n,m}^2 - 1)}{(u_{n,m}u_{n+1,m} + u_{n+1,m} - u_{n,m} + 1)^2} . \tag{220}$$

Substitution of (220) into the conservation law (188) yields

$$\log \frac{-C_{n,m+1}^1}{C_{n,m}^1} = 0 . \tag{221}$$

The last equation is solved by $C_{n,m}^1 = (-1)^m C_n^2$ where C_m^2 is an arbitrary function of one discrete variable.

Therefore by solving equation $z = \log \partial g/\partial u_{n+1,m}$ we find:

$$g = \frac{-(-1)^m C_n^2 u_{n,m}(u_{n,m} - 1)}{u_{n,m}u_{n+1,m} + u_{n+1,m} - u_{n,m} + 1} + g_2(u_{n-1,m}, u_{n,m}) . \tag{222}$$

with g_2 possibly dependent on the lattice variables n, m. For the further specification consider $v(u_{n-1,m}, u_{n,m}) = \log \partial g / \partial u_{n-1,m} = \log \partial g_2 / \partial u_{n-1,m}$ which putted into (201) for v gives:

$$\frac{u_{n-1,m}^2 - 1}{2u_{n,m}} \frac{\partial v}{\partial u_{n-1,m}} + \frac{\partial v}{\partial u_{n,m}} = \frac{2u_{n,m}^2 - 2u_{n,m}u_{n-1,m} + u_{n-1,m}}{u_{n,m}(u_{n,m}^2 - 1)} , \tag{223a}$$

$$\frac{2u_{n-1,m}}{u_{n,m}^2 - 1} \frac{\partial v}{\partial u_{n-1,m}} - \frac{\partial v}{\partial u_{n,m}} = -\frac{1 - u_{n,m}^2 - 2u_{n,m}}{u_{n,m}(u_{n,m}^2 - 1)} . \tag{223b}$$

The solution of this system is given by:

$$v = \log \frac{C_{n,m}^3 u_{n,m}(u_{n,m}^2 - 1)}{(u_{n,m}u_{n-1,m} - u_{n-1,m} + u_{n,m} + 1)^2} . \tag{224}$$

Substituting it into the conservation law (193) we obtain the relation

$$\log \frac{-C_{n,m+1}^3}{C_{n,m}^3} = 0 , \tag{225}$$

whose solution is $C_{n,m}^3 = (-1)^m C_n^4$, where C_n^4 is an arbitrary function of n.

As a result function g takes the form;

$$g = \frac{-(-1)^m C_n^2 u_{n,m}(u_{n,m} - 1)}{u_{n,m}u_{n+1,m} + u_{n+1,m} - u_{n,m} + 1} + \frac{-(-1)^m C_n^4 u_{n,m}(u_{n,m} + 1)}{u_{n,m}u_{n-1,m} - u_{n-1,m} + u_{n,m} + 1} + g^{(1)}(u_{n,m}) . \tag{226}$$

Substituting this definition into (185), applying the operator S defined by (206) and applying the operator:

$$\frac{\partial}{\partial u_{n,m}} \frac{-1}{2u_{n,m}(u_{n+1,m}^2 - 1)(u_{n,m+1}^2 - 1)(u_{n+1,m} + 1 + u_{n,m}u_{n+1,m} - u_{n,m})} \tag{227}$$

we obtain:

$$\frac{\mathrm{d}^2 g^{(1)}}{\mathrm{d}u_{n,m}^2} - \frac{1}{u_{n,m}} \frac{\mathrm{d}g^{(1)}}{\mathrm{d}u_{n,m}} + \frac{g^{(1)}}{u_{n,m}^2} = \frac{(-1)^m (u_{n+1,m}^2 + 1)(C_n^2 - C_{n+1}^4)}{(u_{n,m}u_{n+1,m} - u_{n,m} + u_{n+1,m} + 1)^2} . \tag{228}$$

This equation implies:

$$\frac{\mathrm{d}^2 g^{(1)}}{\mathrm{d}u_{n,m}^2} - \frac{1}{u_{n,m}} \frac{\mathrm{d}g^{(1)}}{\mathrm{d}u_{n,m}} + \frac{g^{(1)}}{u_{n,m}^2} = 0 , \quad C_n^2 = C_{n+1}^4 . \tag{229}$$

Therefore $g^{(1)} = C^5_{n,m}u_{n,m} + C^6_{n,m}u_{n,m}\log u_{n,m}$, where the coefficients do not depend on $u_{n,m}$ but might depend on the lattice variables n, m. Substituting this result again into the determining equations, applying the operator S and taking the coefficients with respect to the independent functions $u_{n,m+1}, u_{n,m}, \log u_{n+1,m}, u_{n+1,m}$ we obtain the three equations:

$$\begin{aligned} C^6_{n+1,m} = 0\,, \quad 2C^5_{n+1,m} + (C^4_{n+2} - C^4_{n+1})(-1)^m = 0\,, \\ 2C^5_{n+1,m} - (3C^4_{n+1} + C^4_{n+2})(-1)^m = 0\,, \end{aligned} \tag{230}$$

which, when solved, give us:

$$C^4_{n,m} = C(-1)^n\,, \quad C^5_{n,m} = C(-1)^{n+m}\,, \quad C^6_{n,m} = 0\,. \tag{231}$$

By plugging these results into (226) we obtain:

$$g = \frac{(-1)^{m+n}Cu_{n,m}(u^2_{n,m} - 1)(u_{n+1,m}u_{n-1,m} + 1)}{(u_{n,m}u_{n+1,m} + u_{n+1,m} - u_{n,m} + 1)(u_{n,m}u_{n-1,m} - u_{n-1,m} + u_{n,m} + 1)}\,. \tag{232}$$

From the direct substitution into (185) we obtain that (232) is a symmetry.

We already discussed how quad equations can be interpreted as Bäcklund transformations of their generalized symmetries through formula (182). In the same spirit as in the case of differential-difference equation generalized symmetries can be used to provide *symmetry reductions*. Suppose we have a three point generalized symmetry in the form (183). We can consider its flux which we recall that it is the solution of the differential-difference equation

$$\frac{\mathrm{d}u_{n,m}}{\mathrm{d}\varepsilon} = g(u_{n+1,m}, u_{n,m}, u_{n-1,m}) \tag{233}$$

and we can consider its *stationary solutions*, i.e., the solutions such that $\mathrm{d}u_{n,m}/\mathrm{d}\varepsilon \equiv 0$:

$$g(u_{n+1,m}, u_{n,m}, u_{n-1,m}) = 0\,. \tag{234}$$

In this equation m plays the rôle of a parameter and we can consider contemporaneous solutions of the stationary equation (234) and the original quad equation (184). This will give raise to families of particular solutions which are known as *symmetry solutions*.

We conclude this section presenting an example of symmetry reduction.

Example 3.5 (Symmetry reduction of the dKdV equation) Consider the dKdV equation as given by formula (207). In Example (3.5) we derived its three point generalized symmetries in both directions. Here we will use the symmetry (214) to derive a family of symmetry solutions. First we start by observing that if we assume

$C^4 \equiv 0$ we cannot have any stationary solution to the equation

$$\frac{C^1}{u_{n-1,m} - u_{n+1,m}} + C^4 = 0 \,, \tag{235}$$

so we must assume $C^4 \neq 0$ and then we can take without loss of generality $C^4 = 1$. This means that the we will have the *linear* stationary equation:

$$u_{n+1,m} - u_{n-1,m} = C^1 \,. \tag{236}$$

This equation has solution:

$$u_{n,m} = U_m^{(0)}(-1)^n + U_m^{(1)} + \tfrac{1}{4}C^1\big((-1)^n - 1 + 2n\big) \,, \tag{237}$$

which substituted into (207) gives us two equations for the coefficients of $(-1)^n$:

$$U_{m+1}^{(0)} + U_m^{(0)} + \frac{C^1}{2} = 0 \,, \tag{238a}$$

$$\begin{aligned}\left(U_{m+1}^{(0)} + U_m^{(0)}\right)^2 - \left(U_{m+1}^{(1)} - U_m^{(1)}\right)^2 + \frac{\left(C^1\right)^2}{2} \\ + C^1 U_m^{(0)} + C^1 U_{m+1}^{(0)} = \alpha_1 - \alpha_2 \,.\end{aligned} \tag{238b}$$

The solution of (238a) is given by:

$$U_m^{(0)} = K_1(-1)^m - \tfrac{1}{4}\big(1 + (-1)^m\big)C^1 \,, \tag{239}$$

which substituted in (238b) gives to the equation:

$$U_{m+1}^{(1)} - U_m^{(1)} = \pm\tfrac{1}{2}\sqrt{-4\alpha_1 + 4\alpha_2 + (C^1)^2} \tag{240}$$

whose solution is given by:

$$U_m^{(1)} = K_2 \pm \tfrac{1}{2}\sqrt{-4\alpha_1 + 4\alpha_2 + (C^1)^2}m \,. \tag{241}$$

So finally putting (239), (241) into (237) we obtain:

$$\begin{aligned}u_{n,m} = (-1)^{n+m}\left(K_1 + \frac{C^1}{4}\right) + K_2 \\ \pm \sqrt{(C^1)^2 - 4\alpha_1 + 4\alpha_2}m - \frac{C^1}{4} + \frac{C^1}{4}n \,.\end{aligned} \tag{242}$$

This is our symmetry solution.

3.4 Master Symmetries

We have stated at the end of Sect. 3.1 that integrability is associated with the existence of an infinite sequence of symmetries. However so far we discussed only how to find certain classes of symmetries, and the existence of a single symmetry cannot be seen as synonymous with integrability (see Fokas' conjecture for the continuous case [13, 34, 64, 69]). However it happens that there might exist some symmetries, which depend on the lattice variables and on their "time" which can generate the whole hierarchy of symmetries of a given equation. These particular symmetries are called *master symmetries*. The notion of master symmetry has been introduced in [36], see also [35, 38, 39, 98]. In the continuous case master symmetries usually are nonlocal, i.e., they contain terms involving integrations. For example the master symmetry for the KdV equation is:

$$X_{\mathrm{M}} = [xu_{xxx} + xuu_x + 4u_{xx} + \tfrac{4}{3}u^2 + \tfrac{1}{3}u_x D_x^{-1}(u)]\partial_u \,, \tag{243}$$

where the integral operator is defined by $D_x^{-1}(u) = \int_{-\infty}^{x} u(t,y)\,\mathrm{d}y$. This means that the master symmetry is not a genuine generalized symmetry, but it belongs to a bigger space. Such master symmetry has been found for the first time in [39] for the Landau-Lifshitz equation. In the semidiscrete and discrete case this would correspond to the presence of operators like $(T - \mathrm{Id})^{-1}$ which gives rise to infinite summations. Fortunately enough in the semidiscrete and discrete case there are many *local* master symmetries [4, 5, 24, 25, 83, 99, 100, 109, 132, 136], i.e., master symmetries with no such dependence.

Let us start the discussion of master symmetries in the case of differential-difference equations of the form (127), since the case for quad equations will follow straightforwardly. We consider local master symmetries of the form:

$$u_{n,\tau} = \varphi_n(\tau, u_{n+1}, u_n, u_{n-1}) \,. \tag{244}$$

If there is here an essential dependence on τ, then the corresponding (127) and its generalized symmetries (128) will also depend on τ which, for these equations, is an external parameter. More details on how to use them will be given at the end of this section. D_τ is defined by:

$$D_\tau = \frac{\partial}{\partial \tau} + \sum_j \varphi_{n+j} \frac{\partial}{\partial u_{n+j}} \,. \tag{245}$$

Let us define a *Lie algebra structure* on the set of functions φ_n of the form (137) and (244). For any functions φ_n and $\hat{\varphi}_n$, we introduce the equations $u_{n,\tau} = \varphi_n$ and $u_{n,\hat{\tau}} = \hat{\varphi}_n$ and the corresponding evolution differentiations D_τ and $D_{\hat{\tau}}$. A new function is defined by:

$$[\varphi_n, \hat{\varphi}_n] \equiv D_\tau \hat{\varphi}_n - D_{\hat{\tau}} \varphi_n \,. \tag{246}$$

Here [,] is a Lie bracket. It is obviously anti-symmetric: $[\varphi_n, \hat{\varphi}_n] = -[\hat{\varphi}_n, \varphi_n]$, and as one can check by a direct calculation, it satisfies the Jacobi identity:

$$\left[[\varphi_n, \hat{\varphi}_n], \tilde{\varphi}_n\right] = \left[[\varphi_n, \tilde{\varphi}_n], \hat{\varphi}_n\right] + \left[\varphi_n, [\hat{\varphi}_n, \tilde{\varphi}_n]\right] . \tag{247}$$

The right-hand side g_n of a generalized symmetry (128) of (127) satisfies (131), i.e., $[g_n, f_n] = 0$. In the case of the master symmetry (244), the function

$$g_n = [\varphi_n, f_n] \tag{248}$$

is the right-hand side of a generalized symmetry. This generalized symmetry must be nontrivial, i.e., in (128) $m > 1$ and $m' < -1$. The function φ_n satisfies the following equation:

$$\left[[\varphi_n, f_n], f_n\right] = 0 . \tag{249}$$

Any generalized symmetry (128) has a trivial solution: $\varphi_n = g_n$. The master symmetry corresponds to a nontrivial solution of (249). Then we say that (244) is a *master symmetry* of (127) if the function φ_n satisfies (249), and the function (248) is the right-hand side of a generalized symmetry (128) with orders $m > 1$ and $m' < -1$.

In the case of the local master symmetry, this definition is constructive because, for any given (127), one can find a master symmetry (244) or prove that it does not exist.

Master symmetries enable us to construct infinite hierarchies of generalized symmetries. Let us introduce an operator ad_{φ_n} corresponding to the master symmetry (244):

$$\mathrm{ad}_{\varphi_n} \hat{\varphi}_n = [\varphi_n, \hat{\varphi}_n] . \tag{250}$$

Then, in terms of its powers $\mathrm{ad}^i_{\varphi_n}$, we can construct generalized symmetries for any $i \geq 1$:

$$u_{n,t_i} = g_n^{(i)} = \mathrm{ad}^i_{\varphi_n} f_n . \tag{251}$$

In spite of the fact that (244) has an explicit dependence on the variable n, the resulting generalized symmetries (251) do not depend on n. Using local master symmetries the generalized symmetries obtained from the application of the operator ad_{φ_n} will never contain nonlocal terms.

In the generic case it is not easy to prove that (251) are generalized symmetries and do not depend explicitly on n. This can be proved only for some integrable equations, using specific additional properties. The definition of master symmetry implies that (251) with $i = 1$ is a generalized symmetry of (127). We only prove here that also (251) with $i = 2$ is a generalized symmetry (see, e.g., [35]).

If (244) is the master symmetry of (127), then (251) with $i = 2$ is a generalized symmetry of this equation. Introducing the notation $g_n^{(0)} = f_n$, we obtain from (250)–(251) the following result for all $i \geq 0$:

$$g_n^{(i+1)} = \mathrm{ad}_{\varphi_n} g_n^{(i)} = [\varphi_n, g_n^{(i)}] \,. \tag{252}$$

Then, using the Jacobi identity (247) and the fact that (251) with $i = 1$ is a generalized symmetry, we have

$$\begin{aligned} [g_n^{(2)}, f_n] &= \left[[\varphi_n, g_n^{(1)}], f_n\right] \\ &= \left[[\varphi_n, f_n], g_n^{(1)}\right] + \left[\varphi_n, [g_n^{(1)}, f_n]\right] \\ &= [g_n^{(1)}, g_n^{(1)}] + [\varphi_n, 0] = 0 \,, \end{aligned} \tag{253}$$

i.e., (251) with $i = 2$ is a generalized symmetry of (127).

Example 3.6 (Master Symmetry for the Volterra equation [25]*)* In this example we derive the form of the master symmetry for the Volterra equation (2) we have considered in Example 3.2. We will construct a master symmetry explicitly dependent on the lattice variable n, but not its "time" τ:

$$u_{n,\tau} = \varphi_n(u_{n+1}, u_n, u_{n-1}) \,. \tag{254}$$

Commuting with the Volterra equation we have the following candidate symmetry:

$$\begin{aligned} g_n^{(1)} &= u_{n+1}(u_{n+2} - u_n)\frac{\partial \varphi_n}{\partial u_{n+1}} + u_n(u_{n+1} - u_{n-1})\frac{\partial \varphi_n}{\partial u_n} \\ &+ u_{n-1}(u_n - u_{n-2})\frac{\partial \varphi_n}{\partial u_{n-1}} - u_n\varphi_{n+1} - (u_{n+1} - u_{n-1})\varphi_n + u_n\varphi_{n-1} \end{aligned} \tag{255}$$

where the functions φ_{n+j} depend on the shifts of u_n. Inserting (255) into the compatibility condition (131) and differentiating twice with respect to u_{n+3} we obtain:

$$\frac{\partial^2 \varphi_{n+2}}{\partial u_{n+3}^2} = 0 \,, \tag{256}$$

which implies:

$$\varphi_n = \alpha_n(u_n, u_{n-1})u_{n+1} + \beta_n(u_n, u_{n-1}) \,. \tag{257}$$

Substituting (257) into the compatibility condition (131) and differentiating this time twice with respect to u_{n-3} we obtain:

$$u_{n-1}\frac{\partial^2 \alpha_{n-2}}{\partial u_{n-3}^2} + \frac{\partial^2 \beta_{n-2}}{\partial u_{n-3}^2} = 0 \tag{258}$$

where both α_{n-2} and β_{n-2} do not depend on u_{n-1}. So:

$$\alpha_n = \gamma_n(u_n)u_{n-1} + \delta(u_n) \ , \quad \beta_n = \varepsilon_n(u_n)u_{n-1} + \eta(u_n) \ . \tag{259}$$

Going back to the compatibility condition and differentiating once with respect to u_{n+3} we obtain:

$$\begin{aligned} &u_{n+2}u_{n+1}\delta_n - 2u_{n+2}u_n^2\gamma_{n+1} - 2u_{n+2}u_n\delta_{n+1} \\ &\qquad + u_{n+1}^2u_n\gamma_{n+2} + u_{n+1}u_n\delta_{n+2} + u_{n+2}u_{n+1}u_{n-1}\gamma_n = 0 \ . \end{aligned} \tag{260}$$

Since in (260) nothing depends on u_{n-1} we can take the coefficient of u_{n-1} and this implies $\gamma_n = 0$. Therefore (260) becomes:

$$u_{n+2}u_{n+1}\delta_n - 2u_{n+2}u_n\delta_{n+1} + u_{n+1}u_n\delta_{n+2} = 0 \ . \tag{261}$$

Dividing by u_{n+2} and differentiating with respect to u_{n+2} we have:

$$u_{n+2}\frac{\mathrm{d}\delta_{n+2}}{\mathrm{d}u_{n+2}} - \delta_{n+2} = 0 \ . \tag{262}$$

The solution is $\delta_n = C_n^1 u_n$, with C_n^1 n dependent function. Inserting δ_n into (260) yields the ordinary difference equation:

$$C_{n+2}^1 - 2C_{n+1}^1 + C_n^1 = (T - \mathrm{Id})^2 C_n^1 = 0 \ , \tag{263}$$

i.e., $C_n^1 = C^{1,0} + C^{1,1}n$, with $C^{1,i}$ arbitrary constants. Returning to the compatibility condition and differentiating with respect to u_{n-3} we have:

$$u_{n-2}u_{n-1}\varepsilon_n - 2u_{n-2}u_n\varepsilon_{n-1} + u_{n-1}u_n\varepsilon_{n+2} = 0 \ , \tag{264}$$

which, proceeding analogously as in the case of δ_n, yields $\varepsilon_n = (C^{2,0} + C^{2,1}n)u_n$ with $C^{2,i}$ arbitrary constants. If we differentiate twice the compatibility conditions with respect to u_{n+2} we obtain the following equation:

$$\frac{\mathrm{d}^2\eta_{n+2}}{\mathrm{d}u_{n+2}^2} = 2C^{1,1} \tag{265}$$

which give us $\eta_n = C^{1,1}u_n^2 + C_n^3 u_n + C_n^4$, where C_n^3 and C_n^4 are arbitrary functions of n.

So we have fixed the functional dependence on u_n and its shifts. We are left to fix the exact form of the coefficients $C^{1,0}, C^{1,1}, C^{2,0}, C^{2,1}, C_n^3$ and C_n^4. To do so we can safely take the coefficients with respect to u_n and its shifts in the compatibility

condition. If we take the coefficient of u_{n+2}^2 we have the restriction $C^{2,1} = -C^{1,1}$. Taking now the coefficient of u_{n+2}, u_n and u_{n-1} we obtain the equations:

$$C^{1,0} - 3C^{1,1} + C^{2,0} = 0 \,, \quad C_{n-1}^3 - C_{n-2}^3 = 0 \,, \quad C_n^4 = 0 \,, \tag{266}$$

which finally yields

$$\begin{aligned} u_{n,\tau} &= C^{1,0} u_n (u_{n+1} - u_{n-1}) \\ &\quad + C^{1,1} u_{n,m} [n u_{n+1} - (n-3) u_{n-1} + u_n] + C^{3,0} u_n \,. \end{aligned} \tag{267}$$

Now some terms are not part of the genuine master symmetry as they are related to point symmetries. The coefficient of $C^{1,0}$ is the Volterra equation itself (166). In the same way we can exclude the coefficient of $C^{3,0}$ as it is a point symmetry again. At the end we conclude that the master symmetry of the Volterra equation (166) is just given by:

$$u_{n,\tau} = u_{n,m} [n u_{n+1} - (n-3) u_{n-1} + u_n] \,. \tag{268}$$

In some cases it not possible to directly construct a master symmetry from the definition (249), but it is still possible to find a master symmetry for the equation under scrutiny. First let us assume that the master symmetry possesses the particular form:

$$u_{n,\tau} = n f_n (u_{n+1}, u_n, u_{n-1}) \tag{269}$$

where f_n is the right-hand side of (127). Then let us assume that f_n depends on some constants, say k_i, $i = 1, \ldots, K$. Let us replace such constants by functions of the master symmetry "time" τ:

$$k_i \to \kappa_i = \kappa_i(\tau) \,, \quad i = 1, \ldots, M \,. \tag{270}$$

Then we can impose the condition that the symmetry (269) is actually a master symmetry. A good strategy is that of imposing the annihilation of the three point part of g_n in (248). Due to the definition of the total derivative D_τ (245) the annihilation will yield a set of first-order differential equations for the new functions with the initial conditions given by the value of the original constants:

$$\kappa_i'(\tau) = G_i\big(\kappa_1(\tau), \ldots, \kappa_M(\tau)\big) \,, \quad i = 1, \ldots, M \,, \tag{271a}$$

$$\kappa_i(0) = k_i \,. \tag{271b}$$

Then we can derive the symmetries for the original equation (127) at any order from the master symmetry (269) by putting $\tau = 0$ in the resulting symmetry. We will see two examples of this technique.

Example 3.7 (A Particular Case of the YdKN Equation [133]*)* Let us start our discussion with the equation:

$$\dot{u}_n = k\frac{u_{n+1}u_{n-1} + u_n^2}{u_{n+1} - u_{n-1}} \,. \tag{272}$$

This equation is a particular case of the YdKN equation (77). Substituting k with an undetermined function $\kappa = \kappa(\tau)$ we search for a master symmetry in the form:

$$u_{n,\tau} = n\kappa\frac{u_{n+1}u_{n-1} + u_n^2}{u_{n+1} - u_{n-1}} \,. \tag{273}$$

Calculating the commutator (248) we obtain:

$$\begin{aligned} g_n = & \frac{\kappa' u_{n+1}u_{n-1} + \kappa^2 u_{n-1}u_n + \kappa' u_n^2 + \kappa^2 u_{n+1}u_n}{u_{n+1} - u_{n-1}} \\ & - \kappa^2\left[\frac{(u_n^4 + u_{n-1}^2u_n^2 + u_{n+1}^2u_n^2 + u_{n+1}^2u_{n-1}^2)}{(u_{n+2} - u_n)(-u_{n+1} + u_{n-1})^2}\right. \\ & \left. - \frac{(u_n^4 + u_{n-1}^2u_n^2 + u_{n+1}^2u_n^2 + u_{n+1}^2u_{n-1}^2)}{(-u_n + u_{n-2})(-u_{n+1} + u_{n-1})^2}\right] . \end{aligned} \tag{274}$$

The three point part of this symmetry is given by the first term in (274), but we see that if we try to annihilate it we have a contradiction:

$$\kappa' = 0 \,, \quad \kappa^2 = 0 \,. \tag{275}$$

This seems to suggest that the Eq. (272) does not possess a master symmetry in the form (273). However we can recall that the Eq. (272) is a particular case of the full YdKN equation [133] which we discussed in the example (2.8). We can then search for an equation with more parameters for which we have a well posed problem. Let us consider instead of (273) the candidate master symmetry with two τ dependent functions κ_1 and κ_2:

$$u_{n,\tau} = n\frac{\kappa_1 u_{n+1}u_{n-1} + \kappa_2 u_n(u_{n+1} + u_{n-1}) + \kappa_1 u_n^2}{u_{n+1} - u_{n-1}} \,, \tag{276}$$

Performing the same computation as we did for (274) we arrive at the following system of equations:

$$\kappa_1' = -\kappa_1\kappa_2 \,, \quad \kappa_2' = -\kappa_1^2 \,, \tag{277}$$

with the initial conditions $\kappa_1 = k$ and $\kappa_2 = 0$. The solution of this system of differential equations is given by:

$$\kappa_1 = -k\tan(k\tau) \,, \quad \kappa_2 = \frac{k}{\cos(k\tau)} \,. \tag{278}$$

The master symmetry (276) is then:

$$u_{n,\tau} = nk\frac{u_{n+1}u_{n-1} - \sin(k\tau)u_n(u_{n+1} + u_{n-1}) + u_n^2}{\cos(k\tau)(u_{n+1} - u_{n-1})}\,, \tag{279}$$

giving the five point symmetry:

$$u_{n,\tau} = -k^2\frac{(u_{n+1}^2 + u_n^2)(u_n^2 + u_{n-1}^2)}{(u_{n+1} - u_{n-1})^2}\left(\frac{1}{u_{n+2} - u_n} + \frac{1}{u_n - u_{n-2}}\right). \tag{280}$$

This shows how the search for master symmetries can be a little bit tricky even with the aid of the ansatz described in this section.

The calculation of the master symmetries in the case of the quad equations in fact depends strongly on the theory we developed for the differential-difference equations. This is because the symmetries of a quad equations as we discussed in Sect. 3.3 is a differential-difference equation.

For a quad equation (4) a symmetry of characteristic φ_n is called a *Master Symmetry* for a generalized symmetry of characteristic symmetry g if it is a symmetry for the quad equation (4), in the sense that it solves the determining equation (177) and it is such that it is a master symmetry in the sense of the differential-difference equations. In the case of quad equations then one should find two separate master symmetries in both direction to have the full hierarchy of symmetries.

We conclude this section on master symmetries with a final example concerning the master symmetries for the equations of the ABS class [6].

Example 3.8 (Master Symmetries for the ABS class [83]*)* In this example we consider the construction of the master symmetries for the whole family of the ABS equations [6]. The symmetries and the master symmetries for the whole family of equations were presented in complete form for the first time in [109]. In [109] the master symmetries were derived through the method of *extended symmetries* which is slightly different from that we presented so far. So in the construction of the master symmetries we will follow [83] where they were derived using the same ideas we discussed above.

The equations in the ABS class, as derived in [6], are divided in two classes: the H class and class Q and arise as classification of the quad equations which possess the property of consistency around the cube.[13]

$$H_1 : (u_{n,m} - u_{n+1,m+1})(u_{n,m+1} - u_{n+1,m}) - \alpha + \beta = 0\,, \tag{281a}$$

$$\begin{aligned} H_2 : (u_{n,m} - u_{n+1,m+1})(u_{n,m+1} - u_{n+1,m}) - \alpha^2 + \beta^2 \\ + (\beta - \alpha)(u_{n,m} + u_{n,m+1} + u_{n+1,m} + u_{n+1,m+1}) = 0\,, \end{aligned} \tag{281b}$$

[13] We briefly discussed this topic also in Example 2.9.

$$
\begin{aligned}
H_3 : \alpha(u_{n,m}u_{n,m+1} + u_{n+1,m}u_{n+1,m+1}) \\
- \beta(u_{n,m}u_{n+1,m} + u_{n,m+1}u_{n+1,m+1}) + \delta(\alpha^2 - \beta^2) = 0 \,,
\end{aligned} \tag{281c}
$$

$$
\begin{aligned}
Q_1 : \alpha(u_{n,m} - u_{n+1,m})(u_{n,m+1} - u_{n+1,m+1}) \\
- \beta(u_{n,m} - u_{n,m+1})(u_{n+1,m} - u_{n+1,m+1}) \\
+ \delta^2\alpha\beta(\alpha - \beta) = 0 \,,
\end{aligned} \tag{281d}
$$

$$
\begin{aligned}
Q_2 : \alpha(u_{n,m} - u_{n+1,m})(u_{n,m+1} - u_{n+1,m+1}) \\
- \beta(u_{n,m} - u_{n,m+1})(u_{n+1,m} - u_{n+1,m+1}) \\
+ \alpha\beta(\alpha - \beta)(u_{n,m} + u_{n,m+1} + u_{n+1,m} + u_{n+1,m+1}) \\
- \alpha\beta(\alpha - \beta)(\alpha^2 - \alpha\beta + \beta^2) = 0 \,,
\end{aligned} \tag{281e}
$$

$$
\begin{aligned}
Q_3 : (\beta^2 - \alpha^2)(u_{n,m}u_{n+1,m+1} + u_{n,m+1}u_{n+1,m}) \\
+ \beta(\alpha^2 - 1)(u_{n,m}u_{n,m+1} + u_{n+1,m}u_{n+1,m+1}) \\
- \alpha(\beta^2 - 1)(u_{n,m}u_{n+1,m} + u_{n+1,m+1}u_{n+1,m+1}) \\
- \frac{\delta^2(\alpha^2 - \beta^2)(\alpha^2 - 1)(\beta^2 - 1)}{4\alpha\beta} = 0 \,,
\end{aligned} \tag{281f}
$$

$$
\begin{aligned}
Q_4 : k_0 u_{n,m}u_{n+1,m}u_{n,m+1}u_{n+1,m+1} \\
- k_1(u_{n,m}u_{n+1,m}u_{n,m+1} + u_{n+1,m}u_{n,m+1}u_{n+1,m+1} \\
+ u_{n,m}u_{n,m+1}u_{n+1,m+1} + u_{n,m}u_{n+1,m}u_{n+1,m+1}) \\
+ k_2(u_{n,m}u_{n+1,m+1} + u_{n+1,m}u_{n,m+1}) \\
- k_3(u_{n,m}u_{n+1,m} + u_{n,m+1}u_{n+1,m+1}) \\
- k_4(u_{n,m}u_{n,m+1} + u_{n+1,m}u_{n+1,m+1}) \\
+ k_5(u_{n,m} + u_{n+1,m} + u_{n,m+1} + u_{n+1,m+1}) + k_6 = 0 \,.
\end{aligned} \tag{281g}
$$

The Eq. (281a) is the same as the dKdV equation (207) and the Q_4 is in the so-called Adler's form as discussed in Example 2.9 and the definition of the coefficients k_i are given in (88)–(89). It can be proved from a direct computation [109] that the three points symmetries of the equations belonging (281) are all particular instances of the YdKN equation, i.e., (77) with the restrictions (83). We can prove that the six arbitrary coefficients a, b, c, d, e and f for the symmetries in the n direction are given in Table 1. Due to the fact that the ABS equations (281) possess the exchange symmetries $n \leftrightarrow m$ and $\alpha \leftrightarrow \beta$ the symmetries in the direction m, can be obtained by the substitutions:

$$
u_{n+1,m} \leftrightarrow u_{n,m+1} \,, \quad u_{n-1,m} \leftrightarrow u_{n,m-1} \,, \quad \alpha \leftrightarrow \beta \,. \tag{282}
$$

Table 1 The identification of the coefficients of the symmetries in the n of the ABS family (281) with those of the YdKN equation

Eq.	a	b	c	d	e	f
H_1	0	0	0	0	0	1
H_2	0	0	0	0	1	2α
H_3	0	0	0	1	0	$2\alpha\delta$
Q_1	0	0	-1	1	0	$\alpha^2\delta^2$
Q_2	0	0	1	-1	$-\alpha^2$	α^4
Q_3	0	0	$-4\alpha^2$	$2\alpha(\alpha^2+1)$	0	$-(\alpha^2-1)^2\delta^2$
Q_4	1	$-\alpha$	α^2	$\frac{g_2}{4}-\alpha^2$	$\frac{\alpha g_2}{4}+\frac{g_3}{2}$	$\frac{g_2^2}{16}+\alpha g_3$

Therefore we can restrict out attention to the symmetries in the direction n, because the discussion in the direction m will be the same.

From our point of view the problem of constructing the master symmetries for the ABS equations (281) is then reduced to the problem of finding the master symmetries of the particular cases of the YdKN equation listed in Table 1. We can proceed in the same way as we did in the preceding example, but in the general case. We start by substituting the constants a, b, c, d, e, and f with the functions $\alpha, \beta, \gamma, \delta, \varepsilon$ and ζ depending on τ and consider the master symmetry given by:

$$\frac{\mathrm{d}u_{n,m}}{\mathrm{d}\tau} = n\frac{A(\tau,u_{n,m})u_{n+1,m}u_{n-1,m}+B(\tau,u_{n,m})(u_{n+1,m}+u_{n-1,m})+C(\tau,u_{n,m})}{u_{n+1,m}-u_{n-1,m}}\,. \tag{283}$$

Calculating the commutator (248) and annihilating the three point part of the commutator and then taking the coefficients with respect to $u_{n+1,m}$, $u_{n,m}$ and $u_{n-1,m}$ we obtain the following system of six equations:

$$\frac{\mathrm{d}\alpha}{\mathrm{d}\tau} = \alpha\delta - 2\beta^2\,, \qquad \alpha(0) = a\,, \tag{284a}$$

$$\frac{\mathrm{d}\beta}{\mathrm{d}\tau} = -\beta\gamma + \alpha\varepsilon\,, \qquad \beta(0) = b\,, \tag{284b}$$

$$\frac{\mathrm{d}\gamma}{\mathrm{d}\tau} = 2\beta\varepsilon - \delta\gamma\,, \qquad \gamma(0) = c\,, \tag{284c}$$

$$\frac{\mathrm{d}\delta}{\mathrm{d}\tau} = -\gamma^2 + \alpha\zeta\,, \qquad \delta(0) = d\,, \tag{284d}$$

$$\frac{\mathrm{d}\varepsilon}{\mathrm{d}\tau} = -\gamma\varepsilon + \beta\zeta\,, \qquad \varepsilon(0) = e\,, \tag{284e}$$

Table 2 Solution of the equations for the master symmetries (285) in the case of the H equations

Eq.	$\delta(\tau)$	$\varepsilon(\tau)$	$\zeta(\tau)$
H_1	0	0	1
H_2	0	1	$2(\alpha-\tau)$
H_3	1	0	$2\alpha\delta e^{\tau}$

$$\frac{\mathrm{d}\zeta}{\mathrm{d}\tau} = \zeta\delta - 2\varepsilon^2 , \qquad \zeta(0) = f . \tag{284f}$$

Solving these equations will yield the desired master symmetry. The system in its general form is difficult to solve, but for example in the case of the H equation deriving the explicit form of the master symmetry is quite simple. From Table 1 we obtain that we can assume $\alpha = \beta = \gamma = 0$ and then the system reduces to:

$$\frac{\mathrm{d}\delta}{\mathrm{d}\tau} = -\gamma^2 , \qquad \delta(0) = d , \tag{285a}$$

$$\frac{\mathrm{d}\varepsilon}{\mathrm{d}\tau} = -\gamma\varepsilon , \qquad \varepsilon(0) = e , \tag{285b}$$

$$\frac{\mathrm{d}\zeta}{\mathrm{d}\tau} = \zeta\delta - 2\varepsilon^2 , \quad \zeta(0) = f , \tag{285c}$$

with d, e and f as given from Table 1. In Table 2 are presented the solutions relative to the H equations of the system (285).

By using the master symmetry constructed above we can construct infinite hierarchies of many-point generalized symmetries of the ABS equations (281) in both directions.

3.5 Some Examples

In this last section we will discuss some particular examples of calculation of symmetries in the case of equations with two-periodic coefficients. These particular nonautonomous equations arise naturally when classifying quad equations consistent on the cube with the *tetrahedron property* only [7, 16–18].

Let us consider a quad equation with two-periodic coefficients. In general such an equation can be written as:

$$F_n^{(+)}F_m^{(+)}Q^{(+,+)} + F_n^{(+)}F_m^{(-)}Q^{(+,-)} + F_n^{(-)}F_m^{(+)}Q^{(+,+)} + F_n^{(-)}F_m^{(-)}Q^{(-,-)} = 0 , \tag{286}$$

where $Q^{(\pm,\pm)} = Q^{(\pm,\pm)}(u_{n,m}, u_{n+1,m}, u_{n,m+1}, u_{n+1,m+1})$ and

$$F_k^{(\pm)} = \frac{1 \pm (-1)^k}{2} \tag{287}$$

[see (107)]. Any point (n, m) on the lattice have coordinates which can be even or odd. Therefore we can first derive (199), (201) for the functions z and v and then use the decomposition:

$$z = F_n^{(+)} F_m^{(+)} z^{(+,+)} + F_n^{(+)} F_m^{(-)} z^{(+,-)} + F_n^{(-)} F_m^{(+)} z^{(+,+)} + F_n^{(-)} F_m^{(-)} z^{(-,-)} \tag{288a}$$

$$v = F_n^{(+)} F_m^{(+)} v^{(+,+)} + F_n^{(+)} F_m^{(-)} v^{(+,-)} + F_n^{(-)} F_m^{(+)} v^{(+,+)} + F_n^{(-)} F_m^{(-)} v^{(-,-)} , \tag{288b}$$

to reduce the problem to the solution of four decoupled systems for the functions $z^{(\pm,\pm)} = z^{(\pm,\pm)}(u_{n+1,m}, u_{n,m}, u_{n-1,m})$ and $v^{(\pm,\pm)} = v^{(\pm,\pm)}(u_{n+1,m}, u_{n,m}, u_{n-1,m})$ by considering the even/odd combinations of discrete variables.

The same decomposition can be used for the function g:

$$g = F_n^{(+)} F_m^{(+)} g^{(+,+)} + F_n^{(+)} F_m^{(-)} g^{(+,-)} + F_n^{(-)} F_m^{(+)} g^{(+,+)} + F_n^{(-)} F_m^{(-)} g^{(-,-)} , \tag{289}$$

with $g^{(\pm,\pm)} = g^{(\pm,\pm)}(u_{n+1,m}, u_{n,m}, u_{n-1,m})$, and the relative compatibility conditions (204). This will yield the following form for g:

$$g = \Omega_{n,m}(u_{n+1,m}, u_{n,m}, u_{n-1,m}) + F_n^{(+)} F_m^{(+)} \varphi^{(+,+)} + F_n^{(+)} F_m^{(-)} \varphi^{(+,-)} + F_n^{(-)} F_m^{(+)} \varphi^{(-,+)} + F_n^{(-)} F_m^{(-)} \varphi^{(-,-)} , \tag{290}$$

where $\Omega_{n,m}$ is a known function derived from the from of z and v and $\varphi^{(\pm,\pm)} = \varphi^{(\pm,\pm)}(u_{n,m})$. These functions can be found using the determining equations with the same decomposition.

In the classification of nonautonomous Consistent Around the Cube equations with only the tetrahedron property presented in [16–18] there exists three families of equations which can be written in the form (286): the rhombic H^4 equations, the trapezoidal H^4 equations and the H^6 equations. The three point generalized symmetries for the rhombic H^4 equations were computed in [132]. The three point generalized symmetries for the trapezoidal H^4 and H^6 equations were instead considered in [49].

Example 3.9 (The D_3 equation [49]) As an explicit example of calculations of symmetries in the case of nonautonomous two-periodic coefficients we discuss the D_3 equation [16–18], which, written on the lattice (n, m), assumes the form [50]:

$$F_n^{(+)} F_m^{(+)} u_{n,m} + F_n^{(-)} F_m^{(+)} u_{n+1,m} + F_n^{(+)} F_m^{(-)} u_{n,m+1} + F_n^{(-)} F_m^{(-)} u_{n+1,m+1} + F_m^{(-)} u_{n,m} u_{n+1,m}$$

$$+ F_n^{(-)} u_{n,m} u_{n,m+1} + F_{n+m}^{(-)} u_{n,m} u_{n+1,m+1} + F_{n+m}^{(+)} u_{n+1,m} u_{n,m+1}$$
$$+ F_n^{(+)} u_{n+1,m} u_{n+1,m+1} + F_m^{(+)} u_{n,m+1} u_{n+1,m+1} = 0 \,, \tag{291}$$

Applying the method explained in Sect. 3.3 we can find the system for the function z from (199). Considering the case in which $n = 2k$ and $m = 2l$ we find from (199) two equations for $z^{(+,+)}$:

$$\frac{u_{n+1,m} + u_{n,m-1}}{u_{n,m} - u_{n,m-1}^2} \frac{\partial z^{(+,+)}}{\partial u_{n+1,m}} + \frac{\partial z^{(+,+)}}{\partial u_{n,m}} + \frac{u_{n-1,m} + u_{n,m-1}}{u_{n,m} - u_{n,m-1}^2} \frac{\partial z^{(+,+)}}{\partial u_{n-1,m}}$$
$$= \frac{2u_{n,m-1}u_{n-1,m} + u_{n,m-1}^2 + u_{n,m}}{(u_{n,m} - u_{n,m-1}^2)(u_{n,m} - u_{n-1,m}^2)} \,, \tag{292a}$$

$$\frac{u_{n+1,m} + u_{n,m+1}}{u_{n,m+1}^2 - u_{n,m}} \frac{\partial z^{(+,+)}}{\partial u_{n+1,m}} - \frac{\partial z^{(+,+)}}{\partial u_{n,m}} + \frac{u_{n-1,m} + u_{n,m+1}}{u_{n,m+1}^2 - u_{n,m}} \frac{\partial z^{(+,+)}}{\partial u_{n-1,m}}$$
$$= \frac{u_{n,m+1}^2 + 2u_{n-1,m}u_{n,m+1} + u_{n,m}}{(u_{n,m} - u_{n-1,m}^2)(u_{n,m} - u_{n,m+1}^2)} \,. \tag{292b}$$

Taking the coefficients with respect to $u_{n,m\pm1}$ and solving we obtain:

$$z^{(+,+)} = \log\left[C_1^{(+,+)} \left(\frac{u_{n,m} - u_{n-1,m}^2}{(u_{n+1,m} - u_{n-1,m})^2} \right) \right] . \tag{293}$$

In an analogous way we obtain the solutions for $z^{(+,-)}$, $z^{(-,+)}$ and $z^{(-,-)}$:

$$z^{(-,+)} = \log\left[C_1^{(-,+)} \left(\frac{u_{n,m}^2 - u_{n-1,m}}{(u_{n+1,m} - u_{n-1,m})^2} \right) \right] , \tag{294a}$$

$$z^{(+,-)} = \log\left[C_1^{(+,-)} \left(\frac{u_{n,m} + u_{n-1,m}}{(u_{n+1,m} - u_{n-1,m})^2} \right) \right] , \tag{294b}$$

$$z^{(-,-)} = \log\left[C_1^{(-,-)} \left(\frac{u_{n,m} + u_{n-1,m}}{(u_{n+1,m} - u_{n-1,m})^2} \right) \right] . \tag{294c}$$

Inserting the resulting value for (288a) into the conservation law (188) we derive the following relation between the constants:

$$C_1^{(+,-)} = -C_1^{(+,+)} \,, \quad C_1^{(-,-)} = C_1^{(-,+)} \,. \tag{295}$$

Proceeding in the same way we can derive the values of the functions $v^{(\pm,\pm)}$ from (201):

$$v^{(+,+)} = \log\left[C_2^{(-,+)}\left(\frac{u_{n,m} - u_{n+1,m}^2}{(u_{n+1,m} - u_{n-1,m})}\right)\right], \tag{296a}$$

$$v^{(-,+)} = \log\left[C_2^{(-,+)}\left(\frac{u_{n,m}^2 - u_{n+1,m}}{(u_{n+1,m} - u_{n-1,m})^2}\right)\right], \tag{296b}$$

$$v^{(+,-)} = \log\left[C_2^{(+,-)}\left(\frac{u_{n+1,m} + u_{n+1,m}}{(u_{n+1,m} - u_{n-1,m})^2}\right)\right], \tag{296c}$$

$$v^{(-,-)} = \log\left[C_2^{(-,-)}\left(\frac{u_{n+1,m} + u_{n,m}}{(u_{n+1,m} - u_{n-1,m})^2}\right)\right]. \tag{296d}$$

Inserting the resulting value for (288b) into the conservation law (193) we derive the following relation between the constants:

$$C_2^{(+,-)} = -C_2^{(+,+)}\,, \quad C_2^{(-,-)} = C_2^{(-,+)}\,. \tag{297}$$

We can now insert (288a), (288b) into the compatibility conditions in order to find g. From these compatibility conditions we obtain the following relations between the remaining constants:

$$C_2^{(+,+)} = -C_1^{(+,+)}, \quad C_2^{(-,+)} = -C_1^{(-,+)}. \tag{298}$$

Integrating (203) we get:

$$\begin{aligned} g = {} & F_n^{(+)}F_m^{(+)}\left[C_1^{(+,+)}\left(\frac{u_{n-1,m}^2 - u_{n,m}}{u_{n+1,m} - u_{n-1,m}} + u_{n-1,m}\right) + \varphi^{(+,+)}\right] \\ & + F_n^{(-)}F_m^{(+)}\left[C_1^{(-,+)}\frac{u_{n-1,m} - u_{n,m}^2}{u_{n+1,m} - u_{n-1,m}} + \varphi^{(-,+)}\right] \\ & + F_n^{(+)}F_m^{(-)}\left[C_1^{(+,+)}\frac{u_{n,m} + u_{n-1,m}}{u_{n+1,m} - u_{n-1,m}} + \varphi^{(+,-)}\right] \\ & + F_n^{(-)}F_m^{(-)}\left[C_1^{(-,+)}\frac{u_{n,m} + u_{n-1,m}}{u_{n-1,m} - u_{n+1,m}} + \varphi^{(-,-)}\right]. \end{aligned} \tag{299}$$

Inserting it in the determining equations (185) and applying the operator (206) we obtain a system of four equations which have to be identically satisfied. The result is $C_1^{(-,+)} = -C_1^{(+,+)}$ and:

$$\begin{aligned} \varphi^{(+,+)} &= K_1 u_{n,m}\,, & \varphi^{(-,+)} &= \tfrac{1}{2}K_1 u_{n,m} - \tfrac{1}{2}C_1^{(+,+)}\,, \\ \varphi^{(+,-)} &= \tfrac{1}{2}K_1 u_{n,m} + \tfrac{1}{2}C_1^{(+,+)}\,, & \varphi^{(-,-)} &= \tfrac{1}{2}K_1 u_{n,m} + \tfrac{1}{2}C_1^{(+,+)}\,, \end{aligned} \tag{300}$$

where K_1 is another arbitrary constant. Note that the symmetry generated by K_1 is a point symmetry, so the Eq. (291) in the direction n possess only the genuine three-point symmetry given by:

$$g = \frac{F_n^{(+)}F_m^{(+)}u_{n+1,m}u_{n-1,m} + \frac{1}{2}(F_m^{(-)} - F_n^{(-)}F_m^{(+)})u_{n,m}(u_{n+1,m} + u_{n-1,m})}{u_{n+1,m} - u_{n-1,m}} + \frac{F_n^{(-)}F_m^{(+)}u_{n,m}^2 + (F_m^{(-)} - F_n^{(+)}F_m^{(+)})u_{n,m}}{u_{n+1,m} - u_{n-1,m}}\,, \tag{301}$$

Note that since (291) is invariant under the exchange $n \leftrightarrow m$ the symmetry in the m direction is given simply by performing such exchange in (301).

The differential-difference equation $\mathrm{d}u_{n,m}/dt = g$ with g given by (301) is a particular instance of the nonautonomous YdKN equation [78]. In fact it was proven in [49] that every differential-difference equation generated by the symmetries of the trapezoidal H^4 and H^6 equation is a particular instance of the nonautonomous YdKN equation. Since an analogous result was previously known for the rhombic H^4 equations we conclude that *every differential-difference equation generated by the symmetries of the equations belonging to the Boll's classification is a particular instance of the nonautonomous YdKN equation*. This result extends that for the ABS classification given in [83] and briefly discussed in Example 3.8.

Example 3.10 (Generalized symmetries depending on arbitrary functions: the case of the ${}_tH_1^{\varepsilon}$ equation) As a final example we will consider the symmetries in the m direction of the ${}_tH_1^{\varepsilon}$ equation. ${}_tH_1^{\varepsilon}$ is still part of the Boll's classification [16–18] and was presented for the first time in [7]. Its symmetries were presented in [49, 51]. For sake of simplicity we will considered its form with n and m exchanged and compute the symmetries in the n direction, i.e., the equation we will study is:

$$(u_{n,m} - u_{n,m+1})(u_{n+1,m} - u_{n+1,m+1}) - \alpha_2 - \varepsilon^2\alpha_2(F_n^{(+)}u_{n+1,m+1}u_{n+1,m} + F_n^{(-)}u_{n,m}u_{n,m+1})\,. \tag{302}$$

Since there are only two two-periodic functions in (302) a function w decompose as:

$$w = F_n^{(+)}w^{(+)} + F_n^{(-)}w^{(-)} \tag{303}$$

instead of the most general decomposition (289). Applying the method explained in Sect. 3.3 we can find the system for the function z decomposed as in (303) from (199). Considering the case $n = 2k$ we find from (199) the system for $z^{(+)}$:

$$-\frac{\alpha_2(1+\varepsilon^2u_{n+1,m}^2)}{(u_{n,m}-u_{n,m-1})^2+\varepsilon^2\alpha_2^2}\frac{\partial z^{(+)}}{\partial u_{n+1,m}}+\frac{\partial z^{(+)}}{\partial u_{n,m}}$$
$$+\frac{\alpha_2(1+\varepsilon^2u_{n-1,m}^2)}{(u_{n,m}-u_{n,m-1})^2+\varepsilon^2\alpha_2^2}\frac{\partial z^{(+)}}{\partial u_{n-1,m}}=\frac{2\varepsilon^2u_{n+1,m}}{(u_{n,m}-u_{n,m-1})^2+\varepsilon^2\alpha_2^2} \tag{304a}$$

$$-\frac{\alpha_2(1+\varepsilon^2u_{n+1,m}^2)}{(u_{n,m}-u_{n,m+1})^2+\varepsilon^2\alpha_2^2}\frac{\partial z^{(+)}}{\partial u_{n+1,m}}+\frac{\partial z^{(+)}}{\partial u_{n,m}}$$
$$+\frac{\alpha_2(1+\varepsilon^2u_{n-1,m}^2)}{(u_{n,m}-u_{n,m+1})^2+\varepsilon^2\alpha_2^2}\frac{\partial z^{(+)}}{\partial u_{n-1,m}}=\frac{2\varepsilon^2u_{n+1,m}}{(u_{n,m}-u_{n,m+1})^2+\varepsilon^2\alpha_2^2}\,. \tag{304b}$$

Taking the coefficients with respect to $u_{n,m\pm1}$ we can solve this system. This time the system is not overdetermined, but it is underdetermined:

$$z^{(+)}=-\log(1+\varepsilon^2u_{n+1,m}^2)+\log Z_{n,m}^{(+)}\left(\frac{\varepsilon(u_{n+1,m}-u_{n-1,m})}{1+\varepsilon^2u_{n+1,m}u_{n-1,m}}\right). \tag{305}$$

The same holds true for $z^{(-)}$:

$$z^{(-)}=\log(1+\varepsilon^2u_{n,m}^2)+\log Z_{n,m}^{(-)}(-u_{n+1,m}+u_{n-1,m})\,. \tag{306}$$

Using (200) we just add equations which are identically satisfied, so all the differential conditions on z are satisfied. Inserting into the conservation law (188) the only condition we get is $Z_{n,m}^{(\pm)}=Z_n^{(\pm)}$ i.e., the two arbitrary functions can depend only on one lattice variable.

For v we can proceed in the same way and we obtain:

$$v^{(+)}=\log\left[\frac{(1+\varepsilon^2u_{n+1,m}u_{n-1,m})^2}{1+\varepsilon^2u_{n+1,m}^2}V_{n,m}^{(+)}\left(\frac{\varepsilon(u_{n+1,m}-u_{n-1,m})}{1+\varepsilon^2u_{n+1,m}u_{n-1,m}}\right)\right], \tag{307a}$$

$$v^{(-)}=\log\left[(1+\varepsilon^2u_{n,m}^2)V_{n,m}^{(-)}(-u_{n+1,m}+u_{n-1,m})\right]. \tag{307b}$$

Using (202) we just add equations which are identically satisfied, so we have satisfied all the differential conditions on v. Inserting v into the conservation law (193) the only condition we get is $V_{n,m}^{(\pm)}=V_n^{(\pm)}$ i.e., the two arbitrary functions depend only on one lattice variable.

Inserting z and v into the compatibility conditions (204) we can reduce the number of independent functions from four to two, since we find the following relations:

$$Z_n^{(+)}(\xi)=C_n^{(1)}-(1+\xi^2)V_n^{(+)}(\xi)\,,\quad V_n^{(-)}(\xi)=C_n^{(2)}-Z^{(-)}(\xi)\,. \tag{308}$$

Then defining:

$$G_n^{(+)}(\xi) = \int V_n^{(+)}(\xi)\,\mathrm{d}\xi\ , \quad G_n^{(-)}(\xi) = \int Z_n^{(-)}(\xi)\,\mathrm{d}\xi\ , \tag{309}$$

we can write the solution for g from (203):

$$\begin{aligned} g = F_n^{(+)}\Bigg[\frac{-1}{\varepsilon}G_n\left(\frac{\varepsilon(u_{n+1,m}-u_{n-1,m}}{(1+\varepsilon^2 u_{n+1,m}u_{n-1,m])}\right) + \frac{C_n^{(1)}}{\varepsilon}\arctan(\varepsilon u_{n+1,m}) + \varphi^{(+)}\Bigg] \\ + F_n^{(-)}[-(1+\varepsilon^2 u_{n,m}^2)G_n^{(-)}(-u_{n+1,m}+u_{n-1,m}) \\ + (1+\varepsilon^2 u_{n,m}^2)C_n^{(2)}u_{n-1,m} + \varphi^{(-)}]\ , \end{aligned} \tag{310}$$

with $\varphi_{n,m}^{(\pm)} = \varphi_{n,m}^{(\pm)}(u_{n,m})$ functions to be determined.

Inserting this form of g into the determining equations we find the following restrictions:

$$C_n^{(1)} = C_n^{(2)} = 0\ , \quad \varphi^{(+)} = C_n^{(3)}\ , \quad \varphi^{(-)} = C_n^{(4)}(1+\varepsilon^2 u_{n,m}^2)\ , \tag{311}$$

where $C_n^{(3)}$ and $C_n^{(4)}$ are arbitrary functions of the lattice variable n. This means that (302) possess generalized symmetries depending on *arbitrary functions*:

$$\begin{aligned} g = F_n^{(+)}\Bigg[\frac{-1}{\varepsilon}G_n^{(+)}\left(\frac{\varepsilon(u_{n+1,m}-u_{n-1,m}}{(1+\varepsilon^2 u_{n+1,m}u_{n-1,m])}\right) + C_n^{(3)}\Bigg] \\ + F_n^{(-)}[-(1+\varepsilon^2 u_{n,m}^2)G_n^{(-)}(-u_{n+1,m}+u_{n-1,m}) + (1+\varepsilon^2 u_{n,m}^2)C_n^{(4)}]\ . \end{aligned} \tag{312}$$

This property is linked with the fact that (302) is *Darboux integrable* [2] as it was proved in [52]. A Darboux integrable equation is *linearizable*, but the differential-difference equation defined by $\mathrm{d}u_{n,m}/\mathrm{d}t = g$ with g as in (312) is clearly nonintegrable for arbitrary values of $G_n^{(\pm)}$. This shows that generalized symmetries of a linearizable equation may not be integrable. Equation (312) possesses the integrable sub-case given by $G^{(+)}(\xi) = -\varepsilon^2/\xi$, $G^{(-)}(\xi) = 1/\xi$ and $C_n^{(3)} = C_n^{(4)} = 0$:

$$g = F_n^{(+)}\frac{1+\varepsilon^2 u_{n+1,m}u_{n-1,m}}{u_{n+1,m}-u_{n-1,m}} + F_n^{(-)}\frac{1+\varepsilon^2 u_{n,m}^2}{u_{n+1,m}-u_{n-1,m}}\ . \tag{313}$$

This symmetry defines a differential-difference equation which is a particular instance of the nonautonomous YdKN equation [49, 78].

Symmetries depending on arbitrary functions are Master Symmetries. Indeed it can be easily seen that the commutator of two symmetries of the form (312) is an higher order symmetry as long as the arbitrary functions are nonconstant [52].

4 Exercises

In this section we collect some exercises that the reader should be able to do after reading this chapter. Exercises are divided by subject so the reader will find in Sect. 4.1 exercises about the Algebraic Entropy and in Sect. 4.2 exercises about Generalized Symmetries.

4.1 Algebraic Entropy

Exercise 4.1 The Riccati equation:

$$u' = u^2 \tag{314}$$

has at least two possible discretizations. One is the trivial one:

$$u_{n+1} - u_n = hu_n^2 , \quad h \in \mathbb{R} \tag{315}$$

and the other one is:

$$u_{n+1} - u_n = hu_n u_{n+1} , \quad h \in \mathbb{R} . \tag{316}$$

Which of the two preserves the property of linearization [59]?

Exercise 4.2 Prove that the dPI equation:

$$u_{n+1} + u_n + u_{n-1} = \frac{a_n}{u_n} , \quad a_n = C_1 + C_2(-1)^n + C_3 n \tag{317}$$

has quadratic growth. Try to change the nonautonomous part on the right-hand side to see if integrability is preserved. What goes wrong [43]?

Exercise 4.3 Prove that the Hietarinta–Viallet equation [60]:

$$u_{n+1} + u_{n-1} = u_n + \frac{a}{u_n} , \tag{318}$$

has exponential growth. If you know the method of singularity confinement prove that (318) confines singularities. Put this fact in relation to what was said about the geometric meaning of the algebraic entropy at the end of Sect. 2.1.

Exercise 4.4 Try to find some other transcendental transformations which do not preserve the integrability of Eq. (60). **Hint:** Try exponential functions [44], hyperbolic functions, etc.

Exercise 4.5 Prove that with respect to the algebraic entropy the semidiscrete Burgers equation (141) has linear growth. Try to find the explicit linearization.

Exercise 4.6 Prove that the semidiscrete KdV equation given (212) has quadratic growth.

Exercise 4.7 The Toda lattice equations [120] can be represented using the Manakov–Flaschka [32, 90] variables as a system of first-order equations:

$$\dot{a}_n = a_n(b_n - b_{n-1}) \,, \tag{319a}$$

$$\dot{b}_n = a_{n+1} - a_n \,. \tag{319b}$$

Introducing nonautonomous functions $F_n^{(\pm)}$ as defined by (287) prove that the system (319) can be written as a single nonautonomous equation [78]:

$$\dot{u}_n = (F_n^{(+)}u_n + F_n^{(-)})(u_{n+1} - u_{n-1}). \tag{320}$$

Prove then that such equation possess quadratic growth. This is a nonautonomous version of the Volterra equation

Exercise 4.8 Consider the discrete Liouville equation of Adler–Startsev [2]:

$$u_{n+1,m+1}\left(1 + \frac{1}{u_{n+1,m}}\right)\left(1 + \frac{1}{u_{n,m+1}}\right)u_{n,m} = 1 \,. \tag{321}$$

Prove that its growth is linear.

Exercise 4.9 Prove that the Eq. (302) possess a principal and a secondary growth in every direction and that they are both linear [50].

Exercise 4.10 Prove that the nonautonomous Q_{V} equation (105) has quadratic growth given by (97) [48].

4.2 Generalized Symmetries

Exercise 4.11 Prove that the generalized symmetry of the Volterra equation (166) with $m = -m' = 2$ is given by (167).

Exercise 4.12 Prove that in the general case the equation of the form (77) does not possess any generalized symmetry with $m = -m' = 2$. Prove then that with the restrictions given by (83) such symmetry exists. Try to obtain such restrictions from the determining equations.

Exercise 4.13 Verify that the symmetries of the ABS equations (281) are given by the YdKN equation with coefficients given by Table 1 [83, 109]. If you are more willing try to make a direct computation of such symmetries using the techniques of Sect. 3.3.

Exercise 4.14 Prove that a three point generalized symmetry in the n direction of the Q_{V} equation can be written in as [131]:

$$\frac{\mathrm{d}u_{n,m}}{\mathrm{d}\varepsilon} = \frac{h(u_{n+1,m}, u_{n,m})}{u_{n+1,m} - u_{n-1,m}} - \frac{1}{2}\frac{\partial h(u_{n+1,m}, u_{n,m})}{\partial u_{n+1,m}} , \tag{322}$$

where h is the biquadratic:

$$h(u_{n+1,m}, u_{n,m}) = Q_{\mathrm{V}} \frac{\partial Q_{\mathrm{V}}}{\partial u_{n,m+1}, u_{n+1,m+1}} - \frac{\partial Q_{\mathrm{V}}}{\partial u_{n,m+1}} \frac{\partial Q_{\mathrm{V}}}{\partial u_{n+1,m+1}} . \tag{323}$$

Find an analogous formula for the m direction with the appropriate biquadratic. Prove that this generalized symmetry is a YdKN equation with $a, b \neq 0$ and find the appropriate connection formulas.

Exercise 4.15 Find a Master Symmetry for the modified Volterra equation (142) with both methods explained in Sect. 3.4.

Exercise 4.16 Find a generalized symmetry with $m = -m' = 2$ for the nonautonomous equation Volterra (320) from Exercise 4.7. Derive a Master Symmetry for it.

Exercise 4.17 Consider the discrete Liouville equation of Adler–Startsev (321) from Exercise 4.8 [2]. Prove that it does not admit three-point Generalized Symmetry.

Exercise 4.18 Show that the equation (a slight modification of an equation from [52, 57]):

$$u_{n,m}u_{n+1,m+1} - u_{n+1,m}u_{n,m+1} = 0 , \tag{324}$$

possesses the following three-point Generalized Symmetries in the n direction:

$$g = u_{n,m}F_n\left(\frac{u_{n+1,m}}{u_{n,m}}, \frac{u_{n,m}}{u_{n-1,m}}\right) + (C_n^1 + C_M^2)u_{n,m} + C^3 u_{n,m}\log u_{n,m} , \tag{325}$$

where $F_n = F_n(\xi, \eta)$ is an arbitrary function of its arguments and of the discrete variable n, C_n^1 is an arbitrary function of the discrete variable n, C_M^2 is an arbitrary function of the discrete variable m and C^3 is a constant.

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References

1. V.E. Adler, Bäcklund transformation for the Krichever–Novikov equation. Int. Math. Res. Not. **1998**(1), 1–4 (1998)
2. V.E. Adler, S.Y. Startsev, On discrete analogues of the Liouville equation. Theor. Math. Phys. **121**(2), 1484–1495 (1999)
3. V.E. Adler, Y.B. Suris, Q_4: integrable master equation related to an elliptic curve. Int. Math. Res. Not. **2004**(47), 2523–2553 (2004)
4. V.E. Adler, S.I. Svinolupov, R.I. Yamilov, Multi-component Volterra and Toda type integrable equations. Phys. Lett. A **254**(1), 24–36 (1999)
5. V.E. Adler, A.B. Shabat, R.I. Yamilov, Symmetry approach to the integrability problem. Theor. Math. Phys. **125**(3), 1603–1661 (2000)
6. V.E. Adler, A.I. Bobenko, Y.B. Suris, Classification of integrable equations on quad-graphs. The consistency approach. Commun. Math. Phys. **233**(3), 513–543 (2003)
7. V.E. Adler, A.I. Bobenko, Y.B. Suris, Discrete nonlinear hyperbolic equations: classification of integrable cases. Funct. Anal. Appl. **43**(1), 3–17 (2009)
8. R.L. Anderson, N.H. Ibragimov, Lie–Bäcklund transformations in applications. Studies in Applied and Numerical Mathematics, vol. 1 (SIAM, Philadelphia, PA, 1979)
9. V.I. Arnol′d, On a theorem of Liouville concerning integrable problems in dynamics. Am. Math. Soc. Transl. (2) **61**, 292–296 (1967)
10. V.I. Arnol′d, *Mathematical Methods of Classical Mechanics*. Graduate Texts in Mathematics, vol. 60, 2nd edn. (Springer, New York, 1997)
11. A.V. Bäcklund, Ueber Flachentransformationen. Math. Ann. **9**, 297–320 (1876)
12. G.A. Baker, P.R. Graves-Morris, *Padé Approximants*. Encyclopedia of Mathematics and Its Applications, vol. 59, 2nd edn. (Cambridge University Press, Cambridge, 1996)
13. I.M. Bakirov, On the symmetries of some system of evolution equations. Preprint, Inst. of Math., Ufa (1991). In Russian
14. M. Bellon, C.-M. Viallet, Algebraic entropy. Commun. Math. Phys. **204**(2), 425–437 (1999)
15. G.W. Bluman, S. Kumei, *Symmetries and Differential Equations*. Applied Mathematical Sciences, vol. 81 (Springer, New York, 1989)
16. R. Boll, Classification of 3*D* consistent quad-equations. J. Nonlinear Math. Phys. **18**(3), 337–365 (2011)
17. R. Boll, Classification and Lagrangian Structure of 3*D* Consistent Quad-Equations. Ph.D. thesis, TU Berlin (2012)
18. R. Boll, Corrigendum: classification of 3*D* consistent quad-equations. J. Nonlinear Math. Phys. **19**(4), 1292001 (2012)
19. S. Butler, M. Hay, Simple identification of fake Lax pairs (2013)
20. F. Calogero, Why are certain nonlinear PDEs both widely applicable and integrable?, in *What Is Integrability*?, ed. by V.E. Zakharov. Springer Series in Nonlinear Dynamics (Springer, Berlin, 1991), pp. 1–62
21. F. Calogero, A. Degasperis, *Spectral Transform and Solitons.* I. Studies in Applied Mathematics, vol. 13 (North Holland, Amsterdam, 1982)
22. F. Calogero, M.C. Nucci, Lax pairs galore. J. Math. Phys. **32**(1), 72–74 (1991)
23. S. Cauchy, *Œuvres complètes*, *Ser.* 1 (Gauthier-Villars, Paris, 1890)
24. I.Y. Cherdantsev, R.I. Yamilov, Master symmetries for differential-difference equations of the Volterra type. Physica D **87**(1–4), 140–144 (1995)
25. I.Y. Cherdantsev, R.I. Yamilov, Local master symmetries of differential-difference equations, in *Symmetries and Integrability of Difference Equations*, ed. by D. Levi, L. Vinet, P. Winternitz. CRM Proceedings and Lecture Notes, vol. 9 (American Mathematical Society, Providence, RI, 1996), pp. 51–61
26. A. de Moivre, *Miscellanea analytica de seriebus et quadraturis* (J. Tonson & J. Watts, London, 1730)

27. D.K. Demskoi, C.-M. Viallet, Algebraic entropy for semi-discrete equations. J. Phys. A **45**(35), 352001 (2012)
28. J. Diller, Dynamics of birational maps of P_2. Indiana Univ. Math. J. **45**(3), 721–772 (1996)
29. J. Diller, C. Favre, Dynamics of bimeromorphic maps of surfaces. Am. J. Math. **123**(6), 1135–1169 (2001)
30. S. Elaydi, *An Introduction to Difference Equations*. Undergraduate Texts in Mathematics, 3rd edn. (Springer, New York, 2005)
31. G. Falqui, C.-M. Viallet, Singularity, complexity, and quasi-integrability of rational mappings. Commun. Math. Phys. **154**(1), 111–125 (1993)
32. H. Flaschka, On Toda lattice. II. Inverse-scattering solution. Prog. Theor. Phys. **51**(3), 703–716 (1974)
33. H. Flaschka, The Toda lattice. I. Existentence of integrals. Phys. Rev. B **9**(4), 1924–1925 (1974)
34. A.S. Fokas, A symmetry approach to exactly solvable evolution equations. J. Math. Phys. **21**(6), 1318–1325 (1980)
35. A.S. Fokas, Symmetries and integrability. Stud. Appl. Math. **77**(3), 253–299 (1987)
36. A.S. Fokas, B. Fuchssteiner, The hierarchy of the Benjamin–Ono equation. Phys. Lett. A **86**(6–7), 341–345 (1981)
37. J. Friš, V. Mandrosov, Y.A. Smorondinski, M. Uhlíř, P. Winternitz, On higher symmetries in quantum mechanics. Phys. Lett. **16**(3), 354–356 (1965)
38. B. Fuchssteiner, Mastersymmetries and higher order time-dependent symmetries and conserved densities of nonlinear evolution equations. Prog. Theor. Phys. **70**(6), 1508–1522 (1983)
39. B. Fuchssteiner, On the hierarchy of the Landau–Lifshitz equation. Physica D **13**(3), 387–394 (1984)
40. V.I. Fushchich, A.G. Nikitin, New and old symmetries of the Maxwell and Dirac equations. Sov. J. Part. Nuclei **14**(1), 1–22 (1983)
41. R.N. Garifullin, E.V. Gudkova, I.T. Habibullin, Method for searching higher symmetries for quad-graph equations. J. Phys. A **44**(32), 325202 (2011)
42. R.N. Garifullin, I.T. Habibullin, R.I. Yamilov, Peculiar symmetry structure of some known discrete nonautonomous equations. J. Phys. A **48**(23), 235201 (2015)
43. B. Grammaticos, A. Ramani, V. Papageorgiou, Do integrable mappings have the Painlevé property? Phys. Rev. Lett. **67**(14), 1825–1828 (1991)
44. B. Grammaticos, A. Ramani, C.-M. Viallet, Solvable chaos. Phys. Lett. A **336**(2–3), 152–158 (2005)
45. B. Grammaticos, R.G. Halburd, A. Ramani, C.-M. Viallet, How to detect the integrability of discrete systems. J. Phys. A **42**(45), 454002 (2009)
46. G. Gubbiotti, M. Hay, A SymPy module to calculate algebraic entropy for difference equations and quadrilateral partial difference equations (2017)
47. G. Gubbiotti, R.I. Yamilov, Darboux integrability of trapezoidal H^4 and H^6 families of lattice equations. I. First integrals (2017)
48. G. Gubbiotti, C. Scimiterna, D. Levi, A non autonomous generalization of the Q_V equation. J. Int. Sys. (2017, in press)
49. G. Gubbiotti, C. Scimiterna, D. Levi, The non autonomous YdKN equation and generalized symmetries of Boll equations. J. Math. Phys. (2017, in press)
50. G. Gubbiotti, C. Scimiterna, D. Levi, Algebraic entropy, symmetries and linearization of quad equations consistent on the cube. J. Nonlinear Math. Phys. **23**(4), 507–543 (2016)
51. G. Gubbiotti, C. Scimiterna, D. Levi, Linearizability and a fake Lax pair for a nonlinear nonautonomous quad-graph equation consistent around the cube. Theor. Math. Phys. **189**(1), 1459–1471 (2016)
52. G. Gubbiotti, C. Scimiterna, D. Levi, On partial differential and difference equations with symmetries depending on arbitrary functions. Acta Polytech. **56**(3), 193–201 (2016)
53. G. Gubbiotti, C. Scimiterna, R.I. Yamilov, Darboux integrability of trapezoidal H^4 and H^6 families of lattice equations. II. General solutions. In preparation

54. I.T. Habibullin, V.V. Sokolov, R.I. Yamilov, Multi-component integrable systems and nonassociative structures, in *Nonlinear Physics: Theory and Experiment*, ed. by E. Alfinito, M. Boiti, L. Martina, F. Pempinelli (World Scientific, Singapore, 1996), pp. 139–168
55. B. Hasselblatt, J. Propp, Degree-growth of monomial maps. Ergodic Theory Dyn. Syst. **27**(5), 1375–1397 (2007)
56. M. Hénon, A two-dimentional mapping with a strange attractor. Commun. Math. Phys. **50**(1), 69–77 (1976)
57. J. Hietarinta, A new two-dimensional lattice model that is 'consistent around the cube'. J. Phys. A **37**(6), L67–L73 (2004)
58. J. Hietarinta, Searching for CAC-maps. J. Nonlinear Math. Phys. **12**(suppl. 2), 223–230 (2005)
59. J. Hietarinta, Definitions and predictions of integrability for difference equations, in *Symmetries and Integrability of Difference Equations*, ed. by D. Levi, P. Olver, Z. Thomova, P. Winternitz. London Mathematical Society Lecture Note Series, vol. 381 (Cambridge University Press, Cambridge, 2011), pp. 83–114
60. J. Hietarinta, C.-M. Viallet, Singularity confinement and chaos in discrete systems. Phys. Rev. Lett. **81**(2), 325–328 (1998)
61. J. Hietarinta, C.-M. Viallet, Searching for integrable lattice maps using factorization. J. Phys. A **40**(42), 12629–12643 (2007)
62. R. Hirota, K. Kimura, H. Yahagi, How to find the conserved quantities of nonlinear discrete equations. J. Phys. A **34**(48), 10377–10386 (2001)
63. N.H. Ibragimov, *Transformation Groups Applied to Mathematical Physics*. Mathematics and Its Applications (Soviet Series) (Reidel, Dordrecht, 1985)
64. N.H. Ibragimov, A.B. Shabat, Evolutionary equations with a nontrivial Lie–Bäcklund group. Funct. Anal. Appl. **14**(1), 19–28 (1980)
65. C.G.J. Jacobi, Über die Darstellung einer Reihe gegebner Werthe durch eine gebrochne rationale Function. J. Reine Angew. Math. **30**, 127–156 (1846)
66. N. Joshi, Singularity analysis and integrability of discrete dynamical systems. J. Math. Anal. Appl. **184**(3), 573–584 (1994)
67. E.I. Jury, *Theory and Applications of the z-Transform Method* (R.E. Krieger, Huntington, 1964)
68. E.G. Kalnins, W. Miller Jr., G.C. Williamns, Matrix operator symmetries of the Dirac equation and separation of variables. J. Math. Phys. **27**(7), 1893–1900 (1986)
69. P.H. van der Kamp, J.A. Sanders, On testing integrability. J. Nonlinear Math. Phys. **8**(4), 561–574 (2001)
70. D.J. Korteweg, G. de Vries, On the change of form of long waves advancing in a rectangular canal, and on a new type of long stationary waves. Philos. Mag. (5) **39**(240), 422–443 (1895)
71. Y. Kosmann-Schwarzbach, Generalized symmetries of nonlinear partial differential equations. Lett. Math. Phys. **3**(5), 395–404 (1979)
72. Y. Kosmann-Schwarzbach, Vector fields and generalized vector fields on fibered manifolds, in *Geometry and Differential Geometry*, ed. by R. Artzy, I. Vaisman. Lecture Notes in Mathematics, vol. 792 (Springer, Berlin, 1980), pp. 307–355
73. I.M. Krichever, S.P. Novikov, Holomorphic bundles over algebraic curves, and nonlinear equations. Russ. Math. Surv. **35**(6), 53–80 (1980)
74. S.K. Lando, *Lectures on Generating Functions*. Student Mathematical Library, vol. 23 (American Mathematical Society, Providence, 2003)
75. P.D. Lax, Integrals of nonlinear equations of evolution and solitary waves. Commun. Pure Appl. Math. **21**(5), 467–490 (1968)
76. D. Levi, M. Petrera, Continuous symmetries of the lattice potential KdV equation. J. Phys. A **40**(15), 4141–4159 (2007)
77. D. Levi, P. Winternitz, Lie point symmetries and commuting flows for equations on lattices. J. Phys. A **35**(9), 2249–2262 (2002)
78. D. Levi, R.I. Yamilov, Conditions for the existence of higher symmetries of the evolutionary equations on the lattice. J. Math. Phys. **38**(12), 6648–6674 (1997)

79. D. Levi, R.I. Yamilov, The generalized symmetry method for discrete equations. J. Phys. A **42**(45), 454,012 (2009)
80. D. Levi, R.I. Yamilov, Generalized symmetry integrability test for discrete equations on the square lattice. J. Phys. A **44**(14), 145,207 (2011)
81. D. Levi, O. Ragnisco, M. Bruschi, Continuous and discrete matrix Burgers' hierarchies. Nuovo Cimento B (11) **74**(1), 33–51 (1983)
82. D. Levi, A. Sym, G.Z. Tu, A working algorithm to isolate integrable surfaces in $E3$. Tech. Rep. DF INFN 761, INFN, Roma (1990)
83. D. Levi, M. Petrera, C. Scimiterna, R.I. Yamilov, On Miura transformations and Volterra-type equations associated with the Adler–Bobenko–Suris equations. SIGMA **4**, 077 (2008)
84. D. Levi, R.I. Yamilov, P. Winternitz, Symmetries of the continuous and discrete Krichever–Novikov equation. SIGMA **7**, 097 (2011)
85. Y.Q. Li, B. Li, S.Y. Lou, Constraints for evolution equations with some special forms of Lax pairs and distinguishing Lax pairs by available constraints (2008)
86. S. Lie, Begründung einer Invarianten-Theorie der Berührungs-Transformationen. Math. Ann. **8**(2), 215–288 (1874)
87. S. Lie, Zur allgemeinen Theorie der partiellen Differentialgleichungen beliebeger Ordnung. Leipzig. Ber. **47**, 53–128 (1895)
88. S. Lie, *Vorlesungen über Differentialgleichungen mit bekannten infinitesimalen Transformationen* (Teubner, Leipzig, 1912)
89. J. Liouville, Note sur l'intégration des équations différentielles de la Dynamique, présentée au Bureau des Longitudes le 29 juin 1853. J. Math. Pures Appl. **20**, 137–138 (1853)
90. S.V. Manakov, Complete integrability and stochastization of discrete dynamical systems. Sov. Phys. JETP **40**(2), 269–274 (1974)
91. M. Marvan, Reducibility of zero curvature representations with application to recursion operators. Acta Appl. Math. **83**(1–2), 39–68 (2004)
92. M. Marvan, On the spectral parameter problem. Acta Appl. Math. **109**(1), 239–255 (2010)
93. A.V. Mikhaĭlov, A.B. Shabat, R.I. Yamilov, A symmetric approach to the classification of nonlinear equations. Complete lists of integrable systems. Russ. Math. Surv. **42**(4), 1–63 (1987)
94. A.V. Mikhaĭlov, A.B. Shabat, V.V. Sokolov, The symmetry approach to classification of integrable equations, in *What Is Integrability*?, ed. by V.E. Zakharov. Springer Series in Nonlinear Dynamics (Springer, Berlin, 1991), pp. 115–184
95. F.W. Nijhoff, Lax pair for the Adler (lattice Krichever–Novikov) system. Phys. Lett. A **297** (1–2), 49–58 (2002)
96. F.W. Nijhoff, H.W. Capel, The discrete Korteweg–de Vries equation. Acta Appl. Math. **39** (1–3), 133–158 (1995)
97. E. Noether, Invariante Variationsprobleme. Nachrichten von der Gesellschaft der Wissenschaften zu Göttingen. Mathematisch-Physikalische Klasse **1918**, 235–257 (1918)
98. W. Oevel, B. Fuchssteiner, Explicit formulas for the symmetries and conservation laws of the Kadomtsev–Petviashvili equation. Phys. Lett. A **88**(7), 323–327 (1982)
99. W. Oevel, B. Fuchssteiner, H. Zhang, O. Ragnisco, Mastersymmetries, angle variables, and recursion operator of the relativistic Toda lattice. J. Math. Phys. **30**(11), 2664–2670 (1989)
100. W. Oevel, H. Zhang, B. Fuchssteiner, Mastersymmetries and multi-hamiltonian formulations for some integrable lattice systems. Prog. Theor. Phys. **81**(2), 295–308 (1989)
101. P.J. Olver, Convervation laws in elasticity. II. Linear homogeneous isotropic elastostatics. Arch. Ration. Mech. Anal. **85**(2), 131–160 (1984)
102. P.J. Olver, *Applications of Lie Groups to Differential Equations*. Graduate Texts in Mathematics, vol. 107 (Springer, New York, 1986)
103. P.J. Olver, Convervation laws in elasticity. III. Planar linear anisotropic elastostatics. Arch. Ration. Mech. Anal. **102**(2), 167–181 (1988)
104. L.V. Ovsiannikov, Groups and invariant-group solutions of differential equations. Dokl. Akad. Nauk SSSR (N.S.) **118**, 439–442 (1958). In Russian

105. L.V. Ovsiannikov, *Group Properties of Differential Equations* (Izdat. Sibirsk. Otdel. Akad. Nauk SSSR, Novosibirsk, 1962). In Russian
106. L.V. Ovsiannikov, *Group Analisys of Differential Equations* (Academic, London, 1982)
107. H. Padé, Sur la représentation approchée d'une fonction par des fractions rationelles. Ann. Sci. École Norm. Sup. (3) **9**, 3–93 (1892)
108. A. Ramani, B. Grammaticos, J. Hietarinta, Discrete version of the Painlevé equations. Phys. Rev. Lett. **67**(14), 1829–1832 (1991)
109. O.G. Rasin, P.E. Hydon, Symmetries of integrable difference equations on the quad-graph. Stud. Appl. Math. **119**(3), 253–269 (2007)
110. S. Rauch-Wojciechovski, Superintegrability of the Calogero–Moser system. Phys. Lett. A **95**(6), 279–281 (1983)
111. A. Russakovskii, B. Shiffman, Value distribution of sequences of rational mappings and complex dynamics. Indiana Univ. Math. J. **46**(3), 897–932 (1997)
112. H. Sakai, Rational surfaces associated with affine root systems and geometry of the Painlevé equations. Commun. Math. Phys. **220**(1), 165–229 (2001)
113. S.Y. Sakovich, Cyclic bases of zero-curvature representations: five illustrations to one concept (2002)
114. S.Y. Sakovich, True and fake Lax pairs: how to distinguish them (2011)
115. E. Schröder, Ueber iterirte Functionen. Math. Ann. **3**(2), 296–322 (1870)
116. A.B. Shabat, A.V. Mikhaĭlov, Symmetries—test of integrability, in *Important Developments in Soliton Theory*, ed. by A.S. Fokas, V.E. Zakharov. Springer Series in Nonlinear Dynamics (Springer, Berlin, 1993), pp. 355–372
117. V.V. Sokolov, Symmetries of evolution equations. Russ. Math. Surv. **43**(5), 165–204 (1988)
118. V.V. Sokolov, A.B. Shabat, Classification of integrable evolution equations, in *Mathematical Physics Reviews*. Soviet Sci. Rev. Sect. C Math. Phys. Rev., vol. 4 (Harwood Academic, Chur, 1984), pp. 221–280
119. T. Takenawa, Discrete dynamical systems associated with root systems of indefinite type. Commun. Math. Phys. **224**(3), 657–681 (2001)
120. M. Toda, Vibration of chain with nonlinear interaction. J. Phys. Soc. Jpn. **22**(2), 431–436 (1967)
121. S. Tremblay, B. Grammaticos, A. Ramani, Integrable lattice equations and their growth properties. Phys. Lett. A **278**(6), 319–324 (2001)
122. A.P. Veselov, Growth and integrability in the dynamics of mappings. Commun. Math. Phys. **145**(1), 181–193 (1992)
123. C.-M. Viallet, Algebraic entropy for differential-delay equations (2014)
124. C.-M. Viallet, Algebraic entropy for lattice equations (2006)
125. C.-M. Viallet, Integrable lattice maps: Q_{V} a rational version of Q_4. Glasg. Math. J. **51**(A), 157–163 (2009)
126. C.-M. Viallet, On the algebraic structure of rational discrete dynamical systems. J. Phys. A **48**(16), 16FT01 (2015)
127. J. von zur Gathen, J. Gerhard, *Modern Computer Algebra*, 3rd edn. (Cambridge University Press, Cambridge, 2013)
128. H. Weyl, *The Theory of Groups and Quantum Mechanics* (Dover, New York, 1950)
129. E.T. Whittaker, *A Treatise on the Analytical Dynamics of Particles and Rigid Bodies* (Cambridge University Press, Cambridge, 1999)
130. E.T. Whittaker, G.N. Watson, *A Course of Modern Analysis*, 4th edn. (Cambridge University Press, Cambridge, 1927)
131. P.D. Xenitidis, Integrability and symmetries of difference equations: the Adler–Bobenko–Suris case, in *Group Analysis of Differential Equations and Integrable Systems*, ed. by C. Sophocleous, R. Popovych, P. Damianou, A.G. Nikitin (2009), pp. 226–242
132. P.D. Xenitidis, V.G. Papageorgiou, Symmetries and integrability of discrete equations defined on a black–white lattice. J. Phys. A **42**(35), 454,025 (2009)
133. R.I. Yamilov, Classification of discrete evolution equations. Usp. Mat. Nauk. **38**, 155–156 (1983). In Russian

134. R.I. Yamilov, Classification of Discrete Integrable Equations. Ph.D. thesis, Ufa (1984). In Russian
135. R.I. Yamilov, Symmetries as integrability criteria for differential difference equations. J. Phys. A **39**(45), R541–R623 (2006)
136. H. Zhang, G.Z. Tu, W. Oevel, B. Fuchssteiner, Symmetries, conserved quantities and hierarchies for some lattice systems with soliton structure. J. Math. Phys. **32**(7), 1908–1918 (1991)

Introduction to Linear and Nonlinear Integrable Theories in Discrete Complex Analysis

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Abstract The field of discrete differential geometry lies on the border of classical differential geometry and discrete geometry. Its aim is to develop discrete geometric theories which respect fundamental aspects of the corresponding smooth ones. Also, these discretizations often clarify structures of the smooth theory.

In our presentation, we focus on the area of discrete complex analysis. In particular, we introduce several concepts of discrete holomorphic functions based on a linear approach and on nonlinear theories concerning cross-ratio systems, circle patterns and discrete conformal equivalence. These examples are used to illustrate some characteristic features in discrete differential geometry like integrability as consistency and Bäcklund–Darboux transformations.

1 Introduction

The field of discrete differential geometry is emerging at the border between differential geometry and discrete geometry. The classical area of differential geometry investigates smooth manifolds. Their study includes important geometric notions like curvature. Also, special classes of surfaces and their transformations are analyzed and characterized, for example minimal surfaces or isothermic surfaces. Parts of this classical theory have been summarized at the beginning of the twentieth century, for example in extensive volumes by Darboux [29, 30], Bianchi [6], etc., see also standard textbooks on differential geometry. In contrast to differential geometry, discrete geometry studies shapes with a finite number of elements, such as polytopes or simplicial complexes. Its history goes back to ancient Greek geometers studying for example Platonic solids which are basic examples of polytopes. Modern discrete geometry has its origins in the late nineteenth century with investigations on density of circle packings or projective configurations. A more detailed history can be found in standard textbooks on discrete geometry, see for example [38].

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Based on these two fields of differential and discrete geometry, the area of discrete differential geometry includes theories, notions and methods for the study of discrete shapes and objects which are discrete equivalents to classical shapes and objects from differential geometry. Its main aim is summarized in the message "Discretize the whole theory, not just the equations." Therefore, discretizations should preserve fundamental properties of the smooth theory. In many cases it also turned out that the discrete theory can clarify structures, for example concerning transformations of special surfaces classes which appear naturally in the discrete context. In this sense, the discrete theory is as rich as the smooth theory and contains more constructive proofs.

An important aspect of discrete differential geometry is its connection to integrability. This can for example be recognized in the existence of Bäcklund–Darboux transformations or zero curvature representations. Our presentation relies in large parts on the textbook [15] by A.I. Bobenko and Yu. Suris. Therefore we consider integrability as multidimensional consistency and emphasize this property in our examples. We focus only on the area of discrete complex analysis and present an introduction to four different discretizations of holomorphic (or conformal) functions. In each of the following sections we explain a certain concept of discrete holomorphicity. In particular, the notion of a 'discrete holomorphic functions' is redefined in every section and these notions are essentially different (although they all carry the same name as they have the same smooth analog) and should not be confused. All our examples illustrate multidimensional consistency as an important general principle in discrete differential geometry.

Note that there exist more approaches to discrete holomorphic functions than the four ideas presented here. For example, Novikov and Dynikov developed a theory based on bicolored triangles, see [34, 37, 61] and also [19].

Discrete holomorphic functions, in particular from the linear theory, have also found applications in other areas of mathematics, for example recently in statistical mechanics and probability theory, see for example [5, 25, 26, 48, 66, 67].

2 Linear Theory of Discrete Holomorphic Functions

Let $U \subset \mathbb{C}$ be open and let $f\colon U \to \mathbb{C}$ be a holomorphic map, that is the complex derivative $f'(z) = \lim_{\eta\to 0} \big(f(z+\eta) - f(z)\big)/\eta$ exists on U. Such maps may be characterized by the *Cauchy–Riemann equations* (1). To this end, fix an orthogonal coordinate system in $\mathbb{C} \cong \mathbb{R}^2$ with coordinates x and y corresponding to the real and imaginary part of the complex numbers $z = x + \mathrm{i}y$. Then we can write $f = u + \mathrm{i}w$ where $u, w\colon U \to \mathbb{R}$ are the real and the imaginary part of f. So f is *holomorphic* if and only if

$$\frac{\partial u}{\partial x} = \frac{\partial w}{\partial y} \text{ and } \frac{\partial u}{\partial y} = -\frac{\partial w}{\partial x} \iff \frac{\partial f}{\partial y} = \mathrm{i}\frac{\partial f}{\partial x}\,. \tag{1}$$

In terms of the Wirtinger derivatives $\partial_z = \partial_x - \mathrm{i}\partial_y$ and $\partial_{\bar{z}} = \partial_x + \mathrm{i}\partial_y$ these conditions (1) read $\partial_{\bar{z}} f = \partial_x f + i\partial_y f = 0$.

Holomorphic functions are naturally connected to harmonic functions, see standard textbooks on complex analysis, for example [3, 36], for details and proofs.

Theorem 2.1 *For any holomorphic function $f = u + \mathrm{i}w$, its real and imaginary part are* harmonic, *that is they satisfy the following Laplace equations*

$$\Delta u := \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 \quad \textit{and} \quad \Delta w = 0 \,.$$

Conversely, for every harmonic function $u\colon U \to \mathbb{R}$ on a simply connected domain U there exists a holomorphic function $f = u + \mathrm{i}w$ which is unique up to an imaginary constant. (That is there exists a conjugate harmonic function $w\colon U \to \mathbb{R}$, which is unique up to a real constant, such that u and w satisfy the Cauchy–Riemann equations.)

The Cauchy–Riemann equations and the Laplace equation for harmonic functions are both linear in u (and w) and build the basis of the linear theory of discrete holomorphic functions.

2.1 Definition of Discrete Harmonic and Discrete Holomorphic Functions

First, we consider discrete Laplacians and then define discrete holomorphic functions based on discrete harmonic function. We start with the square grid lattice (see for example Fig. 1) which provides a simple, but instructive example.

The discrete Laplacian on the square grid lattice $\mathbb{Z}^2$ has already been studied in the beginning of the twentieth century, see for example [28]. In fact, Kirchhoff's circuit law encodes the harmonicity of the potential function. Further investigations on discrete harmonic and discrete holomorphic functions on the square grid lattice are due to Isaacs [47], Ferrand [35] and Duffin [32, 33] who also generalized these notions to planar graphs with rhombic faces. Such graphs are also called *rhombic embeddings*.

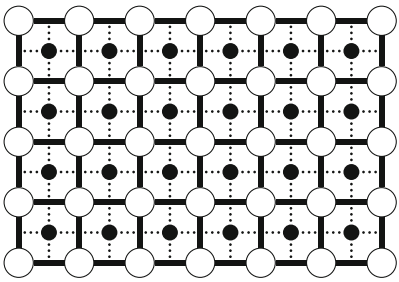

Fig. 1 Regular square grid lattice (*white vertices*) and its dual (*black vertices* and *dotted edges*)

Given a function $u\colon \mathbb{Z}^2 \to \mathbb{R}$, partial derivatives with respect to the coordinates x and y may be replaced by differences $u(m+1,n)-u(n,m)$ and $u(m,n+1)-u(m,n)$ respectively. This leads to the standard *Laplacian on the square grid lattice*

$$\Delta u(m,n) = u(m+1,n) + u(m-1,n) + u(m,n+1) + u(m,n-1) - 4u(m,n)\ .$$

In some contexts, scaled versions of this Laplacian are used, but we are only interested in *discrete harmonic functions* satisfying $\Delta u = 0$, so scaling does not matter in the following.

This Laplacian can easily be generalized for a planar graph $G = (V, E, F)$ where V denotes the vertices, E are the edges and F the faces of G. We always assume that the graph is embedded (or at least immersed) in the plane and identify it with its embedding. At every interior vertex v_0 with adjacent vertices $v_1, v_2, \ldots, v_n$ we define the *Laplacian* on G at v_0 by

$$(\Delta u)(v_0) = \sum_{j=1}^{n} \omega(v_0, v_j)\big(u(v_j) - u(v_0)\big)\ , \tag{2}$$

where $\omega\colon E(G) \to \mathbb{R}$ are *weights* defined on the undirected edges and $u\colon V \to \mathbb{R}$ is some function on the vertices. If $\Delta u = 0$ at all interior vertices, then the function u is called *discrete harmonic*.

Exercise 2.2 (Discrete Maximum Principle) Assume that the weights ω are all positive. Show that a corresponding discrete harmonic function attains its maximum (and its minimum) at a boundary vertex.

This discrete maximum principle is analogous to the maximum principle for harmonic functions in the smooth theory and therefore such positive weights ω may be especially desirable. Note that nonsymmetric weights defined on directed edges are also possible but only rarely used.

Given a harmonic function $u\colon V \to \mathbb{R}$, a natural domain for the conjugate function w is the dual graph $G^* = (V^*, E^*, F^*)$. For the case of the square grid lattice $\mathbb{Z}^2$, we assume that the vertices of the dual graph $(\mathbb{Z}^2)^*$ are the centers of the squares of $\mathbb{Z}^2$. To each edge of $\mathbb{Z}^2$ there corresponds a dual edge (and a square built by two vertices of $\mathbb{Z}^2$ and two corresponding vertices of the dual lattice), see Figs. 1 and 2.

In the notation of Fig. 2 (left) the *discrete Cauchy–Riemann equations* read

$$u_r - u_l = w_u - w_d \quad \text{and} \quad u_u - u_d = -(w_r - w_l) = w_l - w_r\ , \tag{3}$$

where u_r, u_l, u_u, u_d and w_u, w_d, w_r, w_l are the values of the functions u and w respectively on the corresponding vertices. As an immediate consequence we observe that to any harmonic function u on (a simply connected part of) $\mathbb{Z}^2$ there exists a function w on the dual graph (unique up to a constant) such that the discrete Cauchy–Riemann equations hold. Indeed, fix w at some vertex and define its values at the other vertices by the discrete Cauchy–Riemann equations (3). This procedure

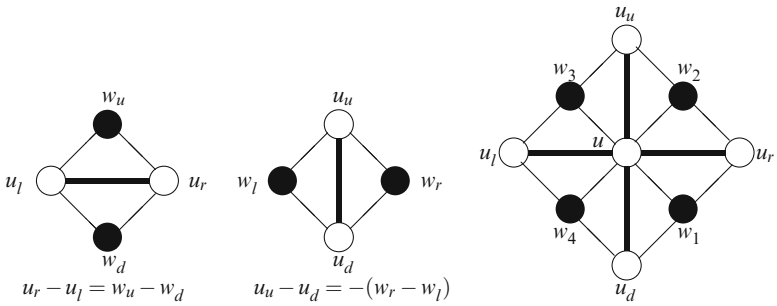

Fig. 2 Discrete Cauchy–Riemann equations (*left*) and dual cycle around a vertex (*right*)

will not cause any ambiguities because for all cycles around a vertex we have with the notation of Fig. 2 (right)

$$\begin{aligned}(w_2 - w_1) + (w_3 - w_2) + (w_4 - w_3) + (w_1 - w_4)\\ = (u_r - u) + (u_u - u) + (u_l - u) + (u_d - u) = \Delta u = 0\,.\end{aligned}$$

The corresponding *discrete holomorphic* function $f^\ell\colon \mathbb{Z}^2 \cup (\mathbb{Z}^2)^* \to \mathbb{C}$ is defined by the formula

$$f^\ell(z) = \begin{cases} u(z) & \text{if } z \text{ is a vertex of } \mathbb{Z}^2,\\ \mathrm{i}w(z) & \text{if } z \text{ is a vertex of } (\mathbb{Z}^2)^*.\end{cases}$$

The superscript ℓ only emphasizes the fact that this is the definition for discrete holomorphicity within the *linear* theory. Remarkably, the discrete Cauchy–Riemann equation for f^ℓ can be summarized as

$$f_4^\ell - f_2^\ell = \mathrm{i}(f_3^\ell - f_1^\ell) \tag{4}$$

for any function $f^\ell\colon \mathbb{Z}^2 \cup (\mathbb{Z}^2)^* \to \mathbb{C}$ where $f_1^\ell, f_2^\ell, f_3^\ell, f_4^\ell$ are the values of f^ℓ on a quadrilateral formed by black and white vertices as in Fig. 2 (left or middle) in cyclic orientation. This corresponds to (1) in the smooth case.

Example 2.3 The function $f^\ell\colon \mathbb{Z}^2 \to \mathbb{C}$ given by $f^\ell(m,n) = (n + \mathrm{i}m)^2$ is discrete holomorphic. This can be easily seen by checking the discrete Cauchy–Riemann equations (4).

The discrete Cauchy–Riemann equation (4) can easily be generalized to an embedded (or immersed) planar graph G with embedded (or immersed) dual graph G^*. Analogously as in Fig. 2 we can build a quadrilateral for every edge of E and obtain a bipartite graph $\mathcal{D}$ with bicolored vertices and quadrilateral faces called *b-quad-graph* as illustrated in Fig. 3 (left).

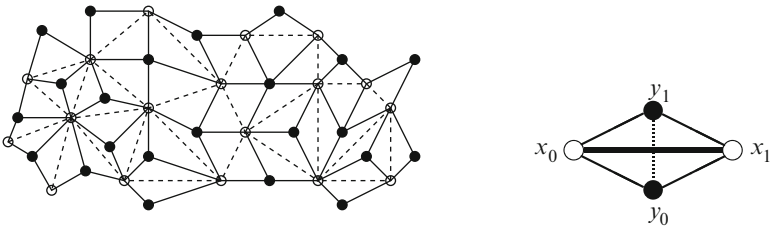

Fig. 3 *Left*: An example of a b-quad-graph $\mathcal{D}$ (*black edges* and *bicolored vertices*) and its associated graph G (*dashed edges* and *white vertices*). *Right*: Quadrilateral of $\mathcal{D}$ with orthogonal diagonals

Note that $V(\mathcal{D}) = V \cup V^*$. On each quad as in Fig. 3 (right) the Cauchy–Riemann equations (3) and (4) generalize to

$$\frac{f^\ell(x_1) - f^\ell(x_0)}{x_1 - x_0} = \frac{f^\ell(y_1) - f^\ell(y_0)}{y_1 - y_0} \,. \tag{5}$$

Note that for every three-connected planar graph (that is G remains connected if one or two edges are removed) there exists an embedding of G and its dual graph G^* such that all dual vertices lie in the interior of the faces of G and every edge intersects the corresponding dual edge orthogonally. This embedding can be constructed using orthogonal circle patterns, see for example [21, 72]. In the following, we restrict ourselves to such orthogonal embeddings. Then corresponding edges of G and G^* are orthogonal and (5) can be rewritten as

$$\frac{f^\ell(y_1) - f^\ell(y_0)}{f^\ell(x_1) - f^\ell(x_0)} = \frac{y_1 - y_0}{x_1 - x_0} = \mathrm{i}\left|\frac{y_1 - y_0}{x_1 - x_0}\right| =: \mathrm{i}\omega(x_0, x_1) = \mathrm{i}\frac{1}{\omega(y_0, y_1)} \,. \tag{6}$$

The weights $\omega\colon E \to \mathbb{R}_+$ and the dual weights $\omega\colon E^* \to \mathbb{R}_+$ are in this case defined geometrically. A function $f^\ell\colon V(\mathcal{D}) \to \mathbb{C}$ which satisfies the discrete Cauchy–Riemann equations (6) is called *discrete holomorphic*. Of course, (6) may also be considered for nongeometric weights and general b-quad-graphs.

Exercise 2.4 Let $\theta_0 \neq \theta_1$ be two complex numbers with same modulus $|\theta_0| = |\theta_1|$. Show that on the b-quad-graph $\theta_0\mathbb{Z} \times \theta_1\mathbb{Z}$ the function defined as

$$f^\ell(m\theta_0 + n\theta_1) = (m\theta_0 + n\theta_1)^3 + \frac{\theta_0^2 - \theta_1^2}{4}(m\theta_0 + n\theta_1)$$

is discrete holomorphic. This can be considered as a discrete analog of z^3.

As for the square grid case, we also observe an analogous connection of discrete harmonic and discrete holomorphic functions.

Theorem 2.5 *Let $\mathcal{D}$ be a simply connected b-quad-graph built from a planar (immersed) graph G and its (immersed) dual G^* such that each edge and its corresponding dual edge intersect orthogonally.*

If $f^\ell\colon V(\mathcal{D}) \to \mathbb{C}$ is discrete holomorphic, then its restrictions $f^\ell|_V$ and $f^\ell|_{V^*}$ are discrete harmonic with respect to the weights ω defined in (6).

Conversely, any discrete harmonic function $u\colon V \to \mathbb{R}$ admits a family of discrete holomorphic extensions $f^\ell\colon V(\mathcal{D}) \to \mathbb{C}$ differing by an additive constant on V^*. That is, f is uniquely determined by the value on an arbitrary vertex $y \in V^*$.

Proof Let $f^\ell\colon V(\mathcal{D}) \to \mathbb{C}$ be discrete holomorphic and let x_0 be an interior vertex. We will only consider the case $x_0 \in V$ and leave the analogous cases $x_0 \in V^*$ as an exercise. Let $x_1, x_2, \dots, x_n$ be the neighboring vertices of x_0 in G. Let $y_0, y_1, \dots, y_{n-1}, y_n = y_0 \in V^*$ be the chain of dual vertices such that $x_0, y_j, x_{j+1}, y_{j+1}$ are quads in $\mathcal{D}$ for $j = 0, 1, \dots, n-1$. Then using the discrete Cauchy–Riemann equations (6) we obtain

$$\begin{aligned} 0 &= f^\ell(y_1) - f^\ell(y_0) + f^\ell(y_2) - f^\ell(y_1) + \cdots + f^\ell(y_0) - f^\ell(y_{n-1}) \\ &= \mathrm{i}\omega(x_0, x_1)\big(f^\ell(x_1) - f^\ell(x_0)\big) + \mathrm{i}\omega(x_0, x_2)\big(f^\ell(x_2) - f^\ell(x_0)\big) + \dots \\ &\qquad\qquad + \mathrm{i}\omega(x_0, x_n)\big(f^\ell(x_n) - f^\ell(x_0)\big) \\ &= \mathrm{i}(\Delta f^\ell|_V)(x_0)\ . \end{aligned}$$

Now given a discrete harmonic function $u : V \to \mathbb{R}$ we can obtain a conjugate harmonic function $w : V^* \to \mathbb{R}$ and a corresponding discrete holomorphic function $f^\ell : V(\mathcal{D}) \to \mathbb{C}$ similarly as for the square grid lattice. Take $f^\ell(x) = u(x)$ at all vertices $x \in V$. Choose a value $f^\ell(y)$ at some fixed vertex $y \in V^*$. Then the discrete Cauchy–Riemann equations (6) uniquely determine the values of f^ℓ at all other vertices of V^* since $\mathcal{D}$ is simply connected and u is harmonic on G with respect to the weights ω defined in (6). □

From a more conceptual perspective, this theorem links the solutions of the quad-equation (6) and to the solutions of a Laplace equation on white (or black) vertices. A similar relation can be established for a broader class of quad-equations, for more details see for example [15, Sect. 6.13] or [1, 14].

2.2 3D-Consistency and Integrability

In the following, we investigate the structure of the discrete Cauchy–Riemann equation (6) in the context of integrability. To this end, we assume given a b-quad-graph $\mathcal{D}$ with weights ω on the faces (more precisely on the edges between black vertices and on the edges between white vertices respectively of any quad). The discrete Cauchy–Riemann equation (6) on the quads of $\mathcal{D}$ defines a *2D-system*. This means that given any three (generic) values of a function f^ℓ on the vertices of a quad,

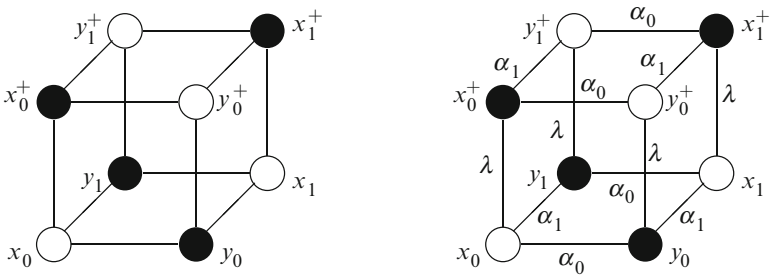

Fig. 4 Elementary cube over a face of $\mathcal{D}$ without (*left*) and with (*right*) labelling on the edges

(6) determines a unique value for f^ℓ on the fourth vertex. These discrete Cauchy–Riemann equations can now be put as condition of the faces on a three-dimensional cube, see Fig. 4 (left).

As we aim at transformations of a given discrete holomorphic function, we assume that opposite faces of the cube carry the same equation. We just need to be careful with the orientation of the faces as the discrete Cauchy–Riemann equations depend on the orientation of the quadrilaterals. Then these equations are consistent if we can prescribe arbitrary values of f^ℓ at one vertex of the cube and its three neighbors and obtain the remaining values uniquely without contradictions using the equations on the faces of the cube.

Example 2.6 (Square Grid Lattice) Let $f^\ell\colon \mathbb{Z}^2 \to \mathbb{C}$ be a discrete holomorphic function (with respect to $\omega \equiv 1$ and bicolored vertices of $\mathbb{Z}^2$). Add an "extra dimension" such that this grid is extended to a subset in $\mathbb{Z}^3$ consisting of two parallel layers of $\mathbb{Z}^2$. Fix the value of f^ℓ at one vertex of the new layer. Determine all remaining values of f^ℓ by using the discrete Cauchy–Riemann equations (4) for $\mathbb{Z}^2$ on the 'vertical faces' of the cubes. On each of these faces we choose the orientation such that the cycle of vertices (x, y, y^+, x^+) is positively oriented in the notation of Fig. 4. This construction will not result in contradictions and furthermore the function defined on the new layer is also discrete holomorphic. It is in fact a *(fundamental) transformation of* f^ℓ, also called *Bäcklund transformation.*

These properties can easily be seen by considering one cube as in Fig. 4. In particular

$$
\begin{aligned}
f^\ell(y_1) - f^\ell(y_0) &= \mathrm{i}\big(f^\ell(x_1) - f^\ell(x_0)\big)\\
f^\ell(y_0^+) - f^\ell(x_0) &= \mathrm{i}\big(f^\ell(y_0) - f^\ell(x_0^+)\big)\\
f^\ell(x_1^+) - f^\ell(y_0) &= \mathrm{i}\big(f^\ell(y_0^+) - f^\ell(x_1)\big)\\
f^\ell(x_1^+) - f^\ell(y_1) &= \mathrm{i}\big(f^\ell(y_1^+) - f^\ell(x_1)\big)\\
f^\ell(y_1^+) - f^\ell(x_0) &= \mathrm{i}\big(f^\ell(y_1) - f^\ell(x_0^+)\big)
\end{aligned}
$$

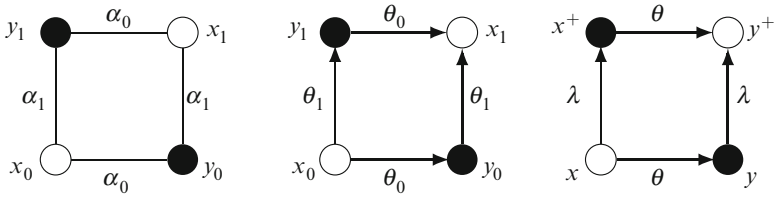

Fig. 5 A fundamental square with labels on the undirected edges (*left*) and on positively oriented directed edges (*middle* and *right*)

These equations show that the values $f^\ell(x_1), f^\ell(x_1^+), f^\ell(y_0^+)$, and $f^\ell(y_1^+)$ are uniquely determined from $f^\ell(x_0), f^\ell(y_0), f^\ell(y_1), f^\ell(x_0^+)$ and also

$$f^\ell(x_1^+) - f^\ell(x_0^+) = \mathrm{i}\big(f^\ell(y_0^+) - f^\ell(y_1^+)\big)$$

holds. Note that on the upper layer the coloring of the vertices is interchanged.

Example 2.7 (Rhombic Embedding) As a more general example we can consider rhombic embeddings, that is planar embedded quad-graphs $\mathcal{D}$ whose faces are all rhombi. In fact, 3D-consistency holds exactly for the rhombic case, see remarks below.

In particular, consider a rhombus which is defined by its two directed edges $\theta_0, \theta_1 \in \mathbb{S}^1 = \{z \in \mathbb{C} : |z| = 1\}$ as illustrated in Fig. 5 (middle). Then the weight $\omega(x_0, x_1)$ can be expressed as

$$\omega(x_0, x_1) = -\mathrm{i}\frac{y_1 - y_0}{x_1 - x_0} = -\mathrm{i}\frac{\theta_1 - \theta_0}{\theta_1 + \theta_0} = \mathrm{i}\frac{\theta_0 - \theta_1}{\theta_0 + \theta_1}\,.$$

On the "vertical" faces of the cube we fix some $\lambda \in \mathbb{S}^1$ as parameter and corresponding weights $\omega(x, y^+) = \mathrm{i}(\theta - \lambda)/(\theta + \lambda)$, see Fig. 5 (right). Then the discrete Cauchy–Riemann equations are 3D-consistent. In particular, a given discrete holomorphic function on a rhombic quad-graph can be transformed into a discrete holomorphic function on the same quad-graph with black and white vertices interchanged. The proof is similar to the square grid case and is left as an exercise to the reader.

The class of rhombic embeddings obviously includes the square grid lattice $\mathbb{Z}^2$ and its "sheared" versions $\theta_0\mathbb{Z} \times \theta_1\mathbb{Z}$ for $\theta_0, \theta_1 \in \mathbb{S}^1$ with $\theta_0/\theta_1 \notin \mathbb{R}$, but also more involved examples like the dual kagome lattice or Penrose tilings (see Figs. 6 (left) and 9 (right) for examples), see also [50].

Remark 2.8 (Rhombic Embeddings and Surfaces in $\mathbb{Z}^d$) For the integrable Cauchy–Riemann equations, rhombic (ramified) embeddings from projections of two-dimensional surfaces in $\mathbb{Z}^d$, $d \geq 2$, are of special importance. In this case, we can lift the discrete holomorphic function from the quad-graph to the vertices of the

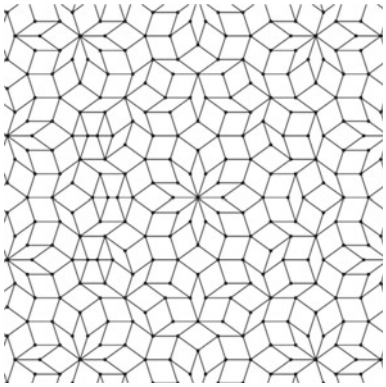

Fig. 6 *Left*: Example of a rhombic embedding (a part of a Penrose tiling). *Right*: A vertical face of the cube with labelled edges

corresponding surface in $\mathbb{Z}^d$. In fact, the directed edges e_k of $\mathbb{Z}^d$ are supposed to carry the corresponding directions θ_k as labelling, such that parallel edges all carry the same label. Then thanks to the 3D-consistency this function can be extended to (a part of) $\mathbb{Z}^d$! Therefore, we call a function $f^\ell\colon \mathbb{Z}^d \to \mathbb{C}$ *discrete holomorphic* if for all quadrilateral faces of $\mathbb{Z}^d$ we have

$$\frac{f^\ell(x+e_k)-f^\ell(x+e_j)}{f^\ell(x+e_k+e_j)-f^\ell(x)} = \mathrm{i}\frac{\theta_k-\theta_j}{\theta_k+\theta_j}\,. \tag{7}$$

In fact, for our geometric choice of the weights ω, it turns out that 3D-consistency of (6) holds for a quad-graph $\mathcal{D}$ if and only if this quad-graph is a rhombic (ramified) embedding. This can be seen by observing, that the discrete Cauchy–Riemann equations are in fact a special reduction (to $\mathbb{R}^2$) of the *discrete Moutard equation*

$$F(x_1)-F(x_0) = a\big(F(y_1)-F(y_0)\big) \tag{8}$$

in the notation of Fig. 5. This equation can be assigned to all two-dimensional faces of the lattice $\mathbb{Z}^m$ analogously as (7), where a is a scalar (real-valued) function on the two-dimensional faces of $\mathbb{Z}^m$. Note that we have to chose an orientation on the quads.

Let $F\colon \mathbb{Z}^m \to \mathbb{R}^n$ be a map satisfying (8) on all 2-dimensional faces (called T-net). Geometrically, (8) means that for each face the points $F(x_1), F(x_0), F(y_1), F(y_0)$ are coplanar (so the net F has planar faces) and furthermore the diagonals of these planar quads are parallel. Analogously as for the Cauchy–Riemann equation in the previous examples we can consider 3D-consistency for the Moutard equation (8). It turned out that this holds if and only if the values of a on the faces are related by the *star-triangle map*, for a proof see for example [15, Sect. 2.3] or [60].

In particular, label the coordinate directions of a three-dimensional fundamental cube with $1, 2, 3$ and the value of a on the face ij incident to x_0 by $a_{ij} = -a_{ji}$ for $i \neq j$. Then (8) reads

$$F(x_0 + e_i + e_j) - F(x_0) = a_{ij}\big(F(x_0 + e_j) - F(x_0 + e_i)\big) \,, \tag{9}$$

where e_k for $k = 1, 2, 3$ are the unit vectors in the three coordinate directions. Let $\tau_k a_{ij} = -\tau_k a_{ji}$ be the value of a on the face ij translated in direction k, that is opposite to ij for $k \neq i, j$. Then the star-triangle equations are:

$$\frac{\tau_1 a_{23}}{a_{23}} = \frac{\tau_2 a_{31}}{a_{31}} = \frac{\tau_3 a_{12}}{a_{12}} = -\frac{1}{a_{12}a_{23} + a_{23}a_{31} + a_{31}a_{12}} \,.$$

Note that solutions a_{ij} of these equations give rise via $a_{ij} = z_i z_j/(z z_{ij})$ to solutions z of the discrete BKP equation (also called Hirota–Miwa equation) on fundamental cubes, which goes back to [59], see [15, Sect. 6.16] or [1]. A geometric interpretation of the discrete Moutard equation and the star-triangle map is given in [53].

Now, for the 3D-consistency of the discrete Cauchy–Riemann equations we want to have the same equation on opposite faces of a fundamental cube as in the examples above. Using the background on the 3D-consistency of the Moutard equation and the star-triangle map we deduce that for any choice of real positive weights ω (corresponding to a), 3D-consistency of the discrete Cauchy–Riemann equations (6) holds for a quad-graph $\mathcal{D}$ if and only if these weights satisfy additional conditions for each flower of faces incident to an interior vertex, as the cubes then share vertical faces. More precisely, the weights need to result from a (ramified) rhombic embedding, see [15, Sect. 7.3] or [17] for a detailed proof of this statement.

2.3 Some Further Topics

The linear theory of discrete holomorphic functions has a long and still developing history. This includes special functions which are analogous to the smooth case like polynomials (see Example 2.3 and Exercise 2.4), discrete exponentials, discrete logarithm and discrete Green's function, see [17, 32, 35, 49, 58]. Also, further properties and theorems of the smooth theory have found discrete analogues, see in particular [8, 41]. As a strong link to the smooth case, convergence issues have been studied, for example in [35, 58].

3 Discrete Holomorphic Functions and Cross-Ratio Systems

Smooth holomorphic maps with nonvanishing derivative are called *conformal*. These are locally injective, preserve angles and may be conceived as infinitesimal scale-rotations. Therefore, on simply connected domains the derivative f' of a conformal map f satisfies $f' = \mathrm{e}^g$ for some holomorphic function g. Note that conformal maps are a subclass of holomorphic mappings, but away from the zeros of the derivative every nonconstant holomorphic map is locally conformal. Therefore, the restriction to conformal mappings is in general not essential.

We will now introduce a nonlinear discrete theory which is based on the preservation of cross-ratios. Note this is essentially different from the linear theory presented in the previous section although some links can be established, see Sect. 3.3.

Recall that the *cross-ratio* of four mutually distinct points $z_1, z_2, z_3, z_4 \in \mathbb{C}$ can be defined as

$$\mathrm{cr}(z_1, z_2, z_3, z_4) = \frac{(z_1 - z_2)(z_3 - z_4)}{(z_2 - z_3)(z_4 - z_1)} \,. \tag{10}$$

Smooth conformal maps f are characterized by the property that they preserve the cross-ratio infinitesimally, in particular

$$\mathrm{cr}\big(f(\varepsilon z_1), f(\varepsilon z_2), f(\varepsilon z_3), f(\varepsilon z_4)\big) = \mathrm{cr}(z_1, z_2, z_3, z_4) + \mathcal{O}(\varepsilon^2)$$

for $\varepsilon > 0$ small enough. The notation $R(f, z_1, z_2, z_3, z_4, \varepsilon) = \mathcal{O}(\varepsilon^2)$ is used as abbreviation for $|R(f, z_1, z_2, z_3, z_4, \varepsilon)| \leq C\varepsilon^2$ where the constant $C = C(f, z_1, z_2, z_3, z_4)$, possibly depends on f and z_1, z_2, z_3, z_4 but not on ε. Recall that fractional linear transformations $m(z) = (az + b)/(cz + d)$ for $a, b, c, d \in \mathbb{C}$ with $ad - bc \neq 0$, also called Möbius transformations, form a special class of examples of conformal maps which exactly preserve the cross-ratio.

As a discrete analog, we consider discrete conformal maps which preserve all cross-ratios of the quadrilaterals of a given quad-graph. This concept was first introduced in [11] in order to define discrete isothermic surfaces, but it already contained discrete conformal maps in the plane. The 3D-consistency of the cross-ratio equation was studied first in [45]. See also Sect. 3.4 for further references.

3.1 Definition of Discrete Conformal Functions

Again, we start with the square grid lattice as an important example.

Exercise 3.1 Check that all quads of the square grid lattice have the same cross-ratio -1, in particular $\mathrm{cr}\big(n + \mathrm{i}m, n + 1 + \mathrm{i}m, n + 1 + \mathrm{i}(m + 1), n + \mathrm{i}(m + 1)\big) = -1$.

Example 3.2 (Square Grid Lattice) Consider the regular square grid lattice together with a cyclic orientation of the vertices in every quad. Then all quads have the same cross-ratio -1. In particular, $f^{\mathrm{cr}}\colon \mathbb{Z}^2 \to \mathbb{C}$ is called *discrete conformal* (or *discrete holomorphic*) if these cross-ratios are preserved, that is

$$\mathrm{cr}\big(f^{\mathrm{cr}}(x_0), f^{\mathrm{cr}}(y_0), f^{\mathrm{cr}}(x_1), f^{\mathrm{cr}}(y_1)\big) = -1 \quad \big(= \mathrm{cr}(x_0, y_0, x_1, y_1)\big) \tag{11}$$

holds for all squares using the notation of Fig. 5 (without any labelling on the edges). The superscript cr again emphasizes the fact that this definition of holomorphicity belongs to the area of *cross-ratio systems*. The reader should keep in mind not to confuse discrete holomorphic functions satisfying (11) with those satisfying (4). A connection between these two different notions of the same name is derived in Sect. 3.3 via linearization of (11).

Equation (11) defines a 2D-system on the quad-graph $\mathbb{Z}^2$.This means that given (generic) values of f^{cr} on three of the four vertices of a quad, (11) determines the fourth value.

Note that every Möbius transformation is an example of a discrete conformal map. This also hints the fact that these discrete conformal maps may (and should) be studied in the context of Möbius geometry.

Discrete conformal maps on the square grid lattice may also be represented as mapping of circle patterns. Recall that four points with real cross-ratio lie on a circle. Thus for every quad there exists a circle where the grid points of $\mathbb{Z}^2$ and their image points are the intersection points of the circles of neighboring quads.

Exercise 3.3 Show that $f^{\mathrm{cr}}\colon \mathbb{Z}^2 \to \mathbb{C}, f^{\mathrm{cr}}(m,n) = (m+\mathrm{i}n)^3 - (m-\mathrm{i}n)$ is discrete conformal.

We now introduce the more general case of *factorizable cross-ratios*. Given a planar b-quad-graph $\mathcal{D}$, we assume that there exists a labelling $\alpha\colon E(\mathcal{D}) \to \mathbb{C}\setminus\{0\}$ on the edges such that in every quad opposite edges carry the same label as in Fig. 5 (left). Then $f^{\mathrm{cr}}\colon V(\mathcal{D}) \to \mathbb{C}$ is called *discrete conformal* (or *discrete holomorphic*) if

$$\mathrm{cr}\big(f^{\mathrm{cr}}(x_0), f^{\mathrm{cr}}(y_0), f^{\mathrm{cr}}(x_1), f^{\mathrm{cr}}(y_1)\big) = \frac{\alpha_0}{\alpha_1} \tag{12}$$

holds for every quad. Instead of the labelling α we can also consider a labelling $\theta\colon \overrightarrow{E}(\mathcal{D}) \to \mathbb{C}\setminus\{0\}$ on the directed edges $\overrightarrow{E}(\mathcal{D})$ such that $\theta^2 = \alpha$. Then all quadrilaterals may be realized as parallelograms (or rhombi in case of equal lengths). Therefore we can start with a parallelogram immersion of $\mathcal{D}$ and take the cross-ratios of the quad to be θ_0^2/θ_1^2. (Again, these discrete holomorphic functions are not to be confused with those defined in (6).)

More generally, given a b-quad-graph with cross-ratios on every face, we can call a map discrete conformal which preserves all these cross-ratios. For a simply connected domain, the existence of a labelling $\alpha\colon E(\mathcal{D}) \to \mathbb{C}\setminus\{0\}$ as above is equivalent to the fact that for every interior vertex the product of the cross-ratios of the adjacent quads equals 1. In this presentation we will confine ourselves to the case of factorizable cross-ratios with a given labelling α or θ.

3.2 3D-Consistency and Bäcklund Transformations

We now want to put the cross-ratio equation on the faces of a cube. The cross-ratio equation (12) defines a 2D-system, since it determines the value of a function f^{cr} at the fourth vertex if the three other (generic) values of f^{cr} on the vertices of a quad are known.

Consider a cube as in Fig. 4 (right) and assume that we put cross-ratio equations on the faces of the cube. Similarly as in Sect. 2.2 we want to have the same equation on opposite faces of the cube. This is guaranteed by the labelling of the edges such that opposite edges carry the same label as in Fig. 4 (right). As for the linear theory we can ask the question, if the four values at x_0, y_0, y_1, x_0^+ determine the value at x_1^+ uniquely.

This is indeed the case. First note that the cross-ratio equation (12) only depends on the differences between the values of f^{cr} at the vertices. Thus we can assume $f^{\mathrm{cr}}(x_0) = 0$ without loss of generality in order to simplify formulas. By (12) we have

$$f^{\mathrm{cr}}(x_1) = \frac{f^{\mathrm{cr}}(y_0)f^{\mathrm{cr}}(y_1)(\alpha_0-\alpha_1)}{f^{\mathrm{cr}}(y_1)\alpha_0 - f^{\mathrm{cr}}(y_0)\alpha_1}\,,$$

$$f^{\mathrm{cr}}(y_0^+) = \frac{f^{\mathrm{cr}}(y_0)f^{\mathrm{cr}}(x_0^+)(\alpha_0-\lambda)}{f^{\mathrm{cr}}(x_0^+)\alpha_0 - f^{\mathrm{cr}}(y_0)\lambda}\,,$$

$$f^{\mathrm{cr}}(y_1^+) = \frac{f^{\mathrm{cr}}(x_0^+)f^{\mathrm{cr}}(y_1)(\lambda-\alpha_1)}{f^{\mathrm{cr}}(y_1)\lambda - f^{\mathrm{cr}}(x_0^+)\alpha_1}\,.$$

Straightforward calculations (which we leave as an exercise) show that

$$f^{\mathrm{cr}}(x_1^+) = \frac{f^{\mathrm{cr}}(y_0)f^{\mathrm{cr}}(y_1)f^{\mathrm{cr}}(x_0^+)(\alpha_0-\alpha_1)(\alpha_0-\lambda)(\alpha_1-\lambda)}{f^{\mathrm{cr}}(x_0^+)f^{\mathrm{cr}}(y_1)\alpha_0^2(\alpha_1-\lambda) + f^{\mathrm{cr}}(y_0)f^{\mathrm{cr}}(x_0^+)\alpha_1^2(\lambda-\alpha_0) + f^{\mathrm{cr}}(y_0)f^{\mathrm{cr}}(y_1)\lambda^2(\alpha_0-\alpha_1)}$$

is uniquely determined. Therefore the cross-ratio equation for factorizable cross-ratios is 3D-consistent.

As a direct consequence we obtain Bäcklund transformations (namely, f^{cr} defined on the 'upper layer' x^+, y^+) for every given discrete conformal map f^{cr}.

Theorem 3.4 *Given a discrete conformal function f^{cr} on a b-quad-graph $\mathcal{D}$ with factorizable cross-ratios given by a labelling α and a parameter $\lambda \in \mathbb{C} \setminus \{0\}$, there exists a discrete conformal function $(f^{\mathrm{cr}})^+$ on the same b-quad-graph with black and white coloring interchanged such that the values on 'vertical faces' are linked via*

$$\mathrm{cr}(f_1^{\mathrm{cr}}, f_2^{\mathrm{cr}}, (f_2^{\mathrm{cr}})^+, (f_1^{\mathrm{cr}})^+) = \frac{\alpha}{\lambda}\,,$$

see Fig. 6 (right) for the notation. $(f^{\mathrm{cr}})^+$ *is called* Bäcklund (*or* Darboux) transformation *and is unique when its value is fixed at one vertex.*

Remark 3.5 If the labelling α only consists of finitely many values $\{\alpha_1, \dots, \alpha_m\}$ we can interpret the b-quad-graph as surface in the multidimensional lattice $\mathbb{Z}^m$. The edges are labelled according to the corresponding unit vectors of the lattice. Thanks to the 3D-consistency a given discrete holomorphic function may be extended to (a part of) $\mathbb{Z}^m$ such that the cross-ratio equation holds on every two-dimensional face.

Remark 3.6 In the special case of real negative cross-ratios all quads are circular. Then the 3D-consistency, that is the uniqueness of the eighth point $f^{\mathrm{cr}}(x_1^+)$, can also be deduced from Miquel's theorem (after a suitable Möbius transformation) as intersection point of three circles, see for example [27] or [15, Sect. 3.1].

Remark 3.7 From a broader perspective on integrability, note that the cross-ratio equation (3) can be considered as an integrable reduction of the integrable multiratio system, also called *discrete Schwarzian KP equation*, see for example [52]. The multiratio equation for a function $h : \mathbb{Z}^3 \to \mathbb{C}$ (actually, h should be defined on the A_3-lattice) reads

$$\frac{\big(h(x_0)-h(y_0)\big)\big(h(x_1)-h(x_1^+)\big)\big(h(y_1^+)-h(x_0^+)\big)}{\big(h(y_0)-h(x_1)\big)\big(h(x_1^+)-h(y_1^+)\big)\big(h(x_0^+)-h(x_0)\big)} = -1$$

in the notation of Fig. 4.

3.3 Linearization

In the following we will establish a link of this nonlinear theory based on the preservation of cross-ratios with the linear theory of discrete holomorphic functions introduced in the previous section.

Theorem 3.8 *Consider a rhombic embedding of a b-quad-graph $\mathcal{D}$ with labelling $\alpha = \theta^2$ where θ are the directed edges of the rhombic embedding as in Fig. 5 (middle). Suppose that $f_\varepsilon^{\mathrm{cr}} : V(\mathcal{D}) \to \mathbb{C}$ is a differentiable one parameter family of discrete conformal functions with respect to the given cross-ratio system where $f_0^{\mathrm{cr}} = \mathrm{id}$ is the identity and $\varepsilon \in (-\varepsilon_0, \varepsilon_0)$. Then $g^\ell = (\mathrm{d}f_\varepsilon^{\mathrm{cr}}/\mathrm{d}\varepsilon)|_{\varepsilon=0}$ solves the discrete Cauchy–Riemann equations for the given rhombic embedding.*

Proof Consider a quad as in Fig. 5 (middle). As $f_\varepsilon^{\mathrm{cr}}$ are discrete conformal

$$\begin{aligned}\mathrm{cr}\big(f_\varepsilon^{\mathrm{cr}}(x_0), f_\varepsilon^{\mathrm{cr}}(y_0), f_\varepsilon^{\mathrm{cr}}(x_1), f_\varepsilon^{\mathrm{cr}}(y_1)\big) &= \frac{\theta_0^2}{\theta_1^2} \\ \iff \big(f_\varepsilon^{\mathrm{cr}}(x_0) - f_\varepsilon^{\mathrm{cr}}(y_0)\big)\big(f_\varepsilon^{\mathrm{cr}}(x_1) - f_\varepsilon^{\mathrm{cr}}(y_1)\big) &\\ = \frac{\theta_0^2}{\theta_1^2}\big(f_\varepsilon^{\mathrm{cr}}(y_0) - f_\varepsilon^{\mathrm{cr}}(x_1)\big)\big(f_\varepsilon^{\mathrm{cr}}(y_1) - f_\varepsilon^{\mathrm{cr}}(x_0)\big)&,\end{aligned}$$

we deduce by taking derivatives by ε at $\varepsilon = 0$ that

$$\begin{aligned}
&\big(g^\ell(x_0) - g^\ell(y_0)\big) \underbrace{\big(f_0^{\mathrm{cr}}(x_1) - f_0^{\mathrm{cr}}(y_1)\big)}_{=\theta_0} \\
&\qquad + \underbrace{\big(f_0^{\mathrm{cr}}(x_0) - f_0^{\mathrm{cr}}(y_0)\big)}_{=-\theta_0} \big(g^\ell(x_1) - g^\ell(y_1)\big) \\
&= \frac{\theta_0^2}{\theta_1^2} \big(g^\ell(y_0) - g^\ell(x_1)\big) \underbrace{\big(f_0^{\mathrm{cr}}(y_1) - f_0^{\mathrm{cr}}(x_0)\big)}_{=\theta_1} \\
&\qquad + \frac{\theta_0^2}{\theta_1^2} \underbrace{\big(f_0^{\mathrm{cr}}(y_0) - f_0^{\mathrm{cr}}(x_1)\big)}_{=-\theta_1} \big(g^\ell(y_1) - g^\ell(x_0)\big) \,.
\end{aligned}$$

Now we easily see that this is equivalent to

$$\frac{g^\ell(y_1) - g^\ell(y_0)}{g^\ell(x_1) - g^\ell(x_0)} = \frac{\theta_1 - \theta_0}{\theta_1 + \theta_0} \,. \qquad \square$$

3.4 Some Further Topics

Cross-ratio systems and their connection to integrability have been studied in many aspects. As we have only touched the basis of this topic we refer the interested reader to [15] and the references therein. In particular, convergence issues have been considered in [57].

4 Circle Patterns as Discrete Holomorphic Functions

The Cauchy–Riemann equations (1) imply that a smooth conformal map, that is a holomorphic map with nonvanishing derivative, is an infinitesimal scale-rotation. In particular, conformal maps can be characterized by the properties that angles are preserved and infinitesimal circles are mapped to infinitesimal circles. Circle patterns can be interpreted as a finite version corresponding to these characterizations.

Circle packings are configurations of touching circles where the underlying combinatorics is a triangulation. These were first connected to conformal mappings, in particular to the Riemann mapping theorem, by Thurston [70], see also [51] and [69] and the references therein.

Circle patterns for given combinatorics and intersection angles have been introduced and studied for example in [13, 21, 62, 64, 65]. Furthermore the definition of immersed circle patterns can be extended allowing cone-like singularities at

vertices; see for example [13] and the references therein. Integrable circle patterns have been studied for example in [10, 16, 17, 65]. Since then there have been various further investigations in this theory, see Sect. 4.6 for some of the questions studied for circle patterns.

As first motivating example we consider the square grid lattice $\mathbb{Z}^2$. If we intend to preserve all (right) angles of the quadrilaterals, the configuration would be rigid up to rescaling of the squares to rectangles (in a 'row' or 'column') and global scaling and Euclidean motions. Therefore, we consider $\mathbb{Z}^2$ with bicolored vertices such that every edge connects vertices of different color. Each quad then has two white and two black vertices. Now we split the two conditions:

- intersection angles should be preserved at black vertices, whereas
- white vertices should be centers of circles, that is all its incident edges have equal length.

For the square grid lattice we then obtain as a first example the regular circle pattern with square grid combinatorics and orthogonally intersecting circles, see Fig. 7 (left). But our definition also applies for other examples like Fig. 7 (right) which have the same combinatorics and intersection angles, but different radii.

In general, we can start with a planar b-quad-graph $\mathcal{D}$. To every (abstract) quadrilateral of $\mathcal{D}$ there corresponds an embedded kite built by two centers of circles and two intersection points as in Fig. 8 (left). In particular, *circle patterns* $\mathcal{C}$ are in one-to-one correspondence with immersed patterns of kites $\mathcal{K}$ with bicolored vertices such that edges incident to a white vertex have the same length. Moreover, the pattern of kites $\mathcal{K}$ is isomorphic to the given b-quad-graph $\mathcal{D}$. Note that there are in general additional intersection points of circles which are not associated to black vertices of $\mathcal{D}$.

The exterior intersection angles $\alpha\colon F(\mathcal{D}) \to (0, \pi)$ of two circles for neighboring white vertices are considered as labelling on the corresponding faces of $\mathcal{D}$ or, equivalently, on the edges connecting the corresponding white vertices. As we consider discrete holomorphic functions we are interested in *planar* circle patterns. This means that the chain of kites incident to a (white or black) vertex 'closes up' such that this configuration is isomorphic to the corresponding configuration of faces in $\mathcal{D}$. Therefore the intersection angles (=labelling) of a planar circle pattern

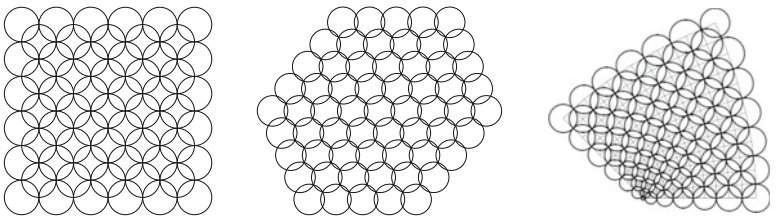

Fig. 7 A regular square grid circle pattern (*left*), a regular hexagonal circle pattern (*middle*) and a more general orthogonal circle pattern (*right*, see also Fig. 10)

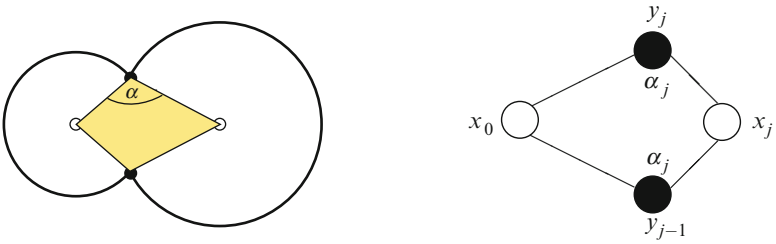

Fig. 8 *Left*: The exterior intersection angle α of two intersecting circles and the associated kite built from centers and intersection points. *Right*: A kite of the circle pattern with labelled vertices and (exterior) intersection angle α_j

cannot be arbitrary. Namely, we call a labelling α of the faces *admissible* if the angles for incident faces sum up to 2π at all interior black vertices v:

$$\sum_{f \text{ incident to } v} \alpha(f) = 2\pi \ .$$

Also, we only consider *immersed* circle patterns which means that for every vertex all incident kites have mutually disjoint interiors and intersect along a straight edge or a vertex if and only if the corresponding quadrilaterals of $\mathcal{D}$ have an edge or a vertex in common, respectively. If this condition holds for all kites of the pattern, that is, not just locally, but globally, then the circle pattern is called *embedded*.

Note that embedded circle patterns are in one-to-one correspondence to *Delaunay decompositions* of (a domain in) $\mathbb{C}$ for a given set of points (= black vertices). This is a cell decomposition such that the boundary of each face is a polygon with straight edges which is inscribed in a circular disc, and these discs have no vertices in their interior. The corresponding embedded circle pattern can be associated to the graph G^*. The Poincaré-dual decomposition of a Delaunay decomposition with the centers of the circles as vertices and straight edges is a *Dirichlet decomposition* (or *Voronoi diagram*) and corresponds to the graph G.

Moreover, circle patterns generalize planar *circle packings* which are configurations of discs corresponding to a triangulation of a planar domain where vertices correspond to discs and for each edge the two corresponding discs touch. Every such circle packing can be understood as an orthogonal circle pattern by adding circles corresponding to the triangular faces through the three touching points. The corresponding intersection angles are all $\pi/2$.

Example 4.1 Every rhombic embedding of a b-quad-graph is in fact the kite pattern of a circle pattern which is even *isoradial*, that is all circles have the same radius. Figure 9 shows an example corresponding to a Penrose tiling. Note that there is a dual isoradial circle pattern corresponding to the b-quad-graph with white and black vertices interchanged.

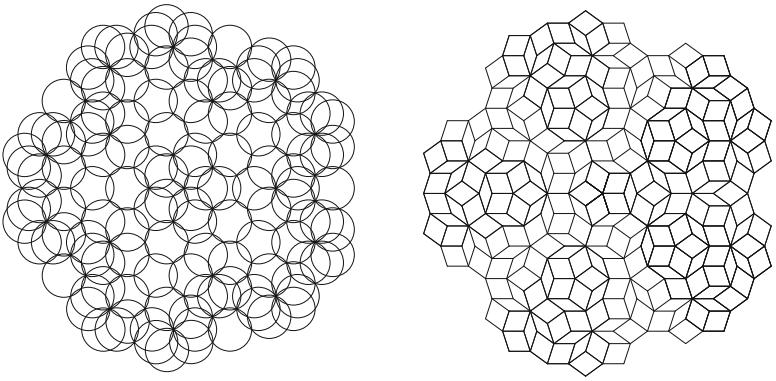

Fig. 9 Example of a circle pattern and corresponding kite pattern (without *bicolored vertices*)

4.1 Definition of Discrete Conformal Functions

Discrete holomorphic functions can now be defined as correspondence of two circle patterns with the same combinatorics (=isomorphic kite patterns) and the same intersection angles.

Definition 4.2 Let $\mathcal{C}_1$ and $\mathcal{C}_2$ be two circle patterns for the same b-quad-graph $\mathcal{D}$ and the same admissible labelling α. We interpret the kite pattern of $\mathcal{C}_1$ as a realization (in fact immersion) of $\mathcal{D}$. The map $f^{\mathcal{C}}: V(\mathcal{D}) \to \mathbb{C}$ which maps the white and black vertices of every kite to their corresponding vertices of the kite pattern of $\mathcal{C}_2$ is called *discrete conformal* (or *discrete holomorphic*). By abuse of notation, we also write this discrete conformal mapping as $f^{\mathcal{C}}: \mathcal{C}_1 \to \mathcal{C}_2$.

Remind that this is yet another definition of discrete holomorphicity which essentially differs from those already introduced in Sects. 2.1 and 3.1. Some connections will be revealed in Sects. 4.4 and 4.5. The superscript $\mathcal{C}$ should hopefully clarify that we here consider discrete holomorphic functions in the context of *circle patterns*.

Example 4.3 As for cross-ratio systems, Möbius transformations are examples of discrete conformal maps because they preserve intersection angles and additionally map circles to circles. A more involved example, which is also connected to integrability, is a discrete analog on of the smooth function z^γ presented and studied in [2, 7, 12] for square grid combinatorics, see Fig. 10 for an illustration.

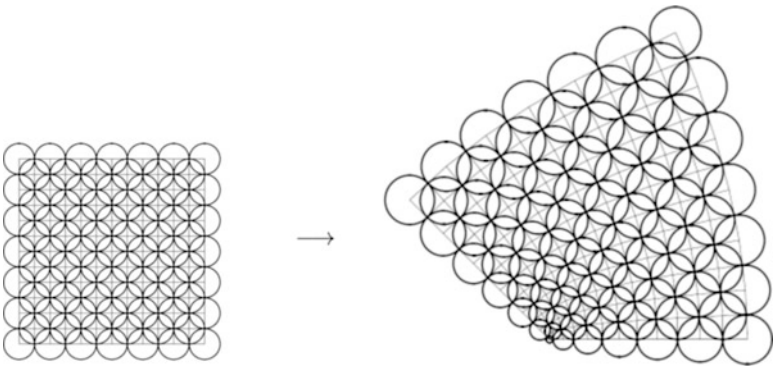

Fig. 10 Illustration of the discrete conformal map corresponding to $z^{2/3}$ via orthogonal circle patterns with square grid combinatorics

4.2 Characterization of Circle Patterns Using Radius Functions

For a given b-quad-graph $\mathcal{D}$ and an admissible labelling α a corresponding circle pattern $\mathcal{C}$ is completely characterized (up to global rotation and translation of the pattern) by the *radius function* $r_{\mathcal{C}} = r$ which assigns to every white vertex x the radius $r_{\mathcal{C}}(x) = r(x)$ of the corresponding circle $\mathcal{C}(x)$. Moreover, a function r defined on the white vertices of $\mathcal{D}$ is the radius function of a circle pattern if and only if at every interior white vertex x_0 the angles at x_0 in the adjacent kites sum up to 2π. Consider in particular a kite with edge lengths $r(x_0)$ and $r(x_j)$ at the white vertices x_0 and x_j respectively and intersection angle $\alpha_j \in (0, \pi)$. Then the angle in this kite at x_0 may be calculated elementary and can be expressed as $2\Phi_{\alpha_j}\big(\log r(x_j) - \log r(x_0)\big)$, where

$$\Phi_\theta(x) := \frac{1}{2\mathrm{i}} \log \frac{1 - \mathrm{e}^{x-\mathrm{i}\theta}}{1 - \mathrm{e}^{x+\mathrm{i}\theta}} \,, \tag{13}$$

and the branch of the logarithm is chosen such that $0 < \Phi_\theta(x) < \pi$.

The following proposition specifies a necessary and sufficient condition for a radius function to originate from a planar circle pattern, see [13] for a proof.

Proposition 4.4 *Let $\mathcal{D}$ be a b-quad-graph and let α be an admissible labelling.*

Suppose that $\mathcal{C}$ is an immersed circle pattern for $\mathcal{D}$ and α with radius function $r = r_{\mathcal{C}}$. Then for every interior white vertex x_0 with neighboring white vertices $x_1, x_2, \ldots, x_n$ (on adjacent kites) we have

$$\left(\sum_{j=1}^{n} 2\Phi_{\alpha_j}\big(\log r(x_j) - \log r(x_0)\big) \right) - 2\pi = 0 \,. \tag{14}$$

Conversely, suppose that $\mathcal{D}$ is simply connected and that $r\colon V_w(\mathcal{D}) \to (0,\infty)$ satisfies (14) for every interior white vertex $x_0 \in V_w(\mathcal{D}) := \{$white vertices of $\mathcal{D}\}$. Then there is an immersed circle pattern for $\mathcal{D}$ and α whose radius function coincides with r. This pattern is unique up to isometries of $\mathbb{C}$.

For the special case of orthogonal circle patterns with the combinatorics of the square grid, there are also other characterizations of radius functions, see for example [65].

Example 4.5 On the square grid lattice $\mathbb{Z}^2$ the radius function $r(z) = \mathrm{e}^{\mathrm{Re}(az)}$ for fixed $a \in \mathbb{C}\setminus\{0\}$ generates an orthogonal circle pattern called *Doyle spiral*, see [65].

Remark 4.6 (Connection to Discrete Harmonic Functions by Linearization) Recall that the local embedding in the plane is ensured by the closing condition (14) for the chain of kites incident to the white vertex x_0. We can interpret this as a nonlinear version of the Laplace equation for $\rho = \log r$, thus $\log r$ may be considered as 'discrete harmonic function'. This is also motivated by the following linearization.

Let r_ε for $\varepsilon \in (-\varepsilon_0, \varepsilon_0)$ be a differentiable family of radius functions for a corresponding family of circle patterns for a b-quad-graph $\mathcal{D}$ and an admissible labelling α. Then (14) implies

$$\left(\sum_{j=1}^{n} 2\Phi_{\alpha_j}\big(\log r_\varepsilon(x_j) - \log r_\varepsilon(x_0)\big)\right) - 2\pi = 0$$

for every interior white vertex x_0 with neighboring white vertices $x_1, x_2, \ldots, x_n$. Differentiating this relation by ε at $\varepsilon = 0$ we obtain for $u = (\mathrm{d}/\mathrm{d}\varepsilon)\log r_\varepsilon|_{\varepsilon=0}$ that

$$0 = \sum_{j=1}^{n} 2\Phi'_{\alpha_j}\big(\log r_0(x_j) - \log r_0(x_0)\big)\big(u(x_j) - u(x_0)\big)\,.$$

This is the linear Laplace equation (2) on the graph built from the white vertices as in Fig. 3 (left). The weights are obtained by an elementary calculation (left as an exercise) as

$$2\Phi'_{\alpha_j}\big(\log r_0(x_j) - \log r_0(x_0)\big) = \frac{|y_{j-1} - y_j|}{|x_j - x_0|}$$

with the notation from Fig. 8 (right). Note that kites have orthogonal diagonals, so these weights also occur in the linear theory of discrete holomorphic functions, see (6).

In analogy to smooth harmonic functions, the radius function of a planar circle pattern satisfies a Dirichlet principle and a maximum principle.

Theorem 4.7 (Maximum Principle) *Let $\mathcal{D}$ be a b-quad-graph with some admissible labelling α. Suppose $\mathcal{C}_1$ and $\mathcal{C}_2$ are two planar circle patterns for $\mathcal{D}$ and α with radius functions r_1, r_2 respectively. Then the maximum and minimum of the quotient r_1/r_2 is attained at the boundary.*

If there exists an isoradial circle pattern for $\mathcal{D}$ and α, the usual maximum principle for the radius function follows by taking $r_2 \equiv 1$.

Proof Assume that the claim is not true, so there is an interior white vertex x_0 with neighboring white vertices $x_1, \dots, x_n$ such that $r_1(x_0)/r_2(x_0)$ is strictly larger than $r_1(x_j)/r_2(x_j)$ for $j = 1, \dots, n$. But then

$$\frac{r_1(x_j)}{r_2(x_j)} < \frac{r_1(x_0)}{r_2(x_0)} \iff \frac{r_1(x_j)}{r_1(x_0)} < \frac{r_2(x_j)}{r_2(x_0)} .$$

From this we will derive a contradiction using the closing condition (14) as r_1 and r_2 are both assumed to be radius functions of circle patterns for $\mathcal{D}$ and α. Note that the derivative of Φ_α, defined in (13), is $\Phi'_\alpha(x) = \sin\alpha/\big(2(\cosh x - \cos\alpha)\big) > 0$. So Φ_α is strictly increasing. Therefore, by Proposition 4.4

$$2\pi = \sum_{j=1}^{n} 2\Phi_{\alpha_j}\big(\log r_1(x_j) - \log r_1(x_0)\big) < \sum_{j=1}^{n} 2\Phi_{\alpha_j}\big(\log r_2(x_j) - \log r_2(x_0)\big) = 2\pi$$

which is a contradiction. □

Theorem 4.8 (Dirichlet Principle) *Let $\mathcal{D}$ be a finite simply connected b-quad-graph with associated graph G and let α be an admissible labelling.*

Let r_∂ be some positive function on the white boundary vertices of $\mathcal{D}$. Then r_∂ can be extended to all white vertices of $\mathcal{D}$ in such a way that (14) holds at every interior vertex x_0 if and only if there exists any immersed circle pattern for $\mathcal{D}$ and α. If it exists, the extension is unique.

Proof The only if part follows directly from the second part of Proposition 4.4.

To show the if part, assume that there exists a circle pattern for G and α with radius function $R\colon V(G) \to (0, \infty)$. A function $\kappa : V(G) \to (0, \infty)$ which satisfies the inequality

$$\left(\sum_{[z,z_0]\in E(G)} \Phi_{\alpha([z,z_0])}\big(\log\kappa(z) - \log\kappa(z_0)\big) \right) - \pi \geq 0$$

at every interior vertex $z \in V_{int}(G)$ will be called *subharmonic* in G. Let b be the minimum of the quotient r/R on $V_\partial(G)$ and let κ_1 be equal to r on $V_\partial(G)$ and to bR on $V_{int}(G)$. Then κ_1 is clearly subharmonic. The maximum of κ_1/R is attained at the boundary, which is a simple generalization of the Maximum Principle 4.7. Let r^* be the supremum of all subharmonic functions on G that coincide with r on $V_\partial(G)$.

Thus r^* is bounded from above by the maximum of r/R on $V_\partial(G)$ which is finite. One easily checks that r^* satisfies condition (14).

The uniqueness claim follows directly from the Maximum Principle 4.7. □

4.3 Characterization of Discrete Conformal Maps in Terms of Radius and Rotation Functions

Similarly as for polar coordinates of the complex plane, a suitably defined rotation function can be interpreted as a "dual" to the radius function.

Consider a discrete conformal map $f^{\mathcal{C}}: \mathcal{C}_1 \to \mathcal{C}_2$ between two circle patterns which are based on the same b-quad-graph $\mathcal{D}$ and have the same labelling α. Then the radius functions r_1 and r_2 of these circle patterns give rise to a scale function $\mathbf{w}(x_0) = r_2(x_0)/r_1(x_0)$ defined at white vertices x_0. At black vertices we can define rotation variables: As the intersection angles and the combinatorics are the same for both patterns, the 'star' of the edges incident to a black vertex y_0 is rotated by $\mathbf{w}(y_0) = e^{i\delta(y_0)} \in \mathbb{S}^1$. This defines a function δ which is the relative turning angle at black vertices. We require additionally that

$$2\Phi_\alpha\left(\log\left(\frac{r_2(x_+)}{r_2(x_-)}\right)\right) - 2\Phi_\alpha\left(\log\left(\frac{r_1(x_+)}{r_1(x_-)}\right)\right) = \delta(y_+) - \delta(y_-) \tag{15}$$

holds. Here the notation is taken from Fig. 11. Then δ is uniquely defined up to addition of a constant $2\pi n$ for $n \in \mathbb{Z}$.

Exercise 4.9 Show that the following relation holds for corresponding diagonals in the circle patterns $\mathcal{C}_1$ and $\mathcal{C}_2$:

$$\frac{f^{\mathcal{C}}(y_+) - f^{\mathcal{C}}(y_-)}{|f^{\mathcal{C}}(y_+) - f^{\mathcal{C}}(y_-)|} = \frac{y_+ - y_-}{|y_+ - y_-|} e^{i(\delta(y_+)+\delta(y_-))/2}.$$

This means that the diagonal connecting the black vertices y_+ and y_- in the circle pattern $\mathcal{C}_1$ is rotated by $e^{i(\delta(y_+)+\delta(y_-))/2}$ to the corresponding diagonal in $\mathcal{C}_2$.

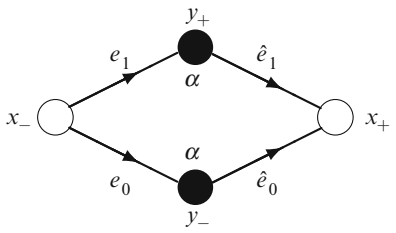

Fig. 11 A face of $\mathcal{D}$ with oriented edges and label α

Remark 4.10 The function $\mathbf{w}$ can be used to characterize discrete holomorphic functions. Assume that $\mathcal{C}_1$ is a planar circle pattern for $\mathcal{D}$ and α with radius function r_1. Let r_2 be a positive function on the white vertices and let δ be a real valued function on the black vertices which satisfies (15) for every face of $\mathcal{D}$. Then r_2 and δ are the radius and rotation function of a planar circle pattern for $\mathcal{D}$ and α. This circle pattern is unique up to translation.

Consider a kite of a circle pattern $\mathcal{C}_1$ as in Fig. 11. The closing condition for the corresponding kite of another circle pattern $\mathcal{C}_2$ with same combinatorics and intersection angles can be expressed as

$$\begin{aligned}(x_- - y_-)\frac{r_2(x_-)}{r_1(x_-)}\mathrm{e}^{\mathrm{i}\delta(y-)} + (y_+ - x_-)\frac{r_2(x_-)}{r_1(x_-)}\mathrm{e}^{\mathrm{i}\delta(y+)} \\ + (y_- - x_+)\frac{r_2(x_+)}{r_1(x_+)}\mathrm{e}^{\mathrm{i}\delta(y-)} + (y_+ - x_+)\frac{r_2(x_+)}{r_1(x_+)}\mathrm{e}^{\mathrm{i}\delta(y+)} = 0\,. \end{aligned} \tag{16}$$

If all kites of the circle pattern $\mathcal{C}_1$ are rhombi (that is, the circle pattern is isoradial), this closing condition yields the *Hirota equation* for the function w, so with the notation of Fig. 5 (middle) we have

$$\theta_0\mathbf{w}(x_0)\mathbf{w}(y_0) + \theta_1\mathbf{w}(x_1)\mathbf{w}(y_0) - \theta_0\mathbf{w}(x_1)\mathbf{w}(y_1) - \theta_1\mathbf{w}(x_0)\mathbf{w}(y_1) = 0 \tag{17}$$

with the additional conditions $\mathbf{w}(x) \in \mathbb{R}_+$ and $\mathbf{w}(y) \in \mathbb{S}^1$.

Note that the Hirota equation (17) can be obtained by the change of variables $\mathbf{w} = \mathrm{e}^{\mathrm{i}\phi/2}$ from an integrable discretization of the sine-Gordon equation, first derived in [46] and also called *Hirota equation*

$$\sin\frac{1}{4}\big(\phi(x_1) - \phi(y_0) - \phi(y_1) + \phi(x_0)\big) = \frac{\theta_0}{\theta_1}\sin\frac{1}{4}\big(\phi(x_1) - \phi(y_0) + \phi(y_1) - \phi(x_0)\big)\,.$$

4.4 3D-Consistency and Bäcklund Transformations

For a link to integrability we use the connection of circle patterns to cross-ratio systems.

Exercise 4.11 Show that the cross-ratio of a kite with intersection angle α corresponding to a face with notation as in Fig. 11 is $\mathrm{cr}(x_-, y_-, x_+, y_+) = \mathrm{e}^{2i\alpha}$.

Recall that integrability of the cross-ratio equation corresponds to factorizable cross-ratios, so $\mathrm{cr}(x_-, y_-, x_+, y_+) = \mathrm{e}^{2i\alpha} = \theta_0^2/\theta_1^2$ with the notation as in Fig. 11 and $\theta_0 = e_0 = \hat{e}_1$, $\theta_1 = e_1 = \hat{e}_0$. Therefore, a circle pattern for a b-quadgraph $\mathcal{D}$ and a labelling α is called *integrable* if and only if there exists a rhombic embedding of $\mathcal{D}$ where the rhombus corresponding to the face $\mathbf{f}$ has an angle $\alpha(\mathbf{f})$

at its black vertices (and $\pi - \alpha(\mathbf{f})$ at its white vertices). The existence of such a rhombic embedding is equivalent to the existence of an isoradial circle pattern for $\mathcal{D}$ and α. Examples of isoradial circle patterns are shown in Figs. 7 and 9. Note that there always exists a *dual isoradial circle pattern* for the same combinatorics, but with intersection angles $(\pi - \alpha)$ and white and black colors interchanged.

The Hirota equation (17) for integrable circle patterns is 3D-consistent and gives rise to Bäcklund transformations. Let $\mathbf{w}$ be the scaling and rotation function corresponding to two integrable circle patterns $\mathcal{C}_1$ and $\mathcal{C}_2$ with the same combinatorics and intersection angles α, so $\mathbf{w}(x) \in \mathbb{R}_+$ for white vertices x and $\mathbf{w}(y) \in \mathbb{S}^1$ for black vertices y. For simplicity we assume that $\mathcal{C}_1$ is an isoradial circle pattern corresponding to a rhombic embedding with directed edges $\theta \in \mathbb{S}^1$, but the same proof also applies in the general integrable case. Let $\lambda \in \mathbb{S}^1$ be a parameter and fix $\mathbf{w}^+(x_0^+) \in \mathbb{S}^1$ for x_0^+ in the upper layer of the cube as in Fig. 4 (left). Analogous reasoning holds for fixed $\mathbf{w}^+(y_0^+) \in \mathbb{R}_+$ instead. Then there exists a solution $\mathbf{w}^+$ of the Hirota equation on all faces of the cube satisfying $\mathbf{w}^+(y^+) \in \mathbb{R}_+$ and $\mathbf{w}^+(x^+) \in \mathbb{S}^1$. This leads to a circle pattern corresponding to the dual isoradial circle pattern.

Proof Assume the values $\mathbf{w}(x_0) \in \mathbb{R}_+$ and $\mathbf{w}(y_0), \mathbf{w}(y_1), \mathbf{w}^+(x_0^+), \in \mathbb{S}^1$ are given. Also we suppose that $\mathrm{Re}(\overline{\mathbf{w}(y_0)}\mathbf{w}(y_1) - \overline{\theta_0}\theta_1) > 0$ such that we obtain a kite. Then the Hirota equation (17) is equivalent to

$$\mathbf{w}(x_1) = \mathbf{w}(x_0)\frac{\theta_0\mathbf{w}(y_0) - \theta_1\mathbf{w}(y_1)}{\theta_0\mathbf{w}(y_1) - \theta_1\mathbf{w}(y_0)}\,.$$

The condition $\mathrm{Re}(\overline{\mathbf{w}(y_0)}\mathbf{w}(y_1) - \overline{\theta_0}\theta_1) > 0$ guarantees $\mathbf{w}(x_1) \in \mathbb{R}_+$. We assume that analogous conditions hold for the 'vertical' faces of the cube which are incident to x_0^+. This shows that the values $\mathbf{w}^+(y_0^+), \mathbf{w}^+(y_1^+)$ obtained from the Hirota equation on the corresponding faces of the cube are also real and positive. Now direct calculations (which we leave as an exercise to the reader) show that

$$\mathbf{w}(x_1^+) = \frac{\mathbf{w}(y_0)\mathbf{w}(x_0^+)\theta_1(\theta_0^2 - \lambda^2) + \mathbf{w}(y_1)\mathbf{w}(x_0^+)\theta_0(\lambda^2 - \theta_1^2) + \mathbf{w}(y_0)\mathbf{w}(y_1)\lambda(\theta_1^2 - \theta_0^2)}{\mathbf{w}(y_0)\theta_0(\lambda^2 - \theta_1^2) + \mathbf{w}(y_1)\theta_1(\theta_0^2 - \lambda^2) + \mathbf{w}(x_0^+)\lambda(\theta_1^2 - \theta_0^2)}$$

is uniquely determined. □

Remark 4.12 As in the previous sections, the 3D-consistency of the Hirota equation (17) for circle patterns shows that the function $\mathbf{w}$ for an integrable circle pattern whose combinatorics and intersection angles are given via a rhombic embedding with only finitely many directions $\{\theta_1, \ldots, \theta_d\}$ can be extended to (a part of) $\mathbb{Z}^d$ such that the Hirota equation (17) holds on all 2-dimensional faces of the corresponding d-dimensional cubes. This has for example been used to generalize the constructions of discrete analogues of z^γ or $\log z$, see [17, 23] and Fig. 12 for an example.

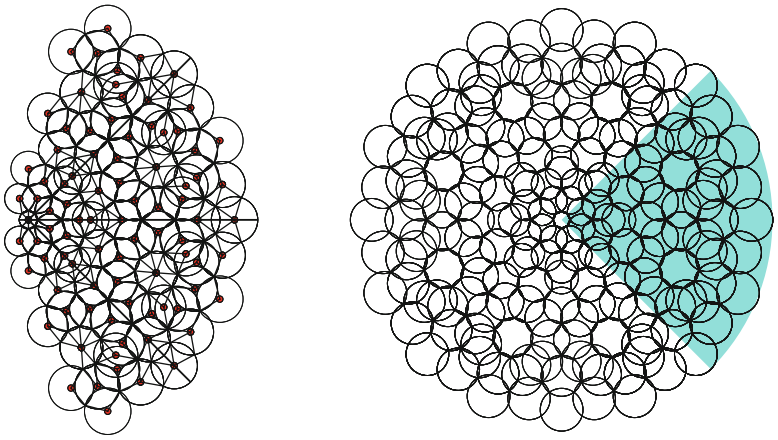

Fig. 12 Example of a circle pattern corresponding to $z^{5/4}$ based on a Penrose tiling (rhombic embedding) with tenfold rotation symmetry

4.5 Linearization

We consider the following linearization of the Hirota equation (17) for integrable circle patterns which will again lead to discrete holomorphic functions from the linear theory.

Theorem 4.13 *For a b-quad-graph $\mathcal{D}$ and a labelling α which corresponds to a rhombic embedding with directed edges $\theta \in \mathbb{S}^1$ let a differentiable one parameter family $\mathbf{w}_\varepsilon : V(\mathcal{D}) \to \mathbb{C}$ for $\varepsilon \in (-\varepsilon_0, \varepsilon_0)$ corresponding to integrable circle patterns be given. In particular, $\mathbf{w}_0 \equiv 1$ and $\mathbf{w}_\varepsilon(x)$ is the radius function at a white vertex x and $\mathbf{w}_\varepsilon(y)$ is the turning angle compared to the given rhombic embedding. Then*

$$
\begin{aligned}
f^\ell &= \left(\mathbf{w}_\varepsilon^{-1}\frac{\mathrm{d}\mathbf{w}_\varepsilon}{\mathrm{d}\varepsilon}\right)\Big|_{\varepsilon=0} = \frac{\mathrm{d}\log\mathbf{w}_\varepsilon}{\mathrm{d}\varepsilon}\Big|_{\varepsilon=0} \\
&= \begin{cases} \left(\dfrac{1}{r_\varepsilon(x)}\dfrac{\mathrm{d}r_\varepsilon(x)}{\mathrm{d}\varepsilon}\right)\Big|_{\varepsilon=0} = \dot{r}(x) & \text{at white vertex } x \\ \left(\mathrm{e}^{-\mathrm{i}\delta_\varepsilon(y)}\dfrac{\mathrm{d}\mathrm{e}^{\mathrm{i}\delta_\varepsilon(y)}}{\mathrm{d}\varepsilon}\right)\Big|_{\varepsilon=0} = \mathrm{i}\dot{\delta}(y) & \text{at black vertex } y \end{cases}
\end{aligned}
$$

solves the discrete Cauchy–Riemann equations for the given rhombic embedding.

Proof Consider a quadrilateral of the rhombic embedding labelled as in Fig. 5 (middle). The Hirota equation (17) then reads

$$\theta_0\mathbf{w}_\varepsilon(x_0)\mathbf{w}_\varepsilon(y_0) + \theta_1\mathbf{w}_\varepsilon(x_1)\mathbf{w}_\varepsilon(y_0) - \theta_0\mathbf{w}_\varepsilon(x_1)\mathbf{w}_\varepsilon(y_1) - \theta_1\mathbf{w}_\varepsilon(x_0)\mathbf{w}_\varepsilon(y_1) = 0\,.$$

Differentiating by ε at $\varepsilon = 0$ and using $\mathbf{w}_0 \equiv 1$ we deduce that

$$\big(f^\ell(x_1) - f^\ell(x_0)\big)(\theta_0 - \theta_1) + \big(f^\ell(y_1) - f^\ell(y_0)\big)(\theta_0 + \theta_1) = 0$$
$$\iff \frac{\theta_1 - \theta_0}{\theta_1 + \theta_0} = \frac{f^\ell(y_1) - f^\ell(y_0)}{f^\ell(x_1) - f^\ell(x_0)} = \frac{\mathrm{i}\dot{\delta}(y_1) - \mathrm{i}\dot{\delta}(y_0)}{\dot{r}(x_1) - \dot{r}(x_0)} .$$

This shows that f^ℓ satisfies the discrete Cauchy–Riemann equations for the rhombic embedding. □

Remark 4.14 The connection to the discrete Cauchy–Riemann equations (6) also holds in the general case. Consider a kite as in Fig. 11 with edge lengths $|e_0| = |e_1| = r_0(x_0)$ and $|\hat{e}_0| = |\hat{e}_1| = r_0(x_1)$ from some circle pattern $\mathcal{C}_0$ with radius function r_0. Assume given a differentiable one-parameter family of circle patterns $\mathcal{C}_\varepsilon$ with the same combinatorics and intersection angles as $\mathcal{C}_0$ and define the corresponding quotient of radius functions and the rotation function by $\mathbf{w}_\varepsilon(x) = r_\varepsilon(x)/r_0(x)$ and $\mathbf{w}_\varepsilon(y) = \mathrm{e}^{\mathrm{i}\delta_\varepsilon(y)}$. Then $\mathbf{w}_0 \equiv 1$ and (16) reads

$$e_0\mathbf{w}_\varepsilon(x_0)\mathbf{w}_\varepsilon(y_0) + \hat{e}_1\mathbf{w}_\varepsilon(x_1)\mathbf{w}_\varepsilon(y_0) - \hat{e}_0\mathbf{w}_\varepsilon(x_1)\mathbf{w}_\varepsilon(y_1) - e_1\mathbf{w}_\varepsilon(x_0)\mathbf{w}_\varepsilon(y_1) = 0 .$$

Define again $f^\ell = (\mathbf{w}_\varepsilon^{-1}\big(\mathrm{d}\mathbf{w}_\varepsilon/\mathrm{d}\varepsilon)\big)\big|_{\varepsilon=0}$. Analogously as in the proof of the previous theorem we obtain

$$\big(f^\ell(x_1) - f^\ell(x_0)\big)(\hat{e}_0 - \hat{e}_1) + \big(f^\ell(y_1) - f^\ell(y_0)\big)(e_0 + e_1) = 0$$
$$\iff \frac{\hat{e}_1 - \hat{e}_0}{e_1 + e_0} = \frac{f^\ell(y_1) - f^\ell(y_0)}{f^\ell(x_1) - f^\ell(x_0)} = \frac{\mathrm{i}\dot{\delta}(y_1) - \mathrm{i}\dot{\delta}(y_0)}{\dot{r}(x_1)/r(x_1) - \dot{r}(x_0)/r(x_0)} .$$

This shows that f^ℓ satisfies the discrete Cauchy–Riemann equations for the immersion of the kite pattern given by the original circle pattern $\mathcal{C}_0$.

4.6 Some Further Topics

During the last 30 years, the theory of circle packings and circle patterns has been developed in many respects. Properties of circle patterns and discrete holomorphic functions which are analogous to properties known from the smooth theory are of special interest. This includes discrete analogs of special functions like polynomials, z^γ, log, erf, see for example [2, 4, 7, 9, 10, 17, 65]. Also, rigidity of circle patterns has been studied, for examples in [23, 42, 63]. A beautiful presentation of the theory of circle packings, including computational aspects, is given by Stephenson in [31].

Convergence issues have first been investigated for circle packings by Rodin and Sullivan in [63] and then further studied by He and Schramm in [43, 44].

Similar results for circle patterns with square grid combinatorics have been obtained in [55, 57, 65]. An approximation result for integrable circle patterns with irregular combinatorics can be found in [22].

5 Conformally Equivalent Triangle Meshes

Recall that a smooth conformal map, that is a holomorphic map with nonvanishing derivative, can be characterized as an infinitesimal scale-rotation. In the discrete theory, this characterization may be translated into different concepts. In the previous section we introduced circle patterns as discrete analogs. Here we consider a discretization coming from a metric viewpoint: Infinitesimally, lengths are scaled by a factor, i.e., by $|f'(z)|$ for a smooth conformal function f. More generally, on a smooth manifold two Riemannian metrics g and $\tilde{g}$ are conformally equivalent if $\tilde{g} = \mathrm{e}^{2s} g$ for some smooth function s.

In the discrete setting, this idea of changing lengths according to scale factors at vertices has been first applied by Luo in [56]. This initiated further research exploring this concept, see for example [18, 40].

5.1 Definition of Discrete Conformal Maps

The smooth complex domain (or manifold) is now replaced in this discrete setting by a triangulation of a connected subset of the plane $\mathbb{C}$ (or a triangulated piecewise Euclidean manifold). A particular case is a (part of a) *triangular lattice*, that is, a lattice triangulation of the whole complex plane $\mathbb{C}$ with congruent triangles, see Fig. 13 (left). We will denote the vertices of the triangulation by $v_i \in V$ and edges will be written as $e = [v_i, v_j] \in E$, where $v_i, v_j \in V$ are its incident vertices. For triangular faces we use the notation $\Delta[v_i, v_j, v_k]$ enumerating the incident vertices with respect to the orientation (counterclockwise) of $\mathbb{C}$. Note that we do not consider a combinatorial structure of a quad-graph (yet) in this theory.

We always identify the given triangulation in $\mathbb{C}$ (or immersed triangulation in $\mathbb{C}$ which is locally an embedding around every vertex) with the corresponding abstract triangulation T. In particular, all (abstract) triangles always correspond to embedded Euclidean triangles and also for every interior vertex the subcomplex consisting of the flower of all incident triangles is embedded. Then we can study

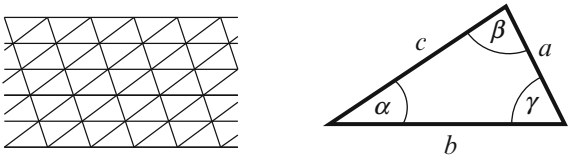

Fig. 13 *Left*: Lattice triangulation of the plane with congruent triangles. *Right*: Triangle with labelled edges and inner angles

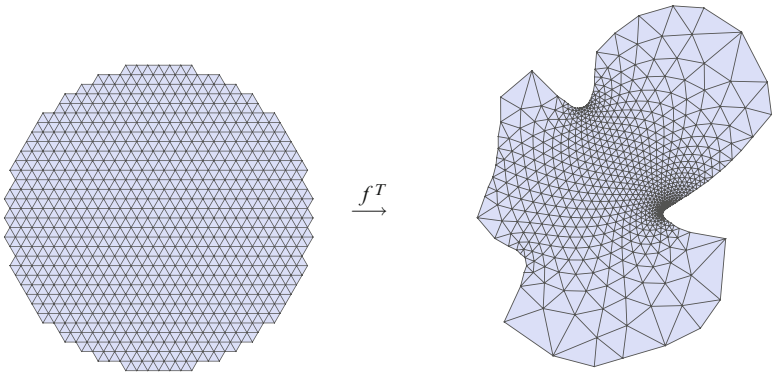

Fig. 14 Example of a discrete conformal map f^T based on conformally equivalent triangulations

a *length function* $l\colon E \to \mathbb{R}_+ := \{x \in \mathbb{R} : x > 0\}$ on the edges by taking for l the edge lengths. This function l plays the role of a discrete metric on T.Thus for an immersed triangulation we write (T, l). In the following, we will always use the Euclidean metric to determine the length of an embedded edge $[v, w] \subset \mathbb{C} \cong \mathbb{R}^2$ of an immersed triangulation T, so $l([v, w]) = |v - w|$.

Now we can 'translate' the idea of changing a given metric by a conformal factor as follows for the discrete case. Given a function $s\colon V \to \mathbb{R}$ we scale the edge length of the edge $[v, w]$ by $\mathrm{e}^{(s(v)+s(w))/2}$ which is the geometric mean of $\mathrm{e}^{s(v)}$ and $\mathrm{e}^{s(w)}$. If this leads to another locally embedded triangulation, this may be considered as discrete holomorphic map. See Fig. 14 for an illustration.

Definition 5.1 Two immersed triangulations (T, l) and $(T, \tilde{l})$ with the same combinatorics of T are called *conformally equivalent triangle meshes* or *conformally equivalent (immersed) triangulations* if the lengths of corresponding edges $e = [v, w]$ satisfy

$$\tilde{l}([v, w]) = l([v, w])\mathrm{e}^{(s(v)+s(w))/2} \tag{18}$$

for some function $s\colon V \to \mathbb{R}$. In this case, the mapping $f^T\colon V \to \mathbb{C}$ is called a *discrete conformal map* (or *discrete holomorphic map*). By abuse of notation, we also call $f^T\colon (T, l) \to (T, \tilde{l})$ a *discrete conformal map* of the corresponding conformally equivalent triangulations. The function s is called *(logarithmic) scale factors*.

Note that (18) expresses a linear relation for the logarithmic lengths, that is

$$2\log\left(\tilde{l}([v, w])\right) = 2\log\left(l([v, w])\right) + s(v) + s(w)\ .$$

Again, the superscript T emphasizes that the previous definition of a discrete holomorphic map refers to conformally equivalent triangulations and is not to be

confused with discrete holomorphic functions considered in the previous sections. Some connections are presented in Sects. 5.3 and 5.4.

In fact, the definition of a discrete conformal map relies on the more general notion of discrete conformal triangle meshes. These have been studied by Luo [56], Gu et al. [39, 40, 56], Bobenko et al. [18] and others.

Recall, that smooth conformal maps infinitesimally preserve length cross-ratios. Also, a smooth function with nonvanishing derivative which preserves all infinitesimal length cross-ratios is conformal or anti-conformal (i.e., $\partial_z f = 0$). Note that conformally equivalent triangle meshes may also be characterized by the fact that they preserve the *length cross-ratios*: For two adjacent triangles $\Delta[v_i, v_j, v_k]$ and $\Delta[v_k, v_j, v_l]$ with common edge $[v_j, v_k]$ define

$$\mathrm{lcr}_{jk} = \frac{l([v_i, v_j])l([v_l, v_k])}{l([v_j, v_l])l([v_k, v_i])} .$$

Note that lcr_{jk} is the absolute value of the cross-ratio $\mathrm{cr}(z_1, z_2, z_3, z_4) = (z_1 - z_2)(z_2 - z_3)^{-1}(z_3 - z_4)(z_4 - z_1)^{-1}$ of the four vertices v_i, v_j, v_l, v_k.

Exercise 5.2 Show that for the equilateral triangular lattice the length cross-ratio for every edge $[v_j, v_k]$ is $lcr_{jk} = 1$. Furthermore, calculate the values of the length cross-ratio lcr_{jk} for a general triangular lattice as in Fig. 13 (left).

Exercise 5.3 Let T be a simply connected triangulation. Show that $f^T\colon (T, l) \to (T, \tilde{l})$ is a discrete conformal map if and only if for any edge $[v_j, v_k]$ with two adjacent triangles $\Delta[v_i, v_j, v_k]$ and $\Delta[v_k, v_j, v_l]$ the length cross-ratios for l and for $\tilde{l}$ agree: $\mathrm{lcr}_{jk} = \widetilde{\mathrm{lcr}}_{jk}$. (See [18, Proposition 2.3.2] for a proof.)

Furthermore, there exists a homeomorphism of two conformally equivalent triangle meshes whose restriction to every triangle is a projective map. In fact, there is a one-parameter family of such homeomorphisms including the piecewise linear map, see [20]. In particular, there exists a homeomorphism between two conformally equivalent triangle meshes whose restriction to every triangle is a projective map onto the corresponding image triangle which also maps the circumcircle of this triangle to the circumcircle of the image triangle. Note that the existence of such a homeomorphism is equivalent to the fact that the corresponding triangle meshes are conformally equivalent, see [18, Theorem 2.7.2].

5.2 *Characterization of Discrete Conformal Maps by Logarithmic Scale Factors*

Similarly as in the case of circle patterns and their radius functions, we can characterize conformally equivalent triangulations in terms of the logarithmic scale factor s on the vertices (up to Euclidean motions). Consider an immersed triangulation (T, l) with edge lengths $l([v, w]) = |v - w|$ where $|\cdot|$ denotes the

Euclidean metric on $\mathbb{C} \cong \mathbb{R}^2$. Given any function $s\colon V \to \mathbb{R}$ we can assign new lengths to the edges according to (18) by

$$\tilde{l}([v,w]) = |v-w|\mathrm{e}^{(s(v)+s(w))/2}. \tag{19}$$

In order to obtain new triangles with these lengths (and ultimately a discrete conformal map) the triangle inequalities need to hold for the edge lengths $\tilde{l}$ on each triangle. If we assume this, we can embed the new triangles (respecting orientation) and immerse sequences of triangles with edge lengths given by $\tilde{l}$ as in (19). In order to obtain a discrete conformal map, in particular a local homeomorphism, the interior angles of these triangles need to sum up to 2π at each interior vertex.

The angle at a vertex of a triangle with given side lengths can be calculated. With the notation of Fig. 13 (right) we have the half-angle formula

$$\tan\left(\frac{\alpha}{2}\right) = \sqrt{\frac{(-b+a+c)(-c+a+b)}{(b+c-a)(a+b+c)}} = \sqrt{\frac{1-(b/a-c/a)^2}{(b/a+c/a)^2-1}}\,. \tag{20}$$

The last expression emphasizes the fact that the angle does not depend on the scaling of the triangle. In particular, we define the function

$$\Theta(x,y) := 2\arctan\sqrt{\frac{1-(\mathrm{e}^{-x/2}-\mathrm{e}^{-y/2})^2}{(\mathrm{e}^{-x/2}+\mathrm{e}^{-y/2})^2-1}}\,,$$

so (20) can be written as

$$\alpha = \Theta(x,y) \quad \text{with } \frac{b}{a} = \mathrm{e}^{-x/2} \text{ and } \frac{c}{a} = \mathrm{e}^{-y/2}\,.$$

Summing up, we have the following characterization of scale factors associated to discrete conformal maps.

Proposition 5.4 *Let T be a triangulation and let $s\colon V \to \mathbb{R}$ be a function satisfying the following two conditions.*

(i) *For every triangle $\Delta[v_1,v_2,v_3]$ of T the* triangle inequalities *for $\tilde{l}$ defined by* (18) *hold, in particular*

$$|v_i-v_j|\mathrm{e}^{(s(v_i)+s(v_j))/2} < |v_i-v_k|\mathrm{e}^{(s(v_i)+s(v_k))/2} + |v_j-v_k|\mathrm{e}^{(s(v_j)+s(v_k))/2}$$

for all permutations (ijk) of (123).

(ii) *For every interior vertex v_0 with neighbors $v_1,v_2,\ldots,v_k,v_{k+1}=v_1$ in cyclic order we have*

$$\sum_{j=1}^{k} \Theta\big(\lambda(v_0,v_j,v_{j+1})+s(v_{j+1})-s(v_0), \lambda(v_0,v_{j+1},v_j)+s(v_j)-s(v_0)\big) = 2\pi\,, \tag{21}$$

where $\lambda(v_a, v_b, v_c) = 2\log(|v_b - v_c|/|v_a - v_b|)$ *for a triangle* $\Delta[v_a, v_b, v_c]$.

Then there is a discrete conformal map (unique up to post-composition with Euclidean motions) such that its associated scale factors are the given function $s: V \to \mathbb{R}$.

Conversely, given a discrete conformal map between two conformally equivalent triangulations, its associated scale factors $s : V \to \mathbb{R}$ *satisfy conditions* (i) *and* (ii).

Example 5.5 (Analogues of Doyle Spirals) Consider the equilateral triangular lattice $\mathbb{Z} + e^{i\pi/3}\mathbb{Z}$. Let $A, B > 0$ such that there exists a nondegenerate triangle with edge lengths A, B and AB. Then $s: \mathbb{Z} + e^{i\pi/3}\mathbb{Z} \to \mathbb{R}$ defined by $s(m + e^{i\pi/3}n) = 2m \log A + 2n \log B$ are the logarithmic scale factors of a discrete conformal map.

This can be easily seen as follows. Consider the triangle Δ_0 with vertices 0, 1 and $e^{i\pi/3}$. By construction, Δ_0 is mapped to a triangle with edge lengths A, B and AB. Any translation of Δ_0, say the triangle with vertices $m + ne^{i\pi/3}$, $m + 1 + ne^{i\pi/3}$ and $m + (n + 1)e^{i\pi/3}$ is mapped to a triangle with edge lengths $A^{2m+1}B^{2n}$, $A^{2m}B^{2n+1}$ and $A^{2m+1}B^{2n+1}$ which is a scaled version of the first image triangle. Note that at any vertex there are three incident triangles which are translations of Δ_0. Thus the three image triangles sharing a common vertex have angles at this vertex which add up to π. An analogous reasoning applies for the triangle $\hat{\Delta}_0$ with vertices 0, 1 and $e^{-i\pi/3}$ and its translates. Therefore the angles of all six image triangles which share a common vertex add up to 2π. Thus we can apply Proposition 5.4.

Note that this example gives an analogue of *Doyle spirals* which have been considered for circle packings for example in [9, 69].

Exercise 5.6 Let $\alpha, \beta, \gamma \in (0, \pi)$ be such that $\alpha + \beta + \gamma = \pi$. Consider the triangular lattice $(\sin\beta)\mathbb{Z} + (e^{i\alpha}\sin\gamma)\mathbb{Z}$ as in Fig. 13 (left). Let $A, B > 0$ such that there exists a nondegenerate triangle with edge lengths $A\sin\beta$, $B\sin\gamma$ and $AB\sin\alpha$. Show that $s: (\sin\beta)\mathbb{Z} + (e^{i\alpha}\sin\gamma)\mathbb{Z} \to \mathbb{R}$ defined by $s(m\sin\beta + e^{i\alpha}\sin\gamma n) = 2m\log A + 2n\log B$ are the logarithmic scale factors of a discrete conformal map. See Fig. 15 for an example.

5.3 Linearization

Discrete holomorphic maps based on conformally equivalent triangle meshes can also be related to the linear theory of discrete harmonic and holomorphic functions via suitable linearization.

Note that (21) may be considered as a nonlinear Laplace equation. This can also be justified by the fact that for the linearization we obtain the well-known cot-Laplacian.

Theorem 5.7 *Consider a differentiable one parameter family of logarithmic scale factors* $s_\varepsilon: V \to \mathbb{R}$, $\varepsilon \in (-\varepsilon_0, \varepsilon_0)$ *for a family of conformally equivalent immersed triangulations* (T, l_ε). *Assume that* $s_0 \equiv 0$. *Then* $u = (\mathrm{d}s_\varepsilon/\mathrm{d}\varepsilon)|_{\varepsilon=0}$ *is harmonic with respect to the* cot*-Laplacian on* (T, l_0). *In particular, let* v_0 *be an interior vertex with*

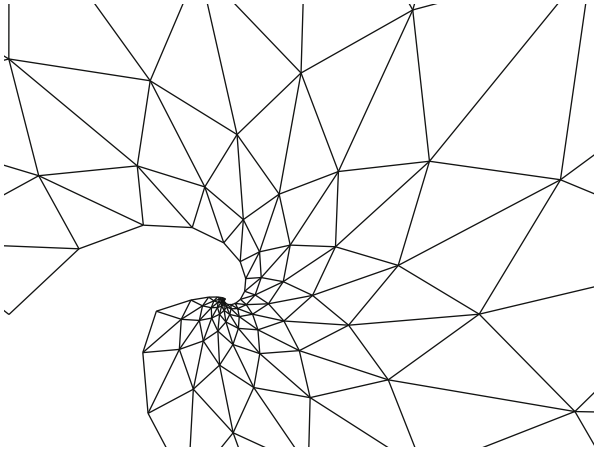

Fig. 15 Example of a part of a "Doyle spiral" for conformally equivalent triangular lattices

neighbors $v_1, v_2, \ldots, v_k, v_{k+1} = v_1$ *in cyclic order. Then*

$$\sum_{k=1}^{n} \frac{1}{2}(\cot \alpha^{k-1}_{[v_0,v_k]} + \cot \alpha^{k+1}_{[v_0,v_k]})\big(u(v_k) - u(v_0)\big) = 0 \,,$$

where $\alpha^{k-1}_{[v_0,v_k]}$ *and* $\alpha^{k+1}_{[v_0,v_k]}$ *are the two angles opposite to the edge* $[v_0, v_k]$ *in the triangles* $\Delta[v_0, v_{k-1}, v_k]$ *and* $\Delta[v_0, v_k, v_{k+1},]$ *in* (T, l_0) *respectively.*

Proof First, consider a single triangle. Observe with the notation of Fig. 13 (right):

$$\frac{\partial \beta}{\partial a} = -\frac{1}{a} \cot \gamma \,.$$

Thus, we easily deduce that

$$\frac{\partial}{\partial \varepsilon} \Theta\left(2 \log\left(\frac{a}{c}\right) + \varepsilon, 2 \log\left(\frac{a}{b}\right)\right)\Big|_{\varepsilon=0} = \frac{1}{2} \cot \gamma \,.$$

Now the claim follows by differentiation of relation (21) for s_ε by ε at $\varepsilon = 0$. □

As in the case of cross-ratio systems and circle patterns, a suitable linearization connects discrete conformal maps for conformally equivalent triangulations to the linear theory. To this end, consider a triangulation (T, l_0) with equilateral triangles, that is (without loss of generality) $l_0 \equiv 1$. Let (T, l_ε) be a differentiable one parameter family of triangulations which are conformally equivalent to (T, l_0) with logarithmic scale factors $s_\varepsilon : V \to \mathbb{R}$. In particular $s_0 \equiv 0$. Define $f^\ell(v) = u(v) = (\mathrm{d}s_\varepsilon(v)/\mathrm{d}\varepsilon)|_{\varepsilon=0}$ as in Theorem 5.7 for vertices v of the triangulation. In order to obtain a discrete Cauchy–Riemann equation we need to define 'dual' variables at the dual vertices located at the centers c of the equilateral triangle, see Fig. 16 (left). (For

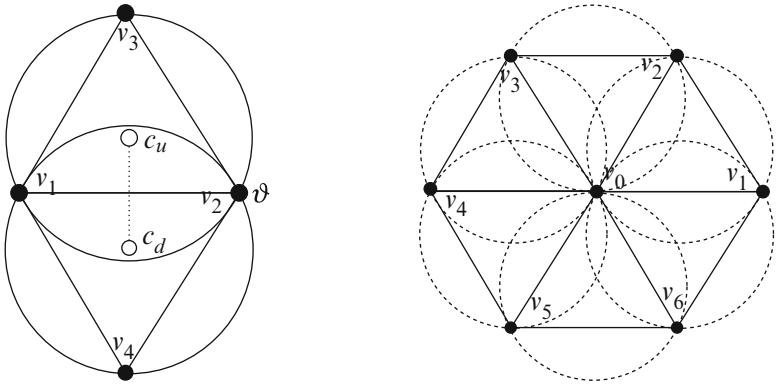

Fig. 16 *Left*: Two adjacent triangles with centers and circumcircles with interior intersection angle ϑ (where $\vartheta = 2\pi/3$ for equilateral triangles). *Right*: A flower of a triangulation, here in particular of an equilateral triangulation

equilateral triangles, the circumcenter coincides with the barycenter and many more triangle centers. Therefore, this regular case does not hint which of these centers might be important in a more general case.) Denote by $p_\varepsilon(v) \in \mathbb{C}$ the location of the vertex v in the triangulation (T, l_ε) and assume that $p_0 = \mathrm{id}$. On an edge $[v_1, v_2]$ we have by assumption

$$p_\varepsilon(v_2) - p_\varepsilon(v_1) = \mathrm{e}^{(s_\varepsilon(v_1)+s_\varepsilon(v_2))/2} = \mathrm{e}^{\mathrm{i}\delta_\varepsilon([v_1,v_2])}(v_2 - v_1) \,,$$

where $\delta_\varepsilon([v_1, v_2])$ is the rotation angle of the edge (which can be chosen to be differentiable in ε). Define $\eta([v_1, v_2]) = (\mathrm{d}\delta_\varepsilon([v_1, v_2])/\mathrm{d}\varepsilon)|_{\varepsilon=0}$ to be the infinitesimal rotation of the edge $[v_1, v_2]$. Summing up,

$$\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\big(p_\varepsilon(v_2) - p_\varepsilon(v_1)\big)\bigg|_{\varepsilon=0} = \left(\frac{u(v_1) + u(v_2)}{2} + \mathrm{i}\eta([v_1, v_2])\right)(v_2 - v_1) \,.$$

The closing condition for the triangle $\Delta_\varepsilon[v_1, v_2, v_3]$ reads

$$p_\varepsilon(v_2) - p_\varepsilon(v_1) + p_\varepsilon(v_3) - p_\varepsilon(v_2) + p_\varepsilon(v_1) - p_\varepsilon(v_3) = 0 \,.$$

Differentiating this equation by ε at $\varepsilon = 0$ gives

$$\left(\frac{u(v_1) + u(v_2)}{2} + \mathrm{i}\eta([v_1, v_2])\right)(v_2 - v_1) + \left(\frac{u(v_2) + u(v_3)}{2} + \mathrm{i}\eta([v_2, v_3])\right)(v_3 - v_2)$$
$$+ \left(\frac{u(v_3) + u(v_1)}{2} + \mathrm{i}\eta([v_3, v_1])\right)(v_1 - v_3) = 0 \,. \qquad (22)$$

As $\Delta_0[v_1, v_2, v_3]$ is an equilateral triangle, elementary geometric considerations yield

$$\begin{aligned} v_2 - v_1 &= -\frac{1}{\sqrt{3}}\mathrm{i}(v_3 - v_2) + \frac{1}{\sqrt{3}}\mathrm{i}(v_1 - v_3) \,, \\ v_3 - v_2 &= -\frac{1}{\sqrt{3}}\mathrm{i}(v_1 - v_3) + \frac{1}{\sqrt{3}}\mathrm{i}(v_2 - v_1) \,, \\ v_1 - v_3 &= -\frac{1}{\sqrt{3}}\mathrm{i}(v_2 - v_1) + \frac{1}{\sqrt{3}}\mathrm{i}(v_1 - v_3) \,. \end{aligned}$$

Inserting these relation into (22), we obtain

$$\begin{aligned} 0 &= \eta([v_1, v_2])\mathrm{i}(v_2 - v_1) + \eta([v_2, v_3])\mathrm{i}(v_3 - v_2) + \eta([v_3, v_1])\mathrm{i}(v_1 - v_3) \\ &\quad + \frac{u(v_1) + u(v_2)}{2}\frac{1}{\sqrt{3}}\big(\mathrm{i}(v_1 - v_3) - \mathrm{i}(v_3 - v_2)\big) \\ &\quad + \frac{u(v_2) + u(v_3)}{2}\frac{1}{\sqrt{3}}\big(\mathrm{i}(v_2 - v_1) - \mathrm{i}(v_1 - v_3)\big) \\ &\quad + \frac{u(v_3) + u(v_1)}{2}\frac{1}{\sqrt{3}}\big(\mathrm{i}(v_3 - v_1) - \mathrm{i}(v_2 - v_1)\big) \\ &= \left(\frac{u(v_2) - u(v_1)}{2\sqrt{3}} + \eta([v_1, v_2])\right)\mathrm{i}(v_2 - v_1) \\ &\quad + \left(\frac{u(v_3) - u(v_2)}{2\sqrt{3}} + \eta([v_2, v_3])\right)\mathrm{i}(v_3 - v_2) \\ &\quad + \left(\frac{u(v_1) - u(v_3)}{2\sqrt{3}} + \eta([v_3, v_1])\right)\mathrm{i}(v_1 - v_3) \,. \end{aligned}$$

Note that any two of $\mathrm{i}(v_2 - v_1)$, $\mathrm{i}(v_3 - v_2)$, $\mathrm{i}(v_1 - v_3)$ are linearly independent over $\mathbb{R}$ and these three terms add up to 0. Therefore, we deduce that all three terms in the big brackets are equal. In particular, we have shown the existence of a variable $f^\ell(c) = w(c)$ which is associated to the center c of $\Delta_0[v_1, v_2, v_3]$ and is defined by

$$\begin{aligned} f^\ell(c) = w(c) &:= \eta([v_1, v_2])\mathrm{i} + \frac{1}{2\sqrt{3}}\big(u(v_2) - u(v_1)\big)\mathrm{i} \\ &= \eta([v_2, v_3])\mathrm{i} + \frac{1}{2\sqrt{3}}\big(u(v_3) - u(v_2)\big)\mathrm{i} \\ &= \eta([v_3, v_1])\mathrm{i} + \frac{1}{2\sqrt{3}}\big(u(v_1) - u(v_3)\big)\mathrm{i} \,. \end{aligned}$$

For two adjacent triangles of T we therefore obtain in the notation of Fig. 16 (left) the discrete Cauchy–Riemann equations for f^ℓ, where $f^\ell(v) = u(v)$ and $f^\ell(c) =$

$w(c)$, so

$$f^\ell(c_u) - f^\ell(c_d) = \mathrm{i}\frac{1}{\sqrt{3}}\big(f^\ell(v_2) - f^\ell(v_1)\big)$$

$$\iff \quad \frac{f^\ell(v_2) - f^\ell(v_1)}{f^\ell(c_d) - f^\ell(c_u)} = \mathrm{i}\left|\frac{v_2 - v_1}{c_d - c_u}\right| .$$

5.4 Towards Integrability for the Equilateral Triangular Lattice

In the following we introduce a characterization of discrete conformal maps based on conformally equivalent triangulations which may lead to a connection to integrability.

First note that any configuration of four mutually distinct points z_1, z_2, z_3, z_4 in the complex plane (respecting this labelling) is determined up to Möbius transformations by the cross-ratio $\mathrm{cr}(z_1, z_2, z_3, z_4)$, as defined for example in (10). For simplicity, we restrict ourselves to immersed triangulations which are conformally equivalent to the equilateral triangular lattice. Therefore, all length cross-ratios are supposed to be one and the cross-ratio $\mathrm{cr}(v_1, v_4, v_2, v_3) =: \mathrm{e}^{\mathrm{i}\vartheta} \in \mathbb{S}^1$ is unitary [with notation of Fig. 16 (left)] and can be associated to the undirected edge $[v_1, v_2]$.

Exercise 5.8 Let v_1, v_2, v_3, v_4 be four mutually distinct points with unitary cross-ratio $\mathrm{cr}(v_1, v_4, v_2, v_3) =: \mathrm{e}^{\mathrm{i}\vartheta} \in \mathbb{S}^1$. Show that ϑ is the interior intersection angle between the circumcircles of the triangles $\Delta[v_1, v_2, v_3]$ and $\Delta[v_1, v_4, v_2]$, see Fig. 16 (left) for the notation.

Now consider an interior vertex v_0 with its six neighbors $v_1, v_2, v_3, v_4, v_5, v_6$ as illustrated in Fig. 16 (right) and the corresponding triangles $\Delta[v_0, v_j, v_{j+1}]$ for $j = 1, \ldots, 6$, where the indices are taken modulo 6. We consider the variables $q_j = \mathrm{cr}(v_0, v_{j-1}, v_j, v_{j+1}) \in \mathbb{S}^1$ defined on the edges $[v_0, v_j]$. As these cross-ratios are invariant under Möbius transformations we can map v_0 to ∞ by a suitable Möbius transformation. Then the circumcircles of the triangles are mapped to lines and form a polygon as illustrated in Fig. 17 (left). As all length cross-ratios are supposed to be one this hexagon has edges of equal length. Now the closing condition for the directed edges of this hexagon translates into the equations

$$1 = q_1 q_2 q_3 q_4 q_5 q_6 , \tag{23}$$

$$0 = 1 - q_2 + q_2 q_3 - q_2 q_3 q_4 + q_2 q_3 q_4 q_5 - q_2 q_3 q_4 q_5 q_6 , \tag{24}$$

$$0 = 1 - q_6 + q_6 q_5 - q_6 q_5 q_4 + q_6 q_5 q_4 q_3 - q_6 q_5 q_4 q_3 q_2 . \tag{25}$$

These are conditions on the variables $q_j \in \mathbb{S}^1$ (defined on the edges) for a cycle in the dual graph T^* of the given equilateral triangulation T. Note that there are additional conditions on the qs in order to obtain an embedded configuration. In

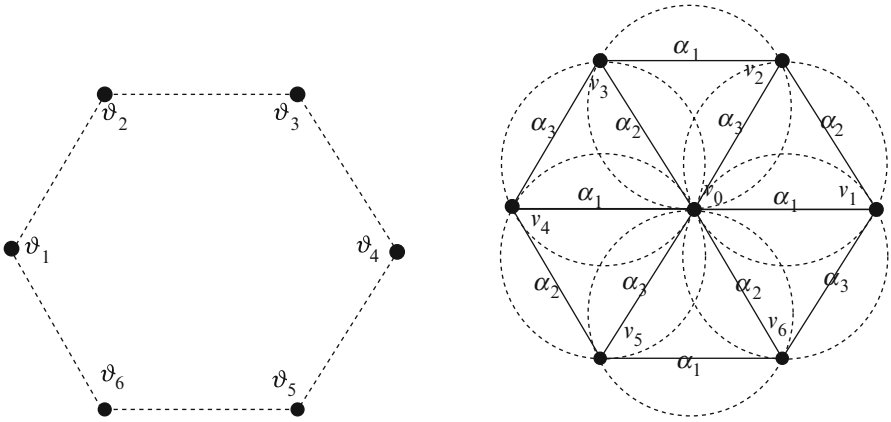

Fig. 17 *Left*: The circumcircles of a flower after a suitable Möbius transformation. *Right*: Integrable labelling $\alpha_j \in \mathbb{S}^1$ of the edges such that $q_j = \alpha_k/\alpha_l$ where (klj) is a cyclic permutation of (123)

particular, $q = \mathrm{e}^{\mathrm{i}\vartheta}$ with $\vartheta \in (0, \pi)$ and condition (23) translates into

$$\sum_{j=1}^{6} (\pi - \vartheta_j) = 2\pi \ .$$

Example 5.9 (Möbius Transformations of Doyle Spirals) A special solution of (23)–(25) is given by the cross-ratio system which provides a first link to integrability. Consider a labelling with labels $\alpha_1, \alpha_2, \alpha_3 \in \mathbb{S}^1$ on the edges of the equilateral triangulation T such that parallel edges carry the same label. Furthermore, the indices of the labelling are chosen with respect to the orientation of the plane, so for a counterclockwise orientation of the edges the labellings $\alpha_k, \alpha_j, \alpha_l$ are a cyclic permutation of $\alpha_1, \alpha_2, \alpha_3$, see Fig. 17 (right).

Similarly as for cross-ratio systems, we now associate the variable $q_l = \alpha_k/\alpha_j$ to the edge carrying the label α_l such that (kjl) is a cyclic permutation of (123). If we set $q_{j+3} = q_j$ for $j = 1, 2, 3$ we obtain a solution of conditions (23)–(25). If additionally $q_j = \mathrm{e}^{\mathrm{i}\vartheta_j}$ with $\vartheta_j \in (0, \pi)$ for $j = 1, 2, 3$, we obtain a solution which corresponds to a conformally equivalent immersed triangulation $\widetilde{T}$. To be precise, we fix the (nondegenerate) image of one triangle and recall that variables q_j then determine the images of the vertices for the whole lattice.

Due to the special construction, these triangulations $\widetilde{T}$ are linked to Example 5.5, in fact they are images of one of these examples by a Möbius transformation.

This can be seen by considering two triangles Δ_0 and Δ_1 sharing a vertex which can be identified in the original equilateral triangulation T by a translation. If we consider the two images $\tilde{\Delta}_0$ and $\tilde{\Delta}_1$ in $\widetilde{T}$ of these triangles and the Möbius transformation M_1 mapping the vertices of triangle $\tilde{\Delta}_0$ onto the corresponding

vertices of $\tilde{\Delta}_1$, we observe that this Möbius transformation maps all vertices of $\widetilde{T}$ onto themselves due to our special (periodic) choice of variables q_j. There is a third triangle Δ_2 sharing a vertex with both Δ_0 and Δ_1 which can be identified with Δ_0 in T by a translation. Analogously as before, we consider the Möbius transformation M_2 mapping the vertices of triangle $\tilde{\Delta}_0$ onto the corresponding vertices of $\tilde{\Delta}_2$. Again we observe that this Möbius transformation maps the whole lattice of vertices of $\widetilde{T}$ onto itself. Furthermore, the two Möbius transformations commute by construction. Therefore, M_1 and M_2 have either both one single fixed point or both two fixed points and these fixed points agree. Mapping one of the fixed points to infinity, the Möbius transformations M_1 and M_2 are changed to a translation in case of only one fixed point and show that the lattice was in fact only the image of the original equilateral triangulation by a Möbius transformation. In the remaining case we obtain an immersed triangulation which covers the whole complex plane except for one point (the image of the second fixed point). Also, all images of the triangle Δ_0 are similar to each other. Therefore, we arrive at the same immersed triangulations as considered in Example 5.5.

5.5 *Some Further Topics*

Discrete conformal maps based on conformally equivalent triangulations are the most recent of the presented discrete analogous of smooth holomorphic mappings. Therefore, this theory is still developing and contains many open questions for further research. In particular, the link to former theories as circle patterns or discrete Cauchy–Riemann equations is not yet fully understood. Some promising connections have been established by Lam in [54] using discrete holomorphic differentials.

As possible application, discrete conformal maps can be used for discrete uniformization. The simplest case is a discrete Riemann mapping theorem, i.e. the problem of finding a discrete conformal mapping of a simply connected domain onto the unit disc. A first answer in this direction has been given in [39] where changes of the combinatorics of the triangulation are allowed. Similarly, we may consider a related Dirichlet problem. Given some function s_∂ on the boundary of a finite triangulation T, find a discrete conformal map whose associated scale factors agree on the boundary with s_∂. For such a Dirichlet problem (with assumptions on s_∂ and T) existence and an approximation result have been proven in [24]. Rigidity questions have first been addressed by Wu, Gu and Sun in [71] who also first described analogs of Doyle spirals. Nevertheless, rigidity and convergence results for irregular triangulations still remain an issue.

Given an immersed triangulation (T, l), the problem of actually computing the scale factors s for given boundary values s_∂ such that s gives rise to a conformally equivalent triangle mesh (in case it exists) can be solved using a variational principle for a convex functional, see [18, 68].

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References

1. V.E. Adler, A.I. Bobenko, Yu.B. Suris, Classification of integrable equations on quad-graphs. The consistency approach. Commun. Math. Phys. **233**(3), 513–543 (2003)
2. S.I. Agafonov, A.I. Bobenko, Discrete z^γ and Painlevé equations. Int. Math. Res. Not. **2000**(4), 165–193 (2000)
3. L.V. Ahlfors, *Complex Analysis*. International Series in Pure and Applied Mathematics, 3rd edn. (McGraw-Hill, New York, 1978)
4. A.F. Beardon, T. Dubejko, K. Stephenson, Spiral hexagonal circle packings in the plane. Geom. Dedicata **49**(1), 39–70 (1994)
5. D. Beliaev, S. Smirnov, Random conformal snowflakes. Ann. Math. (2) **172**(1), 597–615 (2010)
6. L. Bianchi, *Lezioni di geometria differenziale*, 3rd edn. (Enrico Spoerri, Pisa, 1923)
7. A.I. Bobenko, Discrete conformal maps and surfaces, in *Symmetries and Integrability of Difference Equations*, ed. by P.A. Clarkson, F.W. Nijhoff. London Mathematical Society Lecture Note Series, vol. 255 (Cambridge University Press, Cambridge, 1999), pp. 97–108
8. A.I. Bobenko, F. Günther, Discrete complex analysis on planar quad-graphs, in *Advances in Discrete Differential Geometry*, ed. by A.I. Bobenko (Springer, Berlin, 2016), pp. 57–132
9. A.I. Bobenko, T. Hoffmann, Conformally symmetric circle packings. A generalization of Doyle spirals. Exp. Math. **10**, 141–150 (2001)
10. A.I. Bobenko, T. Hoffmann, Hexagonal circle patterns and integrable systems: patterns with constant angles. Duke Math. J. **116**, 525–566 (2003)
11. A.I. Bobenko, U. Pinkall, Discrete isothermic surfaces. J. Reine Angew. Math. **475**, 187–208 (1996)
12. A.I. Bobenko, U. Pinkall, Discretization of surfaces and integrable systems, in *Discrete Integrable Geometry and Physics*, ed. by A.I. Bobenko, R. Seiler. Oxford Lecture Series in Mathematics and Its Applications, vol. 16 (Clarendon Press, New York, 1999), pp. 3–58
13. A.I. Bobenko, B.A. Springborn, Variational principles for circle patterns and Koebe's theorem. Trans. Am. Math. Soc. **356**, 659–689 (2004)
14. A.I. Bobenko, Yu.B. Suris, Integrable systems on quad-graphs. Int. Math. Res. Not. **11**, 573–611 (2002)
15. A.I. Bobenko, Yu.B. Suris, *Discrete Differential Geometry. Integrable Structure*. Graduate Studies in Mathematics, vol. 98 (American Mathematical Society, Providence, 2008)
16. A.I. Bobenko, T. Hoffmann, Yu.B. Suris, Hexagonal circle patterns and integrable systems: patterns with the multi-ratio property and Lax equations on the regular triangular lattice. Int. Math. Res. Not. **3**, 111–164 (2002)
17. A.I. Bobenko, C. Mercat, Yu.B. Suris, Linear and nonlinear theories of discrete analytic functions. Integrable structure and isomonodromic Green's function. J. Reine Angew. Math. **583**, 117–161 (2005)
18. A.I. Bobenko, U. Pinkall, B. Springborn, Discrete conformal maps and ideal hyperbolic polyhedra. Geom. Topol. **19**(4), 2155–2215 (2015)
19. C. Bohle, F. Pedit, U. Pinkall, Discrete holomorphic geometry I. Darboux transformations and spectral curves. J. Reine Angew. Math. **637**, 99–139 (2009)
20. S. Born, U. Bücking, , B.A. Springborn, Quasiconformal distortion of projective transformations and discrete conformal maps. Discrete Comput. Geom. **57**, 305–317 (2017)

21. G.R. Brightwell, E.R. Scheinerman, Representations of planar graphs. SIAM J. Discrete Math. **6**(2), 214–229 (1993)
22. U. Bücking, Approximation of conformal mappings by circle patterns. Geom. Dedicata **137**, 163–197 (2008)
23. U. Bücking, Rigidity of quasicrystallic and z^γ-circle patterns. Discrete Comput. Geom. **46**(2), 223–251 (2011)
24. U. Bücking, Approximation of conformal mappings on triangular lattices, in *Advances in Discrete Differential Geometry*, ed. by A.I. Bobenko (Springer, Berlin, 2016), pp. 133–149
25. D. Chelkak, Robust discrete complex analysis: a toolbox. Ann. Probab. **44**(1), 628–683 (2016)
26. D. Chelkak, S. Smirnov, Universality in the 2D ising model and conformal invariance of fermionic observables. Invent. Math. **189**(3), 515–580 (2012)
27. J. Cieśliński, A. Doliwa, P.M. Santini, The integrable discrete analogues of orthogonal coordinate systems are multi-dimensional circular lattices. Phys. Lett. A **235**(5), 480–488 (1997)
28. R. Courant, K. Friedrichs, H. Lewy, Über die partiellen Differentialgleichungen der mathematischen Physik. Math. Ann. **100**, 32–74 (1928)
29. G. Darboux, *Leçons sur les systèmes orthogonaux et les coordonnées curvilignes*, 2nd edn. (Gauthies-Villars, Paris, 1910)
30. G. Darboux, *Leçons sur la théorie générale des surfaces et les applications géométriques du calcul infinitésimal*, vols. I–IV, 2nd edn. (Gauthies-Villars, Paris, 1914–1927)
31. T. Dubejko, K. Stephenson, Circle packing: experiments in discrete analytic function theory. Exp. Math. **4**, 307–348 (1995)
32. R.J. Duffin, Basic properties of discrete analytic functions. Duke Math. J. **23**, 335–363 (1956)
33. R.J. Duffin, Potential theory on a rhombic lattice. J. Comb. Theory **5**, 258–272 (1968)
34. I.A. Dynnikov, S.P. Novikov, Geometry of the triangle equation on two-manifolds. Mosc. Math. J. **3**(2), 419–438 (2003)
35. J. Ferrand, Fonctions préharmoniques et fonctions préholomorphes. Bull. Sci. Math. (2) **68**, 152–180 (1944)
36. E. Freitag, R. Busam, *Complex Analysis*, 2nd edn. (Springer, Berlin, 2009)
37. P.G. Grinevich, S.P. Novikov, The Cauchy kernel for the Dynnikov–Novikov DN-discrete complex analysis in triangular lattices. Russ. Math. Surv. **62**(4), 799–801 (2007)
38. B. Grünbaum, *Convex Polytopes*. Pure and Applied Mathematics, vol. 16 (Wiley, New York, 1967)
39. X. Gu, R. Guo, F. Luo, J. Sun, T. Wu, A discrete uniformization theorem for polyhedral surfaces. II. arXiv:1401.4594
40. X. Gu, F. Luo, J. Sun, T. Wu, A discrete uniformization theorem for polyhedral surfaces. arXiv:1309.4175
41. F. Günther, Discrete Riemann surfaces and integrable systems. Ph.D. thesis, TU Berlin (2014)
42. Z. -X. He, Rigidity of infinite disk patterns. Ann. Math. **149**, 1–33 (1999)
43. Z. -X. He, O. Schramm, On the convergence of circle packings to the Riemann map. Invent. Math. **125**(2), 285–305 (1996)
44. Z. -X. He, O. Schramm, The C^∞-convergence of hexagonal disk packings to the Riemann map. Acta Math. **180**(2), 219–245 (1998)
45. U. Hertrich-Jeromin, T. Hoffmann, U. Pinkall, A discrete version of the Darboux transformation for isothermic surfaces, in *Discrete Integrable Geometry and Physics*, ed. by A.I. Bobenko, R. Seiler, Oxford Lecture Series in Mathematics and Its Applications, vol. 16 (Clarendon Press, New York, 1999), pp. 59–81
46. R. Hirota, Nonlinear partial difference equations. III. Discrete sine-Gordon equation. J. Phys. Soc. Jpn. **43**, 2079–2086 (1977)
47. R.P. Isaacs, A finite difference function theory. Univ. Nac. Tucumán Revista A **2**, 177–201 (1941)
48. R. Kenyon, Conformal invariance of domino tiling. Ann. Probab. **28**(2), 759–795 (2000)
49. R. Kenyon, The Laplacian and Dirac operators on critical planar graphs. Invent. Math. **150**(2), 409–439 (2002)

50. R. Kenyon, J. -M. Schlenker, Rhombic embeddings of planar quad-graphs. Trans. Am. Math. Soc. **357**(9), 3443–3458 (2005)
51. P. Koebe, Kontaktprobleme der konformen Abbildung. Abh. Sächs. Akad. Wiss. Leipzig Math.-Natur. Kl. **88**, 141–164 (1936)
52. B.G. Konopelchenko, W.K. Schief, Menelaus' theorem, Clifford configurations and inversive geometry of the Schwarzian KP hierarchy. J. Phys. A **35**(29), 6125–6144 (2002)
53. B.G. Konopelchenko, W.K. Schief, Reciprocal figures, graphical statics, and inversive geometry of the Schwarzian BKP hierarchy. Stud. Appl. Math. **109**(1), 89–124 (2002)
54. W.Y. Lam, U. Pinkall, Holomorphic vector fields and quadratic differentials on planar triangular meshes, in *Advances in Discrete Differential Geometry*, ed. by A.I. Bobenko (Springer, Berlin, 2016), pp. 241–265
55. S.-Y. Lan, D.-Q. Dai, The C^∞-convergence of SG circle patterns to the Riemann mapping. J. Math. Anal. Appl. **332**(2), 1351–1364 (2007)
56. F. Luo, Combinatorial Yamabe flow on surfaces. Commun. Contemp. Math. **6**(5), 765–780 (2004)
57. D. Matthes, Convergence in discrete Cauchy problems and applications to circle patterns. Conform. Geom. Dyn. **9**, 1–23 (2005)
58. C. Mercat, Discrete Riemann surfaces and the Ising model. Commun. Math. Phys. **218**, 177–216 (2001)
59. T. Miwa, On Hirota's difference equations. Proc. Jpn. Acad. Ser. A Math. Sci. **58**, 9–12 (1982)
60. J.J.C. Nimmo, W.K. Schief, Superposition principles associated with the Moutard transformation: an integrable discretization of a $(2 + 1)$-dimensional sine-Gordon system. Proc. Math. Phys. Eng. Sci. **453**(1957), 255–279 (1997)
61. S.P. Novikov, New discretization of complex analysis: the Euclidean and hyperbolic planes. Proc. Steklov Inst. Math. **273**(1), 238–251 (2011)
62. I. Rivin, Euclidean structures on simplicial surfaces and hyperbolic volume. Ann. Math. (2) **139**(3), 553–580 (1994)
63. B. Rodin, D. Sullivan, The convergence of circle packings to the Riemann mapping. J. Differ. Geom. **26**(2), 349–360 (1987)
64. O. Schramm, How to cage an egg. Invent. Math. **107**(3), 543–560 (1992)
65. O. Schramm, Circle patterns with the combinatorics of the square grid. Duke Math. J. **86**, 347–389 (1997)
66. O. Schramm, S. Sheffield, Harmonic explorer and its convergence to SLE_4. Ann. Probab. **33**(6), 2127–2148 (2005)
67. S. Smirnov, H. Duminil-Copin, Conformal invariance of lattice models, in *Probability and Statistical Physics in Two and More Dimensions*, ed. by D. Ellwood, C. Newman, V. Sidoravicius, W. Werner. Clay Mathematics Proceedings, vol. 15 (American Mathematical Society, Providence, 2012), pp. 213–276
68. B. Springborn, P. Schröder, U. Pinkall, Conformal equivalence of triangle meshes. ACM Trans. Graph. **27**(3), 77 (2008)
69. K. Stephenson, *Introduction to Circle Packing* (Cambridge University Press, Cambridge, 2005)
70. W.P. Thurston, The finite Riemann mapping theorem. Invited address at the International Symposium in Celebration of the Proof of the Bieberbach Conjecture, Purdue University (1985)
71. T. Wu, D. Gu, J. Sun, Rigidity of infinite hexagonal triangulation of the plane. Trans. Am. Math. Soc. **367**(9), 6539–6555 (2015)
72. G.M. Ziegler, Convex polytopes: extremal constructions and f-vector shapes, in *Geometric Combinatorics*, ed. by E. Miller, V. Reiner, B. Sturmfels. IAS/Park City Mathematics Series, vol. 13 (American Mathematical Society, Providence, 2007), pp. 617–692

Discrete Integrable Systems, Darboux Transformations, and Yang–Baxter Maps

Deniz Bilman and Sotiris Konstantinou-Rizos

Abstract This chapter is devoted to the integrability of discrete systems and their relation to the theory of Yang–Baxter (YB) maps. Lax pairs play a significant role in the integrability of discrete systems. We introduce the notion of Lax pair by considering the well-celebrated doubly-infinite Toda lattice. In particular, we present solution of the Cauchy initial value problem via the method of the inverse scattering transform, provide a review of scattering theory of Jacobi matrices, and give the Riemann–Hilbert formulation of the inverse scattering transform. On the other hand, the Lax–Darboux scheme constitutes an important tool in the theory of integrable systems, as it relates several concepts of integrability. We explain the role of Darboux and Bäcklund transformations in the theory of integrable systems, and we show how they can be used to construct discrete integrable systems via the Lax–Darboux scheme. Moreover, we give an introduction to the theory of Yang–Baxter maps and we show its relation to discrete integrable systems. Finally, we demonstrate the construction of Yang–Baxter maps via Darboux transformations, using the Nonlinear Schrödinger (NLS) equation as illustrative example.

1 Introduction

Discrete systems, namely systems with their independent variables taking discrete values, are of particular interest and have many applications in several sciences as physics, biology, financial mathematics, as well as several other branches of mathematics, since they are essential in numerical analysis. Initially, they were appearing as discretizations of continuous equations, but now discrete integrable systems, and in particular those defined on a two-dimensional lattice, are appreciated in their own right from a theoretical perspective.

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As in the continuous case, the definition of integrability for discrete systems is itself highly nontrivial; there are several opinions on what "integrable" should mean, which makes the definition of integrability elusive, rather than tangible. In fact, a comprehensive definition of integrability is not yet available. As working definitions we often use the existence of a Lax pair, the solvability of the system by the inverse scattering transform method, the existence of infinitely many symmetries or conservation laws, or the existence of a sufficient number of first integrals which are in involution (Liouville integrability). For infinite dimensional systems, the existence of a Lax pair provides a change of variables (through "scattering data" associated to the Lax operator) which linearizes the flow. Thus, existence of a Lax pair can be taken as a practical definition for integrability for systems with infinite dimensional phase space, e.g., PDEs. For more information on *what is integrability* one can consult [128] and the references therein.

Historically, the study of discrete systems and their integrability earned its interest in late seventies; Hirota studied particular discrete systems in 1977, in a series of papers [58–61] where he derived discrete analogues of many already famous PDEs. In the early eighties, semidiscrete and discrete systems started appearing in field-theoretical models in the work of Jimbo and Miwa; they also provided a method of generating discrete soliton equations [25–29]. Shortly after, Ablowitz and Taha in a series of papers [113–115] are using numerical methods in order to find solutions for known integrable PDEs, using as basis of their method some partial difference equations, which are integrable in their own right. Moreover, Capel, Nijhoff, Quispel and collaborators provided some of the first systematic tools for studying discrete integrable systems and, in particular, for the direct construction of integrable lattice equations (we indicatively refer to [95, 104]); that was a starting point for new systems of discrete equations to appear in the literature.

In 1991 Grammaticos et al. proposed the first discrete integrability test, known as *singularity confinement* [52], which is similar to that of the Painlevé property for continuous integrability. However, as mentioned in [53], it is not sufficient criterion for predicting integrability, as it does not furnish any information about the rate of growth of the solutions of the discrete integrable system.

As in the continuous case, the usual integrability criterion being used for discrete systems is the existence of a Lax pair. The existence of such pair is the key point to the integrability of a nonlinear system under the inverse scattering transform. On the other hand, Darboux transformations (DTs) associated to Lax operators constitute very important tools in the theory of integrable systems, since they link continuous integrable systems to discrete integrable ones. Moreover, the study of Darboux transformations gives rise to several other notions of integrability, such as Bäcklund transformations (BTs), conservation laws, symmetries etc. Additionally, the associated Darboux matrices can be used to construct Yang–Baxter maps. Yet another significant integrability criterion for difference equations and systems of difference equations is the so-called 3D-*consistency* and, by extension, the *multidimensional consistency*, which were proposed independently by Nijhoff in 2001 [94] and Bobenko and Suris in 2002 [19]. As we shall see later on, there is a strict relation between the 3D-consistency and the Yang–Baxter equation.

This chapter splits into two logical parts: In the first part, namely Sect. 2, we explain the basic steps of the inverse scattering transform method for solution of the Cauchy initial value problem for an integrable equation, using as illustrative example the famous doubly-infinite Toda lattice: a discrete space–continuous time system. More specifically, we begin with the classical problem of a doubly-infinite one-dimensional chain of interacting particles, which becomes completely integrable (the Toda lattice) if the interaction potential is the Toda potential. As is well-known, the Toda lattice equations can be recast as an isospectral deformation on Jacobi matrices and this gives rise to the existence of a Lax pair. Thus, we move on to cover scattering theory for doubly-infinite Jacobi matrices, introduce the direct scattering transform and scattering data associated with a Jacobi matrix. Then, we cover the time evolution of the scattering data under the dynamics induced by the Toda lattice equations, and discuss the Riemann–Hilbert formulation of the inverse scattering transform. We finally give a brief description and literature survey of analogous techniques applied to the finite Toda lattice and periodic Toda lattice systems.

In the second part, namely Sects. 3 and 4, we introduce the Darboux–Lax (or Lax–Darboux) scheme [16, 70, 87, 89] and we show the relation between Darboux transformations and discrete integrable systems. Moreover, we show the relation between the 3D-consistency and the Yang–Baxter equation, and we show how, using Darboux transformations, we can construct Yang–Baxter maps which can be restricted to completely integrable ones on invariant leaves. More specifically, in Sect. 3 we give a brief introduction to Darboux and Bäcklund transformations and their role in the theory of integrable systems. Then, we explain the basic points of the Darboux-Lax scheme, and we demonstrate them using the nonlinear Schrödinger (NLS) equation as an illustrative example. In particular, studying the Darboux transformations associated to the NLS equation we first derive a discrete integrable system, for which we present the initial value problem on the staircase. Then, using certain first integrals we reduce this discrete system to an Adler–Yamilov type of system [8]. Moreover, in the same way we construct the discrete Toda equation [108]. In Sect. 4 we give an introduction to equations on quad graphs & the 3D-consistency criterion, and we present some recent classification results. Then, we give and introduction to the theory of Yang–Baxter maps, namely set-theoretical solutions of the Yang–Baxter equation, and we explain their relation with 3D-consistent equations. We focus on those Yang–Baxter maps which possess Lax-representation and we show how one can construct them using Darboux transformations. As an illustrative example we use the Darboux transformation of the NLS equation, which was presented in Sect. 3, and we use it to construct a six-dimensional Yang–Baxter map [68]. The former can be restricted to the completely integrable Adler–Yamilov map on symplectic leaves [68].

2 The Toda Lattice

2.1 One-Dimensional Chain of Particles

Consider the classical problem of one-dimensional chain of particles on a line with nearest neighbor interactions as depicted in Fig. 1. Assume that each particle has unit mass, and that there are no impurities, i.e., the potential energies of the springs between the particles are identical. In this treatment, our focus is going to be the doubly-infinite lattices. Therefore, unless otherwise noted, we assume that there are infinitely many particles on a line. We let $V\colon \mathbb{R} \to \mathbb{R}$ denote the uniform interaction potential between the neighboring particles. With the aforementioned assumptions, the equations of motion that govern this system are given by

$$\frac{\mathrm{d}^2 q_n}{\mathrm{d}t^2} = V'(q_{n+1} - q_n) - V'(q_n - q_{n-1}) \,, \quad n \in \mathbb{Z} \,, \tag{1}$$

where q_n stands for the displacement of the nth particle from its equilibrium position. If $V'(r) = \mathrm{d}V(r)/\mathrm{d}r$, that is if $V'(r)$ is proportional to r, that is V is a harmonic potential, then the force which governs the interaction between the particles is linear. In this case, the solutions are given by superpositions of normal modes and there is no transfer of energy between these modes.

The general belief in the early 1950s was that if a nonlinearity is introduced in the interaction of these particles, then energy would flow between the different modes, eventually leading to a stable state of statistical equilibrium, i.e., thermalization. In the summer of 1953 at Los Alamos National Laboratory, E. Fermi, J. Pasta, and S. Ulam, together with M. Tsingou, set out to numerically study the thermalization process in solids by conducting one of the first-ever numerical experiments using the first electronic computer **MANIAC**—**M**athematical **A**nalyzer, **N**umerical **I**ntegrator and **C**omputer. To model solids, they used the aforementioned one-dimensional chain of particles with 32 particles and 64 particles, equipped interaction potentials which had weak nonlinear terms. More explicitly, they considered the potentials

$$V_\alpha(r) = \tfrac{1}{2} r^2 + \alpha r^3 \,, \quad V_\beta(r) = \tfrac{1}{2} r^2 + \beta r^4 \,, \tag{2}$$

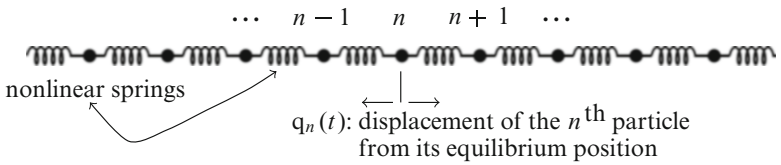


Fig. 1 One-dimensional chain of particles with nearest neighbor interactions

with α and β being small and positive constants. The expectation was to observe equipartition of energy as time elapses due to the presence of nonlinear contributions in the potentials. One day, they forgot to terminate the experiment and it went on over the weekend. To their surprise, they found that the system exhibited quasiperiodic behavior. The energy of the system revisited the initially excited modes and the initial state was almost exactly recovered. This phenomenon, known as the FPU recurrence, has been studied from various perspectives, including ergodicity, Poincaré recurrence theory, and KAM theory (see [31] for a survey article on the so-called FPU Experiment, [46] for an earlier article and the references therein.) Ten years after the experiment, Kruskal and Zabusky made the groundbreaking discovery of the "soliton" solution of the Korteweg–de Vries (KdV) equation in their pioneering work [127]. Zabusky and Kruskal coined the name 'soliton' to these traveling "solitary wave" solutions of the KdV equation because they retained their speed and shape upon interacting with such other waves—they interacted as particles. The observation that the lattices used in the FPU Experiment approximated KdV equation [127], which exhibited solitonic behavior, in an appropriate continuum limit provided an explanation for the FPU recurrence. This work led to a big growth in research on nonlinear waves, particularly on solitons. It also triggered a search for an interaction potential for which the resulting lattice system possesses traveling solitary wave solutions. In 1972, while working on elliptic functions, M. Toda considered the exponential interaction potential (see Fig. 2)

$$V_{\text{Toda}}(r) = \mathrm{e}^{-r} + r - 1 \,, \tag{3}$$

and found out that the resulting lattice, now known as the Toda lattice, has soliton solutions.

The Toda potential (3) leads to an explicit form of the evolution equations (1), namely:

$$\frac{\mathrm{d}^2 q_n}{\mathrm{d}t^2} = \mathrm{e}^{q_n - q_{n+1}} - \mathrm{e}^{q_{n-1} - q_n} \,, \quad n \in \mathbb{Z} \,, \tag{4}$$

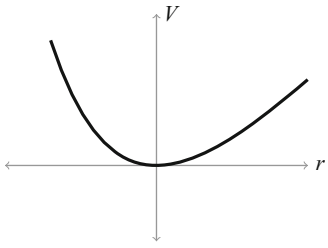


Fig. 2 The graph $V = V_{\text{Toda}}(r)$

where we suppressed the time dependence of q.[1] If we denote the momentum of the nth particle at a time t by $p_n(t)$, then we can rewrite (4) as the first-order system:

$$\frac{\mathrm{d}p_n}{\mathrm{d}t} = \mathrm{e}^{-(q_n - q_{n-1})} - \mathrm{e}^{-(q_{n+1} - q_n)} , \quad \frac{\mathrm{d}q_n}{\mathrm{d}t} = p_n , \tag{5}$$

for each $n \in \mathbb{Z}$. If we assume that $q_{n+1} - q_n \to 0$ and $p_n \to 0$ sufficiently fast as $|n| \to \infty$, we can recast (5) as a Hamiltonian system of equations

$$\frac{\mathrm{d}p_n}{\mathrm{d}t} = -\frac{\partial \mathcal{H}(p,q)}{\partial q_n} , \quad \frac{\mathrm{d}q_n}{\mathrm{d}t} = \frac{\partial \mathcal{H}(p,q)}{\partial p_n} , \tag{6}$$

with the Hamiltonian $\mathcal{H}(p,q)$:

$$\mathcal{H}(p,q) = \mathcal{H}_{\mathrm{Toda}}(p,q) := \sum_{n\in\mathbb{Z}} \frac{1}{2}p_n^2 + V_{\mathrm{Toda}}(q_{n+1} - q_n) . \tag{7}$$

2.2 Solitons

As mentioned earlier, the doubly-infinite Toda lattice has soliton solutions. Solitons are localized traveling waves (solitary waves) which interact like particles: they preserve their shapes and speeds after interacting with another wave. If two 1-solitons interact, no dispersive wave is generated after the interaction. A 1-soliton solution travels with a constant speed and constant amplitude, which are proportional. 1-soliton solutions for the displacements in the Toda lattice are given explicitly by the following 2-parameter family:

$$q_n^{[1]}(t) = q_{\mathrm{R}} + \log\left(\frac{1 + \big(\gamma/(1-\mathrm{e}^{-2\kappa})\big)\mathrm{e}^{-2\kappa(n-1)-2k\sigma ct}}{1 + \big(\gamma/(1-\mathrm{e}^{-2\kappa})\big)\mathrm{e}^{-2\kappa n-2\kappa\sigma ct}}\right) , \tag{8}$$

where $\gamma > 0$, $\kappa > 0$ is the wave number, $c = (\sinh\kappa)/\kappa > 1$ is the speed of propagation, and $\sigma = \pm 1$ is the constant determining direction of propagation. Here $q_{\mathrm{R}} = \lim_{n\to+\infty} q_n(t)$ for all finite t. See Fig. 3 for a plot of such a solution.

In fact there are N-soliton solutions, for $N \in \mathbb{N}$, whose formulae are of the form

$$q_n^{[N]}(t) = q_{\mathrm{R}} + \log\left(\frac{\det\big(\mathbb{I}_n + \mathbf{C}^{[N]}(n,t)\big)}{\det\big(\mathbb{I} + \mathbf{C}^{[N]}(n+1,t)\big)}\right) , \tag{9}$$

[1] We employ two notational conventions in this section. We use bold capital letters to denote a matrix, say $\mathbf{A}$, and use the regular capital type of the same letter to denote its entries: A_{ij}. Whenever it is clear from the context, we use x to denote a sequence $\{x_n\}_{n\in\mathbb{Z}}$.

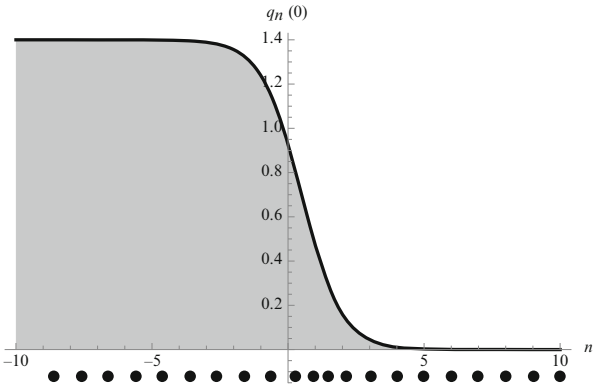


Fig. 3 One-soliton solution of the Toda lattice at time $t = 0$

where $\mathbb{I}_n$ is the $N \times N$ identity matrix. The entries of the $N \times N$ matrices $\mathbf{C}^{[N]}(n,t)$ are given by

$$C_{ij}^{[N]}(n,t) = \left(\frac{\sqrt{\hat{\gamma}_j(n,t)\hat{\gamma}_k(n,t)}}{1 - \mathrm{e}^{-(\kappa_j+\kappa_k)}} \right), \quad \hat{\gamma}_j(n,t) = \gamma_j \mathrm{e}^{-2\kappa_j n - 2\sigma_j \sinh(\kappa_j)t},$$

for $\gamma_j > 0$, $\kappa_j > 0$, and $\sigma_j \in \{-1, 1\}$. The case $N = 1$ coincides with the 1-soliton solution (8). Asymptotically, as $t \to \infty$, the N-soliton solution can be written as a sum of 1-soliton solutions as was proved in [78].

We shall see below that these solutions are *reflectionless* solutions since the reflection coefficient in the associated scattering data is identically zero.

2.3 Complete Integrability and Scattering Theory

Complete integrability of the Toda lattice equations (7) can be established by considering an eigenvalue problem for a second order linear difference operator.

2.3.1 Existence of a Lax Pair

In 1974, Flaschka [43, 44] and Manakov [82] independently and simultaneously introduced the following variables to obtain a first-order system of differential equations that is equivalent to the Toda lattice:

$$a_n := \tfrac{1}{2}\mathrm{e}^{-(q_{n+1}-q_n)/2}, \quad b_n := -\tfrac{1}{2}p_n. \tag{10}$$

If $q_n \to q_{\mathrm{R,L}} \in \mathbb{R}$ sufficiently fast as $n \to \pm\infty$, the inverse map is given by

$$q_n = q_{\mathrm{R}} + 2\log\left(\prod_{k=n}^{\infty} 2a_n \right), \quad p_n = -2b_n,$$

and (10) is a bijection. Note that $q_n \to q_{\mathrm{R,L}}$ and $p_n \to 0$ as $n \to \pm\infty$ corresponds to $a_n \to \frac{1}{2}$ and $b_n \to 0$ as $|n| \to \infty$. It is immediately verified that the pair of sequences (p, q) satisfies (5) if and only if the pair (a, b) defined via (10) satisfies the equations

$$\frac{\mathrm{d}a_n}{\mathrm{d}t} = a_n(b_{n+1} - b_n) \,, \quad \frac{\mathrm{d}b_n}{\mathrm{d}t} = 2(a_n^2 - a_{n-1}^2) \,. \tag{11}$$

Using the pair of sequences introduced in (10), define the operators $\mathbf{L}$ and $\mathbf{P}$ on the Hilbert space $\ell^2(\mathbb{Z})$ of square-summable sequences:

$$\begin{aligned} (\mathbf{L}\phi)_n &:= a_{n-1}\phi_{n-1} + b_n\phi_n + a_n\phi_{n+1} \,, \\ (\mathbf{P}\phi)_n &:= -a_{n-1}\phi_{n-1} + a_n\phi_{n+1} \,. \end{aligned} \tag{12}$$

In the standard basis, $\mathbf{L}$ and $\mathbf{P}$ have doubly-infinite matrix representations.They are given explicitly by:

$$\mathbf{L} = \begin{pmatrix} \ddots & \ddots & \ddots & & \\ \ddots & b_{n-1} & a_{n-1} & 0 & \\ \ddots & a_{n-1} & b_n & a_n & \ddots \\ & 0 & a_n & b_{n+1} & \ddots \\ & & \ddots & \ddots & \ddots \end{pmatrix} \,, \quad \mathbf{P} = \begin{pmatrix} \ddots & \ddots & \ddots & & \\ \ddots & 0 & a_{n-1} & 0 & \\ \ddots & -a_{n-1} & 0 & a_n & \ddots \\ & 0 & -a_n & 0 & \ddots \\ & & \ddots & \ddots & \ddots \end{pmatrix} \,. \tag{13}$$

Note that $\mathbf{L}$ is a doubly-infinite Jacobi matrix: symmetric, tridiagonal with positive off-diagonal entries. The following proposition gives the existence of a Lax pair for the Toda lattice.

Proposition 2.1 (Flaschka [43, 44], Manakov [82]) *The Toda lattice equations* (11) *are equivalent to the matrix equation*

$$\frac{\mathrm{d}\mathbf{L}}{\mathrm{d}t} = [\mathbf{P}, \mathbf{L}], \tag{14}$$

where $[\mathbf{P}, \mathbf{L}]$ *denotes the matrix commutator*, $[\mathbf{P}, \mathbf{L}] := \mathbf{PL} - \mathbf{LP}$.

Proof By direct calculation. Left as an exercise. □

Equation (14) is called the Lax equation after Lax [79]; and the pair $(\mathbf{L}, \mathbf{P})$ is called a Lax pair. We will call $\mathbf{L}$ the Lax operator for the Toda lattice. Note that the matrix $\mathbf{P}$ defined in (13) depends on $\mathbf{L}$: $\mathbf{P} = \mathbf{L}_+ - \mathbf{L}_-$, where $\mathbf{L}_\pm$ stands for the upper $(+)$ and the lower $(-)$ diagonal parts of $\mathbf{L}$.

At this point, it must be stressed out, that (14), namely the *Lax formulation*, on one hand constitutes a basis for the inverse scattering method, but it also possesses a deeper property, i.e., the so-called *Hamiltonian formulation*. An equation

(or system of equations) is said to have a Hamiltonian formulation if they can be written as a (perhaps infinite-dimensional) classical Hamiltonian system. In general, Hamiltonian formulation is a characteristic of all equations (or systems of equations) which are solvable by the inverse scattering transform. Moreover, in our case, the inverse scattering transform can be understood as a canonical transformation of the associated Hamiltonian structure. The first example demonstrating the relation between the Lax pair and the Hamiltonian formulation was the famous KdV equation—to which we shall come back in the next subsection—in 1971 [129]. Just as the KdV equation, the Toda lattice also possesses infinitely many conserved quantities (see Exercise 2.3). For further study on Hamiltonian structure of Lax equations for integrable systems, the reader may consult [1, 3], or [42] (and the references therein) which is a self-contained textbook.

Remark 2.2 Proposition 2.1 holds for the finite Toda lattice with the boundary condition $a_{-1} = a_{N-1} = 0$ for some integer $N > 0$. In fact, complete integrability was first proved [43, 44, 82] for this finite version of the Toda lattice, and was later generalized to the infinite lattice. The equations of motion in the (a, b) variables for the finite the Toda lattice are given by:

$$\begin{aligned} \frac{\mathrm{d}b_0}{\mathrm{d}t} &= 2a_0^2 \,, \\ \frac{\mathrm{d}b_n}{\mathrm{d}t} &= 2(a_n^2 - a_{n-1}^2) \,, \qquad n = 1, 2, \ldots, N-2 \,, \\ \frac{\mathrm{d}a_n}{\mathrm{d}t} &= a_n(b_{n+1} - b_n) \,, \qquad n = 0, 1, 2, \ldots, N-2 \,, \\ \frac{\mathrm{d}b_{N-1}}{\mathrm{d}t} &= -2a_{N-2}^2 \,. \end{aligned} \tag{15}$$

Note that the condition $a_{-1} = a_{N-1} = 0$ corresponds to setting the relative displacements $q_N - q_{N-1}$ and $q_0 - q_{-1}$ to be infinite. This is sometimes called a *reservoir* condition in the literature.

Exercise 2.3 Show that if the Lax equation (14) holds for $\mathbf{L}(t)$, then it also holds for the matrix power $\mathbf{L}(t)^m$, for any $m \in \mathbb{N}$. Using this, find an infinite sequence of conserved quantities for the Toda lattice equations: $\operatorname{trace}(\mathbf{L}(t)^m - \mathbf{L}_\infty{}^m)$, where $\mathbf{L}_\infty$ is the doubly infinite Jacobi matrix with $\lim_{|n|\to\infty} b_n = 0$ on its diagonal and $\lim_{|n|\to\infty} a_n = 1/2$ on its off-diagonal.

Exercise 2.4 (Teschl [117]) For two sequences $\psi, \phi \in \ell(\mathbb{Z})$ define

$$\mathcal{G}(\psi, \phi)(n) = \psi_n(\mathbf{L}\phi)_n - \phi_n(\mathbf{L}\psi)_n \,.$$

Prove Green's formula:

$$\sum_{j=m}^{n} \mathcal{G}(\phi, \psi)(j) = \mathcal{W}_n(\psi, \phi) - \mathcal{W}_{m-1}(\psi, \phi) \,, \tag{16}$$

where $\mathcal{W}_n(\phi, \psi)$ stands for the Wronskian which is defined by

$$\mathcal{W}_n(\psi, \phi) = a_n(\psi_n \phi_{n+1} - \psi_{n+1}\phi_n) \,. \tag{17}$$

Before we cover scattering data associated with $\mathbf{L}$ we have the following theorem that summarizes its basic properties.

Theorem 2.5 (from [117, Theorem 1.5]) *Assume that $a, b \in \ell^\infty(\mathbb{Z})$, with $a_n > 0$ for all $n \in \mathbb{Z}$. Then $\mathbf{L}$ defined in (12) is a bounded self-adjoint operator on $\ell^2(\mathbb{Z})$. Moreover, $a, b \in \ell^\infty(\mathbb{Z})$ if and only if $\mathbf{L}$ is bounded on $\ell^2(\mathbb{Z})$.*

Proof For $\psi, \phi \in \ell^2(\mathbb{Z})$ we have $\lim_{n\to\pm\infty} \mathcal{W}_n(\psi, \phi) = 0$, where $\mathcal{W}_n(\cdot, \cdot)$ is the Wronskian defined in (17). Using this together with Green's formula (16) from Exercise 2.4 implies that

$$\langle \phi, \mathbf{L}\psi \rangle_{\ell^2} = \langle \mathbf{L}\phi, \psi \rangle_{\ell^2} \,,$$

for all $\phi, \psi \in \ell^2(\mathbb{Z})$, proving that $\mathbf{L}$ is self-adjoint. Now, if $a, b \in \ell^\infty(\mathbb{Z})$, then for any $\phi \in \ell^2(\mathbb{Z})$

$$|\langle \phi, \mathbf{L}\phi \rangle_{\ell^2}| \leq (2\|a\|_\infty + \|b\|_\infty)\|\phi\|_2^2 \,,$$

which implies that $\|\mathbf{L}\| \leq 2\|a\|_\infty + \|b\|_\infty$, where $\|\cdot\|$ denotes the operator norm. On the other hand, assume that $\mathbf{L}$ is bounded. Let $\left\{\delta_n^{[k]}\right\}_{n\in\mathbb{Z}}$ denote the sequence defined by $\delta_n^{[k]} = 0$ if $n \neq k$ and $\delta_k^{[k]} = 1$. Then for any $k \in \mathbb{Z}$

$$a_k^2 + a_{k-1}^2 + b_k^2 = \left\|\mathbf{L}\delta^{[k]}\right\|_2^2 \leq \|\mathbf{L}\|^2 \,,$$

which implies that a and b belong to $\ell^\infty(\mathbb{Z})$. This completes the proof. □

For a detailed treatment on Jacobi matrices and the associated difference operators we refer the reader to [117].

As is well-known, the integrability of the Toda lattice can be exploited via the bijective correspondence between the Lax operator, which in this case is the Jacobi matrix $\mathbf{L}$, and its scattering data. This correspondence goes under the name of direct and inverse scattering theory, and has already been studied in detail. While we do not attempt to give a comprehensive survey of the relevant references, the interested reader may enter the subject, for example, through [117] or [17], and the references therein. We now proceed with the spectral properties of the Lax operator $\mathbf{L}$ and definition of the scattering data.

2.3.2 Spectral Properties of the Lax Operator L

For the moment, we forget about the time dependence and begin with a brief study of the spectrum associated with the doubly-infinite Jacobi matrix $\mathbf{L}$ given in (13). First,

recall from Theorem 2.5 that $\mathbf{L}$ is a bounded self-adjoint operator on $\ell^2(\mathbb{Z})$. Thus it bears no residual spectrum and its spectrum $\sigma(\mathbf{L})$ is a subset of $\mathbb{R}$. Let $\mathcal{M}$ denote the *Marchenko* class of Jacobi matrices whose coefficients $(a, b) \in \ell^\infty(\mathbb{Z}) \oplus \ell^\infty(\mathbb{Z})$ satisfy

$$\sum_{n\in\mathbb{Z}} (1+|n|)\big(\big|a_n - \tfrac{1}{2}\big| + |b_n|\big) < \infty \,. \tag{18}$$

Throughout this section, we assume that $a_n > 0$ for all $n \in \mathbb{Z}$ and that (18) holds. We later present the theorem which states that these two conditions are preserved by the Toda lattice equations (11).

The following theorem from [117] locates the essential spectrum of $\mathbf{L}$ under an assumption that is weaker than (18). We present it in a version that is simplified for our setting and purposes.

Theorem 2.6 (from [117, Theorem 3.19]) *Suppose that the sequences $(a, b) \in \ell^\infty(\mathbb{Z}) \oplus \ell^\infty(\mathbb{Z})$, with $a_n > 0$ for all $n \in \mathbb{Z}$, satisfy*

$$\sum_{n\in\mathbb{Z}} |a_{n+1} - a_n| + |b_{n+1} - b_n| < \infty \,. \tag{19}$$

Suppose further that $\lim_{|n|\to\infty} a_n = \frac{1}{2}$ and $\lim_{|n|\to\infty} b_n = 0$. Then the following are true for the essential spectrum $\sigma_{\mathrm{ess}}(\mathbf{L})$ and the pure point spectrum $\sigma_{\mathrm{pp}}(\mathbf{L})$ of the associated Jacobi matrix $\mathbf{L}$:

$$\sigma_{\mathrm{ess}}(\mathbf{L}) = \sigma_{\mathrm{ac}}(\mathbf{L}) = [-1, 1] \,, \quad \sigma_{\mathrm{pp}}(\mathbf{L}) \subset \overline{\mathbb{R} \setminus \sigma_{\mathrm{ess}}(\mathbf{L})} \,. \tag{20}$$

Note that due to the closure present in (20), Theorem 2.6 does not exclude eigenvalues at the boundary of the essential spectrum, but it does prevent eigenvalues embedded in the interior of the essential spectrum. Here is an example illustrating presence of eigenvalues at the edge of the essential spectrum.

Example 2.7 (Teschl [117]) Consider the sequences (a, b) with

$$a_n = \frac{1}{2} \,, \quad b_n = \frac{2 - 3n^2}{4 + n^4} \,. \tag{21}$$

Then the associated Jacobi matrix has indeed an eigenvalue at $\lambda = 1$ with the corresponding eigenfunction $\phi \in \ell^2(\mathbb{Z})$ given by

$$\phi_n = \frac{1}{1 + n^2} \,. \tag{22}$$

The reason for this is that (18) is violated: the first moment $\sum_{n\in\mathbb{Z}} |n b_n|$ is divergent.

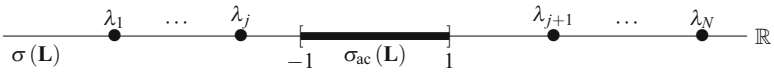


Fig. 4 Spectrum $\sigma(\mathbf{L})$ of $\mathbf{L}$ on the λ-plane, consisting of finitely many real simple eigenvalues $\{\lambda_j\}_{j=1}^N$ and the absolutely continuous part $\sigma_{\mathrm{ac}}(\mathbf{L}) = [-1, 1]$

Under the assumption (18), $\mathbf{L}$ has finitely many simple eigenvalues with associated eigenvectors in $\ell^2(\mathbb{Z})$. $\sigma(\mathbf{L})$ consists of an absolutely continuous part $\sigma_{\mathrm{ac}}(\mathbf{L}) = [-1, 1]$ and a finite simple pure point part $\sigma_{\mathrm{pp}}(\mathbf{L})$:

$$\sigma_{\mathrm{pp}}(\mathbf{L}) = \{\lambda_j : j = 1, 2, \ldots, N\} \subset (-\infty, -1) \cup (1, +\infty),$$

for some $N \in \mathbb{N}$. The spectrum of $\mathbf{L}$ typically is of the form depicted in Fig. 4.

We close this section with a series of remarks.

Remark 2.8 A Jacobi matrix $\mathbf{J}$ with bounded sequences b on the diagonal and a, with $a_n \neq 0$ for all $n \in \mathbb{Z}$, on the off-diagonal, is unitarily equivalent to the Jacobi matrix $\widetilde{\mathbf{J}}$ with b on the diagonal and $\{|a_n|\}_{n\in\mathbb{Z}}$ on the off-diagonal. Therefore, the assumption that $a_n > 0$ made in this section makes no difference from a spectral theory point of view. If $a_n = 0$ for some n however, $\mathbf{J}$ is decomposed in to a direct sum of two half-line (infinite) Jacobi matrices. The assumption that $a_n \neq 0$ for all n guarantees that the equation

$$\mathbf{J}\psi = \lambda\psi$$

has exactly two linearly independent solutions in $\ell(\mathbb{Z})$ for any $\lambda \in \mathbb{C}$, and that the spectrum of $\mathbf{J}$ has multiplicity at most two [117]. Thus, we need the assumption $a_n \neq 0$ to have a well defined, bijective direct and inverse scattering theory to solve the Cauchy initial value problem. Noting that the dynamics given in (11) preserve the signs of a_n, we can make the assumption $a_n > 0$.

Remark 2.9 The spectral problem

$$\mathbf{L}\psi = \lambda\psi$$

is a discrete analogue of the Sturm–Liouville eigenvalue problem. For a discrete version of Sturm oscillation theory, see [116] or [106] and the references therein.

Remark 2.10 The spectral properties of the Lax operator $\mathbf{L}$ are similar to the Schrödinger operator

$$H := -\frac{\mathrm{d}}{\mathrm{d}x} + u(x) \tag{23}$$

on the line, which arises as the Lax operator for the KdV equation

$$u_t + uu_x + u_{xxx} = 0 \,,$$

as was discovered by Gardner et al. in [48] (see also the seminal work of Lax [79]). Just as in the Toda case, if u in the Marchenko class

$$\int_{\mathbb{R}} (1 + |x|)|u(x)| \, \mathrm{d}x \,, \tag{24}$$

then H has finitely many real simple L^2-eigenvalues $-E_j^2$ on $(-\infty, 0)$ and an absolutely continuous spectrum $[0, +\infty)$. A difference is that the Jacobi matrix $\mathbf{L}$ has two sides to its continuous spectrum, where the Schrödinger operator has only one side. This manifests itself in the fact that Toda solitons can propagate in two directions whereas KdV solitons propagate in only one direction on the line.

2.3.3 Scattering Data

Our aim in this section is to define "spectral data" from the spectral problem

$$\mathbf{L}\psi = \lambda\psi \,, \tag{25}$$

that is enough to reconstruct $\mathbf{L}$ from. First, it is convenient to map the spectrum of $\mathbf{L}$ via the Joukowski transformation:

$$\lambda = \tfrac{1}{2}(z + z^{-1}) \,, \quad z = \lambda - \sqrt{\lambda^2 - 1} \,, \quad \lambda \in \mathbb{C}, \quad |z| \leq 1 \,.$$

Here the square root $\sqrt{\lambda^2 - 1}$ is defined to be positive for $\lambda > 1$ with $\sigma_{\mathrm{ac}}(\mathbf{L}) = [-1, 1]$ being its only branch cut. This is, of course, a 1-to-2 map. Under this transformation, the absolutely continuous spectrum is mapped to the unit circle, denoted by $\mathbb{T}$, and the eigenvalues λ_j are mapped to $\zeta_j^{\pm 1}$, with $\zeta_j \in (-1, 0) \cup (0, 1)$ via

$$\lambda_j = \tfrac{1}{2}(\zeta_j + \zeta_j^{-1}) \,, \tag{26}$$

for $j = 1, 2, \ldots, N$. In these new coordinates the spectrum of $\mathbf{L}$, which is depicted in Fig. 4, takes the form of the set of points illustrated in Fig. 5.

It is a standard result (see, for example,[117, Theorem 10.2]) that for any $z \in \mathbb{C}$ with $0 < |z| \leq 1$, the linear problem (the 3-term recurrence relation)

$$\mathbf{L}\psi = \frac{z + z^{-1}}{2}\psi \tag{27}$$

has two unique solutions, $\varphi_+(z, \cdot)$ and $\varphi_-(z, \cdot)$, normalized such that

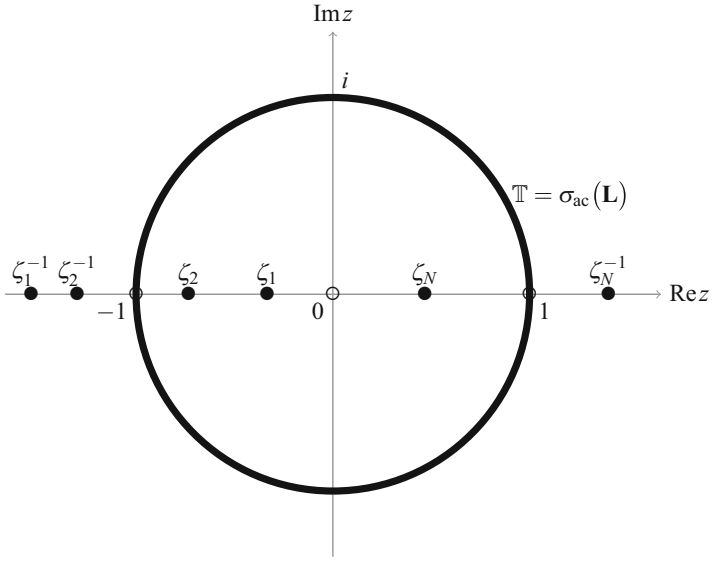


Fig. 5 $\sigma(\mathbf{L})$ in the z-plane, $z = \lambda - \sqrt{\lambda^2 - 1}$

$$\lim_{n\to\pm\infty} z^{\mp n}\varphi^{\pm}(z;n) = 1 \, .$$

These are called *Jost* solutions, named after Swiss theoretical physicist R. Jost. Moreover, the functions $z \mapsto \varphi_{\pm}(z;n)$ are analytic for $0 < |z| < 1$ (for each value of the parameter n) with continuous boundary values for $z = 1$. The Jost solutions have the following asymptotic expansions near $z = 0$:

$$\varphi_{\pm}(z;n) = \frac{z^{\pm n}}{A_{\pm}(n)}\big(1 + 2B_{\pm}(n)z + O(z^2)\big) \, , \quad \text{as } z \to 0 \, , \tag{28}$$

where

$$\begin{aligned} A_+(n,t) &= \prod_{j=n}^{\infty} 2a_j(t) \qquad \text{and} \qquad B_+(n,t) = -\sum_{j=n+1}^{\infty} b_j(t) \, , \\ A_-(n,t) &= \prod_{j=-\infty}^{n-1} 2a_j(t) \qquad \text{and} \qquad B_-(n,t) = -\sum_{-\infty}^{n-1} b_j(t) \, . \end{aligned} \tag{29}$$

Note that the functions $z \mapsto A_{\pm}(n)z^{\mp n}\varphi_{\pm}(z;n)$ are analytic for $|z| < 1$ and they extend continuously to the boundary $|z| = 1$. Moreover, $\mu_{\pm}(z;n) := A_{\pm}(n)z^{\mp n}\varphi_{\pm}(z;n)$ satisfies $\mu_{\pm}(0;n) = 1$.

Before we proceed with the definition of scattering data, we have an exercise.

Exercise 2.11 Suppose that $\phi(z)$ and $\psi(z)$ are two different solutions of (27) for the same value of $z+z^{-1}$. Show that their Wronskian $\mathcal{W}_n(\phi,\psi)$ is independent of n. **Hint:** Use Green's identity.

From here on, we drop the subscript n in the Wronskian whenever it is independent of n. In addition to the result of the above exercise, $\mathcal{W}(\phi,\psi)=0$ holds if and only if $\phi=c\psi$ for some constant $c\in\mathbb{C}$. Now, $\varphi_+(z;\cdot)$ and $\varphi_+(z^{-1};\cdot)$ solve (27) for the same value of $z+z^{-1}$. Evaluating their Wronskian as $n\to+\infty$ gives

$$\mathcal{W}\big(\varphi_+(z;\cdot),\varphi_+(z^{-1};\cdot)\big)=\frac{1}{2}(z^n z^{-(n+1)}-z^{n+1}z^{-n})=\frac{z^{-1}-z}{2}\,. \tag{30}$$

It similarly follows that

$$\mathcal{W}\big(\varphi_-(z;\cdot),\varphi_-(z^{-1};\cdot)\big)=\frac{z-z^{-1}}{2}\,. \tag{31}$$

Equations (30) and (31) show that $\{\varphi_-(z;\cdot),\varphi_-(z^{-1};\cdot)\}$ and $\{\varphi_+(z;\cdot),\varphi_+(z^{-1};\cdot)\}$ both form a set of linearly independent solutions of (27) for $|z|=1$ with $z^2\neq 1$. Therefore, we can write

$$\varphi_+(z;n)=\beta_-(z)\varphi_-(z;n)+\alpha_+(z)\varphi_-(z^{-1};n)\,, \tag{32}$$

$$\varphi_-(z;n)=\beta_+(z)\varphi_+(z;n)+\alpha_-(z)\varphi_+(z^{-1};n)\,. \tag{33}$$

Note that $\alpha_\pm(z)$ and $\beta_\pm(z)$ are independent of n. Now, using (32) and the asymptotics for the Jost solutions as $n\to-\infty$ we calculate

$$\mathcal{W}\big(\varphi_+(z;\cdot),\varphi_-(z;\cdot)\big)=\alpha_+(z)\frac{z^{-1}-z}{2}\neq 0 \tag{34}$$

for $|z|=1$ and $z^2\neq 1$. On the other hand, using (33) and the asymptotics as $n\to+\infty$ we obtain

$$\mathcal{W}\big(\varphi_+(z;\cdot),\varphi_-(z;\cdot)\big)=\alpha_-(z)\frac{z^{-1}-z}{2}\neq 0\,. \tag{35}$$

These imply that

$$\alpha_+(z)\equiv\alpha_-(z)\,,$$

hence we rename these quantities as $\Delta(z):=\alpha_+(z)=\alpha_-(z)$. Then

$$\Delta(z)=\frac{2z}{1-z^2}\mathcal{W}\big(\varphi_+(z;\cdot),\varphi_-(z;\cdot)\big)\,. \tag{36}$$

The above formula tells us that $\Delta(z)$ has no zeros on the unit circle, for $z^2 \neq 1$. We will come back to zeros of $\Delta(z)$ later. Now we move on to obtain formulae for $\beta_\pm(z)$. Using (33) and the asymptotics for the Jost solutions as $n \to +\infty$ yields

$$\mathcal{W}\big(\varphi_-(z;\cdot),\varphi_+(z^{-1};\cdot)\big) = \beta_+(z)\frac{z^{-1}-z}{2} \neq 0\,, \tag{37}$$

for $|z| = 1$, $z^2 \neq 1$. Similarly, using (32) and the asymptotics for the Jost solutions as $n \to -\infty$ gives us

$$\mathcal{W}\big(\varphi_-(z^{-1};\cdot),\varphi_+(z;\cdot)\big) = \beta_-(z)\frac{z^{-1}-z}{2}\,. \tag{38}$$

Hence

$$\begin{aligned}\beta_+(z) &= \frac{2z}{1-z^2}\mathcal{W}\big(\varphi_-(z;\cdot),\varphi_+(z^{-1};\cdot)\big)\,,\\ \beta_-(z) &= \frac{2z}{1-z^2}\mathcal{W}\big(\varphi_-(z^{-1};\cdot),\varphi_+(z;\cdot)\big)\,.\end{aligned} \tag{39}$$

Moreover, it follows that

$$\begin{aligned}\varphi_-(z;\cdot) = \big(1-\beta_+(z)\beta_-(z)-\Delta(z)\Delta(z^{-1})\big)\varphi_-(z;\cdot)\\ +\big(\beta_+(z)\Delta(z)+\beta_+(z)\beta^+(z^{-1})\big)\varphi_-(z^{-1};\cdot)\,,\end{aligned}$$

and by linear independence we obtain the following relations:

$$\beta_-(z)\beta_+(z)+\Delta(z)\Delta(z^{-1}) = 1\,, \quad -\beta_+(z) = \beta_-(z^{-1})\,. \tag{40}$$

A straightforward calculation shows that $\varphi_+(z;\cdot)$ and its Schwarz reflection $\varphi_+(z^*;\cdot)^*$, where z^* denotes the complex conjugate of z, solve (27) for the same value of z, and both of these solutions have the same asymptotic behavior:

$$\lim_{n\to+\infty}\varphi_+(z^*;n)^* z^{-n} = 1\,, \quad \lim_{n\to+\infty}\varphi_+(z;n)z^{-n} = 1\,. \tag{41}$$

Therefore, by uniqueness, $\varphi_+(z^*;\cdot)^* = \varphi_+(z;\cdot)$ for $0 < |z| \leq 1$. It follows by the same argument that $\varphi_-(z^*;\cdot)^* = \varphi_-(z;\cdot)$ for $0 < |z| \leq 1$. We can use these two facts to deduce the symmetries of $\Delta(z)$ and $\beta_\pm(z)$. Taking complex conjugates of both sides in (32) for $|z| = 1$ gives

$$\varphi_+(z^*;\cdot)^* = \beta_-(z^*)^*\varphi_-(z;\cdot) + \Delta(z^*)^*\varphi_-(z^{-1};\cdot)\,.$$

Then, by independence, we have

$$\beta_-(z^*)^* = \beta_-(z) \ , \quad \Delta(z^*)^* = \Delta(z) \ . \tag{42}$$

By an analogous argument using (33) we deduce that

$$\beta_+(z^*)^* = \beta_+(z) \ . \tag{43}$$

Then using (40), (42), and (43) yields

$$|\Delta(z)|^2 = 1 + |\beta_-(z)|^2 \ , \quad |\Delta(z)|^2 = 1 + |\beta_+(z)|^2 \ . \tag{44}$$

Now we define a new quantity $T(z)$ by

$$T(z) = \frac{1}{\Delta(z)} \ ,$$

and rewrite (32) and (33) as

$$T(z)\varphi_+(z;\cdot) = \frac{\beta_-(z)}{\Delta(z)}\varphi_-(z;\cdot) + \varphi_-(z^{-1};\cdot) \ , \tag{45}$$

and

$$T(z)\varphi_-(z;\cdot) = \frac{\beta_+(z)}{\Delta(z)}\varphi_+(z;\cdot) + \varphi_+(z^{-1};\cdot) \tag{46}$$

respectively. In addition to these, (44) takes the form:

$$1 = |T(z)|^2 + \frac{|\beta_-(z)|^2}{|\Delta(z)|^2} \ , \quad 1 = |T(z)|^2 + \frac{|\beta_+(z)|^2}{|\Delta(z)|^2} \ . \tag{47}$$

For $|z| = 1$, (45) has the following wave reflection interpretation. Since

$$\lim_{n\to-\infty} \varphi_-(z^{-1};n)z^n = 1 \ ,$$

we imagine $\varphi_-(z^{-1};n)$ to be a left incident wave with unit amplitude placed at the left end ($n \to -\infty$) of the lattice. Then we picture that the wave $\varphi_-(z^{-1};n)$ is incident from the left end of the lattice, gets reflected by the lattice potential and $\frac{\beta_-(z)}{\Delta(z)}\varphi_-(z;n)$ is the reflected wave moving left. Seen from the right end of the lattice ($n \to +\infty$), we have the transmitted wave $T(z)\varphi_+(z;n)$. In light of this interpretation, we define

$$R_-(z) := \frac{\beta_-(z)}{\Delta(z)} \tag{48}$$

to be the *left reflection coefficient* and $T(z)$ is called the *transmission coefficient*. The analogous interpretation for (46) has $\big(\beta_+(z)/\Delta(z)\big)\varphi_+(z;n)$ as the reflected wave moving right, and we define

$$R_+(z) := \frac{\beta_+(z)}{\Delta(z)} \tag{49}$$

to be the *right reflection coefficient*. With these definitions, we have the following scattering relations:

$$\begin{gathered} |T(z)|^2 + |R_+(z)|^2 = 1\,, \quad |T(z)|^2 + |R_-(z)|^2 = 1\,, \\ T(z)R_+(z^*) + T(z^*)R_-(z) = 0\,, \end{gathered} \tag{50}$$

and

$$T(z)^* = T(z^*), \quad R_\pm(z)^* = R_\pm(z^*)\,. \tag{51}$$

Exercise 2.12 Using the Laurent expansion of $\Delta(z)$ at $z = 0$, show that

$$T(z) = A\left(1 + z\sum_{n\in\mathbb{Z}} 2b_n + O(z^2)\right), \tag{52}$$

where $A = \prod_{n\in\mathbb{Z}} 2a_n$.

Proposition 2.13 *$T(z)$ has a meromorphic extension inside the unit disk. The only poles of $T(z)$ inside the unit circle are at $z = \zeta_j$, $j = 1, 2, \ldots, N$, for which $\lambda_j := (\zeta_j + \zeta_j^{-1})/2$ is an eigenvalue of* $\mathbf{L}$.

Proof Since both $\varphi_\pm(z;\cdot)$ are both analytic for $0 < |z| < 1$, $\Delta(z)$ has an analytic extension inside the punctured unit disk, given by the formula (36), and we define $\Delta(0) = 1/A$ using the series expansion in Exercise 2.12. The poles of $T(z)$ are precisely the zeros of $\Delta(z)$. Suppose that $\Delta(\xi) = 0$ for some fixed $\xi \in \mathbb{C}$ with $0 < |\xi| < 1$. Then

$$\mathcal{W}\big(\varphi_+(\xi;\cdot), \varphi_-(\xi;\cdot)\big) = 0\,,$$

implying that $\varphi_+(\xi;\cdot) = c(\xi)\varphi_-(\xi;\cdot)$ for some constant $c(\xi) \in \mathbb{C}$. Then we have

$$\lim_{n\to+\infty} \varphi_+(\xi;n)\xi^{-n} = 1\,, \tag{53}$$

and

$$\lim_{n\to-\infty} \varphi_+(\xi;n)\xi^{n} = \lim_{n\to-\infty} c(\xi)\varphi_-(\xi;n)\xi^{n} = c(\xi). \tag{54}$$

Equations (53) and (54) imply that $\varphi_+(\xi;n) \to 0$ exponentially fast as $|n| \to +\infty$, hence $\varphi_\pm(\xi;\cdot) \in \ell^2(\mathbb{Z})$. This means that $T(z)$ has a pole at $z = \xi$ inside the unit disk if and only if $\mathbf{L}$ has an eigenvalue at

$$\lambda = \tfrac{1}{2}(\xi + \xi^{-1}) ,$$

with the associated eigenfunction $\varphi(\xi,\cdot) := \varphi_+(\xi,\cdot) = c(\xi)\varphi_-(\xi;\cdot)$ in $\ell^2(\mathbb{Z})$. □

Note that positive ζ_js correspond to the eigenvalues above 1, while negative ζ_j's correspond to the eigenvalues below -1. By analyticity, the zeros of $\Delta(z)$ inside the unit disk are isolated and they cannot have an accumulation point inside the unit disk. Note that if the zeros of $\Delta(z)$ do not have an accumulation point on the boundary $|z| = 1$, then the zero set of $\Delta(z)$ is finite. The following exercise addresses this.

Exercise 2.14 Prove that $\Delta(z)$ has finitely many isolated simple zeros inside the unit disk by showing that the zero set does not have an accumulation point on the boundary $|z| = 1$. **Hint:** It might be useful to treat the cases $\mathcal{W}\big(\varphi_+(z;\cdot), \varphi_-(z;\cdot)\big) = 0$ and $\mathcal{W}\big(\varphi_+(z;\cdot), \varphi_-(z;\cdot)\big) \neq 0$ separately.

Now let $c_j \in \mathbb{C}$, for $j = 1, 2, \ldots, N$, be the proportionality constants given by $\varphi_+(\zeta_j;\cdot) = c_j\varphi_-(\zeta_j;\cdot)$. The residues of $T(z)$ at $z = \zeta_j, j = 1, 2, \ldots, N$, are given by

$$\operatorname*{Res}_{\zeta_j} T(z) = -c_j\zeta_j\gamma_{j,+} = -\frac{\zeta_j\gamma_{j,-}}{c_j} , \tag{55}$$

where

$$\gamma_{j,\pm} := \|\varphi_\pm(\zeta_j;\cdot)\|_2^{-2} . \tag{56}$$

The constants $\gamma_{j,-}$ are called the *left norming constants* and the constants $\gamma_{j,+}$ are called the *right norming constants*. The sets

$$\mathcal{S}_\pm(\mathbf{L}) := \{R_\pm(z) \text{ for } |z| = 1, \{\zeta_j\}_{j=1}^N, \{\gamma_{j,\pm}\}_{j=1}^N\}$$

are called the *right and the left scattering data* for $\mathbf{L}$, respectively. In fact, a symmetry calculation shows that either of these sets determine the other and the transmission coefficient $T(z)$ via an application of the Poisson–Jensen formula [117, Lemma 10.7]. Therefore it is enough to work with only one of these sets. We set

$$R(z) := R_+(z) , \quad \gamma_j := \gamma_{j,+}$$

and call

$$\mathcal{S}(\mathbf{L}) := \{R(z) \text{ for } |z| = 1, \{\zeta_j\}_{j=1}^N, \{\gamma_j\}_{j=1}^N\}$$

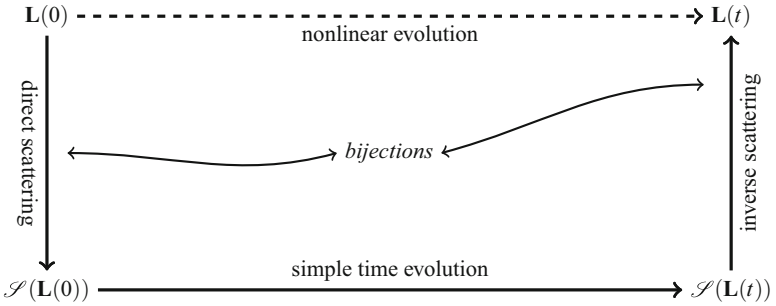


Fig. 6 Inverse scattering transform method for solving the Cauchy initial value problem for the Toda lattice

the *scattering data* for $\mathbf{L}$. The mapping $\mathbf{L} \mapsto \mathcal{S}(\mathbf{L})$ is called the *direct scattering transform*.

It is a fundamental fact of scattering theory that Jacobi matrices $\mathbf{L}$ whose coefficients satisfy (18) are in bijective correspondence with their scattering data $\mathcal{S}(\mathbf{L})$ (see, for example,[117, Chap. 11]). Thus, there exists an inverse mapping $\mathcal{S}(\mathbf{L}) \mapsto \mathbf{L}$, which is called the *inverse scattering transform*. Moreover, as we shall see in the next section, time evolution of the scattering data for $\mathbf{L}(t)$ is governed by simple linear ordinary differential equations when $\mathbf{L}(t)$ evolves according to the Toda lattice equations (14). This fact equips us with a method to solve the Cauchy initial value problem for the Toda lattice as depicted in Fig. 6:

1. Given initial data (a^0, b^0) satisfying (18), compute the scattering data $\mathcal{S}\big(\mathbf{L}(0)\big)$ for the Jacobi matrix $\mathbf{L}(0)$ with coefficients (a^0, b^0).
2. Compute the time evolution of the scattering data $\mathcal{S}\big(\mathbf{L}(t)\big)$ at a desired time $t \in \mathbb{R}$.
3. Compute the inverse scattering transform to reconstruct $\mathbf{L}(t)$ from $\mathcal{S}\big(\mathbf{L}(t)\big)$, hence obtaining $(a(t), b(t))$.

Following this procedure transfers the inherent difficulty of dealing with a nonlinear equation into the study of the scattering and inverse scattering transform for an operator. The latter can be approached with the specific and powerful methods, mainly with the method of nonlinear steepest descent introduced by Deift and Zhou [34], developed for Riemann–Hilbert problems.

We end the section with a theorem which establishes that one generically has $R(\pm 1) = -1$ for Jacobi matrices in the Marchenko class $\mathcal{M}$ [see (18)].

Theorem 2.15 ([18, Theorem 1]) *The set of doubly infinite Jacobi matrices* $\mathbf{J}(a, b)$ *(with the sequence* a *in the off-diagonal entries and the sequence* b *in the diagonal entries) in* $\mathcal{M}$ *with the associated reflection coefficient satisfying* $R(\pm 1) = -1$ *forms an open and dense subset of* $\mathcal{M}$ *in the topology induced by the norm*

$$\|\mathbf{J}(a, b)\|_{\mathcal{M}} = \sum_{n \in \mathbb{Z}} (1 + |n|)\big(\big|a_n - \tfrac{1}{2}\big| + |b_n|\big) \, .$$

2.3.4 Time Dependence of Scattering Data

Existence of a Lax pair has several important consequences. We begin with the one that concerns the spectrum of the Lax operator.

Proposition 2.16 *The Lax equation* (14) *is an isospectral evolution on Jacobi matrices.*

Proof Let $\mathbf{Q}(t)$ be the unique solution of the matrix Cauchy initial value problem

$$\frac{\mathrm{d}\mathbf{Q}}{\mathrm{d}t} = \mathbf{P}\mathbf{Q}\,, \quad \mathbf{Q}(0) = \mathbb{I}\,, \tag{57}$$

where $\mathbb{I}$ is the identity. Solutions for the initial value problem exist locally and they are unique (see, for example,[6, Theorem 4.1.5]). Since $\|\mathbf{P}(t)\|$ is uniformly bounded on any compact time interval, the solution is global. The skew-symmetry of $\mathbf{P}$ implies that $\mathrm{d}\mathbf{Q}^*/\mathrm{d}t = -\mathbf{Q}^*\mathbf{P}$. Therefore

$$\frac{\mathrm{d}}{\mathrm{d}t}(\mathbf{Q}^*\mathbf{Q}) = -\mathbf{Q}^*\mathbf{P}\mathbf{Q} + \mathbf{Q}^*\mathbf{P}\mathbf{Q} = 0\,, \tag{58}$$

implying that $\mathbf{Q}(t)$ is unitary for all $t \in \mathbb{R}$. Furthermore,

$$\frac{\mathrm{d}}{\mathrm{d}t}(\mathbf{Q}^*\mathbf{L}\mathbf{Q}) = -\mathbf{Q}^*\mathbf{P}\mathbf{L}\mathbf{Q} + \mathbf{Q}^*(\mathbf{P}\mathbf{L} - \mathbf{L}\mathbf{P})\mathbf{Q} + \mathbf{Q}^*\mathbf{L}\mathbf{P}\mathbf{Q} = 0\,, \tag{59}$$

which means $(\mathbf{Q}^*\mathbf{L}\mathbf{Q})(t) = \mathbf{L}(0)$, hence

$$\mathbf{L}(t) = \mathbf{Q}(t)\mathbf{L}(0)\mathbf{Q}(t)^*\,. \tag{60}$$

We showed that $\mathbf{L}(t)$ is unitarily equivalent to $\mathbf{L}(0)$ for all $t \in \mathbb{R}$. This completes the proof. □

By proving Proposition 2.16 we established the fact that $\sigma\big(\mathbf{L}(0)\big) = \sigma\big(\mathbf{L}(t)\big)$ for all time $t \in \mathbb{R}$ if $\mathbf{L}(t)$ evolves according to (14). We have the corollary:

Corollary 2.17 *Each eigenvalue* λ_j, $j = 1, 2, \ldots, N$, *of* $\mathbf{L}$ *is a constant of motion of the Toda lattice equations* (11).

Another consequence of Proposition 2.16 is

$$\|\mathbf{L}(t)\| = \|\mathbf{L}(0)\|\,, \quad \text{for all } t \geq 0\,, \tag{61}$$

which implies that the solution (a, b) of the Cauchy initial value problem in $\ell^\infty(\mathbb{Z}) \oplus \ell^\infty(\mathbb{Z})$ for the Toda lattice equations (11) is global in time since

$$\|a\|_\infty + \|b\|_\infty \leq 2\|\mathbf{L}(t)\| = 2\|\mathbf{L}(0)\|\,.$$

We know present the time evolution of the scattering data.

Proposition 2.18 ([117, Theorem 13.4]) *The time evolutions of the quantities in the scattering data are as follows*:

$$\begin{aligned} \zeta_j(t) &= \zeta_j \,, & &\text{for } j = 1, 2, \ldots, N \,, \\ \gamma_j(t) &= \gamma_j \mathrm{e}^{(\zeta_j - \zeta_j^{-1})t} \,, & &\text{for } j = 1, 2, \ldots, N \,, \\ R(z;t) &= R(z)\mathrm{e}^{(z-z^{-1})t} \,, & &\text{for } \|z\| = 1 \,, \end{aligned}$$

where $R(z) = R(z;0)$, $\zeta_j = \zeta_j(0)$, *and* $\gamma_j = \gamma_j(0)$.

Exercise 2.19 Prove Proposition 2.18. Define the *scattering matrix* $\mathbf{S}(z)$ by

$$\mathbf{S}(z) := \begin{pmatrix} \Delta(z) & -\beta_+(z) \\ \beta_-(z) & \Delta(z^{-1}) \end{pmatrix} \,,$$

and then the "$\infty \times 2$" matrices $\boldsymbol{\Psi}(z)$ and $\boldsymbol{\Phi}(z)$ whose nth rows are

$$\begin{aligned} \boldsymbol{\Psi}(z;n) &= \begin{pmatrix} \varphi_+(z;n) & \varphi_+(z^{-1};n) \end{pmatrix} \,, \\ \boldsymbol{\Phi}(z;n) &= \begin{pmatrix} \varphi_-(z^{-1};n) & \varphi_-(z;n) \end{pmatrix} \,, \end{aligned} \tag{62}$$

respectively, so that we have $\boldsymbol{\Psi}(z;n) = \boldsymbol{\Phi}(z;n)\mathbf{S}(z)$ for all $n \in \mathbb{Z}$. Differentiate both sides of (27) and obtain the time evolution $\mathbf{S}(z;t)$.

Exercise 2.20 (Moser [91]) Consider the finite version of the Toda lattice as described in (15). Show that the time evolution of the first component $\psi_1^{[k]}$ of the normalized eigenvector $\psi^{[k]}$ associated to the eigenvalue λ_k is given explicitly by:

$$\psi_1^{[k]}(t)^2 = \frac{\mathrm{e}^{2\lambda_k t}\psi_1^{[k]}(0)^2}{\sum_{j=1}^{N} \mathrm{e}^{2\lambda_j t}\psi_1^{[j]}(0)^2} . \tag{63}$$

See also [90] *for a detailed proof of* (63).

We close this section with a calculation which is due to Moser [91] and dates back to 1975.

Exercise 2.21 (Moser [91]) For the finite Toda lattice (15) considered in Remark 2.2 show that the off-diagonal elements $L_{j+1,j}(t) = L_{j,j+1}(t)$ of $\mathbf{L}(t)$ converge to zero as t tends to infinity.

2.4 Inverse Problem

The problem of reconstructing $\mathbf{L}$ from its scattering data is often called the inverse problem (and the mapping that achieves this is called the inverse scattering transform). This problem can be formulated as a Riemann–Hilbert factorization problem. Before giving a brief description of a Riemann–Hilbert problem, we need to introduce some notation. For an oriented contour Σ in the complex plane, its $+$ side is to the left of Σ as it is traversed in the direction of orientation, and its $-$ side is to the right. Given this convention, we denote by ϕ^+ and ϕ^- the nontangential limits of a function ϕ on Σ from $+$ side and $-$ side of Σ, respectively. Loosely speaking, a Riemann–Hilbert problem is the problem of finding a *sectionally analytic* (or *sectionally meromorphic*) function ϕ that is discontinuous across an oriented contour $\Sigma \subset \mathbb{C}$ with the jump condition

$$\phi^+(z) = \phi^-(z)G(z) + F(z) \ , \quad \text{for } z \in \Sigma \ .$$

In case the sought after function ϕ is sectionally meromorphic, say, with simple poles, there are prescribed residue conditions along with the jump condition. To assure that the problem at hand is uniquely solvable, one specifies normalization of ϕ at a point $\alpha \in \mathbb{C} \cup \{\infty\}$ and, perhaps, a symmetry condition. A detailed overview and discussion on Riemann–Hilbert problems is beyond the scope of these lectures. The interested reader is encouraged to see [2, 23, 32, 119]. We now proceed with presenting the Riemann–Hilbert formulation of the inverse scattering transform for the Toda lattice.

Based on the domains of analyticity of the Jost solutions $z \mapsto \varphi_\pm(z;\cdot,\cdot)$, we define the following row-vector valued meromorphic function in the complex plane:

$$m(z;n,t) := \begin{cases} \big(T(z)\varphi_-(z;n,t)z^n \ \varphi_+(z;n,t)z^{-n}\big) \ , & |z| < 1 \ , \\ \big(\varphi_+(z^{-1};n,t)z^n \ T(z^{-1})\varphi_-(z^{-1};n,t)z^{-n}\big) \ , & |z| > 1 \ , \end{cases} \tag{64}$$

We first find what jump condition $m(z;n,t)$ satisfies on the unit circle $\mathbb{T}$. Using the notation given above for the nontangential limits, define

$$m^\pm(z_0;n,t) := \lim_{\substack{z \to z_0 \\ |z|^\pm < 1}} m(z) \ , \quad \text{for } |z_0| = 1 \ .$$

We note here that these $\pm$ superscripts should not be confused with the $\pm$ signs used in subscripts for labeling the asymptotic behavior of Jost solutions $\varphi_\pm$.

From the relations (32) and (33) we see that the jump condition satisfied by m across the unit circle $\mathbb{T}$ is

$$m^+(z;n,t) \ = \ m^-(z;n,t) \begin{pmatrix} 1-|R(z)|^2 & -R(z)^* \mathrm{e}^{-\theta(z;n,t)} \\ R(z)\mathrm{e}^{\theta(z;n,t)} & 1 \end{pmatrix}, \quad \text{for } z \in \mathbb{T} \ , \tag{65}$$

where

$$\theta(z;n,t) = t(z - z^{-1}) + 2n\log z\,.$$

We have arrived at the following fact [78, Theorem 3.3]. $m(z;n,t)$ is a solution of the following vector Riemann–Hilbert problem:

RH Problem 1 Find a row vector-valued function $m(\cdot;n,t)\colon \mathbb{C}\setminus\mathbb{T}\to\mathbb{C}^{1\times 2}$ which satisfies the following conditions:

- *Analyticity condition*: $m(z;n,t)$ is sectionally meromorphic away from the unit circle $\mathbb{T}$ with simple poles at $\zeta_j^{\pm 1}, j = 1,2,\ldots,N$.
- *Jump condition*:

$$m^+(z;,n,t) = m^-(z;n,t)\begin{pmatrix} 1-|R(z)|^2 & -R(z)^*\mathrm{e}^{-\theta(z;n,t)} \\ R(z)\mathrm{e}^{\theta(z;n,t)} & 1\end{pmatrix}, \quad \text{for } z\in\mathbb{T}\,,$$

- *Residue conditions*:

$$\operatorname*{Res}_t \zeta_j m(z;n,t) = \lim_{z\to\zeta_j} m(z)\begin{pmatrix} 0 & 0 \\ -\zeta_j\gamma_j\mathrm{e}^{\theta(\zeta_j;n,t)} & 0\end{pmatrix}\,,$$

$$\operatorname*{Res}_{\zeta_j^{-1}} m(z;n,t) = \lim_{z\to\zeta_j} m(z)\begin{pmatrix} 0 & \zeta_j^{-1}\gamma_j\mathrm{e}^{\theta(\zeta_j;n,t)} \\ 0 & 0\end{pmatrix}\,,$$

- *Symmetry condition*:

$$m(z^{-1}) = m(z)\begin{pmatrix} 0 & 1 \\ 1 & 0\end{pmatrix}\,,$$

- *Normalization condition*:

$$\lim_{z\to\infty} m(z;n,t) =: m(\infty;n,t) = \begin{pmatrix} m_1 & m_2\end{pmatrix}\,, \quad m_1\cdot m_2 = 1\,, \quad m_1 > 0\,.$$

The solution of this Riemann–Hilbert problem is unique (see [77]) and the symmetry condition is essential for uniqueness in presence of poles. Note that once $m(z;n,t)$ is obtained, we can extract the solution $\big(a_n(t), b_n(t)\big)$ of the Cauchy initial value problem for the Toda lattice equations from the asymptotic expansion of $m(z;n,t)$ as $z\to\infty$:

$$m(z;n,t) = \frac{1}{A_+(n,t)}(1+2B_+(n,t)z)A_+(n,t)(1-2B_+(n-1,t)z) + O(z^{-2}). \tag{66}$$

We recover (a, b) from the formulae

$$a_n(t) = \frac{A_+(n+1,t)}{A_+(n,t)} \quad \text{and} \quad b_n(t) = B_+(n) - B_+(n-1)\ . \tag{67}$$

As can be seen, solving the Cauchy initial value problem for sufficiently decaying initial data for the Toda lattice equations is equivalent to solving RH Problem 1 which depends parametrically on the independent variables (n, t) of the nonlinear evolution equations (11). However, obtaining an explicit formula for the solution $m(z; n, t)$ for any given values of (n, t) is difficult, if possible. One can, on the other hand, obtain rigorous long-time asymptotics (as $t \to \infty$) for the solutions of the Cauchy initial value problem through the analysis of Riemann–Hilbert formulation of the inverse scattering transform as $t \to \infty$. Note that as $t \to \infty$, the jump matrix in RH Problem 1 becomes highly oscillatory since the coefficient of the t-term in $\theta(z; n, t)$ is purely imaginary for $|z| = 1$. One can approach this problem by the method of nonlinear stationary phase/steepest descent (see [34]). Loosely speaking, this method involves finding the stationary phase points of the exponential terms in the jump matrix, and then deforming the jump contours so that the deformed contours pass locally from the directions of steepest descent of these exponential terms at the stationary phase points and that the new jump matrices on those deformed contours tend to the identity matrix as $t \to \infty$ exponentially fast away from the stationary phase points.

This method has yielded a large number of rigorous asymptotic results for various completely integrable partial differential equations (see, for example, [36] and [35], among many others) as well as for the Toda lattice (see [77, 78]). Moreover, recent advances in numerical solution of the Riemann–Hilbert problems [97–99] has led to numerical implementations of the inverse scattering transform method for integrable PDEs [118, 120] and for the Toda lattice [18]. Therefore, it is possible to numerically compute and plot solutions accurately in arbitrarily long time scales without using any time-stepping methods.

The deformations that are employed in the process of analyzing the solutions of the Riemann–Hilbert problem in the long time regime are determined by the asymptotic region that (n, t) lies in as $t \to \infty$ (see Fig. 7 for asymptotic regions for the Toda lattice).

The Toda lattice has the following asymptotic regions [18]: for constants $k_j > 0$:

1. *The dispersive region.* This region is defined for $|n| \leq k_1 t$, with $0 < k_1 < 1$. Asymptotics in this region were obtained in [78].
2. *The collisionless shock region*. This region is defined by the relation $c_1 t \leq |n| \leq t - c_2 t^{1/3} (\log t)^{2/3}$. For the behavior of the solutions obtained via the numerical inverse scattering transform see [18].
3. *The transition region*. This region is also not present in the literature for the Toda lattice. The region is defined by the relation $t - c_2 t^{1/3} (\log t)^{2/3} \leq |n| \leq t - c_3 t^{1/3}$ [18]. An analogue of this region was first introduced for KdV in [120].

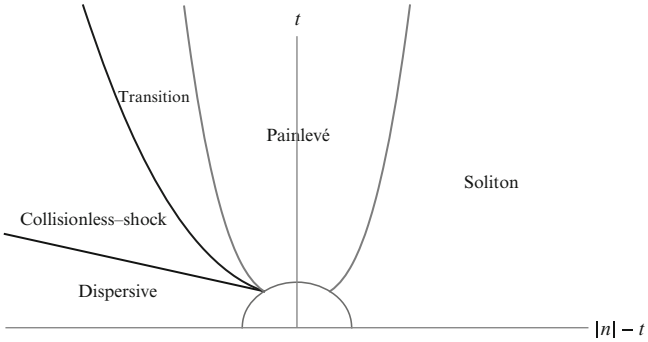


Fig. 7 Asymptotic regions for the Toda lattice, figure taken from [18]

4. *The Painlevé region*. This region is defined for $t - c_3 t^{1/3} \leq |n| \leq t + c_3 t^{1/3}$. Asymptotics in this region were obtained in [64] in absence of solitons and under the additional assumption that $|R(z)| < 1$.
5. *The soliton region*. This region is defined for $|n| > t + c_3 t^{1/3}$. Let $v_k > 1$ denote the velocity of the kth soliton and choose $\nu > 0$ so that the intervals $(v_k - \nu, v_k + \nu)$, $k = 1, 2, \ldots, N$, are disjoint. If $|n/t - v_k| < \nu$, the asymptotics in this region were obtained in [77] and [78].

For the deformations used in each region for the Toda lattice we refer the reader to [78] and [18].

Remark 2.22 The collisionless shock region and the transition region appear as $t \to \infty$ only if the reflection coefficient $R(z)$ corresponding to the initial data attains the value -1 at the edges of the continuous spectrum $z = \pm 1$. Theorem 2.15 tells us that this is generically the case: for an open dense subset of initial data inside the Marchenko class (18), the long time behavior of the solution exhibits behavior that is different than the behavior in the Painlevé region. If $|R(\pm 1)| < 1$ the collisionless shock and the transition regions are absent.

The following rigorous results were obtained in [77, 78]. The solution corresponding to sufficiently decaying [as in (18)] splits into a sum of N independent solitons (N being the number of eigenvalues of the Lax operator) and radiation. This result shows that in the region $n/t > 1$, the solution is asymptotically given by an N_--soliton solution, where N_- is the number of $\zeta_j \in (-1, 0)$. Similarly, in the region $n/t < -1$ the solution is asymptotically given by an N_+-soliton solution, where N_+ is the number of $\zeta_j \in (0, 1)$. Each soliton is formed by a distinct pair of eigenvalue and the associated norming constant, that is, by a (ζ_j, γ_j), for some $j \in \{1, 2, \ldots \mathbb{N}\}$. In the dispersive region $n/t < 1$, the solution (radiation) decays to the background, i.e., $a_n(t) \to \frac{1}{2}$ and $b_n(t) \to 0$ in the sup-norm as $t \to \infty$.

We close this subsection with a special case that leads to an explicit formula for the solution. If the potential Jacobi matrix is reflectionless, that is if $R(z) \equiv 0$ on the entire unit circle, then RH Problem 1 can be solved explicitly. Below we present the

solution $m(z;n,t)$ in the case where there is only one eigenvalue $\zeta \in (-1,0)\cup(0,1)$ and the associated norming constant $\gamma > 0$ in the scattering data. Such scattering data results in a pure 1-soliton solution of the Toda lattice.

Proposition 2.23 ([77, Lemma 2.6]) *If $\mathcal{S}(\mathbf{L}) = \{R(z) \equiv 0 \text{ for } |z| = 1, \zeta, \gamma\}$, then the unique solution of RH Problem 1 is given by*

$$m(z;n,t) = \begin{pmatrix} f(z) & f(1/z) \end{pmatrix}, \tag{68}$$

where

$$f(z) = \frac{1}{\sqrt{1-\zeta^2+\gamma e^{\theta(\zeta;n,t)}}\sqrt{1-\zeta^2+\zeta^2\gamma e^{\theta(\zeta;n,t)}}} \times \left(1-\zeta^2+\zeta^2\gamma e^{\theta(\zeta;n,t)}\frac{z-\zeta^{-1}}{z-\zeta}\right). \tag{69}$$

Proof The symmetry condition forces the solution to be of the form

$$m(z;n,t) = \begin{pmatrix} f(z;n,t) & f(1/z;n,t) \end{pmatrix},$$

where $f(z;n,t)$ is meromorphic in $\mathbb{C}\cup\infty$ with simple pole at $z=\zeta$. Therefore f must be of the form

$$f(z) = \frac{1}{G(n,t)}\left(1+2\frac{H(n,t)}{z-\zeta}\right), \tag{70}$$

where the unknown constants (in z) G and H are uniquely determined by the residue condition

$$\operatorname*{Res}_{\zeta} m(z;n,t) = -f(\zeta^{-1})\zeta\gamma e^{\theta(\zeta;n,t)}$$

and the normalization $f(0)f(\infty) = 1, f(0) > 0$. □

From Proposition 2.23 we obtain

$$\begin{aligned} A_+(n,t) &= \sqrt{\frac{1-\zeta^2+\gamma e^{\theta(\zeta;n,t)}}{1-\zeta^2+\zeta^2\gamma e^{\theta(\zeta;n,t)}}}, \\ B_+(n,t) &= \frac{\zeta^2\gamma e^{\theta(\zeta;n,t)}\zeta(\zeta^2-1)}{2\left(1-\zeta^2+\zeta^2\gamma e^{\theta(\zeta;n,t)}\right)}, \end{aligned} \tag{71}$$

from which the solution $\begin{pmatrix} a_n(t), b_n(t) \end{pmatrix}$ to the Cauchy initial value problem can be extracted using (67).

The solutions (a, b) that correspond to reflectionless Jacobi matrices (Lax operators) $\mathbf{L}$ are precisely the N-soliton solutions of the Toda lattice given in (9), where N is the number of eigenvalues $\lambda_j = \frac{1}{2}(\zeta_j + 1/\zeta_j)$ of $\mathbf{L}$, i.e., the number of pole pairs (ζ_j, ζ_j^{-1}) in the Riemann–Hilbert formulation of the inverse scattering transform.

The inverse scattering transform method for solution of the initial value problem also applies to the finite Toda lattice and the periodic Toda lattice. While it is not possible to give a full exposure to these cases here, we provide a summary and references below for the interested reader.

2.4.1 The Solution of the Finite Toda Lattice

For the finite $N \times N$ version[2] of the Toda lattice given in (15), the Lax operator becomes

$$\mathbf{L} = \begin{pmatrix} b_0 & a_0 & & & & \\ a_0 & b_1 & a_1 & & & \\ & a_1 & b_2 & a_2 & & \\ & & \ddots & \ddots & \ddots & \\ & & & a_{N-3} & b_{N-2} & a_{N-2} \\ & & & & a_{N-2} & b_{N-1} \end{pmatrix} \tag{72}$$

and the scattering data consists of N real simple eigenvalues $\lambda_j, j = 1, 2, \ldots, N$ of the Jacobi matrix $\mathbf{L}(t)$ and

$$w_j(t) := \left(\psi_1^{[j]}(t)\right)^2 ,$$

where $\psi_1^{[j]}$ is the first component of the jth normalized eigenvector (associated with λ_j). As mentioned in Exercise 2.20, $w_j(t)$ has simple time evolution:

$$w_j(t) = \frac{\mathrm{e}^{2\lambda_j t} w_j(0)}{\sum_{k=1}^{N} \mathrm{e}^{2\lambda_k t} w_k(0)} , \quad j = 1, 2, \ldots, N , \tag{73}$$

when $\mathbf{L}(t)$ evolves under the finite Toda dynamics (observed by Moser [91]) and λ_j remain constant in time [44]:

$$\lambda_j(t) = \lambda_j(0) , \quad j = 1, 2, \ldots, N .$$

It is well-known that $\mathbf{L}(t)$ can be reconstructed from the data $\{\lambda_j, w_j(t)\}_{j=1}^{N}$ (see [33, 112], or [32] and the references therein.) Moreover, the inverse scattering transform

[2] Finite Toda lattice is sometimes called the open Toda lattice.

method to solve the initial value problem for the finite Toda equations becomes the Gram–Schmidt orthogonalization process:

1. Given initial data $\mathbf{L}(0)$ and some time $t > 0$ at which the solution $\mathbf{L}(t)$ is desired, compute the QR-factorization:

$$e^{t\mathbf{L}(0)} = \mathbf{Q}(t)\mathbf{R}(t).$$

2. The solution of the Toda lattice is then obtained via

$$\mathbf{L}(t) = \mathbf{Q}(t)^{\top}\mathbf{L}(0)\mathbf{Q}(t),$$

where $\mathbf{Q}(t)^{\top}$ is the transpose of the orthogonal matrix $\mathbf{Q}(t)$. For details, we refer the reader to [91] and [110, 111].

2.4.2 The Periodic and Quasi-Periodic Solutions of the Toda Lattice

The inverse scattering transform methods in the context of nonlinear evolution equations are not limited to spatially decaying solutions. Beginning with the seminal works of Novikov [96], Lax [79], Dubrovin [38, 40], Its and Matveev [62, 63], and McKean and van Moerbeke [86], the inverse scattering transform methods were extended to construct spatially periodic and quasi-periodic solutions of the KdV equation in the late 1970s. These methods make extensive use of the algebro-geometric theory of Riemann surfaces. By the early 1980s analogous methods were developed for other integrable nonlinear evolution equations such as the nonlinear Schrödinger equation. Explicit formulae for periodic and quasi-periodic solutions, which give soliton solutions as certain limiting cases, became available in terms of the Riemann theta function (see [39] for a survey article on theta functions and nonlinear equations). The fundamental object of the algebro-geometric approach to integrate nonlinear evolution equations is the Baker–Akheizer function (a function with certain analyticity properties on a Riemann surface) [11, 12, 14]. Such a connection between nonlinear evolution equations and algebro-geometric methods led to rapid developments both in algebraic geometry and in the theory of integrable PDEs. While it is not possible to list here the vast literature, the interested reader is encouraged to see the recent survey article of Matveev [84] on finite gap theory, a not so recent survey article by Krichever [76] and his previous work [73, 75].

Integrability of the periodic Toda lattice consisting of N particles, with

$$a_{n+N} = a_n, \quad b_{n+N} = b_n \tag{74}$$

was first established by Hénon [55] in 1974 (see also [45], where Flaschka and McLaughlin obtained the action-angle variables, and [121]). In 1976 Dubrovin et al. [41] and Date and Tanaka [30] simultaneously gave the explicit formula for the diagonal elements $b_n(t)$ of the solution of the periodic Toda lattice in terms of

Riemann theta functions. Three years after this development Krichever gave the explicit formulae (again in terms of theta functions) for the off-diagonal elements $a_n(t)$ [74]. In his work, Krichever provides the solution for both quasi-periodic and the periodic Toda lattices. In these cases the spectrum of the Lax operator consists of finitely many bands on the real line and the scattering data is generally referred as "algebro-geometric" data obtained from the resulting Riemann surface. For a detailed treatment on algebro-geometric solution methods for the periodic and quasi-periodic Toda lattice (and the entire Toda hierarchy), we refer the reader to [49] and the references therein.

3 Darboux and Bäcklund Transformations. Derivation of Discrete Systems

Bäcklund and Darboux (or Darboux type) transformations originate from differential geometry of surfaces in the nineteenth century, and they constitute an important and very well studied connection with the modern soliton theory and the theory of integrable systems. In the modern theory of integrable systems, these transformations are used to generate solutions of partial differential equations, starting from known solutions, even trivial ones. In fact, Darboux transformations apply to systems of linear equations, while Bäcklund transformations are generally related to systems of nonlinear equations.

For further information on Bäcklund and Darboux transformations we indicatively refer to [54, 85, 105] (and the references therein).

3.1 Darboux Transformations

In 1882 Jean-Gaston Darboux [24] presented the so-called "Darboux theorem" which states that a Sturm-Liouville problem is covariant with respect to a linear transformation. In the recent literature, this is called the *Darboux transformation* [85, 105]. The first book devoted to the relation between Darboux transformations and the soliton theory is that of Matveev and Salle [85].

3.1.1 Darboux's Theorem

Darboux's original result is related to the so-called *one-dimensional, time-independent Schrödinger* equation, namely

$$y'' + (\lambda - u)y = 0 \,, \quad u = u(x) \,, \tag{75}$$

which can be found in the literature as a *Sturm–Liouville problem* of finding eigenvalues and eigenfunctions. Moreover, we refer to u as a *potential function*, or just *potential*.

In particular we have the following.

Theorem 3.1 (Darboux) *Let $y_1 = y_1(x)$ be a particular integral of the Sturm–Liouville problem (75), for the value of the spectral parameter $\lambda = \lambda_1$. Consider also the following (Darboux) transformation*

$$y \mapsto y[1] := \left(\frac{\mathrm{d}}{\mathrm{d}x} - l_1\right) y \,, \tag{76}$$

of an arbitrary solution, y, of (75), where $l_1 = l_1(y_1) = y_{1,x} y_1^{-1}$ is the logarithmic derivative of y_1. Then, $y[1]$ obeys the following equation

$$y''[1] + (\lambda - u[1]) y[1] = 0 \,, \tag{77a}$$

where $u[1]$ is given by

$$u[1] = u - 2l_1' \,. \tag{77b}$$

Darboux's theorem states that function $y[1]$ given in (76) obeys a Sturm–Liouville problem of the same structure with (75), namely the same (75) but with an updated potential $u[1]$. In other words, (75) is covariant with respect to the Darboux transformation, $y \mapsto y[1]$, $u \mapsto u[1]$.

3.1.2 Darboux Transformation for the KdV Equation

The significance of the Darboux theorem lies in the fact that transformation (76) maps solutions of a Sturm–Liouville equation (75) to other solutions of the same equation, which allows us to construct hierarchies of such solutions. At the same time, the theorem provides us with a relation between the "old" and the "new" potential. In fact, if the potential u obeys a nonlinear ODE (or more importantly a nonlinear PDE[3]), then relation (77) may allow us to construct new nontrivial solutions starting from trivial ones, such as the zero solution.

Example 3.2 Consider the Sturm–Liouville equation (75) in the case where the potential, u, satisfies the KdV equation. Therefore, both the eigenfunction y and the potential u depend on t, which slips into their expressions as a parameter.

In this case, (75) is nothing else but the spatial part of the Lax pair for the KdV equation, namely:

$$\mathbf{L}y = \lambda y \quad \text{or} \quad y_{xx} + \big(\lambda - u(x,t)\big) y = 0 \,. \tag{78}$$

[3]Potential u may depend on a temporal parameter t, namely $u = u(x,t)$.

Now, according to Theorem 3.1, for a known solution of the KdV equation, say u, we can solve (75) to obtain $y = y(x,t;\lambda)$. Evaluating at $\lambda = \lambda_1$, we get $y_1(x,t) = y(x,t;\ \lambda_1)$ and thus, using (77b), a new potential $u[1]$. Therefore, we simultaneously obtain new solutions, $(y[1], u[1])$, for both the linear equation (78) and the KdV equation,[4] which are given by

$$y[1] = (\partial_x - l_1)y\ , \tag{79a}$$

$$u[1] = u - 2l_{1,x}\ , \tag{79b}$$

respectively.

Now, applying the Darboux transformation once more, we can construct a second solution of the KdV equation in a fully algebraic manner. Specifically, first we consider the solution $y_2[1]$, which is $y[1]$ evaluated at $\lambda = \lambda_2$, namely

$$y_2[1] = (\partial_x - l_1)y_2\ . \tag{80}$$

where $y_2 = y(x,t;\lambda_2)$ Then, we obtain a second pair of solutions, $(y[2], u[2])$, for (78) and the KdV equation, given by

$$y[2] = (\partial_x - l_2)y[1] \overset{(79a)}{=} (\partial_x - l_2)(\partial_x - l_1)y\ , \tag{81a}$$

$$u[2] = u[1] - 2l_{2,x} \overset{(79b)}{=} u - 2(l_{1,x} + l_{2,x})\ . \tag{81b}$$

This procedure can be repeated successively, in order to construct hierarchies of solutions for the KdV equation, namely

$$(y[1], u[1]) \to (y[2], u[2]) \to \cdots \to (y[n], u[n]) \to \cdots\ , \tag{82}$$

where $(y[n], u[n])$ are given by

$$y[n] = \left(\prod_{k=1}^{\curvearrowleft n}(\partial_x - l_k)\right)y\ , \quad u[n] = u - 2\sum_{k=1}^{n}(l_{k,x})\ , \tag{83}$$

where "$\curvearrowleft$" indicates that the terms of the above "product" are arranged from the right to the left.

In these notes, we understand Darboux transformations as gauge-like transformations which depend on a spectral parameter. In fact, as we shall see in the next chapter, their dependence on the spectral parameter is essential to construct discrete integrable systems.

[4] Potential $u[1]$ is a solution of the KdV equation, since it can be readily shown that the pair $(y[1], u[1])$ also satisfies the temporal part of the Lax pair for KdV.

3.2 Bäcklund Transformations

As mentioned earlier, Bäcklund transformations originate in differential geometry in the 1880s and, in particular, they arose as certain transformations between surfaces.

In the theory of integrable systems, they are seen as relations between solutions of the same PDE (auto-BT) or as relations between solutions of two different PDEs (hetero-BT). Regarding the nonlinear equations which have Lax representation, Darboux transformations apply to the associated linear problem (Lax pair), while Bäcklund transformations are related to the nonlinear equation itself. Therefore, unlike DTs, BTs do not depend on the spectral parameter which appears in the definition of the Lax pair. Yet, both DTs and BTs serve the same purpose; they are used to construct nontrivial solutions starting from trivial ones.

Definition 3.3 (BT-Loose Definition) Consider the following partial differential equations for u and v:

$$F(u, u_x, u_t, u_{xx}, u_{xt}, \dots) = 0 \,, \tag{84a}$$

$$G(v, v_x, v_t, v_{xx}, v_{xt}, \dots) = 0 \,. \tag{84b}$$

Consider also the following pair of relations

$$\mathcal{B}_i(u, u_x, u_t, \dots, v, v_x, v_t, \dots) = 0 \,, \tag{85}$$

between u, v and their derivatives. If $\mathcal{B}_i = 0$ is integrable for v, $\mathrm{mod}\langle F = 0\rangle$, and the resulting v is a solution of $G = 0$, and vice versa, then it is an hetero-Bäcklund transformation. Moreover, if $F \equiv G$, the relations $\mathcal{B}_i = 0$ is an auto-Bäcklund transformation.

The simplest example of BT are the well-known Cauchy-Riemann relations in complex analysis, for the analyticity of a complex function, $f = u(x,t) + v(x,t)i$.

Example 3.4 (Laplace Equation) Functions $u = u(x,t)$ and $v = v(x,t)$ are harmonic, namely

$$\nabla^2 u = 0 \,, \quad \nabla^2 v = 0 \,, \tag{86}$$

if the following Cauchy–Riemann relations hold

$$u_x = v_t \,, \quad u_t = -v_x \,. \tag{87}$$

The latter equations constitute an auto-BT for the Laplace equation (86) and can be used to construct solutions of the same equations, starting with known ones. For instance, consider the simple solution $v(x,t) = xt$. Then, according to (87), a second solution of (86), u, has to satisfy $u_x = x$ and $u_t = -t$. Therefore, u is given by

$$u = \tfrac{1}{2}(x^2 - t^2) \ . \tag{88}$$

However, even though Laplace's equation is linear, the same idea works for nonlinear equations.

3.2.1 Bäcklund Transformation for the PKdV Equation

An auto-Bäcklund transformation associated to the PKdV equation,

$$u_t = 6u_x^2 - u_{xxx} \ , \tag{89}$$

is given by the following relations

$$\mathcal{B}_\alpha : \begin{cases} (u+v)_x = 2\alpha + \tfrac{1}{2}(u-v)^2 \ , \\ (u-v)_t = 3(u_x^2 - v_x^2) - (u-v)_{xxx} \ , \end{cases} \tag{90}$$

which was first presented in 1973 in a paper of Wahlquist and Estabrook [125]. In this section we show how we can construct algebraically a solution of the PKdV equation, using Bianchi's permutability.

Remark 3.5 We shall refer to the first equation of (90) as the *spatial part* (or *x-part*) of the BT, while we refer to the second one as the *temporal part* (or *t-part*) of the BT.

Exercise 3.6 Show that relations (90) constitute an auto-Bäcklund transformation for the PKdV equation (89).

Now, let $u = u(x,t)$ be a function satisfying the PKdV equation. Focusing on the spatial part of the BT (90), we can construct a new solution of the PKdV equation, $u_1 = \mathcal{B}_{\alpha_1}(u)$, i.e.

$$(u_1 + u)_x = 2\alpha_1 + \tfrac{1}{2}(u_1 - u)^2 \ . \tag{91}$$

Moreover, using another parameter, α_2, we can construct a second solution $u_2 = \mathcal{B}_{\alpha_2}(u)$, given by

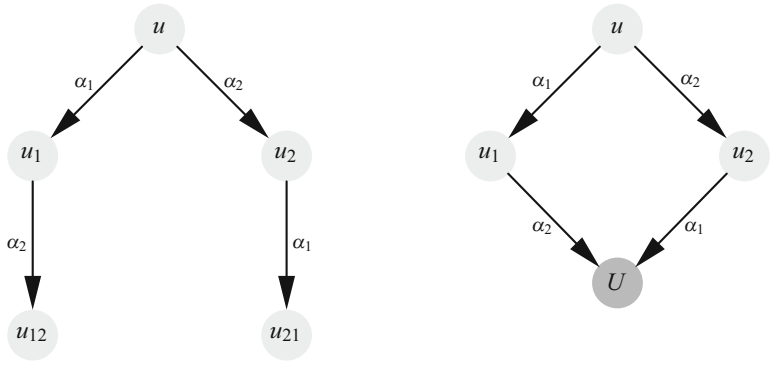
$$(u_2 + u)_x = 2\alpha_2 + \tfrac{1}{2}(u_2 - u)^2 \ . \tag{92}$$

Starting with the solutions u_1 and u_2, we can construct two more solutions from relations $u_{12} = \mathcal{B}_{\alpha_2}(u_1)$ and $u_{21} = \mathcal{B}_{\alpha_1}(u_2)$, namely

$$(u_{12} + u_1)_x = 2\alpha_2 + \tfrac{1}{2}(u_{12} - u_1)^2 \ , \tag{93a}$$

$$(u_{21} + u_2)_x = 2\alpha_1 + \tfrac{1}{2}(u_{21} - u_2)^2 \ , \tag{93b}$$

as represented in Fig. 8a.



(a) *Construction of solutions using BT* (b) *Bianchi's diagram*

Fig. 8 Bianchi's permutability. (**a**) Construction of solutions using BT. (**b**) Bianchi's diagram

Nevertheless, the above relations need integration in order to derive the actual solutions u_1, u_2 and, in retrospect, solutions u_{12} and u_{21}. Yet, having at our disposal solutions u_1 and u_2, a new solution can be constructed using Bianchi's permutativity (see Fig. 8b) in a purely algebraic way. Specifically, we have the following.

Proposition 3.7 *Imposing the condition* $u_{12} = u_{21}$, *the BTs* (91)–(93b) *imply the following solution of the PKdV equation*:

$$U = u - 4\frac{\alpha_1 - \alpha_2}{u_1 - u_2} \,. \tag{94}$$

Proof It is straightforward calculation; one needs to subtract (92) and (93b) by (91) and (93a), respectively, and subtract the resulting equations. □

Later on we study the Darboux transformations for the NLS equation, and we shall see that BT arise naturally in the derivation of DT.

Exercise 3.8 (Bäcklund Transform for the sine-Gordon Equation) Show that the following relations

$$\mathcal{B}_\alpha : \begin{cases} \left(\dfrac{u+v}{2}\right)_x = \alpha \sin\left(\dfrac{u-v}{2}\right) , \\ \left(\dfrac{u-v}{2}\right)_t = \dfrac{1}{\alpha} \sin\left(\dfrac{u+v}{2}\right) , \end{cases} \tag{95}$$

between functions $u = u(x,t)$ and $v = v(x,t)$, constitute an auto-BT for the sine-Gordon equation:

$$u_{xt} = \sin u \,. \tag{96}$$

Following the same procedure as for the PKdV equation, namely using the BT (95) and Bianchi's permutability, show that:

$$U = u + 4\arctan\left[\frac{\alpha_1 + \alpha_2}{\alpha_2 - \alpha_1}\tan\left(\frac{u_1 - u_2}{4}\right)\right], \tag{97}$$

where u satisfies (96), is also a solution of (96).

3.3 *From Darboux Transformations to Discrete Systems*

In this section, we shall show how one can derive discrete integrable systems using Darboux transformations. In particular, our starting point will be continuous Lax operators, and by considering the associated Darboux transformations, we derive semidiscrete and fully discrete Lax operators. That is, in the derivation of Darboux transformations, we derive differential-difference (Bäcklund transformations, [80, 81]) and difference-difference integrable systems.

3.3.1 Lax–Darboux Scheme

With the single term *Lax–Darboux scheme*, we describe several structures which are related to each other and all of them are related to integrability. To be more precise, the Lax–Darboux scheme incorporates Lax operators, corresponding Darboux matrices and Darboux transformations, as well as the Bianchi permutability of the latter transformations.

In what follows we present the basic points of the scheme:

- We consider Lax operators of the following AKNS form:

$$\mathbf{L} := D_x + U(p, q; \lambda)\,, \quad p = p(x)\,,\ q = q(x)\,,$$

where U is a matrix which belongs in the Lie algebra $\mathfrak{sl}(2, \mathbb{C})$.

Remark 3.9 The abbreviation AKNS is due to Ablowitz, Kaup, Newell and Segur who solved the sine-Gordon equation (96) (see [4]) writing it as compatibility condition of a set of Lax operators in the form $\mathbf{L} = D_x + U$ and $\mathbf{T} = D_t + V$, where U and V are certain matrices. Moreover, they generalized this method to cover a number of PDEs [5]. It is worth mentioning that the authors of Ablowitz et al. [4, 5] were motivated by Zakharov and Shabat [130] who applied the inverse scattering method to the nonlinear Schrödinger equation.

- By *Darboux transformation*, here, we understand a map

$$\mathbf{L} \to M\mathbf{L}M^{-1} = \mathbf{L}_1 := D_x + \underbrace{U(p_{10}, q_{10}; \lambda)}_{U_{10}} . \tag{98}$$

Matrix M is called *Darboux matrix* and satisfies the following equation (see Exercise 3.11).

$$D_x M + U_{10} M - MU = 0 , \quad M = M(p, q, p_{10}, q_{10}, f; \lambda) . \tag{99}$$

The Darboux matrix M depends on the "old" potentials, p, q and the "updated" ones, p_{10}, q_{10}. It also depends on the spectral parameter and may depend on an auxiliary function, as we shall see later in the example.

Darboux transformations consist of *Darboux matrices* M along with corresponding *Bäcklund transformations* (or dressing chains).

Remark 3.10 It is obvious from relations (98)–(99) that, for a given operator $\mathbf{L}$ we cannot determine M in full generality, and we need to make an ansatz. In what follows, we shall be assuming that M has the same dependence on the spectral parameter as $\mathbf{L}$.

Exercise 3.11 Show that according to (98) for a Darboux transformation, the corresponding Darboux matrix satisfies (99).

- The associated Bäcklund transformation is a set of differential equations relating the potentials and the auxiliary functions involved in $\mathbf{L}$ and $\widetilde{\mathbf{L}}_1$. It can be regarded as integrable systems of differential-difference equations DΔEs [80, 81]. This follows from the interpretation of the corresponding Darboux transformation defining a sequence

$$\cdots \xrightarrow{M} (p_{-10}, q_{-10}) \xrightarrow{M} (p, q) \xrightarrow{M} (p_{10}, q_{10}) \cdots .$$

- A Darboux matrix M maps a fundamental solution of the equation $\mathbf{L}\Psi = 0$, where $\Psi = \Psi(x, \lambda)$ to a fundamental solution Ψ_{10} of $\mathbf{L}_1\Psi_{10} = 0$ according to $\Psi_{10} = M\Psi$. In general, matrix M is invertible and depends on p and q, their updates p_{10} and q_{10}, the spectral parameter λ, and some auxiliary functions, i.e., $M = M(p, q, p_{10}, q_{10}; \lambda)$.

  Moreover, the determinant of the Darboux matrix is independent of x (see Exercise 3.12).

Exercise 3.12 Using (98), where $U \in \mathfrak{sl}(2, \mathbb{C})$ show that matrix M:

1. maps fundamental solutions of $\mathbf{L}\Psi = 0$ to fundamental solutions of $\mathbf{L}_1\Psi = 0$.
2. has determinant independent of x, namely $\partial_x(\det M) = 0$. **Hint:** Use Liouville's well-known formula for the determinant of the solution of the equation $(\mathrm{d}/\mathrm{d}x)\Psi = M\Psi$).

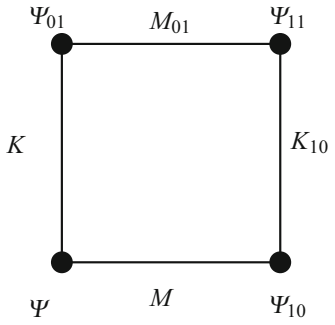


Fig. 9 Bianchi commuting diagram

- We employ Darboux matrices to derive two new fundamental solutions Ψ_{10} and Ψ_{01}:

$$\Psi_{10} = M(p, q, p_{10}, q_{10}; \lambda)\Psi \equiv M\Psi \ , \quad \Psi_{01} = M(p, q, p_{01}, q_{01}; \lambda)\Psi \equiv K\Psi \ .$$

- Considering compatibility around the square, a third solution can be derived as described in the *Bianchi-type diagram* Fig. 9, where $M_{01} := M(p_{01}, q_{01}, p_{11}, q_{11}; \lambda)$ and $K_{10} := M(p_{10}, q_{10}, p_{11}, q_{11}; \lambda)$.

  The compatibility around the square yields the following condition:

$$M_{01}K - K_{01}M = 0 \ , \tag{100}$$

  If the latter condition is written out explicitly, it results in algebraic relations among the various potentials involved, namely a system of PΔE equations.

  We can interpret the above construction in a discrete way. Particularly, let us assume that p and q are functions depending not only on x but also on two discrete variables n and m, i.e., $p = p(x; n, m)$ and $q = q(x; n, m)$. Furthermore, we define the *shift operators* $\mathcal{S}$ and $\mathcal{T}$ acting on a function $f = f(n, m)$ as

$$f_{10} := \mathcal{S}f(n, m) = f(n + 1, m) \ , \quad f_{01} := \mathcal{T}f(n, m) = f(n, m + 1) \ . \tag{101}$$

  In general,

$$f_{ij} := \mathcal{S}^i \mathcal{T}^j f(n, m) = f(n + i, m + j) \tag{102}$$

  We shall refer to $\mathcal{S}$ and $\mathcal{T}$ as the *shift operators in the n* and the *m-direction*, respectively.

3.3.2 An Example: Lax–Darboux Scheme for the Nonlinear Schrödinger Equation

Consider the following Lax operator

$$\mathbf{L} := D_x + U(p, q; \lambda) = D_x + \lambda U^1 + U^0 \ , \tag{103a}$$

where U^1 and U^0 are given by

$$U^1 \equiv \sigma_3 = \mathrm{diag}(1,-1)\ , \quad U^0 = \begin{pmatrix} 0 & 2p \\ 2q & 0 \end{pmatrix}\ . \tag{103b}$$

Operator (103) constitutes the spatial part of the Lax pair for the nonlinear Schrödinger equation,

$$p_t = p_{xx} + 4p^2 q\ , \quad q_t = -q_{xx} - 4pq^2\ .$$

Now, we seek *elementary* Darboux transformation, namely Darboux transformation that cannot be decomposed to others. We assume that the associated Darboux matrix, M, has linear λ-dependence, namely it is of the form $M = \lambda M_1 + M_0$. Substitution of the latter to (99) implies a second order algebraic equation in λ. Equating the coefficients of the several powers of λ equal to zero, we obtain the following system of equations

$$\lambda^2: \quad [\sigma_3, M_1] = 0\ , \tag{104a}$$

$$\lambda^1: \quad M_{1,x} + [\sigma_3, M_0] + U^0_{10} M_1 - M_1 U^0 = 0\ , \tag{104b}$$

$$\lambda^0: \quad M_{0,x} + U^0_{10} M_0 - M_0 U^0 = 0\ , \tag{104c}$$

where with $[\sigma_3, M_1]$ we denote the commutator of σ_3 and M_1.

Equation (104a) implies that M_1 must be diagonal, i.e., $M_1 = \mathrm{diag}(c_1, c_2)$. Then, we substitute M_1 to (104b).

Now, for simplicity of the notation, we denote the $(1,1)$ and $(2,2)$ entries of M_0 by f and g respectively. Then, it follows from (104c) that the entries of matrix M_0 must satisfy the following equations

$$\partial_x f = 2(M_{0,12} q - p_{10} M_{0,21})\ , \tag{105a}$$

$$\partial_x g = 2(M_{0,21} p - q_{10} M_{0,12})\ , \tag{105b}$$

$$\partial_x M_{0,12} = 2(pf - g p_{10})\ , \tag{105c}$$

$$\partial_x M_{0,21} = 2(qg - q_{10} f)\ . \tag{105d}$$

The off-diagonal part of (104b) implies that the $(1,2)$ and $(2,1)$ entries of matrix M_0 are given by

$$M_{0,12} = c_1 p - c_2 p_{10}\ , \quad M_{0,21} = c_1 q_{10} - c_2 q\ . \tag{106}$$

Additionally, from the diagonal part of (104b) we deduce that $c_{1,x} = c_{2,x} = 0$. Therefore, c_i, $i = 1, 2$ can be either zero or nonzero. Thus, after rescaling we can choose either $c_1 = 1$, $c_2 = 0$ ($\mathrm{rank}\, M_1 = 1$), or $c_1 = 0$, $c_2 = -1$ ($\mathrm{rank}\, M_1 = 1$), or $c_1 = 1, c_2 = -1$ ($\mathrm{rank}\, M_1 = 2$). The first two choices correspond to gauge

equivalent elementary Darboux matrices and the third one leads to a Darboux matrix which can be given as a composition of the two previous elementary matrices.

Indeed, the choice $c_1 = 1, c_2 = 0$ implies $M_{0,12} = p$ and $M_{0,21} = q_{10}$. Moreover, (105b) implies that $g = \text{const.} = \alpha$, i.e.,

$$M_0 = \begin{pmatrix} f & p \\ q_{10} & \alpha \end{pmatrix} . \tag{107}$$

In this case the Darboux matrix is given by

$$\lambda \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} f & p \\ q_{10} & \alpha \end{pmatrix} , \tag{108}$$

where, according to (105), its entries satisfy

$$\partial_x f = 2(pq - p_{10}q_{10})/;\,, \quad \partial_x p = 2(pf - \alpha p_{10})/;\,, \quad \partial_x q_{10} = 2(cq - q_{10}f)/;\,. \tag{109}$$

Now, if $\alpha \neq 0$, it can be rescaled to $\alpha = 1$.

In the case where $\alpha = 0$, from (109) we deduce

$$p_x = 2fp\,, \quad q_{10,x} = -2fq_{10}\,. \tag{110}$$

Thus, the Darboux matrix in this case is given by

$$M(p, q_{10}, f) := \lambda \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} f & p \\ q_{10} & 0 \end{pmatrix} . \tag{111}$$

In addition, after an integration with respect to x, (110) imply that $q_{10} = c/p$.

In general, we have the following.

Proposition 3.13 *Let M be an elementary Darboux matrix for the Lax operator (103) and suppose it is linear in λ. Then, up to a gauge transformation, M is given by*

$$M(p, q_{10}, f) := \lambda \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} f & p \\ q_{10} & 1 \end{pmatrix} , \tag{112}$$

where the potentials p and q satisfy the following differential-difference equations

$$\partial_x f = 2(pq - p_{10}q_{10})\,, \tag{113a}$$

$$\partial_x p = 2(pf - p_{10})\,, \tag{113b}$$

$$\partial_x q_{10} = 2(q - q_{10}f)\,. \tag{113c}$$

Moreover, matrix (112) *degenerates to*

$$M_c(p,f) = \lambda \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} f & p \\ c/p & 0 \end{pmatrix} , \quad f = \frac{p_x}{2p} . \tag{114}$$

It is straightforward to show that system (113) admits the following first integral

$$\partial_x (f - p\, q_{10}) = 0 . \tag{115}$$

which implies that $\partial_x \det M = 0$.

Exercise 3.14 Show that the choice $c_1 = 0, c_2 = -1$ in (106) leads to a Darboux matrix gauge equivalent to (112), and, in particular, show that matrix $\sigma_1 N(p_{10}, q, g)\sigma_1^{-1}$ is of the form Eq. (112).

Remark 3.15 In this case, of the nonlinear Schrödinger equation, an elementary Darboux transformation consists of an elementary Darboux matrix (112), which is λ-depended, and a system of DΔEs, namely system (113). The latter is nothing else but the spatial part of a Bäcklund transformation associated to the nonlinear Schrödinger equation, and it does not depend on the spectral parameter, λ.

3.4 Derivation of Discrete Systems and Initial Value Problems

In this section we employ the Darboux matrices derived in the previous section to derive discrete integrable systems. We shall present only the pairs of Darboux matrices which lead to genuinely nontrivial discrete integrable systems. For these systems we consider an initial value problem on the staircase.

3.4.1 Nonlinear Schrödinger Equation and Related Discrete Systems

Having derived two Darboux matrices for operator (103), we focus on the one given in (112) and consider the following discrete Lax pair

$$\Psi_{10} = M\Psi , \quad \Psi_{01} = K\Psi , \tag{116}$$

where M and K are given by

$$M \equiv M(p, q_{10}, f) = \lambda \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} f & p \\ q_{10} & 1 \end{pmatrix} , \tag{117a}$$

$$K \equiv M(p, q_{01}, g) = \lambda \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} g & p \\ q_{01} & 1 \end{pmatrix} . \tag{117b}$$

The compatibility condition of (117) results to

$$f_{01} - f - (g_{10} - g) = 0 \,, \tag{118a}$$

$$f_{01}\, g - f g_{10} - p_{10} q_{10} + p_{01} q_{01} = 0 \,, \tag{118b}$$

$$p(f_{01} - g_{10}) - p_{10} + p_{01} = 0 \,, \tag{118c}$$

$$q_{11}(f - g) - q_{01} + q_{10} = 0 \,. \tag{118d}$$

This system can be solved either for $(p_{01}, q_{01}, f_{01}, g)$ or for $(p_{10}, q_{10}, f, g_{10})$. In either of these cases, we derive two solutions. The first one is

$$p_{10} = p_{01} \,, \quad q_{10} = q_{01} \,, \quad f = g \,, \quad g_{10} = f_{01} \,, \tag{119}$$

which is trivial and corresponds to $M(p, q_{10}, f) = M(p, q_{01}, g)$.

The second solution is given by

$$p_{01} = \frac{q_{10} p^2 + (g_{10} - f) p + p_{10}}{1 + p q_{11}} \,, \qquad q_{01} = \frac{p_{10} {q_{11}}^2 + (f - g_{10}) q_{11} + q_{10}}{1 + p q_{11}} \,, \tag{120a}$$

$$f_{01} = \frac{q_{11}(p_{10} + p g_{10}) + f - p q_{10}}{1 + p q_{11}} \,, \qquad g = \frac{q_{11}(p f - p_{10}) + g_{10} + p q_{10}}{1 + p q_{11}} \,. \tag{120b}$$

The above system has some properties which take their rise in the derivation of the Darboux matrix. In particular, we have the following.

Proposition 3.16 *System* (120) *admits two first integrals,* $\mathcal{F} := f - p q_{10}$ *and* $\mathcal{G} := g - p q_{01}$*, and the following conservation law*

$$(\mathcal{T} - 1)\mathcal{F} = (\mathcal{S} - 1)\mathcal{G} \,. \tag{121}$$

Proof Relation (115) suggests that

$$(\mathcal{T} - 1)(f - p q_{10}) = 0 \quad \text{and} \quad (\mathcal{S} - 1)(g - p q_{01}) = 0 \,, \tag{122}$$

which can be shown by straightforward calculation, and it is left as an exercise. Thus, $F = f - p q_{10}$ and $G := g - p q_{01}$ are first integrals. Moreover, (118a) can be written in the form of the conservation law (121). □

Corollary 3.17 *The following relations hold.*

$$f - p q_{10} = \alpha(n) \quad \textit{and} \quad g - p q_{01} = \beta(m) \,. \tag{123}$$

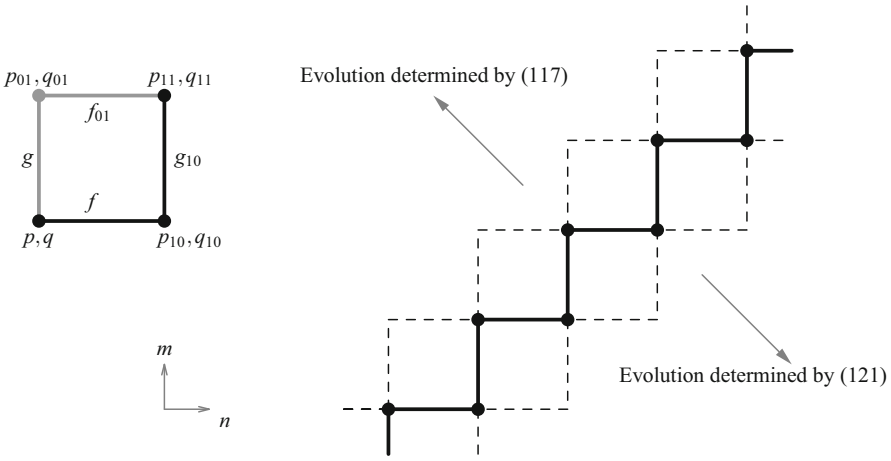


Fig. 10 Initial value problem and direction of evolution

Remark 3.18 In view of relations (123), we can interpret functions f and g as being given on the edges of the quadrilateral where system (120) is defined, and, consequently, consider system (120) as a vertex-bond system [56].

Exercise 3.19 Show relations (122) using (118).

Our choice to solve system (118) for p_{01}, q_{01}, f_{01} and g is motivated by the initial value problem related to system (120). Suppose that the initial values for p and q are given on the vertices along a staircase as shown in Fig. 10. Functions f and g are given on the edges of this initial value configuration in a consistent way with the first integrals (123). In particular, horizontal edges carry the initial values of f and vertical edges the corresponding ones of g.

With these initial conditions, the values of p and q can be uniquely determined at every vertex of the lattice, while f and g on the corresponding edges. This is obvious from the rational expressions (120) defining the evolution above the staircase, cf. Fig. 10.

For the evolution below the staircase, one has to use

$$p_{10} = \frac{q_{01}p^2 + (f_{01} - g)p + p_{01}}{1 + p\,q_{11}}, \qquad q_{10} = \frac{p_{01}{q_{11}}^2 + (g - f_{01})q_{11} + q_{01}}{1 + pq_{11}}, \tag{124a}$$

$$g_{10} = \frac{q_{11}(p_{01} + pf_{01}) + g - pq_{01}}{1 + pq_{11}}, \qquad f = \frac{q_{11}(pg - p_{01}) + f_{01} + pq_{01}}{1 + p\,q_{11}}, \tag{124b}$$

which uniquely defines the evolution below the staircase as indicated in Fig. 10.

Remark 3.20 We could consider more general initial value configurations of staircases of lengths ℓ_1 and ℓ_2 in the n and m lattice direction, respectively. Such initial value problems are consistent with evolutions (120), (124) determining the values of all fields uniquely at every vertex and edge of the lattice.

Now, using first integrals we can reduce system (120) to an *Adler–Yamilov type* of system as those in [8]. Specifically, we have the following.

Proposition 3.21 *System* (120) *can be reduced to the following nonautonomous Adler–Yamilov type of system for p and q:*

$$p_{01} = p_{10} - \frac{\alpha(n) - \beta(m)}{1 + pq_{11}} p \,, \quad q_{01} = q_{10} + \frac{\alpha(n) - \beta(m)}{1 + pq_{11}} q_{11} \,. \tag{125}$$

Proof The proof is straightforward if one uses relations (123) to replace f and g in system (120). □

Now, we will use two different Darboux matrices associated with the NLS equation to construct the discrete Toda equation [108].

In fact, we introduce a discrete Lax pair as (116), with $M = M_1(p,f)$ in (114) and $K = M(p, q_{01}, g)$ in (112). That is, we consider the following system

$$\Psi_{10} = \left(\lambda \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} f & p \\ \frac{1}{p} & 0 \end{pmatrix} \right) \Psi \,, \tag{126a}$$

$$\Psi_{01} = \left(\lambda \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} g & p \\ q_{01} & 1 \end{pmatrix} \right) \Psi \,, \tag{126b}$$

and impose its compatibility condition.

From the coefficient of the λ-term in the latter condition we extract the following equations

$$f - f_{01} = g - g_{10} \,, \tag{127a}$$

$$p_{01} = \frac{1}{q_{11}} \,. \tag{127b}$$

Additionally, the λ^0-term of the compatibility condition implies

$$f_{01} g - g_{10} f = \frac{p_{10}}{p} - p_{01} q_{01} \,, \tag{128a}$$

$$g_{10} - f_{01} = \frac{p_{01}}{p} \,, \tag{128b}$$

$$g - f = \frac{p_{01}}{p} \,. \tag{128c}$$

Now, recall from the previous section that, using (123), the quantities g and g_{10} are given by

$$g = \beta(m) + pq_{01} \quad \text{and} \quad g_{10} = \beta(m) + p_{10}q_{11} \ . \tag{129}$$

We substitute g and g_{10} into (128b) and (128c), and then replace p and its shifts using (127b). Then, we can express f and f_{01} in terms of the potential q and its shifts:

$$f = \frac{q_{01}}{q_{10}} - \frac{q_{10}}{q_{11}} + \beta(m) \ , \tag{130a}$$

$$f_{01} = \frac{q_{11}}{q_{20}} - \frac{q_{10}}{q_{11}} + \beta(m) \ . \tag{130b}$$

Proposition 3.22 *The compatibility of system* (130) *yields a fully discrete Toda type equation.*

Proof Applying the shift operator $\mathcal{T}$ on both sides of (130a) and demanding that its right-hand side agrees with that of (130b), we obtain

$$\frac{q_{11}}{q_{20}} - \frac{q_{02}}{q_{11}} + \frac{q_{11}}{q_{12}} - \frac{q_{10}}{q_{11}} = \beta(m+1) - \beta(m) \ . \tag{131}$$

Then, we make the transformation

$$q \to \exp(-w_{-1,-1}) \ , \tag{132}$$

which implies the following discrete Toda type equation

$$\mathrm{e}^{w_{1,-1}-w} - \mathrm{e}^{w-w_{-1,1}} + \mathrm{e}^{w_{0,1}-w} - \mathrm{e}^{w-w_{0,-1}} = \beta(m+1) - \beta(m) \ , \tag{133}$$

and proves the statement. □

Exercise 3.23 Show that the discrete Toda equation (133) can be written in the form of a conservation law.

3.5 Lax–Darboux Scheme for NLS Type Equations

In the previous section we used the NLS equation as an illustrative example to describe the Lax–Darboux scheme. The NLS equation was not selected randomly, but as a simple example of recent classification results of automorphic Lie algebras. In particular, finite groups of fractional-linear transformations of a complex variable were classified by Klein [66], and they correspond to the cyclic groups $\mathbb{Z}_n$, the

dihedral groups $\mathbb{D}_n$, the tetrahedral group $\mathbb{T}$, the octahedral group $\mathbb{O}$ and the icosahedral group $\mathbb{I}$. Following Klein's classification, in [21, 22] it has been shown that in the case of 2×2 matrices ($n = 2$), the essentially different reduction groups are

- the trivial group (with no reduction);
- the cyclic reduction group $\mathbb{Z}_2$ (leading to the Kac–Moody algebra A_1^1);
- the Klein reduction group $\mathbb{Z}_2 \times \mathbb{Z}_2 \cong \mathbb{D}_2$.

Now, the following Lax operators

$$\mathbf{L} = D_x + \lambda \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} + \begin{pmatrix} 0 & 2p \\ 2q & 0 \end{pmatrix}, \tag{134a}$$

$$\mathbf{L} = D_x + \lambda^2 \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} + \lambda \begin{pmatrix} 0 & 2p \\ 2q & 0 \end{pmatrix}, \tag{134b}$$

$$\mathbf{L} = D_x + (\lambda^2 - \lambda^{-2}) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} + \lambda \begin{pmatrix} 0 & 2p \\ 2q & 0 \end{pmatrix} + \lambda^{-1} \begin{pmatrix} 0 & 2q \\ 2p & 0 \end{pmatrix}, \tag{134c}$$

constitute all the essential different Lax operators, with poles of minimal order, invariant with respect to the generators of $\mathbb{Z}_2$ and $\mathbb{D}_2$ groups with degenerate orbits.[5] In what follows, we study the Darboux transformations for all the above cases.

Operator (134a) is associated with the NLS equation [131], while (134b) and (134c) are associated with the DNLS equation [65], and a deformation of the DNLS equation [88], respectively.

In [67, 70], the Lax–Darboux scheme was applied to all cases (134a), (134b) and (134c). As a result, for all these cases, Darboux transformations were studied and novel discrete integrable systems were constructed.

4 Discrete Integrable Systems and Yang–Baxter Maps

As we mentioned in the introduction, a very important integrability criterion is that of the 3D-*consistency* and, by extension, the *multidimensional consistency* [19, 94].

In what follows, we briefly explain what is the 3D-consistency property and we review some recent classification results. For more information we refer to [57, 92] which are two of the few self-contained books on the integrability of discrete systems, as well as [53] for a collection of results.

[5] These are orbits corresponding to the fixed points of the fractional linear transformations of the spectral parameter.

4.1 *Equations on Quad-Graphs: 3D-Consistency*

Let us consider a discrete equation of the form

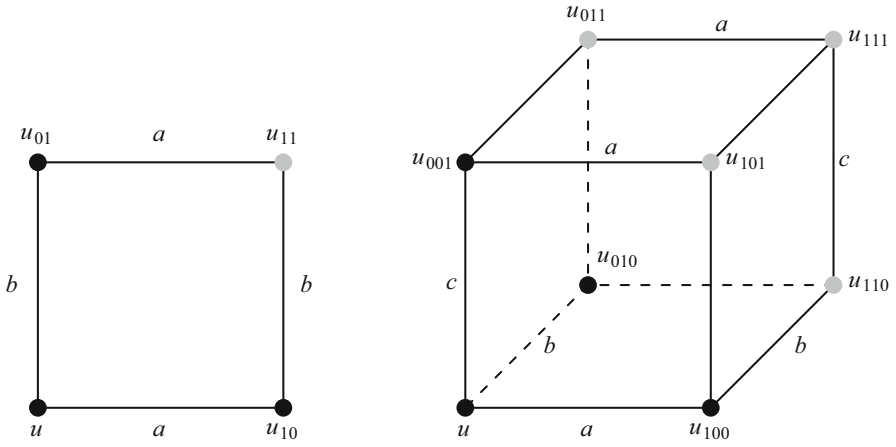
$$Q(u, u_{10}, u_{01}, u_{11}; a, b) = 0 \,, \tag{135}$$

where u_{ij}, $i,j = 0,1$, $u \equiv u_{00}$, belong in a set $\mathcal{A}$ and the parameters $a, b \in \mathbb{C}$. Moreover, we assume that (135) is uniquely solvable for any u_i in terms of the rest. We can interpret the fields u_i to be attached to the vertices of a square as in Fig. 11a.

If (135) can be generalized in a consistent way on the faces of a cube, then it is said to be *3D-consistent*. In particular, suppose we have the initial values u, u_{100}, u_{010} and u_{001} attached to the vertices of the cube as in Fig. 11b. Now, since (135) is uniquely solvable, we can uniquely determine values u_{110}, u_{101} and u_{011}, using the bottom, front and left face of the cube. Then, there are three ways to determine value u_{111}, and we have the following.

Definition 4.1 If for any choice of initial values u, u_{100}, u_{010} and u_{001}, equation $Q = 0$ produces the same value u_{111} when solved using the left, back or top face of the cube, then it is called 3D-consistent.

Note 4.2 In the above interpretation, we have adopted similar notation to (101)–(102): We consider the square in Fig. 11a to be an elementary square in a two-dimensional lattice. Then, we assume that field u depends on two discrete variables n and m, i.e., $u = u(n,m)$. Therefore, u_{ij}s on the vertices of Fig. 11a are



(a) Quad-Graph (b) Cube

Fig. 11 3D-consistency. (**a**) Quad-graph. (**b**) Cube

$$\begin{aligned} u_{00} &= u(n,m)\ , & u_{10} &= u(n+1,m)\ , \\ u_{01} &= u(n,m+1)\ , & u_{11} &= u(n+1,m+1)\ . \end{aligned} \tag{136}$$

Moreover, for the interpretation on the cube we assume that u depends on a third variable k, such that

$$u_{000} = u(n,m,k)\ , \quad u_{100} = u(n+1,m,k)\ , \ldots \quad , u_{111} = u(n+1,m+1,k+1)\ . \tag{137}$$

Now, as an illustrative example we use the discrete potential KdV equation which first appeared in [58].

Example 4.3 (Discrete Potential KdV Equation) Consider (135), where Q is given by

$$Q(u,u_{10},u_{01},u_{11};a,b) = (u-u_{11})(u_{10}-u_{01}) + b - a. \tag{138}$$

Now, using the bottom, front and left faces of the cube Fig. 11b, we can solve equations

$$Q(u,u_{100},u_{010},u_{110};a,b) = 0\ , \tag{139a}$$

$$Q(u,u_{100},u_{001},u_{101};a,c) = 0\ , \tag{139b}$$

$$Q(u,u_{010},u_{001},u_{011};b,c) = 0\ , \tag{139c}$$

to obtain solutions for u_{110}, u_{101} and u_{011}, namely

$$u_{110} = u + \frac{a-b}{u_{010}-u_{100}}\ , \tag{140a}$$

$$u_{101} = u + \frac{a-c}{u_{001}-u_{100}}\ , \tag{140b}$$

$$u_{011} = u + \frac{b-c}{u_{001}-u_{010}}\ , \tag{140c}$$

respectively.

Now, if we shift (140a) in the k-direction, and then substitute u_{101} and u_{011} (which appear in the resulting expression for u_{11}) by (140), we deduce

$$u_{111} = -\frac{(a-b)u_{100}u_{010} + (b-c)u_{010}u_{001} + (c-a)u_{100}u_{001}}{(a-b)u_{001} + (b-c)u_{100} + (c-a)u_{010}}\ . \tag{141}$$

It is obvious that, because of the symmetry in the above expression, we would obtain exactly the same expression for u_{111} if we had alternatively shifted u_{101} in the m-direction and substituted u_{110} and u_{011} by (140), or if we had shifted u_{011} in the n-direction and substituted u_{110} and u_{101}. Thus, the dpKdV equation is 3D-consistent.

4.2 ABS Classification of Maps on Quad-Graphs

In 2003 [9] Adler et al. classified all the 3D-consistent equations in the case where $\mathcal{A} = \mathbb{C}$. In particular, they considered all the equations of the form (135), where $u, u_{10}, u_{01}, u_{11}, a, b \in \mathbb{C}$, that satisfy the following properties:

I. Multilinearity. Function $Q = Q(u, u_{10}, u_{01}, u_{11}; a, b)$ is a first order polynomial in each of its arguments, namely linear in each of the fields $u, u_{10}, u_{01}, u_{11}$. That is,

$$\begin{aligned} &Q(u, u_{10}, u_{01}, u_{11}; a, b) \\ &\qquad = a_1 u u_{10} u_{01} u_{11} + a_2 u u_{10} u_{01} + a_3 u u_{10} u_{11} + \cdots + a_{16} \,, \end{aligned} \tag{142}$$

where $a_i = a_i(a, b)$, $i = 1, \ldots, 16$.

II. Symmetry. Function Q satisfies the following symmetry property

$$\begin{aligned} Q(u, u_{10}, u_{01}, u_{11}; a, b) &= \epsilon Q(u, u_{01}, u_{10}, u_{11}; b, a) \\ &= \sigma Q(u_{10}, u, u_{11}, u_{01}; a, b) \,, \end{aligned} \tag{143}$$

with $\epsilon, \sigma = \pm 1$.

III. Tetrahedron property. That is, the final value u_{111} is independent of u.

ABS proved that all the equations of the form (135) which satisfy the above conditions, can be reduced to seven basic equations, using Möbius (fraction linear) transformations of the independent variables and point transformations of the parameters. These seven equations are distributed into two lists known as the *Q-list* (list of 4 equations) and the *H-list* (list of three equations).

Remark 4.4 The discrete potential KdV (dpKdV) equation, which we shall consider in Eq. (161), is the first member of the H-list (H_I).

Those equations of the form (135) which satisfy the multilinearity condition (I), admit Lax representation. In fact, in this case, introducing an auxiliary spectral parameter, λ, there is an algorithmic way to find a matrix L such that (135) can be written as the following *zero-curvature* equation

$$L(u_{11}, u_{01}; a, \lambda) L(u_{01}, u; b, \lambda) = L(u_{11}, u_{10}; b, \lambda) L(u_{10}, u; a, \lambda) \,. \tag{144}$$

We shall see later on that 1. equations of the form (135) with the fields on the edges of the square Fig. 11a are related to Yang–Baxter maps and 2. Yang–Baxter maps may have Lax representation as (144).

4.2.1 Classification of Quadrirational Maps: The F-List

A year after the classification of the 3D-consistent equations, ABS in [10] classified all the quadrirational maps in the case where $\mathcal{A} = \mathbb{CP}^1$; the associated list of maps is known as the F-list. Recall that, a map $Y\colon (x, y) \mapsto \big(u(x, y), v(x, y)\big)$ is called *quadrirational*, if the maps

$$u(., y)\colon \mathcal{A} \to \mathcal{A}\ , \quad v(x, .)\colon \mathcal{A} \to \mathcal{A}\ , \tag{145}$$

are birational. In particular, we have the following.

Theorem 4.5 (ABS, F-List) *Up to Möbius transformations, any quadrirational map on $\mathbb{CP}^1 \times \mathbb{CP}^1$ is equivalent to one of the following maps*

$$u = ayP\ , \qquad v = bxP\ , \qquad P = \frac{(1-b)x + b - a + (a-1)y}{b(1-a)x + (a-b)xy + a(b-1)y}\ ; \tag{$\mathrm{F_I}$}$$

$$u = \frac{y}{a}P\ , \qquad v = \frac{x}{b}P\ , \qquad P = \frac{ax - by + b - a}{x - y}\ ; \tag{$\mathrm{F_{II}}$}$$

$$u = \frac{y}{a}P\ , \qquad v = \frac{x}{b}P\ , \qquad P = \frac{ax - by}{x - y}\ ; \tag{$\mathrm{F_{III}}$}$$

$$u = yP\ , \qquad v = xP\ , \qquad P = 1 + \frac{b-a}{x-y}\ ; \tag{$\mathrm{F_{IV}}$}$$

$$u = y + P\ , \qquad v = x + P\ , \qquad P = \frac{a-b}{x-y}\ , \tag{$\mathrm{F_V}$}$$

up to suitable choice of the parameters a and b.

We shall come back to the F-list in Sect. 4, where we shall see that all the equations of the F-list have the Yang–Baxter property; yet, the other members of their equivalence classes may not satisfy the Yang–Baxter equation. However, we shall present a more precise list given in [103].

4.3 The Yang–Baxter Equation

The original (quantum) Yang–Baxter equation originates in the works of Yang [126] and Baxter [15], and it has a fundamental role in the theory of quantum and classical integrable systems.

Here, we are interested in the study of the set-theoretical solutions of the Yang–Baxter equation. The first examples of such solutions appeared in 1988, in a paper of Sklyanin [107]. However, the study of the set-theoretical solutions was formally proposed by Drinfiel'd in 1992 [37], and gained a more algebraic flavor in [20].

Veselov, in [123], proposed the more elegant term "Yang–Baxter maps" for this type of solutions and, moreover, he connected them with integrable mappings [123, 124].

Let V be a vector space and $Y \in \mathrm{End}(V \otimes V)$ a linear operator. The Yang–Baxter equation is given by the following

$$Y^{12} \circ Y^{13} \circ Y^{23} = Y^{23} \circ Y^{13} \circ Y^{12} \,, \tag{146}$$

where Y^{ij}, $i, j = 1, 2, 3$, $i \neq j$, denotes the action of Y on the ij factor of the triple tensor product $V \otimes V \otimes V$. In this form, (146) is known in the literature as the *quantum YB equation*.

4.3.1 Parametric Yang–Baxter Maps

Let us now replace the vector space V by a set A, and the tensor product $V \otimes V$ by the Cartesian product $A \times A$. In what follows, we shall consider A to be a finite-dimensional algebraic variety in K^N, where K is any field of zero characteristic, such as $\mathbb{C}$ or $\mathbb{Q}$.

Now, let $Y \in \mathrm{End}(A \times A)$ be a map defined by

$$Y\colon (x, y) \mapsto \big(u(x, y), v(x, y)\big) \,. \tag{147}$$

Furthermore, we define the maps $Y^{ij} \in \mathrm{End}(A \times A \times A)$ for $i, j = 1, 2, 3$, $i \neq j$, which appear in (146), by the following relations

$$Y^{12}(x, y, z) = \big(u(x, y), v(x, y), z\big) \,, \tag{148a}$$

$$Y^{13}(x, y, z) = \big(u(x, z), y, v(x, z)\big) \,, \tag{148b}$$

$$Y^{23}(x, y, z) = \big(x, u(y, z), v(y, z)\big) \,. \tag{148c}$$

Let also $Y^{21} = \pi Y \pi$, where $\pi \in \mathrm{End}(A \times A)$ is the permutation map: $\pi(x, y) = (y, x)$.

Map Y is a YB map, if it satisfies the YB equation (146). Moreover, it is called *reversible* if the composition of Y^{21} and Y is the identity map, i.e.,

$$Y^{21} \circ Y = \mathrm{Id} \,. \tag{149}$$

Now, let us consider the case where parameters are involved in the definition of the YB map. In particular we define the following map

$$Y_{a,b}\colon (x, y) \mapsto (u, v) \equiv \big(u(x, y; a, b), v(x, y; a, b)\big) \,. \tag{150}$$

This map is called *parametric YB map* if it satisfies the *parametric YB equation*

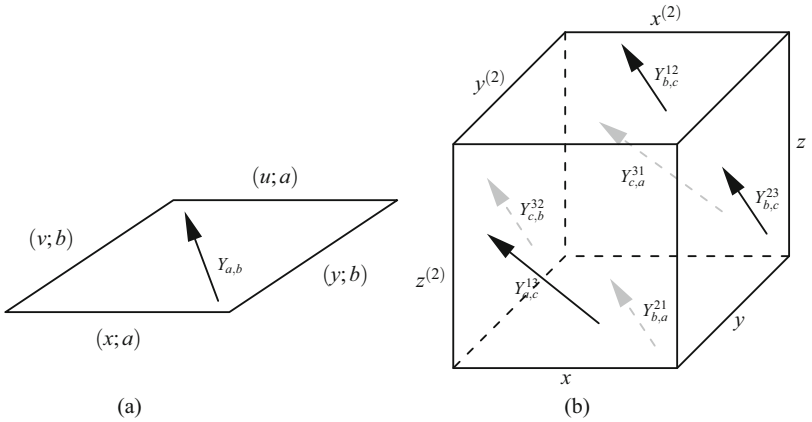


Fig. 12 Cubic representation of (**a**) the parametric YB map and (**b**) the corresponding YB equation

$$Y^{12}_{a,b} \circ Y^{13}_{a,c} \circ Y^{23}_{b,c} = Y^{23}_{b,c} \circ Y^{13}_{a,c} \circ Y^{12}_{a,b} \, . \tag{151}$$

One way to represent the map $Y_{a,b}$ is to consider the values x and y taken on the sides of the quadrilateral as in Fig. 12a; the map $Y_{a,b}$ maps the values x and y to the values placed on the opposite sides of the quadrilateral, u and v.

Moreover, for the YB equation, we consider the values x, y and z taken on the sides of the cube as in Fig. 12b. Specifically, by the definition (148) of the functions Y^{ij}, the map $Y^{23}_{b,c}$ maps

$$(x, y, z) \xrightarrow{Y^{23}_{b,c}} (x, y^{(1)}, z^{(1)}) \, , \tag{152}$$

using the right face of the cube. Then, map $Y^{13}_{a,c}$ maps

$$(x, y^{(1)}, z^{(1)}) \xrightarrow{Y^{13}_{a,c}} (x^{(1)}, y^{(1)}, z^{(2)}) \equiv Y^{13}_{a,c} \circ Y^{23}_{b,c}(x, y, z) \, , \tag{153}$$

using the front face of the cube. Finally, map $Y^{12}_{a,b}$ maps

$$(x^{(1)}, y^{(1)}, z^{(2)}) \xrightarrow{Y^{12}_{a,b}} (x^{(2)}, y^{(2)}, z^{(2)}) \equiv Y^{12}_{a,b} \circ Y^{13}_{a,c} \circ Y^{23}_{b,c}(x, y, z) \, , \tag{154}$$

using the top face of the cube.

On the other hand, using the bottom, the back and the left face of the cube, the values x, y and z are mapped to the values $\hat{x}^{(2)}, \hat{y}^{(2)}$ and $\hat{z}^{(2)}$ via the map $Y^{23}_{b,c} \circ Y^{13}_{a,c} \circ Y^{12}_{a,b}$ which consists with the right-hand side of equation, namely (147)

$$Y^{23}_{b,c} \circ Y^{13}_{a,c} \circ Y^{12}_{a,b}(x, y, z) = (\hat{x}^{(2)}, \hat{y}^{(2)}, \hat{z}^{(2)}) \, . \tag{155}$$

Therefore, the map $Y_{a,b}$ satisfies the YB equation (151) if and only if $x^{(2)} = \hat{x}^{(2)}$, $y^{(2)} = \hat{y}^{(2)}$ and $z^{(2)} = \hat{z}^{(2)}$.

Most of the examples of YB maps which appear in these lecture notes are parametric.

Example 4.6 One of the most famous parametric YB maps is Adler's map [7]

$$(x, y) \xrightarrow{Y_{a,b}} (u, v) = \left(y - \frac{a-b}{x+y}, x + \frac{a-b}{x+y} \right) , \tag{156}$$

which is related to the 3D consistent discrete potential KDV equation [93, 101].

Exercise 4.7 By straightforward substitution, show that Adler's map (156) satisfies the YB equation (146).

4.3.2 Matrix Refactorization Problems and the Lax Equation

Let us consider the matrix L depending on a variable x, a parameter c and a *spectral parameter* λ, namely $L = L(x; c, \lambda)$, such that the following matrix refactorization problem

$$L(u; a, \lambda)L(v; b, \lambda) = L(y; b, \lambda)L(x; a, \lambda) , \quad \text{for any } \lambda \in \mathbb{C} , \tag{157}$$

is satisfied whenever $(u, v) = Y_{a,b}(x, y)$. Then, L is called Lax matrix for $Y_{a,b}$, and (157) is called the *Lax-equation* or *Lax-representation* for $Y_{a,b}$.

Note 4.8 In the rest of this thesis we use the letter "L" when referring to Lax matrices of the refactorization problem (157) and the bold "$\mathbf{L}$" for Lax operators. Moreover, for simplicity of the notation, we usually omit the dependence on the spectral parameter, namely $L(x; a, \lambda) \equiv L(x; a)$.

Since the Lax equation (157) does not always have a unique solution for (u, v), Kouloukas and Papageorgiou in [72] proposed the term *strong Lax matrix* for a YB map. This is when the Lax equation is equivalent to a map

$$(u, v) = Y_{a,b}(x, y) . \tag{158}$$

The uniqueness of refactorization (157) is a sufficient condition for the solutions of the Lax equation to define a reversible YB map of the form (158). In particular, we have the following.

Proposition 4.9 (Veselov) *Let $u = u(x, y)$, $v = v(x, y)$ and $L = L(x; \alpha)$ a matrix such that the refactorization (157) is unique. Then, the map defined by (158) satisfies the Yang–Baxter equation and it is reversible.*

In the case where the map (158) admits Lax representation (157), but it is not equivalent to (157), one may need to check the YB property separately.

In these lecture notes, we are interested in those YB maps whose Lax representation involves matrices with rational dependence on the spectral parameter, as the following.

Example 4.10 In terms of Lax matrices, Adler's map (156) has the following strong Lax representation [109, 124]

$$L(u;a,\lambda)L(v;b,\lambda) = L(y;b,\lambda)L(x;a,\lambda)\ , \quad \text{for any } \lambda \in \mathbb{C}\ , \tag{159}$$

where

$$L(x;a,\lambda) = \begin{pmatrix} x & 1 \\ x^2 - a & x \end{pmatrix} - \lambda \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\ . \tag{160}$$

4.4 Yang–Baxter Maps and 3D Consistent Equations

From the representation of the YB equation on the cube, as in Fig. 12b, it is clear that the YB equation is essentially the same with the 3D consistency condition with the fields lying on the edges of the cube. Therefore, one would expect that we can derive YB maps from equations having the 3D consistency property.

The connection between YB maps and the multidimensional consistency condition for equations on quad graphs originates in the paper of Adler et al. in 2003 [9]. However, a more systematic approach was presented in the paper of Papageorgiou et al. [102] a couple of years later and it is based on the symmetry analysis of equations on quad-graphs. In particular, the YB variables constitute invariants of their symmetry groups.

We present the example of the discrete potential KdV (dpKdV) equation [93, 101] which was considered in [102].

Example 4.11 The dpKdV equation is given by

$$(f_{11} - f)(f_{10} - f_{01}) - a + b = 0\ , \tag{161}$$

where the fields are placed on the vertices of the square as in Fig. 13. We consider the values on the edges to be the difference of the values on the vertices, namely

$$x = f_{10} - f\ , \quad y = f_{11} - f_{10}\ , \quad u = f_{11} - f_{01}\ , \quad \text{and} \quad v = f_{01} - f\ , \tag{162}$$

as in Fig. 13. This choice of the variables is motivated by the fact that the dpKdV equation is invariant under the translation $f \to f + \text{const}$. Now, the invariants (162) satisfy the following equation

$$x + y = u + v\ . \tag{163}$$

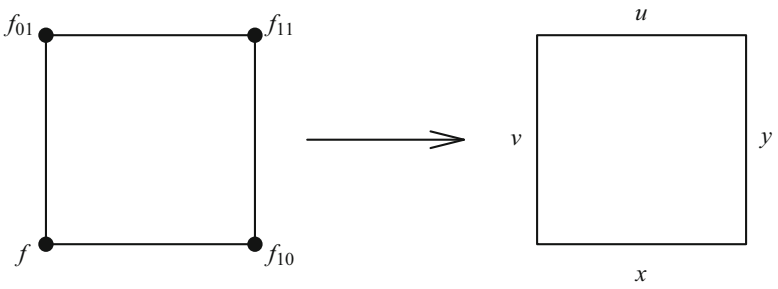


Fig. 13 (**a**) dpKdV equation: fields placed on vertices. (**b**) Adler's map: fields placed on the edges

Moreover, (161) can be rewritten as

$$(x+y)(x-v) = a-b\ . \tag{164}$$

Solving (163) and (164), we obtain the Adler's map (156).

4.5 Classification of Quadrirational YB Maps: The H-List

All the quadrirational maps in the F-list presented in the first chapter satisfy the YB equation. However, in principle, their Möbius-equivalent maps do not necessarily have the YB property, as in the following.

Example 4.12 Consider the map $\mathrm{F_V}$ of the F-list. Under the change of variables

$$(x,y,u,v) \to (-x,-y,u,v)\ , \tag{165}$$

it becomes

$$(x,y) \to \left(-y-\frac{a-b}{x-y}, -x-\frac{a-b}{x-y}\right)\ . \tag{166}$$

The above map does not satisfy the YB equation.

In fact, all the maps of the F-list lose the YB property under the transformation (165).

The quadrirational maps which satisfy the YB equation were classified in [103]. Particularly, their classification is based on the following.

Definition 4.13 Let $\rho_\lambda : X \to X$ be a λ-parametric family of bijections. The parametric YB maps $Y_{a,b}$ and $\widetilde{Y}_{a,b}$ are called equivalent, if they are related as follows

$$\widetilde{Y}_{a,b} = \rho_a^{-1} \times \rho_b^{-1}\, Y_{a,b}\, \rho_a \times \rho_b \ . \tag{167}$$

Remark 4.14 It is straightforward to show that the above equivalence relation is well defined; if $Y_{a,b}$ has the YB property, so does the map $\widetilde{Y}_{a,b}$.

The representative elements of the equivalence classes, with respect to the equivalence relation (167), are given by the following list.

Theorem 4.15 *Every quadrirational parametric YB map is equivalent* (*in the sense* (167)) *to one of the maps of the F-list or one of the maps of the following list*

$$u = yQ^{-1}\ , \quad v = xQ\ , \qquad Q = \frac{(1-b)xy + (b-a)y + b(a-1)}{(1-a)xy + (a-b)x + a(b-1)}\ ; \tag{$\mathrm{H_I}$}$$

$$u = yQ^{-1}\ , \quad v = xQ, \qquad Q = \frac{a + (b-a)y - bxy}{b + (a-b)x - axy}\ ; \tag{$\mathrm{H_{II}}$}$$

$$u = \frac{y}{a}Q\ , \quad v = \frac{x}{b}Q\ , \qquad Q = \frac{ax + by}{x + y}\ ; \tag{$\mathrm{H_{III}}$}$$

$$u = yQ^{-1} \qquad v = xQ\ , \qquad Q = \frac{axy + 1}{bxy + 1}; \tag{$\mathrm{H_{IV}}$}$$

$$u = y - P, \quad v = x + P\ , \quad P = \frac{a-b}{x+y}. \tag{$\mathrm{H_V}$}$$

We refer to the above list as the H-list. Note that, the map $\mathrm{H_V}$ is the Adler's map (156).

4.6 Derivation of Yang–Baxter Maps from Darboux Transformations

In this section we shall show how we can use Darboux transformations of particular Lax operators to construct Yang–Baxter maps, which can then be restricted to completely integrable ones (in the Liouville sense) on invariant leaves.

4.6.1 Invariants and Integrability of Yang–Baxter Maps

Proposition 4.16 *If $L = L(x, a; \lambda)$ is a Lax matrix with corresponding YB map, $Y : (x, y) \mapsto (u, v)$, then the* $\mathrm{tr}(L(y, b; \lambda)L(x, a; \lambda))$ *is a generating function of invariants of the YB map.*

Proof Since,

$$\begin{aligned} \mathrm{tr}\big(L(u,a;\lambda)L(v,b;\lambda)\big) &\overset{(157)}{=} \mathrm{tr}\big(L(y,b;\lambda)L(x,a;\lambda)\big) \\ &= \mathrm{tr}\big(L(x,a;\lambda)L(y,b;\lambda)\big)\ , \end{aligned} \tag{168}$$

and the function $\mathrm{tr}\big(L(x,a;\lambda)L(y,b;\lambda)\big)$ can be written as $\mathrm{tr}(L\big(x,a;\lambda)L(y,b;\lambda)\big) = \sum_k \lambda^k I_k(x,y;a,b)$, from (168) follows that

$$I_i(u,v;a,b) = I_i(x,y;a,b)\ , \tag{169}$$

which are invariants for Y. □

The invariants of a YB map are essential towards its integrability in the Liouville sense. Note that, the generated invariants, $I_i(x,y;a,b)$, in Proposition 4.16, may not be functionally independent. In what follows, we define the complete (Liouville) integrability of a YB map, following [47, 122]. However, for Liouville integrability, the reader is expected to have some basic knowledge of Poisson geometry [13, 83].

Definition 4.17 A $2N$-dimensional Yang–Baxter map,

$$Y\colon (x_1,\ldots,x_{2N}) \mapsto (u_1,\ldots,u_{2N})\ ,\quad u_i = u_i(x_1,\ldots,x_{2N})\ ,\ i=1,\ldots,2N\ ,$$

is said to be completely integrable or Liouville integrable if

1. there is a Poisson matrix, $J_{ij} = \{x_i, x_j\}$, of rank $2r$, which is invariant under the action of the YB map, namely J_{ij} and $J_{ij} = \{u_i, u_j\}$ have the same functional form of their respective arguments,
2. map Y has r functionally independent invariants, I_i, namely $I_i \circ Y = I_i$, which are in involution with respect to the corresponding Poisson bracket, i.e., $\{I_i, I_j\} = 0$, $i,j = 1,\ldots,r$, $i \neq j$,
3. there are $k = 2N - 2r$ Casimir functions, namely functions C_i, $i = 1,\ldots,k$, such that $\{C_i, f\} = 0$, for any arbitrary function $f = f(x_1,\ldots,x_{2N})$. These are invariant under Y, namely $C_i \circ Y = C_i$.

4.6.2 Example: From the NLS Equation to the Adler–Yamilov YB Map

Recall that, in the case of NLS equation, the Lax operator is given by

$$\mathbf{L}(p,q;\lambda) = D_x + \lambda U_1 + U_0,\quad \text{where } U_1 = \sigma_3,\ U_0 = \begin{pmatrix} 0 & 2p \\ 2q & 0 \end{pmatrix}, \tag{170}$$

where σ_3 is the standard Pauli matrix, i.e., $\sigma_3 = \mathrm{diag}(1,-1)$.

Moreover, a Darboux matrix for $\mathbf{L}$ is given by

$$M = \lambda \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} f & p \\ q_{10} & 1 \end{pmatrix} . \tag{171}$$

The entries of (171) must satisfy the following system of equations

$$\partial_x f = 2(pq - p_{10}q_{10}), \qquad \partial_x p = 2(pf - p_{10}) , \quad \partial_x q_{10} = 2(q - q_{10}f) , \tag{172}$$

which admits the following first integral

$$\partial_x(f - pq_{10}) = 0 . \tag{173}$$

This integral implies that $\partial_x \det M = 0$.

In correspondence with (171), we define the matrix

$$M(\mathbf{x};\lambda) = \lambda \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} X & x_1 \\ x_2 & 1 \end{pmatrix} , \quad \mathbf{x} = (x_1, x_2, X) , \tag{174}$$

and substitute it into the Lax equation (157)

$$M(\mathbf{u};\lambda)M(\mathbf{v};\lambda) = M(\mathbf{y};\lambda)M(\mathbf{x};\lambda) \tag{175}$$

to derive the following system of equations

$$v_1 = x_1 , \quad u_2 = y_2 , \quad U + V = X + Y , \quad u_2 v_1 = x_1 y_2 ,$$
$$u_1 + U v_1 = y_1 + x_1 Y , \; u_1 v_2 + UV = x_2 y_1 + XY , \; v_2 + u_2 V = x_2 + X y_2 .$$

The corresponding algebraic variety is a union of two six-dimensional components. The first one is obvious from the refactorization problem (175), and it corresponds to the permutation map

$$\mathbf{x} \mapsto \mathbf{u} = \mathbf{y} , \quad \mathbf{y} \mapsto \mathbf{v} = \mathbf{x} ,$$

which is a (trivial) YB map. The second one can be represented as a rational six-dimensional noninvolutive map of $K^3 \times K^3 \to K^3 \times K^3$

$$x_1 \mapsto u_1 = \frac{y_1 + x_1^2 x_2 - x_1 X + x_1 Y}{1 + x_1 y_2} , \qquad y_1 \mapsto v_1 = x_1 , \tag{176a}$$

$$x_2 \mapsto u_2 = y_2 , \qquad y_2 \mapsto v_2 = \frac{x_2 + y_1 y_2^2 + y_2 X - y_2 Y}{1 + x_1 y_2} , \tag{176b}$$

$$X \mapsto U = \frac{y_1y_2 - x_1x_2 + X + x_1y_2Y}{1 + x_1y_2}\,, \quad Y \mapsto V = \frac{x_1x_2 - y_1y_2 + x_1y_2X + Y}{1 + x_1y_2}\,, \tag{176c}$$

which, one can easily check that, satisfies the YB equation.

The trace of $M(\mathbf{y};\lambda)M(\mathbf{x};\lambda)$ is a polynomial in λ whose coefficients are

$$\operatorname{tr}\big(M(\mathbf{y};\lambda)M(\mathbf{x};\lambda)\big) = \lambda^2 + \lambda I_1(\mathbf{x},\mathbf{y}) + I_2(\mathbf{x},\mathbf{y})\,,$$

where

$$I_1(\mathbf{x},\mathbf{y}) = X + Y \quad \text{and} \quad I_2(\mathbf{x},\mathbf{y}) = x_2y_1 + x_1y_2 + XY\,, \tag{177}$$

and those, according to Proposition 4.16, are invariants for the YB map (176).

In the following section we show that the YB map (176) can be restricted to a four-dimensional YB map which has Poisson structure.

Now, we show that map (176) can be restricted to the Adler–Yamilov map on symplectic leaves, by taking into account the first integral, (173), of the system (172).

In particular, we have the following.

Proposition 4.18 *For the six-dimensional map* (176) *we have the following*:

1. *The quantities* $\Phi = X - x_1x_2$ *and* $\Psi = Y - y_1y_2$ *are its invariants* (*first integrals*).
2. *It can be restricted to a four-dimensional map* $Y_{a,b} : A_a \times A_b \to A_a \times A_b$, *where* A_a, A_b *are level sets of the first integrals* Φ *and* Ψ, *namely*

$$A_a = \{(x_1, x_2, X) \in K^3 \mid X = a + x_1x_2\}\,, \tag{178a}$$

$$A_b = \{(y_1, y_2, Y) \in K^3 \mid Y = b + y_1y_2\}\,. \tag{178b}$$

Moreover, map $Y_{a,b}$ *is the Adler–Yamilov map.*

Proof 1. It can be readily verified that (176) implies $U - u_1u_2 = X - x_1x_2$ and $V - v_1v_2 = Y - y_1y_2$. Thus, Φ and Ψ are invariants, i.e., first integrals of the map.

2. The existence of the restriction is obvious. Using the conditions $X = x_1x_2 + a$ and $Y = y_1y_2 + b$, one can eliminate X and Y from (176). The resulting map, $\mathbf{x} \to \mathbf{u}(\mathbf{x},\mathbf{y})$, $\mathbf{y} \to \mathbf{v}(\mathbf{x},\mathbf{y})$, is given by

$$(\mathbf{x},\mathbf{y}) \xrightarrow{Y_{a,b}} \left(y_1 - \frac{a-b}{1+x_1y_2}x_1, y_2, x_1, x_2 + \frac{a-b}{1+x_1y_2}y_2\right)\,. \tag{179}$$

Map (179) coincides with the Adler–Yamilov map. □

Map (179) originally appeared in the work of Adler and Yamilov [8]. Moreover, it appears as a YB map in [71, 100].

Now, one can use the condition $X = x_1x_2 + a$ to eliminate X from the Lax matrix (174), i.e.,

$$M(\mathbf{x}; a, \lambda) = \lambda \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} a + x_1x_2 & x_1 \\ x_2 & 1 \end{pmatrix} , \quad \mathbf{x} = (x_1, x_2) . \tag{180}$$

The form of Lax matrix (180) coincides with the well-known Darboux transformation for the NLS equation (see [105] and references therein). Now, Adler–Yamilov map follows from the strong Lax representation

$$M(\mathbf{u}; a, \lambda)M(\mathbf{v}; b, \lambda) = M(\mathbf{y}; b, \lambda)M(\mathbf{x}; a, \lambda) . \tag{181}$$

Therefore, the Adler–Yamilov map (179) is a reversible parametric YB map with strong Lax matrix (180). Moreover, it is easy to verify that it is not involutive.

For the integrability of this map we have the following

Proposition 4.19 *The Adler–Yamilov map* (179) *is completely integrable.*

Proof The 4×4 Poisson matrix associated to the following Poisson bracket

$$\{x_1, x_2\} = \{y_1, y_2\} = 1 , \quad \text{and all the rest } \{x_i, y_j\} = 0 , \tag{182}$$

is invariant under the YB map (179), namely the latter is a Poisson map with respect to the Poisson bracket $\pi = (\partial/\partial x_1) \wedge (\partial/\partial x_2) + (\partial/\partial y_1) \wedge (\partial/\partial y_2)$. Now, from the trace of $M(\mathbf{y}; b, \lambda)M(\mathbf{x}; a, \lambda)$ we obtain the following invariants for the map (179)

$$I_1(\mathbf{x}, \mathbf{y}) = x_1x_2 + y_1y_2 + a + b , \tag{183}$$

$$I_2(\mathbf{x}, \mathbf{y}) = (a + x_1x_2)(b + y_1y_2) + x_1y_2 + x_2y_1 + 1 . \tag{184}$$

It is easy to check that I_1, I_2 are in involution with respect to (182), namely $\{I_1, I_2\} = 0$. Therefore the map (179) is completely integrable. □

The above proposition implies the following.

Corollary 4.20 *The invariant leaves A_a and B_b, given in* (178), *are symplectic.*

4.7 Yang–Baxter Maps for NLS Type Equations. Noncommutative Extensions

In the previous section we showed how one can use Darboux transformations to construct Yang–Baxter maps which can restrict to completely integrable ones on invariant leaves. In particular, using a Darboux transformation for the NLS equation, namely matrix (171), we constructed the six-dimensional Yang–Baxter map (176) which was restricted to the completely integrable Adler–Yamilov map (179) on the

invariant (symplectic) leaves (178). In [67, 68], all Yang–Baxter maps related to the cases (134a), (134b) and (134c), as well as their integrability, were studied, using the associated Darboux transformations.

Motivated by some results on noncommutative extensions (in a Grassmann setting) of Darboux transformations and their use in the construction of noncommutative discrete integrable systems [50], in [51, 69], the first steps towards extending the theory of Yang–Baxter maps were made.

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References

1. M.J. Ablowitz, P.A. Clarkson, *Soliton, Nonlinear Evolution Equations and Inverse Scattering*. London Mathematical Society Lecture Note Series, vol. 149 (Cambridge University Press, Cambridge, 1991)
2. M.J. Ablowitz, A.S. Fokas, *Complex Variables*, 2nd edn. Cambridge Texts in Applied Mathematics, vol. 36 (Cambridge University Press, Cambridge, 2003)
3. M.J. Ablowitz, H. Segur, *Solitons and the Inverse Scattering Transform*. SIAM Studies in Applied Mathematics, vol. 4 (SIAM, Philadelphia, 1981)
4. M.J. Ablowitz, D.J. Kaup, A.C. Newell, H. Segur, Method for solving the sine-Gordon equation. Phys. Rev. Lett. **30**, 1262–1264 (1973)
5. M.J. Ablowitz, D.J. Kaup, A.C. Newell, H. Segur, The inverse scattering transform-Fourier analysis for nonlinear problems. Stud. Appl. Math. **53**(4), 249–315 (1974)
6. R. Abraham, J.E. Marsden, T. Ratiu, *Manifolds, Tensor Analysis, and Applications*. Global Analysis, Pure and Applied Series B, vol. 2 (Addison-Wesley, Reading, 1983)
7. V.E. Adler, Recuttings of polygons. Funct. Anal. Appl. **27**(2), 141–143 (1993)
8. V.E. Adler, R. Yamilov, Explicit auto-transformations of integrable chains. J. Phys. A **27**(2), 477–492 (1994)
9. V.E. Adler, A.I. Bobenko, Yu.B. Suris, Classification of integrable equations on quad-graphs. The consistency approach. Commun. Math. Phys. **233**(3), 513–543 (2003)
10. V.E. Adler, A.I. Bobenko, Yu.B. Suris, Geometry of Yang–Baxter maps: pencils of conics and quadrirational mappings. Commun. Anal. Geom. **12**(5), 967–1007 (2004)
11. N.I. Akhiezer, Orthogonal polynomials on several intervals. Sov. Math. Dokl. **1**, 989–992 (1960)
12. N.I. Akhiezer, Continuous analogues of the polynomials orthogonal on the system of intervals. Dokl. Akad. Nauk SSSR **141**, 263–266 (1961). In Russian
13. V.I. Arnol'd, *Mathematical Methods of Classical Mechanics*, 2nd edn. Graduate Texts in Mathematics, vol. 60 (Springer, New York, 1989)
14. H.F. Baker, Note on the foregoing paper "commutative ordinary differential operators" by J. L. Burchnall and J. W. Chaundy. Proc. R. Soc. Ser. A **118**(780), 584–593 (1928)
15. R.J. Baxter, Partition function of the eight-vertex lattice model. Ann. Phys. **70**(1), 193–228 (1972)
16. G. Berkeley, A.V. Mikhailov, P. Xenitidis, Darboux transformations with tetrahedral reduction group and related integrable systems. J. Math. Phys. **57**(9), 092701 (2016)
17. D. Bilman, On long-time asymptotics for the Toda lattice and its Hamiltonian perturbations. Ph.D. thesis, University of Illinois at Chicago (2015)
18. D. Bilman, T. Trogdon, Numerical inverse scattering for the Toda lattice. Comm. Math. Phys. **352**(2), 805–879 (2017)

19. A.I. Bobenko, Yu.B. Suris, Integrable systems on quad-graphs. Int. Math. Res. Not. **2002**(11), 573–611 (2002)
20. V.M. Bukhshtaber, The Yang–Baxter transformation. Russ. Math. Surv. **53**(6), 1343–1345 (1998)
21. R. Bury, Automorphic Lie algebras, corresponding integrable systems and their soliton solutions. Ph.D. thesis, University of Leeds (2010)
22. R. Bury, A.V. Mikhailov. Automorphic Lie algebras and corresponding integrable systems (2009). Draft (unpublished)
23. K.F. Clancey, I. Gohberg, *Factorization of Matrix Functions and Singular Integral Operators*. Operator Theory: Advances and Applications, vol. 3 (Birkhäuser, Basel, 1981)
24. G. Darboux, Sur une proposition relative aux équations linéaires. C. R. Acad. Sci. **94**, 1456–1459 (1882)
25. E. Date, M. Jimbo, T. Miwa, Method for generating discrete soliton equations. I. J. Phys. Soc. Jpn. **51**(12), 4116–4124 (1982)
26. E. Date, M. Jimbo, T. Miwa, Method for generating discrete soliton equations. II. J. Phys. Soc. Jpn. **51**(12), 4125–4131 (1982)
27. E. Date, M. Jimbo, T. Miwa, Method for generating discrete soliton equations. III. J. Phys. Soc. Jpn. **52**(2), 388–393 (1983)
28. E. Date, M. Jimbo, T. Miwa, Method for generating discrete soliton equations. IV. J. Phys. Soc. Jpn. **52**(3), 761–765 (1983)
29. E. Date, M. Jimbo, T. Miwa, Method for generating discrete soliton equations. V. J. Phys. Soc. Jpn. **52**(3), 766–771 (1983)
30. E. Date, S. Tanaka, Analogue of inverse scattering theory for the discrete Hill's equation and exact solutions for the periodic Toda lattice. Prog. Theor. Phys. **55**(2), 457–465 (1976)
31. T. Dauxois, M. Peyrard, S. Ruffo, The Fermi–Pasta–Ulam 'numerical experiment': history and pedagogical perspectives. Eur. J. Phys. **26**(5), S3–S11 (2005)
32. P. Deift, *Orthogonal Polynomials and Random Matrices*: *A Riemann–Hilbert Approach*. Courant Lecture Notes in Mathematics, vol. 3 (American Mathematical Society, Providence, 1999)
33. P. Deift, K.T.-R. McLaughlin, A continuum limit of the Toda lattice. Mem. Am. Math. Soc. **131**(624) (1998)
34. P. Deift, X. Zhou, A steepest descent method for oscillatory Riemann–Hilbert problems. Asymptotics for the MKdV equation. Ann. Math. (2) **137**(2), 295–368 (1993)
35. P. Deift, X. Zhou, Asymptotics for the Painlevé II equation. Commun. Pure Appl. Math. **48**(3), 277–337 (1995)
36. P. Deift, S. Venakides, X. Zhou, The collisionless shock region for the long-time behavior of solutions of the KdV equation. Commun. Pure Appl. Math. **47**(2), 199–206 (1994)
37. V.G. Drinfel'd, On some unsolved problems in quantum group theory, in *Quantum Groups* (Springer, Berlin, 1992), pp. 1–8
38. B.A. Dubrovin, The inverse scattering problem for periodic short-range potentials. Funct. Anal. Appl. **9**(1), 61–62 (1975)
39. B.A. Dubrovin, Theta functions and non-linear equations. Russ. Math. Surv. **36**(2), 11–92 (1981)
40. B.A. Dubrovin, S.P. Novikov, A periodic problem for the Korteweg–de Vries and Sturm–Liouville equations. Their connection with algebraic geometry. Sov. Math. Dokl. **15**(6), 1597–1601 (1974)
41. B.A. Dubrovin, V.B. Matveev, S.P. Novikov, Nonlinear equations of Korteweg–de Vries type, finite-band linear operators and Abelian varieties. Uspehi Mat. Nauk **31**(187), 55–136 (1976). In Russian
42. L.D. Faddeev, L.A. Takhtajan, *Hamiltonian Methods in the Theory of Solitons*. Classics in Mathematics (Springer, Berlin, 2007)
43. H. Flaschka, On the Toda lattice. II. Inverse-scattering solution. Prog. Theor. Phys. **51**, 703–716 (1974)
44. H. Flaschka, The Toda lattice. I. Existence of integrals. Phys. Rev. B **9**(3), 1924–1925 (1974)

45. H. Flaschka, D.W. McLaughlin, Canonically conjugate variables for the Korteweg–de Vries equation and the Toda lattice with periodic boundary conditions. Prog. Theor. Phys. **55**(2), 438–456 (1976)
46. J. Ford, The Fermi–Pasta–Ulam problem: paradox turns discovery. Phys. Rep. **213**(5), 271–310 (1992)
47. A.P. Fordy, Periodic cluster mutations and related integrable maps. J. Phys. A **47**(47), 474003 (2014)
48. C.S. Gardner, J.M. Greene, M.D. Kruskal, R.M. Miura, Method for solving the Korteweg–de Vries equation. Phys. Rev. Lett. **19**(19), 1095–1097 (1967)
49. F. Gesztesy, H. Holden, J. Michor, G. Teschl, *Soliton Equations and Their Algebro-Geometric Solutions*, vol. II. Cambridge Studies in Advanced Mathematics (Cambridge University Press, Cambridge, 2008)
50. G.G. Grahovski, A.V. Mikhailov, Integrable discretisations for a class of nonlinear Schrödinger equations on Grassmann algebras. Phys. Lett. A **377**(45–48), 3254–3259 (2013)
51. G.G. Grahovski, K.-S. Rizos, A. Mikhailov, Grassmann extensions of Yang–Baxter maps. J. Phys. A **49**(14), 145202 (2016)
52. B. Grammaticos, A. Ramani, V.G. Papageorgiou, Do integrable mappings have the Painlevé property? Phys. Rev. Lett. **67**(14), 1825–1828 (1991)
53. B. Grammaticos, K.-Y. Schwarzbach, T. Tamizhmani (eds.), *Discrete Integrable Systems*. Lecture Notes in Physics (Springer, Berlin, 2004)
54. C. Gu, H. Hu, Z. Zhou, *Darboux Transformations in Integrable Systems*. Mathematical Physics Studies (Springer, New York, 2005)
55. M. Hénon, Integrals of the toda lattice. Phys. Rev. B (3) **9**(4), 1921–1923 (1974)
56. J. Hietarinta, C. Viallet, Integrable lattice equations with vertex and bond variables. J. Phys. A **44**(38), 385201 (2011)
57. J. Hietarinta, N. Joshi, F.W. Nijhoff, *Discrete Systems and Integrability*. Cambridge Texts in Applied Mathematics, vol. 54 (Cambridge University Press, Cambridge, 2016)
58. R. Hirota, Nonlinear partial difference equations. I. A difference analogue of the Korteweg–de Vries equation. J. Phys. Soc. Jpn. **43**(4), 1424–1433 (1977)
59. R. Hirota, Nonlinear partial difference equations. II. Discrete-time Toda equation. J. Phys. Soc. Jpn. **43**(6), 2074–2078 (1977)
60. R. Hirota, Nonlinear partial difference equations. III. Discrete sine-Gordon equation. J. Phys. Soc. Jpn. **43**(6), 2079–2086 (1977)
61. R. Hirota, Nonlinear partial difference equations. IV. Bäcklund transformations for the discrete-time Toda equation. J. Phys. Soc. Jpn. **45**(1), 321–332 (1978)
62. A.R. Its, V.B. Matveev, Hill's operator with finitely many gaps. Funct. Anal. Appl. **9**(1), 65–66 (1975)
63. A.R. Its, V.B. Matveev, Schrödinger operators with finite-gap spectrum and N-soliton solutions of the Korteweg–de Vries equation. Theor. Math. Phys. **23**(1), 343–355 (1975)
64. S. Kamvissis, On the long time behavior of the doubly infinite Toda lattice under initial data decaying at infinity. Commun. Math. Phys. **153**(3), 479–519 (1993)
65. D.J. Kaup, A.C. Newell, An exact solution for a derivative nonlinear Schrödinger equation. J. Math. Phys. **19**(4), 798–801 (1978)
66. F. Klein, Ueber binäre formen mit linearen transformationen in sich selbst. Math. Ann. **9**(2), 183–208 (1875)
67. S. Konstantinou-Rizos, Darboux transformations, discrete integrable systems and related Yang–Baxter maps. Ph.D. thesis, University of Leeds (2014)
68. S. Konstantinou-Rizos, A.V. Mikhailov, Darboux transformations, finite reduction groups and related Yang–Baxter maps. J. Phys. A **46**(42), 425201 (2013)
69. S. Konstantinou-Rizos, A.V. Mikhailov, Anticommutative extension of the Adler map. J. Phys. A **49**(30), 30LT3 (2016)
70. S. Konstantinou-Rizos, A.V. Mikhailov, P. Xenitidis, Reduction groups and related integrable difference systems of nonlinear Schrödinger type. J. Math. Phys. **56**(8), 082701 (2015)

71. T.E. Kouloukas, V.G. Papageorgiou, Yang–Baxter maps with first-degree-polynomial 2×2 Lax matrices. J. Phys. A **42**(40), 404012 (2009)
72. T.E. Kouloukas, V.G. Papageorgiou, Poisson Yang–Baxter maps with binomial Lax matrices. J. Math. Phys. **52**(7), 073502 (2011)
73. I.M. Krichever, Integration of nonlinear equations by the methods of algebraic geometry. Funct. Anal. Appl. **11**(1), 12–26 (1977)
74. I.M. Krichever, Algebraic curves and non-linear difference equations. Russ. Math. Surv. **33**4), 255–256 (1978)
75. I.M. Krichever, Nonlinear equation and elliptic curves, in *Current Problems in Mathematics*, vol. 23. Itogi Nauki i Tekhniki (Akad. Nauk SSSR, VINITI, Moscow, 1983), pp. 79–136. In Russian
76. I.M. Krichever, Algebraic-geometrical methods in the theory of integrable equations and their perturbations. Acta Appl. Math. **39**, 93–125 (1995)
77. H. Krüger, G. Teschl, Long-time asymptotics for the Toda lattice in the soliton region. Math. Z. **262**(3), 585–602 (2009)
78. H. Krüger, G. Teschl, Long-time asymptotics of the Toda lattice for decaying initial data revisited. Rev. Math. Phys. **21**(1), 61–109 (2009)
79. P.D. Lax, Integrals of nonlinear equations of evolution and solitary waves. Commun. Pure Appl. Math. **21**, 467–490 (1968)
80. D. Levi, Nonlinear differential-difference equations as Bäcklund transformations. J. Phys. A **14**(5), 1083–1098 (1981)
81. D. Levi, R. Benguria, Bäcklund transformations and nonlinear differential difference equations. Proc. Natl. Acad. Sci. USA **77**(9), 5025–5027 (1980)
82. S.V. Manakov, Complete integrability and stochastization of discrete dynamical systems. Sov. Phys. JETP **40**(2), 269–274 (1974)
83. J.E. Marsden, T.S. Ratiu, *Introduction to Mechanics and Symmetry*, 2nd edn. Texts in Applied Mathematics, vol. 17 (Springer, New York, 1999)
84. V.B. Matveev, 30 years of finite-gap integration theory. Philos. Trans. R. Soc. Lond. Ser. A Math. Phys. Eng. Sci. **366**(1867), 837–875 (2008)
85. V.B. Matveev, M.A. Salle, *Darboux Transformations and Solitons*. Springer Series in Nonlinear Dynamics (Springer, Berlin, 1991)
86. H.P. McKean Jr., P. van Moerbecke, The spectrum of Hill's equation. Invent. Math. **30**(3), 217–274 (1975)
87. A.V. Mikhailov, Formal diagonalisation of Lax–Darboux schemes. Model. Anal. Inf. Sist. **22**(6), 795–817 (2015)
88. A.V. Mikhailov, A.B. Shabat, R.I. Yamilov, Extension of the module of invertible transformations. Classification of integrable systems. Commun. Math. Phys. **115**(1), 1–19 (1988)
89. A.V. Mikhailov, G. Papamikos, J.P. Wang, Darboux transformation with dihedral reduction group. J. Math. Phys. **55**(11), 113507 (2014)
90. P.D. Miller, Topics in pde: integrable systems and Riemann–Hilbert problems. Lecture Notes, University of Michigan (2015)
91. J. Moser, Finitely many mass points on the line under the influence of an exponential potential—an integrable system, in *Dynamical Systems, Theory and Applications*. Lecture Notes in Physics (Springer, Berlin, 1975)
92. F.W. Nijhoff, Discrete systems and integrability. Lecture Notes, University of Leeds (2006)
93. F.W. Nijhoff, H.W. Capel, The discrete Korteweg–de Vries equation. Acta Appl. Math. **39**(1–3), 133–158 (1995)
94. F.W. Nijhoff, A.J. Walker, The discrete and continuous Painlevé VI hierarchy and the Garnier systems. Glasg. Math. J. **43**(A), 109–123 (2001)
95. F.W. Nijhoff, H.W. Capel, G.L. Wiersma, Integrable lattice systems in two and three dimensions. in *Geometric Aspects of the Einstein Equations and Integrable Systems*, ed. by R. Martini. Lecture Notes in Physics, vol. 239 (Springer, Berlin, 1984), pp. 263–302
96. S.P. Novikov, A periodic problem for the Korteweg–de Vries equation. Funct. Anal. Appl. **8**(3), 236–246 (1974)

97. S. Olver, Numerical solution of Riemann–Hilbert problems: Painlevé II. Found. Comput. Math. **11**(2), 153–179 (2011)
98. S. Olver, A general framework for solving Riemann–Hilbert problems numerically. Numer. Math. **122**(2), 305–340 (2012)
99. S. Olver, T. Trogdon, Nonlinear steepest descent and the numerical solution of Riemann–Hilbert problems. Commun. Pure Appl. Math. **67**(8), 1353–1389 (2014)
100. V.G. Papageorgiou, A.G. Tongas, Yang–Baxter maps and multi-field integrable lattice equations. J. Phys. A **40**(42), 12677–12690 (2007)
101. V.G. Papageorgiou, F.W. Nijhoff, H.W. Capel, Integrable mappings and nonlinear integrable lattice equations. Phys. Lett. A **147**(2–3), 106–114 (1990)
102. V.G. Papageorgiou, A.G. Tongas, A.P. Veselov, Yang–Baxter maps and symmetries of integrable equations on quad-graphs. J. Math. Phys. **47**(8), 083502 (2006)
103. V.G. Papageorgiou, S.B. Suris, A.G. Tongas, A.P. Veselov, On quadrirational Yang–Baxter maps. SIGMA **6**, 033 (2010)
104. G.R.W. Quispel, F.W. Nijhoff, H.W. Capel, J. van der Linden, Linear integral equations and nonlinear difference-difference equations. Phys. A **125**(2–3), 344–380 (1984)
105. C. Rogers, W.K. Schief, *Bäcklund and Darboux Transformations*. Cambridge Texts in Applied Mathematics, vol. 30 (Cambridge University Press, Cambridge, 2016)
106. B. Simon, Sturm oscillation and comparison theorems, in *Sturm–Liouville Theory*, ed. by W.O. Amrein, A.M. Hinz, D.P. Pearson (Birkhäuser, Basel, 2005)
107. E.K. Sklyanin, Classical limits of the SU(2)-invariant solutions of the Yang–Baxter equation. J. Sov. Math. **40**(1), 93–107 (1988)
108. Yu.B. Suris, Bi-Hamiltonian structure of the *qd* algorithm and new discretizations of the Toda lattice. Phys. Lett. A **206**(3–4), 153–161 (1995)
109. Yu.B. Suris, A.P. Veselov, Lax matrices for Yang–Baxter maps. J. Nonlinear Math. Phys. **10**(2), 223–230 (2003)
110. W.W. Symes, Hamiltonian group actions and integrable systems. Phys. D **1**(4), 339–374 (1980)
111. W.W. Symes, The *qr* algorithm and scattering for the finite nonperiodic toda lattice. Phys. D **4**(2), 275–280 (1981/82)
112. G. Szegő, *Orthogonal Polynomials*, 4th edn. American Mathematical Society Colloquium-Publications, vol. 23 (American Mathematical Society, Providence, 1975)
113. T.R. Taha, M.J. Ablowitz, Analytical and numerical aspects of certain nonlinear evolution equations. I. Analytical. J. Comput. Phys. **55**(2), 192–202 (1984)
114. T.R. Taha, M.J. Ablowitz, Analytical and numerical aspects of certain nonlinear evolution equations. II. Numerical, nonlinear Schrödinger equation. J. Comput. Phys. **55**(2), 203–230 (1984)
115. T.R. Taha, M.J. Ablowitz, Analytical and numerical aspects of certain nonlinear evolution equations. III. Numerical, Korteweg-de Vries equation. J. Comput. Phys. **55**(2), 231–253 (1984)
116. G. Teschl, Oscillation theory and renormalized oscillation theory for Jacobi operators. J. Differ. Equ. **129**(2), 532–558 (1996)
117. G. Teschl, *Jacobi Operators and Completely Integrable Nonlinear Lattices*. Mathematical Surveys and Monographs, vol. 72 (American Mathematical Society, Providence, 2000)
118. T. Trogdon, S. Olver, Numerical inverse scattering for the focusing and defocusing nonlinear Schrödinger equations. Proc. R. Soc. Lond. Ser. A Math. Phys. Eng. Sci. **469**(2149), 20120330 (2013)
119. T. Trogdon, S. Olver, *Riemann–Hilbert Problems*, *Their Numerical Solution and the Computation of Nonlinear Special Functions* (SIAM, Philadelphia, 2016)
120. T. Trogdon, S. Olver, B. Deconinck, Numerical inverse scattering for the Korteweg–de Vries and modified Korteweg–de Vries equations. Phys. D **241**(11), 1003–1025 (2012)
121. P. van Moerbeke, The spectrum of Jacobi matrices. Invent. Math. **37**(1), 45–81 (1976)
122. A.P. Veselov, Integrable maps. Russ. Math. Surv. **46**(5), 1–51 (1991)

123. A.P. Veselov, Yang–Baxter maps and integrable dynamics. Phys. Lett. A **314**(3), 214–221 (2003)
124. A.P. Veselov, Yang–Baxter maps: dynamical point of view, in *Combinatorial Aspect of Integrable Systems*. MSJ Memoirs, vol. 17, pp. 145–167 (Mathematical Society of Japan, Tokyo, 2007)
125. H.D. Wahlquist, F.B. Estabrook, Bäcklund transformation for solutions of the Korteweg–de Vries equation. Phys. Rev. Lett. **31**(23), 1386–1390 (1973)
126. C.N. Yang, Some exact results for the many-body problem in one dimension with repulsive delta-function interaction. Phys. Rev. Lett. **19**(23), 1312–1315 (1967)
127. N.J. Zabusky, M.D. Kruskal, Interaction of "solitons" in a collisionless plasma and the recurrence of initial states. Phys. Rev. Lett. **15**(6), 240–243 (1963)
128. V.E. Zakharov (ed.), *What Is Integrability*? Springer Series in Nonlinear Dynamics (Springer, Berlin, 1991)
129. V.E. Zakharov, L.D. Faddeev, Korteweg–de Vries equation: a completely integrable Hamiltonian system. Funct. Anal. Appl. **5**(4), 280–287 (1971)
130. V.E. Zakharov, A.B. Shabat, Exact theory of two-dimensional self-focusing and one-dimensional self-modulation of waves in nonlinear media. Sov. Phys. JETP **61**(1), 62–69 (1972)
131. V.E. Zakharov, A.B. Shabat, A scheme for integrating the nonlinear equations of mathematical physics by the method of the inverse scattering problem. I. Funct. Anal. Appl. **8**(3), 226–235 (1974)

Symmetry-Preserving Numerical Schemes

Alexander Bihlo and Francis Valiquette

Abstract In these lectures we review two procedures for constructing finite difference numerical schemes that preserve symmetries of differential equations. The first approach is based on Lie's infinitesimal symmetry generators, while the second method uses the novel theory of equivariant moving frames. The advantages of both techniques are discussed and illustrated with the Schwarzian differential equation, the Korteweg–de Vries equation and Burgers' equation. Numerical simulations are presented and innovative techniques for obtaining better invariant numerical schemes are introduced. New research directions and open problems are indicated at the end of these notes.

1 Introduction

The aim of geometric numerical integration is to develop numerical integrators that preserve geometric properties of the system of differential equations under investigation. Classical examples include symplectic integrators [36, 51], energy preserving methods [77], and schemes that preserve a Lie–Poisson structure [88]. The motivation behind geometric numerical integration is that, as a rule of thumb, such integrators will typically give better global or long term numerical results than standard methods since they incorporate qualitative properties of the system under consideration.

In mathematical physics, most fundamental differential equations are invariant under a certain collection of symmetry transformations. These symmetries can be point transformations, contact transformations, or generalized transformations [68]. In all cases, the symmetries of a differential equation encapsulate important proper-

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ties of the equation and its solutions. Furthermore, Lie group techniques are amongst the most effective methods for obtaining explicit solutions and conservation laws of nonlinear differential equations [11, 68, 76].

When discretizing differential equations invariant under a certain symmetry group, there are different incentives for preserving the symmetries of these equations. From a physical standpoint, discrete spacetime models should preserve the symmetries of their continuous counterparts. Mathematically, Lie group techniques could then be used to find explicit solutions and compute conservation laws of the discrete models. From a more practical point of view, symmetry-preserving discretizations should share some exact solutions with the original differential equations, or at least provide better approximations than noninvariant numerical schemes.

In the last 30 years, the application of Lie group techniques to finite difference equations has become a very active field of research. To the best of our knowledge, Yanenko and Shokin were the first to use group theoretical methods to study finite difference schemes by introducing first differential approximations of difference equations [82, 87]. The application of Lie group methods to finite difference equations, as we know it today, was first introduced by Dorodnitsyn in 1989 [23]. Early on, one of the main focuses in the field was to construct Lie point symmetry-preserving finite difference approximations of differential equations. Beside Dorodnitsyn, early contributors include Bakirova, Kozlov, Levi, and Winternitz who constructed symmetry-preserving schemes for heat transfer equations [2, 3, 26], variable coefficient Korteweg–de Vries equations [27], Burgers' equation [37], the nonlinear Schrödinger equation [17], and second-order ordinary differential equations [28]. Symmetry-preserving approximation of Euler–Lagrange equations and their corresponding Lagrangian have also been considered in [29, 30], and the application of Noether's theorem to compute conservation laws has been extensively studied in the discrete setting [24, 44, 45]. The applications of Lie point symmetries to finite difference equations have also been extended to generalized symmetries [54, 55], λ-symmetries [53, 59], and contact transformations [62].

In recent years, more systematic efforts have been directed towards investigating the numerical performance of symmetry-preserving schemes. For ordinary differential equations, symmetry-preserving schemes have proven to be very promising. For solutions exhibiting sharp variations or singularities, symmetry-preserving schemes systematically appear to outperform standard numerical schemes [13, 14, 18, 50]. For partial differential equations, the improvement of symmetry-preserving schemes versus traditional integrators is not as clear [9, 49, 61, 78]. On one hand, it was shown in [85] that symmetry-preserving schemes do much better in tracking sharp interfaces in Hamilton–Jacobi equations. On the other hand, invariant numerical schemes for evolution equations generally require the use of time-evolving meshes which can lead to mesh tangling and thereby severely limit the use of symmetry-preserving schemes. In this case, special techniques have to be developed to avoid mesh singularities. For example, new ideas relying on r-adaptivity have been implemented to improve the performance of invariant integrators [7]. Also, in [5, 6]

an invariant evolution–projection strategy was introduced and invariant meshless discretization schemes were considered in [4].

The preceding references only provide a short bibliographical overview of the field. Many papers had to be omitted. More references on the subject can be found in the survey papers [56, 86], and the books [25, 44].

Given a differential equation with symmetry group G, the first step in constructing a symmetry-preserving numerical scheme is to compute difference invariants of the product action of G on a chosen stencil. There are mainly two approaches for constructing those invariants. Most of the references cited above use the infinitesimal symmetry generators of the group action and Lie's infinitesimal invariance criterion to construct difference invariants. Alternatively, the difference invariants can be constructed using the novel method of equivariant moving frames mainly developed by Olver, which was done in [4, 21, 50, 70, 78, 79]. Given sufficiently many difference invariants, an invariant numerical scheme is, in general, obtained by finding a suitable combination of these invariants that converges to the original differential equation in the continuous limit. When using Lie's infinitesimal generator approach, a suitable combination is found by taking the Taylor expansion of the difference invariants and combining them in such a way to obtained the desired invariant scheme. With the method of moving frames, a suitable combination is found more systematically by invariantizing a noninvariant numerical scheme. Since the symmetry group of a differential equation will, in general, act on both the independent and dependent variables, a symmetry-preserving numerical scheme will usually not be defined on a uniform orthogonal mesh.

The application of Lie groups to finite difference equations is a vast and very dynamic field of study. While preparing these lecture notes we had to omit many interesting applications and important results. The focus of these notes will be on the theoretical construction of invariant numerical schemes and their numerical implementation. At the heart of all our considerations are differential equations, finite difference equations, symmetry groups, and invariants. These familiar notions are all reviewed in Sects. 2, 3, and 4. As outlined above, there are two different approaches for computing invariants of a Lie group action. The infinitesimal approach based on Lie's symmetry generators is introduced in Sect. 4.1, while the equivariant moving frame approach is explained in Sect. 4.2. Section 5 is devoted to weakly invariant equations, which can play an important role in the construction of symmetry-preserving schemes. The construction of symmetry-preserving numerical schemes is carefully explained in Sect. 6. To illustrate the implementation, we consider the Schwarzian differential equation and the Korteweg–de Vries (KdV) equation. In Sect. 7 we carry out numerical simulations for the Schwarzian equation, the KdV equation and Burgers' equation. For partial differential equations, the invariance of a numerical scheme does not, in general, guarantee better numerical results. We will show that symmetry-preserving schemes can lead to mesh tangling, which limit their practical scope. To circumvent this shortcoming, we discuss new invariant numerical strategies. For the Korteweg–de Vries equation, we introduce *invariant evolution–projection schemes* and *invariant adaptive numerical schemes*.

Unlike the KdV equation, solutions to Burgers' equation can exhibit shocks. For these shock solutions we propose a new *invariant finite volume* type scheme. Finally, in Sect. 8 we identify some open problems and challenges in the field of symmetry-preserving numerical integrators.

2 Differential and Difference Equations

In this section we review the definitions of differential equations and finite difference equations. We take this opportunity to introduce some of the notation used throughout these notes.

2.1 Differential Equations

Let M be an m-dimensional manifold. For $0 \leq \ell \leq \infty$, let $\mathrm{J}^{(\ell)} = \mathrm{J}^{(\ell)}(M,p)$ denote the *extended ℓth order jet space* of $1 \leq p < m$ dimensional submanifolds $S \subset M$ defined as the space of equivalence classes of submanifolds under the equivalence relation of ℓth order contact at a point [68]. Local coordinates on $\mathrm{J}^{(\ell)}$ are given by the ℓ-jet

$$\left(x, u^{(\ell)}\right), \tag{1}$$

where $x = (x^1, \dots, x^p)$ correspond to the independent variables and $u^{(\ell)}$ denotes the derivatives

$$u^\alpha_{x^J} = \frac{\partial^k u^\alpha}{(\partial x^1)^{j_1} \cdots (\partial x^p)^{j_p}}$$

$$\text{with } 1 \leq \alpha \leq q = m - p \text{ and } 0 \leq k = j_1 + \cdots + j_p \leq \ell\,.$$

In the above notation, $J = (j_1, \dots, j_p)$ is an ordered p-tuple of nonnegative integers, with entries $j_i \geq 0$ indicating the number of derivatives taken in the variable x^i. The order of the multi-index, denoted by $\#J = k$, indicates how many derivatives are being taken.

Example 2.1 In the case where $p = 2$ and $q = 1$, we have two independent variables $(x^1, x^2) = (t, x)$ and one dependent variable $u^1 = u$. Then, the second order jet space is parametrized by

$$(t, x, u, u_t, u_x, u_{tt}, u_{tx}, u_{xx})\,.$$

Definition 2.2 A *differential equation* of order n is the zero locus of a differential map $\Delta\colon \mathrm{J}^{(\ell)} \to \mathbb{R}$. That is,

$$\Delta\big(x, u^{(\ell)}\big) = 0\ . \tag{2}$$

For later use, we introduce two regularity requirements on differential equations.

Definition 2.3 A differential equation $\Delta\big(x, u^{(\ell)}\big) = 0$ is said to be *regular* if the rank of its differential

$$\mathrm{d}\Delta = \sum_{i=1}^{p} \frac{\partial \Delta}{\partial x^i}\mathrm{d}x^i + \sum_{J} \sum_{\alpha=1}^{q} \frac{\partial \Delta}{\partial u^{\alpha}_{x^J}}\mathrm{d}u^{\alpha}_{x^J}$$

is constant on the domain of definition of $\Delta\colon \mathrm{J}^{(\ell)} \to \mathbb{R}$.

Example 2.4 Any evolutionary partial differential equation

$$\Delta\big(t, x, u^{(\ell)}\big) = u_t - f(t, x, u, u_x, u_{xx}, \dots, u_{x^\ell}) = 0$$

is regular since the rank of $\mathrm{d}\Delta = \mathrm{d}u_t - \mathrm{d}f$ is one.

Definition 2.5 A differential equation $\Delta\big(x, u^{(\ell)}\big) = 0$ is *locally solvable* at a point $\big(x_0, u_0^{(\ell)}\big)$ if there exists a smooth solution $u = f(x)$, defined in the neighborhood of x_0, such that $u_0^{(\ell)} = f^{(\ell)}(x_0)$. A differential equation which is both regular and locally solvable is said to be *fully regular*.

The above description assumes that a submanifold $S \subset M$ is locally represented as the graph of a function $S = \big\{\big(x, f(x)\big)\big\}$. Alternatively, when no distinction between independent and dependent variables is made, a submanifold $S \subset M$ is locally parameterized by p variables $s = (s^1, \dots, s^p) \in \mathbb{R}^p$ such that

$$\big(x(s), u(s)\big) \in S\ .$$

In numerical analysis, the independent variables $s = (s^1, \dots, s^p)$ are called *computational variables* [39]. These are the variables that are discretized when finite difference equations are introduced in Sect. 2.2. We let $\mathcal{J}^{(\ell)}$ denote the ℓth order jet space of submanifolds $S \subset M$ parametrized by computational variables. Local coordinates on $\mathcal{J}^{(\ell)}$ are given by

$$\big(s, x^{(\ell)}, u^{(\ell)}\big) = \big(\dots s^i \dots x^i_{s^A} \dots u^{\alpha}_{s^A} \dots\big)\ , \tag{3}$$

with $1 \le i \le p$, $1 \le \alpha \le q$, and $0 \le \#A \le \ell$.

Remark 2.6 We hope that the jet notations $\big(x, u^{(\ell)}\big)$ and $\big(s, x^{(\ell)}, u^{(\ell)}\big)$ will not confuse the reader. The independent variable, that is x and s, respectively, indicates with

respect to which variables the dependent variables u (and x in the second case) are differentiated in $u^{(\ell)}$.

Example 2.7 In the case where $p = 2$ and $m = 3$, let $(s^1, s^2) = (\tau, s)$ denote the two computational variables and let (t, x, u) be a local parametrization of M. Then the second order jet space $\mathcal{J}^{(2)}$ is parametrized by

$$(\tau, s, t, x, u, t_\tau, t_s, x_\tau, x_s, u_\tau, u_s, t_{\tau\tau}, t_{\tau s}, t_{ss}, x_{\tau\tau}, x_{\tau s}, x_{ss}, u_{\tau\tau}, u_{\tau s}, u_{ss}).$$

The transition between the jet coordinates (1) and (3) is given by the chain rule. Provided

$$\det\left(\frac{\partial x^j}{\partial s^i}\right) \neq 0\,, \quad \text{where } 1 \leq i, j \leq p\,, \tag{4}$$

the implicit total derivative operators

$$D_{x^i} = \sum_{j=1}^{p} W_i^j D_{s^j}, \quad \left(W_i^j\right) = \left(\frac{\partial x^j}{\partial s^i}\right)^{-1}, \quad i = 1, \ldots, p\,,$$

are well-defined, and successive application of those operators to the dependent variables u^α will give the coordinate expressions for the x-derivatives of u in terms of the s-derivatives of x and u:

$$u^\alpha_{x^J} = (D_{x^1})^{j_1} \cdots (D_{x^p})^{j_p} u^\alpha = \left(\sum_{l=1}^{p} W_1^l D_{s^l}\right)^{j_1} \cdots \left(\sum_{l=1}^{p} W_p^l D_{s^l}\right)^{j_p} u^\alpha\,. \tag{5}$$

We note that the nondegeneracy constraint (4) implies that the change of variables $x = x(s)$ is invertible.

Example 2.8 Combining Examples 2.1 and 2.7, assume that $x = x(\tau, s)$ and $t = t(\tau, s)$ are functions of the computational variables (τ, s). Provided

$$\det\begin{bmatrix} t_\tau & t_s \\ x_\tau & x_s \end{bmatrix} = t_\tau x_s - t_s x_\tau \neq 0\,, \tag{6}$$

the implicit derivative operators

$$D_x = \frac{t_\tau D_s - t_s D_\tau}{x_s t_\tau - x_\tau t_s}\,, \quad D_t = \frac{x_s D_\tau - x_\tau D_s}{x_s t_\tau - x_\tau t_s}\,. \tag{7}$$

are well-defined. It follows that

$$u_x = \frac{t_\tau u_s - t_s u_\tau}{x_s t_\tau - x_\tau t_s}\,, \quad u_t = \frac{x_s u_\tau - x_\tau u_s}{x_s t_\tau - x_\tau t_s}\,. \tag{8}$$

Relations for the higher order derivatives are obtained by applying (7) to (8).

Given a differential equation (2), the chain rule (5) can be used to re-express (2) in terms of $x^i = x^i(s)$, $u^\alpha = u^\alpha(s)$ and their computational derivatives $x^i_{s^A}$, $u^\alpha_{s^A}$:

$$\bar{\Delta}\big(s, x^{(\ell)}, u^{(\ell)}\big) = \Delta\big(x, u^{(\ell)}\big) = 0 \,. \tag{9a}$$

Recall that $\big(s, x^{(\ell)}, u^{(\ell)}\big) = (s, \dots x^i_{s^A} \dots u^\alpha_{s^A} \dots) \in \mathcal{J}^{(\ell)}$ for $\bar{\Delta} = 0$ in (9a) while $\big(x, u^{(\ell)}\big) = (x, \dots u^\alpha_{x^J} \dots) \in \mathrm{J}^{(\ell)}$ in $\Delta = 0$. Equation (9a) can be supplemented by *companion equations* [64],

$$\tilde{\Delta}\big(s, x^{(\ell)}, u^{(\ell)}\big) = 0 \,. \tag{9b}$$

The latter are introduced to impose restrictions on the change of variables $x = x(s)$. The system of differential equations (9) is called an *extended system* of the differential equation (2). For the extended system of differential equations (9) to share the same solution space as the original equation (2), the companion equations (9b) cannot introduce differential constraints on the derivatives $u^\alpha_{s^A}$.

Definition 2.5 is readily adapted to the computational variable framework.

Definition 2.9 A differential equation $\bar{\Delta}\big(s, x^{(\ell)}, u^{(\ell)}\big) = 0$ (or system of differential equations) is *regular* if the rank of its differential

$$\mathrm{d}\bar{\Delta} = \sum_{i=1}^{p} \frac{\partial \bar{\Delta}}{\partial s^i} \mathrm{d}s^i + \sum_J \sum_{i=1}^{p} \frac{\partial \bar{\Delta}}{\partial x^i_{s^J}} \mathrm{d}x^i_{s^J} + \sum_J \sum_{\alpha=1}^{q} \frac{\partial \bar{\Delta}}{\partial u^\alpha_{s^J}} \mathrm{d}u^\alpha_{s^J}$$

is constant on the domain of definition. The equation (or system of equations) is *locally solvable* at a point $(s_0, x_0^{(\ell)}, u_0^{(\ell)})$ if there exists a smooth solution $x = f(s)$, $u = g(s)$, defined in the neighborhood of s_0, such that $x_0^{(\ell)} = f^{(\ell)}(s_0)$ and $u_0^{(\ell)} = g^{(\ell)}(s_0)$. The differential equation (or system of differential equations) is said to be *fully regular* if it is both regular and locally solvable.

Example 2.10 As one of our main examples in these notes, we consider the Korteweg–de Vries (KdV) equation

$$u_t + uu_x + u_{xxx} = 0 \,. \tag{10}$$

We introduce the computational variables (τ, t) so that $x = x(\tau, s)$, $t = t(\tau, s)$. Then the implicit total derivative operators are given by (7). Before proceeding any further, we assume that

$$t_s = 0 \,, \quad t_{\tau\tau} = 0 \,. \tag{11}$$

In other words,

$$t = k\tau + t^0 \,, \tag{12}$$

where $k \neq 0$ and t^0 are constants. The reasons for imposing the constraints (11) are explained in Example 3.10. The operators of implicit differentiation (7) then simplify to

$$D_x = \frac{1}{x_s} D_s \,, \quad D_t = \frac{1}{t_\tau}\left(D_\tau - \frac{x_\tau}{x_s} D_s\right) .$$

Therefore,

$$u_x = \frac{u_s}{x_s} \,, \quad u_{xx} = \frac{1}{x_s}\left(\frac{u_s}{x_s}\right)_s \,, \quad u_{xxx} = \frac{1}{x_s}\left(\frac{1}{x_s}\left(\frac{u_s}{x_s}\right)_s\right)_s \,, \quad u_t = \frac{u_\tau}{t_\tau} - \frac{x_\tau}{t_\tau} \cdot \frac{u_s}{x_s}$$

and the KdV equation (10) becomes

$$\frac{u_\tau}{t_\tau} + \left(u - \frac{x_\tau}{t_\tau}\right)\frac{u_s}{x_s} + \frac{1}{x_s}\left(\frac{1}{x_s}\left(\frac{u_s}{x_s}\right)_s\right)_s = 0 \,, \tag{13}$$

together with the companion equations (11). The differential equation (13) is reminiscent of the equation one obtains when writing the KdV equation in *Lagrangian form* [9]. In the classical Lagrangian framework, the differential constraint

$$\frac{x_\tau}{t_\tau} = u \,, \tag{14}$$

is also imposed. The KdV equation then reduces to

$$\bar{\Delta} = \frac{u_\tau}{t_\tau} + \frac{1}{x_s}\left(\frac{1}{x_s}\left(\frac{u_s}{x_s}\right)_s\right)_s = 0 \,, \tag{15}$$

together with the companion equations (11), (14). In particular, when $k = 1$ in (12), we obtain the system of differential equations

$$u_\tau + \frac{1}{x_s}\left(\frac{1}{x_s}\left(\frac{u_s}{x_s}\right)_s\right)_s = 0 \,, \quad x_\tau = u \,.$$

2.2 *Finite Difference Equations*

We now move on to the discrete setting, which is the main focus of these lecture notes. In the previous section, we introduced two different jets spaces, namely $\mathrm{J}^{(\ell)}$ and $\mathcal{J}^{(\ell)}$. The motivation for introducing computational variables and the

corresponding jet space $\mathcal{J}^{(\ell)}$ stems from the fact that the discrete framework is more closely related to $\mathcal{J}^{(\ell)}$ than $\mathrm{J}^{(\ell)}$.

Let $N = (n^1, \dots, n^p) \in \mathbb{Z}^p$ denote an integer-valued multi-index. Thinking of the multi-index N as sampling the computational variables $s = (s^1, \dots, s^p) \in \mathbb{R}^p$ at integer values, the discrete notation (x_N, u_N) should be understood as sampling the submanifold $S = \{(x(s), u(s))\} \subset M$ at the integer-valued points $s = N \in \mathbb{Z}^p \subset \mathbb{R}^p$. In other words $(x_N, u_N) = \big(x(N), u(N)\big)$. To approximate the ℓ-jet $\big(s, x^{(\ell)}, u^{(\ell)}\big) \in \mathcal{J}^{(\ell)}$ at $s = N$, we consider a finite collection of points

$$(N, x_N^{[\ell]}, u_N^{[\ell]}) = (N, \dots, x_{N+K}, \dots, u_{N+K}, \dots) \,, \tag{16}$$

where $K \in \mathbb{Z}^p$. We require that the point (x_N, u_N) is always included and that

$$x_{N+K_1} \neq x_{N+K_2} \quad \text{whenever } K_1 \neq K_2 \,,$$

so that no two discrete independent variables are the same. We refer to (16) as the *ℓth order discrete jet at N*. In numerical analysis, a point in (16) is also called a *stencil*. For theoretical purposes, one can assume that the multi-index $K \in (\mathbb{Z}^{\geq 0})^p$ only takes nonnegative values and that $0 \leq \# K = k^1 + \cdots + k^p \leq \ell$. The latter provides the minimal number of points required to approximate the ℓ-jet $\big(x, u^{(\ell)}\big)$ (or $\big(s, x^{(\ell)}, u^{(\ell)}\big)$) by first order forward differences. In applications, especially when constructing numerical schemes, it is generally preferable to consider points centered around (x_N, u_N) and to include more than the minimum number of points in $\big(N, x_N^{[\ell]}, u_N^{[\ell]}\big)$ required to approximate $\big(x, u^{(\ell)}\big)$ for better numerical accuracy and stability. From now on, we will assume that a certain stencil (16) has been chosen. We denote by

$$\mathcal{J}^{[\ell]} = \bigcup_{N \in \mathbb{Z}^p} \Big(N, x_N^{[\ell]}, u_N^{[\ell]}\Big)$$

the union over all the stencils and call $\mathcal{J}^{[\ell]}$ the ℓth *order discrete jet space* as $\mathcal{J}^{[\ell]}$ provides an approximation of $\mathcal{J}^{(\ell)}$. Since the jet coordinates of $\mathrm{J}^{(\ell)}$ can be expressed in terms of the jet coordinates of $\mathcal{J}^{(\ell)}$ using (5), it follows that the points in $\mathcal{J}^{[\ell]}$ can be used to approximate $\mathrm{J}^{(\ell)}$.

Example 2.11 Consider the case where $p = 2$ and the dimension of the manifold M is $\dim M = m = 3$. Let (t, x, u) be local coordinates on M. In the continuous case, see Example 2.7, we introduced the computational variables (τ, s). In the discrete case, let $N = (n, i) \in \mathbb{Z}^2$, which can be thought of as evaluating the computational variables (τ, s) at integer values. To make the multi-index notation more compact, we let

$$(t_N, x_N, u_N) = (t_i^n, x_i^n, u_i^n) \,, \quad N = (n, i) \in \mathbb{Z}^2 \,.$$

Working with forward differences, the simplest first order discrete jet is parametrized by

$$\left(t_N^{[1]}, x_N^{[1]}, u_N^{[1]}\right) = (t_i^n, x_i^n, u_i^n, t_i^{n+1}, x_i^{n+1}, u_i^{n+1}, t_{i+1}^n, x_{i+1}^n, u_{i+1}^n) \, .$$

First order approximations of the first order derivatives (t_τ, x_τ, u_τ) and (t_s, x_s, u_s) on a grid with unit spacing are then given by

$$\begin{aligned} (t_\tau, x_\tau, u_\tau) &\approx (t_i^{n+1} - t_i^n, x_i^{n+1} - x_i^n, u_i^{n+1} - u_i^n) \, , \\ (t_s, x_s, u_s) &\approx (t_{i+1}^n - t_i^n, x_{i+1}^n - x_i^n, u_{i+1}^n - u_i^n) \, . \end{aligned} \tag{17}$$

Referring to (8) for the expressions of the t and x derivatives of u in terms of the computational variable derivatives, and using (17) we have that

$$\begin{aligned} u_x &= \frac{t_\tau u_s - t_s u_\tau}{x_s t_\tau - x_\tau t_s} \approx \frac{(t_i^{n+1} - t_i^n)(u_{i+1}^n - u_i^n) - (t_{i+1}^n - t_i^n)(u_i^{n+1} - u_i^n)}{(x_{i+1}^n - x_i^n)(t_i^{n+1} - t_i^n) - (x_i^{n+1} - x_n^i)(t_{i+1}^n - t_i^n)} \, , \\ u_t &= \frac{x_s u_\tau - x_\tau u_s}{x_s t_\tau - x_\tau t_s} \approx \frac{(x_{i+1}^n - x_i^n)(u_i^{n+1} - u_i^n) - (x_i^{n+1} - x_i^n)(u_{i+1}^n - u_i^n)}{(x_{i+1}^n - x_i^n)(t_i^{n+1} - t_i^n) - (x_i^{n+1} - x_n^i)(t_{i+1}^n - t_i^n)} \, . \end{aligned} \tag{18}$$

The latter expressions are first order forward approximations of the first order partial derivatives u_x and u_t on any mesh that satisfies

$$\begin{aligned} &\det \begin{bmatrix} (t_i^{n+1} - t_i^n) & (t_{i+1}^n - t_i^n) \\ (x_i^{n+1} - x_i^n) & (x_{i+1}^n - x_i^n) \end{bmatrix} \\ &\qquad = (x_{i+1}^n - x_i^n)(t_i^{n+1} - t_i^n) - (x_i^{n+1} - x_i^n)(t_{i+1}^n - t_i^n) \neq 0 \, , \end{aligned}$$

the latter being a discrete version of the nondegeneracy condition (6). The procedure can be repeated to obtain approximations of higher order derivatives on arbitrary meshes. For example, applying the implicit derivative operators (7) to the first order derivative expressions (8) one obtains formulas for the second order derivatives u_{xx}, u_{xt}, and u_{tt} expressed in terms of the computational derivatives. Substituting the approximations (17) and the second order derivative approximations

$$\begin{aligned} t_{\tau\tau} &\approx t_i^{n+2} - 2t_i^{n+1} + t_i^n \, , & x_{\tau\tau} &\approx x_i^{n+2} - 2x_i^{n+1} + x_i^n \, , \\ t_{\tau s} &\approx t_{i+1}^{n+1} - t_i^{n+1} - t_{i+1}^n + x_i^n \, , & x_{\tau s} &\approx x_{i+1}^{n+1} - x_i^{n+1} - x_{i+1}^n + x_i^n \, , \\ t_{ss} &\approx t_{i+2}^n - 2t_{i+1}^n + t_i^n \, , & x_{ss} &\approx x_{i+2}^n - 2x_{i+1}^n + x_i^n \, , \end{aligned}$$

into the formulas obtained yields discrete approximations for u_{xx}, u_{xt}, and u_{tt} in the computational variables on an orthogonal grid with unit spacing.

Definition 2.12 A *finite difference equation* is the zero locus of a discrete map $E\colon \mathcal{J}^{[\ell]} \to \mathbb{R}$. That is,

$$E\Big(N, x_N^{[\ell]}, u_N^{[\ell]}\Big) = 0\ .$$

Definition 2.13 A finite difference equation $E\colon \mathcal{J}^{[\ell]} \to \mathbb{R}$ is said to be *regular* if the rank of the differential

$$\mathrm{d}E = \sum_K \left[\sum_{i=1}^{p} \frac{\partial E}{\partial x_{N+K}^i} \mathrm{d}x_{N+K}^i + \sum_{\alpha=1}^{q} \frac{\partial E}{\partial u_{N+K}^\alpha} \mathrm{d}u_{N+K}^\alpha \right]$$

is constant for all N in the domain of definition of the equation.

Finite difference equations can be studied as mathematical objects of interest in their own [31, 44, 63]. In the following we are interested in finite difference equations that approximate differential equations.

Definition 2.14 A finite difference equation $E(N, x_N^{[\ell]}, u_N^{[\ell]}) = 0$ is said to be *consistent* with the differential equation $\Delta\big(x, u^{(\ell)}\big) = 0$ (or $\bar{\Delta}\big(s, x^{(\ell)}, u^{(\ell)}\big) = 0$) if in the continuous limit $(x_{N+K}, u_{N+K}) \to (x_N, u_N)$,

$$E(N, x_N^{[\ell]}, u_N^{[\ell]}) \to \Delta\big(x, u^{(\ell)}\big) \quad \big(\text{or } E(N, x_N^{[\ell]}, u_N^{[\ell]}) \to \bar{\Delta}\big(s, x^{(\ell)}, u^{(\ell)}\big)\big)\ .$$

Remark 2.15 The process of taking continuous limits is discussed in more details in Sect. 6.

Definition 2.16 Let $\Delta\big(x, u^{(\ell)}\big) = 0$ be a differential equation with extended system $\{\bar{\Delta}\big(s, x^{(\ell)}, u^{(\ell)}\big) = 0,\ \tilde{\Delta}\big(s, x^{(\ell)}, u^{(\ell)}\big) = 0\}$. A *numerical scheme* is a system of finite difference equations

$$\overline{E}(N, x_N^{[\ell]}, u_N^{[\ell]}) = 0\ , \quad \widetilde{E}(N, x_N^{[\ell]}, u_N^{[\ell]}) = 0\ ,$$

where $\overline{E}(N, x_N^{[\ell]}, u_N^{[\ell]}) = 0$ approximates the differential equation

$$\Delta\big(x, u^{(\ell)}\big) = \bar{\Delta}\big(s, x^{(\ell)}, u^{(\ell)}\big) = 0$$

and the equations $\widetilde{E}(N, x_N^{[\ell]}, u_N^{[\ell]}) = 0$ provide an approximation of the companion equations

$$\tilde{\Delta}\big(s, x^{(\ell)}, u^{(\ell)}\big) = 0\ .$$

Intuitively, the difference equations $\widetilde{E}(N, x_N^{[\ell]}, u_N^{[\ell]}) = 0$ provide constraints on the mesh used to approximate the differential equation $\Delta = 0$. The latter should not yield any restrictions on the discrete dependent variables $u_N^{[\ell]}$.

Example 2.17 To illustrate Definition 2.16, let us consider the KdV equation (10). Assume the equation is to be discretized on the orthogonal mesh

$$t^n = k\,n + t^0\,, \quad x_i = h\,i + x_0\,, \tag{19}$$

where $k, h > 0$, $(n, i) \in \mathbb{Z}^2$, and t^0, x_0 are arbitrary constants. The mesh (19) can be encapsulated in a system of finite difference equations in different ways. For example, it is not difficult to see that (19) is the solution to the system of equations

$$\begin{aligned} t_i^{n+1} - t_i^n &= k\,, & x_i^{n+1} - x_i^n &= 0\,,\\ t_{i+1}^n - t_i^n &= 0\,, & x_{i+1}^n - x_i^n &= h\,. \end{aligned} \tag{20}$$

The mesh (19) is also a solution to

$$\begin{aligned} t_i^{n+1} - 2t_i^n + t_i^{n-1} &= 0, & x_i^{n+1} - x_i^n &= 0\,,\\ t_{i+1}^n - t_i^n &= 0, & x_{i+1}^n - 2x_i^n + x_{i-1}^n &= 0\,. \end{aligned} \tag{21}$$

The difference between the two systems of mesh equations is that in (20) the time step k and the spatial step h are fixed by the system whereas in (21) those steps corresponds to constants of integration. In both cases, the KdV equation can be approximated by

$$\frac{u_i^{n+1} - u_i^n}{k} + u_i^n \cdot \frac{u_{i+1}^n - u_{i-1}^n}{2h} + \frac{u_{i+2}^n - 2u_{i+1}^n + 2u_{i-1}^n - u_{i-2}^n}{2h^3} = 0\,. \tag{22}$$

The systems of equations (20)–(22) or (21)–(22) provide two examples of Definition 2.16. They also illustrate the fact that, in general, the equations $\widetilde{E} = 0$ specifying the mesh are not unique.

3 Lie Symmetries

Let G be an r-dimensional Lie group, and let $\mathcal{M}$ be a d-dimensional manifold with local coordinates $z = (z^1, \dots, z^d)$. In the following, the manifold $\mathcal{M}$ can represent the submanifold jet spaces $\mathrm{J}^{(\ell)}$ or $\mathcal{J}^{(\ell)}$ or the discrete jet space $\mathcal{J}^{[\ell]}$. In the latter case, $\mathcal{M}$ should in fact be called a *lattifold* or *lattice variety*, that is a manifold-like structure modeled on $\mathbb{Z}^p$ [65, 67].

Definition 3.1 A *transformation group* acting on a manifold $\mathcal{M}$ is given by a Lie group G and a smooth map $\Phi\colon G\times\mathcal{M} \to \mathcal{M}$, such that $\Phi(g, z) = g\cdot z$, which satisfies the following two properties

$$e \cdot z = z\,, \quad g \cdot (h \cdot z) = (gh) \cdot z\,, \quad \text{for all } z \in \mathcal{M},\, g,\, h \in G\,, \tag{23}$$

and where $e \in G$ denotes the identity element.

It follows from (23) that the inverse of the transformation defined by the group element g is given by the inverse group element g^{-1}. Therefore g induces a diffeomorphism from $\mathcal{M}$ to itself.

Remark 3.2 Definition 3.1 assumes that the group action is *global*, meaning that $g \cdot z$ is defined for every $g \in G$ and every $z \in \mathcal{M}$. In practice, group actions may only be defined *locally*, meaning that for a given $z \in \mathcal{M}$, the transformation $g \cdot z$ is only defined for group elements g sufficiently near the identity. For a *local transformation group*, the map Φ is defined on an open subset $\mathcal{B}$ with $\{e\} \times \mathcal{M} \subset \mathcal{B} \subset G \times \mathcal{M}$, and the conditions (23) of Definition 23 are imposed wherever they are defined.

In the following, we use capital letters to denote the image of a point under a group transformation. For example,

$$Z = g \cdot z \quad \text{where } g \in G \text{ and } z \in \mathcal{M} \ .$$

At the infinitesimal level, let $\mathfrak{g}$ denote the Lie algebra of vector fields corresponding to the infinitesimal generators of the group action. A vector field

$$\mathbf{v} = \sum_{a=1}^{d} \zeta^a(z) \frac{\partial}{\partial z^a}$$

will be in $\mathfrak{g}$ if it is tangent to the orbits of a one-parameter subgroup of transformations of G. The *flow* through the point $z \in \mathcal{M}$ generated by a vector field $\mathbf{v} \in \mathfrak{g}$, is found by solving the initial value problem

$$\frac{\mathrm{d}Z^a}{\mathrm{d}\epsilon} = \zeta^a(Z) \ , \quad Z^a(0) = z^a \ , \qquad a = 1, \dots, d \ .$$

The maximal integral curve is denoted $\exp[\epsilon \mathbf{v}] \cdot z$, and is called the *exponentiation* of the infinitesimal generator $\mathbf{v}$.

Definition 3.3 Let G be a local Lie group of transformations acting on $\mathcal{M}$. The Lie group G is a (local) *symmetry group* of the (fully) regular equation[1] $F(z) = 0$ if and only if

$$F(g \cdot z) = 0 \quad \text{whenever } F(z) = 0 \ ,$$

for all $g \in G$ such that the local action is defined. Infinitesimally, a connected Lie group of transformations G acting on $\mathcal{M}$ is a local symmetry group of $F(z) = 0$ if and only if

[1] Depending whether $\mathcal{M}$ represents $\mathrm{J}^{(\ell)}$, $\mathcal{J}^{(\ell)}$, or $\mathcal{J}^{[\ell]}$, we refer to Definitions 2.5, 2.9, or 2.13 for the notion of (fully) regular equation.

$$\mathbf{v}(F)\big|_{F=0} = 0 \quad \text{for all } \mathbf{v} \in \mathfrak{g} \,. \tag{24}$$

Remark 3.4 Definition 3.3 extends to systems of equations and more general local groups of transformations by including discrete transformations as well [10, 40, 42, 43]. In the following we restrict all our considerations to Lie point symmetries and omit the interesting case of discrete symmetries.

3.1 Symmetries of Differential Equations

Symmetries of differential equations are covered extensively in many excellent textbooks such as [11, 12, 43, 68, 71, 76]. We refer to these references for a more detailed exposition.

If $\mathcal{M} = \mathrm{J}^{(\ell)}$, then the local group action is given by the *prolonged action* $(X, U^{(\ell)}) = g \cdot \big(x, u^{(\ell)}\big)$ on the submanifold ℓ-jet $\big(x, u^{(\ell)}\big)$. Let

$$X^i = g \cdot x^i \,, \quad i = 1, \dots, p \,, \qquad U^\alpha = g \cdot u^\alpha \,, \quad \alpha = 1, \dots, q \tag{25}$$

denote the local group action of G on the manifold M locally coordinatized by (x, u). To compute the prolonged action, we introduce the *implicit differentiation operators* [33],

$$D_{X^i} = \sum_{j=1}^{p} W_i^j D_{x^j} \,, \quad \text{where } (W_i^j) = \left(\frac{\partial X^j}{\partial x^i}\right)^{-1} \tag{26}$$

denotes the entries of the inverse Jacobian matrix and

$$D_{x^j} = \frac{\partial}{\partial x^j} + \sum_{J} \sum_{\alpha=1}^{q} u^\alpha_{x^J + e_j} \frac{\partial}{\partial u^\alpha_{x^J}}$$

is the total differentiation operator with respect to the independent variable x^j. In the above formula, $e_j = (0, \dots, 0, 1, 0, \dots, 0) \in \mathbb{R}^p$ denotes the unit vector with zeros everywhere except in the jth component. We note that the operators (26) mutually commute

$$[D_{X^i}, D_{X^j}] = 0 \,, \quad 1 \le i, j \le p \,.$$

Successively applying the implicit differentiation operators (26) to $U^\alpha = g \cdot u^\alpha$ yields the expressions for the prolonged action

$$U^\alpha_{X^J} = (D_{X^1})^{j_1} \cdots (D_{X^p})^{j_p} U^\alpha \,, \quad \alpha = 1, \dots, q, \quad \#J \ge 0 \,.$$

At the infinitesimal level, let

$$\mathbf{v} = \sum_{i=1}^{p} \xi^i(x,u)\frac{\partial}{\partial x^i} + \sum_{\alpha=1}^{q} \phi^\alpha(x,u)\frac{\partial}{\partial u^\alpha} \tag{27}$$

denote an infinitesimal generator of the group action (25). The prolongation of (27) to $\mathrm{J}^{(\ell)}$ is given by

$$\mathbf{v}^{(\ell)} = \sum_{i=1}^{p} \xi^i \frac{\partial}{\partial x^i} + \sum_{\alpha=1}^{q} \sum_{J} \phi^{\alpha;J} \frac{\partial}{\partial u^\alpha_{x^J}} \ ,$$

where the prolonged vector field coefficients are defined recursively by the standard prolongation formula

$$\phi^{\alpha;J+e_j} = D_{x^j}\phi^{\alpha;J} - \sum_{i=1}^{p} (D_{x^j}\xi^i)\, u^\alpha_{x^{J+e_i}} \ .$$

Given a differential equation $\Delta\big(x,u^{(\ell)}\big) = 0$, the Lie point symmetries of the equation are found from the *infinitesimal invariance criterion*

$$\mathbf{v}^{(\ell)}(\Delta)\big|_{\Delta=0} = 0 \quad \text{for all } \mathbf{v} \in \mathfrak{g} \ . \tag{28}$$

The latter yields a differential equation in x, u and the derivatives of u with respect to x, as well as $\xi^i(x,u)$ and $\phi^\alpha(x,u)$ and their partial derivatives with respect to x and u. After eliminating any dependencies among the derivatives of the us due to the equation $\Delta\big(x,u^{(\ell)}\big) = 0$, one can equate the coefficients of the remaining unconstrained partial derivatives of u to zero. This yields a system of linear partial differential equations for the coefficients ξ^i and ϕ^α, called the *determining equations* of the (maximal) Lie symmetry algebra. The procedure for obtaining and solving the determining equations has been implemented in all major computer algebra systems such as MACSYMA, MAPLE, MATHEMATICA, MUMATH and REDUCE. An extensive list of references on the subject can be found in [19].

Example 3.5 To illustrate the algorithm outlined above, we compute the infinitesimal generators of the KdV equation (10). Let $\mathbf{v} = \xi(t,x,u)\partial_x + \eta(t,x,u)\partial_t + \phi(t,x,u)\partial_u$ denote a general vector field on $\mathbb{R}^3$. The third order prolongation of $\mathbf{v}$ is

$$\mathbf{v}^{(3)} = \xi\frac{\partial}{\partial x} + \eta\frac{\partial}{\partial t} + \phi\frac{\partial}{\partial u} + \phi^x\frac{\partial}{\partial u_x} + \phi^t\frac{\partial}{\partial u_t} + \phi^{xx}\frac{\partial}{\partial u_{xx}} + \phi^{xt}\frac{\partial}{\partial u_{xt}} + \phi^{tt}\frac{\partial}{\partial u_{tt}}$$
$$+ \phi^{xxx}\frac{\partial}{\partial u_{xxx}} + \phi^{xxt}\frac{\partial}{\partial u_{xxt}} + \phi^{xtt}\frac{\partial}{\partial u_{xtt}} + \phi^{ttt}\frac{\partial}{\partial u_{ttt}},$$

where

$$\begin{aligned}
\phi^t &= D_t\phi - u_x D_t\xi - u_t D_t\eta \,,\\
\phi^x &= D_x\phi - u_x D_x\xi - u_t D_x\eta \,,\\
\phi^{xx} &= D_x(\phi^x) - u_{xx} D_x\xi - u_{xt} D_x\eta\\
&= D_x^2\phi - u_x D_x^2\xi - u_t D_x^2\eta - 2u_{xx} D_x\xi - 2u_{xt} D_x\eta \,,\\
\phi^{xxx} &= D_x(\phi^{xx}) - u_{xxx} D_x\xi - u_{xxt} D_t\eta\\
&= D_x^3\phi - u_x D_x^3\xi - u_t D_x^3\eta - 3u_{xx} D_x^2\xi - 3u_{xt} D_x^2\eta\\
&\qquad - 3u_{xxx} D_x\xi - 3u_{xxt} D_x\eta \,.
\end{aligned} \tag{29}$$

Applying the infinitesimal invariance criterion (24) to the KdV equation (10) we obtain

$$\phi^t + u\phi^x + u_x\phi + \phi^{xxx} = 0 \,, \tag{30}$$

where u satisfies (10). Substituting the expressions (29) into (30) and replacing u_t by $-uu_x - u_{xxx}$, we obtain the determining equations of the Lie symmetry algebra, which we now solve. Firstly, the coefficient of u_{xxt} is $D_x\eta = \eta_x + u_x\eta_u$ which implies that $\eta_x = \eta_u = 0$. In other words, $\eta = \eta(t)$ is a function of t only[2]. Secondly, the coefficient of u_{xx}^2 yields $\xi_u = 0$ and thus $\xi = \xi(t,x)$, implying that the admitted Lie symmetries are projectable. Next, the coefficient of u_{xxx} gives $\eta_t - 3\xi_x = 0$. Integrating the latter with respect to x, we find that $\xi = \frac{1}{3}x\,\eta_t + \chi(t)$. The coefficient of u_{xx} implies that $\phi_{uu} = \phi_{xu} = 0$ so that $\phi = \sigma(t)u + \varphi(t,x)$. Next the coefficient in u_x yields the equation

$$-\xi_t + u(\eta_t - \xi_x) + \phi = 0 \,.$$

Substituting the expressions for ξ and ϕ, we find

$$\sigma = -\tfrac{2}{3}\eta_t \quad \text{and} \quad \varphi = \tfrac{1}{3}x\,\eta_{tt} + \chi_t \quad \text{so that} \quad \phi = -\tfrac{2}{3}u\,\eta_t + \tfrac{1}{3}x\,\eta_{tt} + \chi_t \,.$$

Finally, the term with no derivatives of u gives $\phi_t + \phi_{xxx} + u\,\phi_x = 0$, which after substitution yields

$$-\tfrac{1}{3}u\,\eta_{tt} + \tfrac{1}{3}x\,\eta_{ttt} + \chi_{tt} = 0 \,.$$

Since $\eta = \eta(t)$ and $\chi = \chi(t)$ are functions of t, the latter equation holds for all (t,x,u) provided that $\eta_{tt} = \chi_{tt} = 0$. Therefore,

$$\xi = c_1 + c_2\,t + c_3\,x \,, \quad \eta = c_4 + 3c_3\,t \,, \quad \phi = c_2 - 2c_3\,u \,,$$

[2]This is true for all evolution equations.

and the maximal Lie symmetry algebra is spanned by the four vector fields

$$\begin{aligned} \mathbf{v}_1 &= \frac{\partial}{\partial x}, && \longrightarrow \quad \text{space translations}, \\ \mathbf{v}_2 &= \frac{\partial}{\partial t}, && \longrightarrow \quad \text{time translations}, \\ \mathbf{v}_3 &= t\frac{\partial}{\partial x} + \frac{\partial}{\partial u}, && \longrightarrow \quad \text{Galilean boosts}, \\ \mathbf{v}_4 &= x\frac{\partial}{\partial x} + 3t\frac{\partial}{\partial t} - 2u\frac{\partial}{\partial u}, && \longrightarrow \quad \text{scalings}. \end{aligned} \tag{31}$$

Exercise 3.6 Show that the symmetry group of the ordinary differential equation $u_{xx} = 0$ is eight-dimensional, and generated by

$$\begin{aligned} &\frac{\partial}{\partial x}, \quad x\frac{\partial}{\partial x}, \quad u\frac{\partial}{\partial x}, \quad x^2\frac{\partial}{\partial x} + xu\frac{\partial}{\partial u}, \\ &\frac{\partial}{\partial u}, \quad x\frac{\partial}{\partial u}, \quad u\frac{\partial}{\partial u}, \quad xu\frac{\partial}{\partial x} + u^2\frac{\partial}{\partial u}. \end{aligned} \tag{32}$$

Show that the corresponding group of local transformations is the projective group $SL(3, \mathbb{R})$ acting via fractional linear transformations

$$X = \frac{\epsilon_1 x + \epsilon_2 u + \epsilon_3}{\epsilon_7 x + \epsilon_8 u + \epsilon_9}, \quad U = \frac{\epsilon_4 x + \epsilon_5 u + \epsilon_6}{\epsilon_7 x + \epsilon_8 u + \epsilon_9}, \quad \det \begin{bmatrix} \epsilon_1 & \epsilon_2 & \epsilon_3 \\ \epsilon_4 & \epsilon_5 & \epsilon_6 \\ \epsilon_7 & \epsilon_8 & \epsilon_9 \end{bmatrix} = 1,$$

where $\epsilon_1, \ldots, \epsilon_9 \in \mathbb{R}$ are group parameters.

Exercise 3.7 Consider the Schwarzian differential equation

$$\frac{u_x\, u_{xxx} - (3/2)u_{xx}^2}{u_x^2} = F(x), \tag{33}$$

where $F(x)$ is an arbitrary function.

1. Find the determining equations for the vector fields spanning the maximal Lie symmetry algebra and show that a basis is given by

$$\mathbf{v}_1 = \frac{\partial}{\partial u}, \quad \mathbf{v}_2 = u\frac{\partial}{\partial u}, \quad \mathbf{v}_3 = u^2\frac{\partial}{\partial u}. \tag{34}$$

2. Show that the corresponding local Lie group of transformations is

$$X = x, \qquad U = \frac{au + b}{cu + d}, \quad \text{with } ad - bc = 1. \tag{35}$$

3. When $F(x) \equiv 0$ is identically zero, show that the maximal Lie symmetry algebra is four-dimensional and determine a basis. Also find the corresponding finite group transformations.

Exercise 3.8 Show that the maximal Lie symmetry algebra of Burgers' equation

$$u_t + uu_x = \nu u_{xx} \,, \tag{36}$$

where $\nu > 0$ denotes the viscosity, is spanned by the vector fields

$$\begin{gathered} \mathbf{v}_1 = \frac{\partial}{\partial x} \,, \quad \mathbf{v}_2 = \frac{\partial}{\partial t} \,, \quad \mathbf{v}_3 = t\frac{\partial}{\partial x} + \frac{\partial}{\partial u} \,, \\ \mathbf{v}_4 = x\frac{\partial}{\partial x} + 2t\frac{\partial}{\partial t} - u\frac{\partial}{\partial u} \,, \quad \mathbf{v}_5 = tx\frac{\partial}{\partial x} + t^2\frac{\partial}{\partial t} + (x - tu)\frac{\partial}{\partial u} \,. \end{gathered} \tag{37}$$

In the computational variable framework, the local transformation group G acting on the manifold M is trivially extended to the computational variables. That is,

$$g \cdot (s, x, u) = (s, g \cdot x, g \cdot u) \,.$$

The prolongation of an infinitesimal generator (27) to $\mathcal{G}^{(\ell)}$ is then simply given by

$$\mathbf{v}^{(\ell)} = \sum_{i=1}^{p} \sum_{J} D_s^J \xi^i \frac{\partial}{\partial x^i_{s^J}} + \sum_{\alpha=1}^{q} \sum_{J} D_s^J \phi^\alpha \frac{\partial}{\partial u^\alpha_{s^J}} \,,$$

where $D_s^J = (D_{s^1})^{j_1} \cdots (D_{s^p})^{j_p}$ denotes the total differentiation operator in the computational variables $s = (s^1, \dots, s^p)$ with

$$D_{s^j} = \frac{\partial}{\partial s^j} + \sum_{i=1}^{p} \sum_{J} x^i_{s^{J+e_j}} \frac{\partial}{\partial x^i_{s^J}} + \sum_{\alpha=1}^{q} \sum_{J} u^\alpha_{s^{J+e_j}} \frac{\partial}{\partial u^\alpha_{s^J}} \,, \quad j = 1, \dots, p.$$

Definition 3.9 Let G be a symmetry group of the differential equation $\Delta\big(x, u^{(\ell)}\big) = 0$. The extended system of differential equations

$$\{\bar{\Delta}\big(s, x^{(\ell)}, u^{(\ell)}\big) = 0,\ \tilde{\Delta}\big(s, x^{(\ell)}, u^{(\ell)}\big) = 0\} \tag{38}$$

is said to be *G-compatible* if G is a symmetry group of (38). That is,

$$\begin{cases} \bar{\Delta}(s, g \cdot x^{(\ell)}, g \cdot u^{(\ell)}) = 0, \\ \tilde{\Delta}(s, g \cdot x^{(\ell)}, g \cdot u^{(\ell)}) = 0, \end{cases} \quad \text{whenever} \quad \begin{cases} \bar{\Delta}\big(s, x^{(\ell)}, u^{(\ell)}\big) = 0, \\ \tilde{\Delta}\big(s, x^{(\ell)}, u^{(\ell)}\big) = 0, \end{cases}$$

and where the prolonged action is defined. At the infinitesimal level,

$$\mathbf{v}^{(\ell)}(\bar{\Delta})\big|_{\{\bar{\Delta}=0,\tilde{\Delta}=0\}} = 0 \quad \text{and} \quad \mathbf{v}^{(\ell)}(\tilde{\Delta})\big|_{\{\bar{\Delta}=0,\tilde{\Delta}=0\}} = 0$$

for all infinitesimal generators $\mathbf{v} \in \mathfrak{g}$.

Example 3.10 Recall from Example 3.5 that the KdV equation (10) is invariant under a four-dimensional maximal Lie symmetry group whose associated algebra of infinitesimal generators is spanned by the vector fields (31). In the computational variables (τ, s) introduced in Example 2.10, the first prolongation of the infinitesimal generators (31) is given by

$$\mathbf{v}_1^{(1)} = \frac{\partial}{\partial x}\,, \quad \mathbf{v}_2^{(1)} = \frac{\partial}{\partial t}\,, \quad \mathbf{v}_3^{(1)} = t\frac{\partial}{\partial x} + \frac{\partial}{\partial u} + t_s\frac{\partial}{\partial x_s} + \frac{\partial}{\partial u_s} + t_\tau\frac{\partial}{\partial x_\tau} + \frac{\partial}{\partial u_\tau},$$
$$\mathbf{v}_4^{(1)} = x\frac{\partial}{\partial x} + 3t\frac{\partial}{\partial t} - 2u\frac{\partial}{\partial u} + x_s\frac{\partial}{\partial x_s} + 3t_s\frac{\partial}{\partial t_s} - 2u_s\frac{\partial}{\partial u_s} + x_\tau\frac{\partial}{\partial x_\tau} + 3t_\tau\frac{\partial}{\partial t_\tau} - 2u_\tau\frac{\partial}{\partial u_\tau}\,.$$

By direct computation, it is not hard to verify that for the differential equation (15)

$$\mathbf{v}_1^{(2)}[\bar{\Delta}]\big|_{\bar{\Delta}=0} = \mathbf{v}_2^{(2)}[\bar{\Delta}]\big|_{\bar{\Delta}=0} = \mathbf{v}_3^{(2)}[\bar{\Delta}]\big|_{\bar{\Delta}=0} = \mathbf{v}_4^{(2)}[\bar{\Delta}]\big|_{\bar{\Delta}=0} = 0\,.$$

Therefore, Eq. (15) is invariant under the symmetry group of the KdV equation. Also,

$$\mathbf{v}_\kappa^{(2)}(t_s) = 0\,, \quad \mathbf{v}_\kappa^{(2)}(t_{\tau\tau}) = 0\,, \quad \mathbf{v}_\kappa^{(2)}\left(\frac{x_\tau}{t_\tau} - u\right) = 0\,, \qquad \kappa = 1,2,3,4,$$

whenever

$$t_s = 0\,, \quad t_{ss} = 0\,, \quad \frac{x_\tau}{t_\tau} - u = 0\,.$$

Therefore, the companion equations (11), (14) are invariant under the symmetry group of the KdV equation. The extended system of differential equations (11), (14), (15) is therefore G-compatible with the symmetry group of the KdV equation.

3.2 Symmetries of Finite Difference Equations

As in Sect. 3.1, let G be a local Lie group of transformations acting smoothly on the manifold M. The induced action on the discrete n-jet $(N, x_N^{[\ell]}, u_N^{[\ell]})$ is given by the product action

$$g \cdot (N, x_N^{[\ell]}, u_N^{[\ell]}) = (N, \dots, g \cdot x_{N+K}, \dots, g \cdot u_{N+K}, \dots) \,, \tag{39}$$

where each point (x_{N+K}, u_{N+K}) is transformed by the same group transformation g. At the infinitesimal level, given the vector field

$$\mathbf{v} = \sum_{i=1}^{p} \xi_N^i \frac{\partial}{\partial x_N^i} + \sum_{\alpha=1}^{q} \phi_K^\alpha \frac{\partial}{\partial u_N^\alpha} \,, \tag{40}$$

where $\xi_N^i = \xi^i(x_N, u_N)$ and $\phi_N^\alpha = \phi^\alpha(x_N, u_N)$, the prolonged vector field is given by

$$\mathbf{v}^{[\ell]} = \sum_K \left[\sum_{i=1}^{p} \xi_{N+K}^i \frac{\partial}{\partial x_{N+K}^i} + \sum_{\alpha=1}^{q} \phi_{N+K}^\alpha \frac{\partial}{\partial u_{N+K}^\alpha} \right],$$

which is obtained by adding copies of $\mathbf{v}$ evaluated at the different points in the discrete jet $(N, x_N^{[\ell]}, u_N^{[\ell]})$.

Remark 3.11 The above considerations can be generalized by allowing the group action (39) or the infinitesimal generator (40) to depend on the multi-index N. For example, in (40), the vector field coefficients could be functions of N so that $\xi_N^i = \xi^i(N, x_N, u_N)$ and $\phi_N^\alpha = \phi^\alpha(N, x_N, u_N)$. When constructing symmetry-preserving schemes, this more general case does not occur as the transformation group that one considers is the group of point symmetries of the differential equation $\Delta\big(x, u^{(\ell)}\big) = 0$, which only contains point transformations in the x, u variables.

Using the infinitesimal invariance criterion

$$\mathbf{v}^{[\ell]}(E)\big|_{E=0} = 0 \quad \text{for all } \mathbf{v} \in \mathfrak{g} \,, \tag{41}$$

the symmetries of finite difference equations can be computed in a manner similar to the differential case. Equation (41) yields a finite difference equation for the vector field coefficients ξ_N^i and ϕ_N^α. Since the invariance condition (41) only has to hold on the solution of the difference equation, one must eliminate any dependencies among (x_N, u_N) and their shifts due to the equation $E(N, x_N^{[\ell]}, u_N^{[\ell]}) = 0$. Differentiating the resulting equation with respect to the remaining variables sufficiently many times, one obtains a system of differential equations for the vector field coefficients. Once the differential equations are solved, one will, in general, have to substitute the solution into the original difference equation for the vector field coefficients, or an intermediate equation obtained along the way, and solve the resulting equation to obtain the symmetry generators.

Example 3.12 As a first example, let us compute the admitted infinitesimal generators of the ordinary difference equation

$$u_{i+2} = a(i)u_{i+1} + b(i)u_i \quad \text{where } a(i)b(i) \neq 0 \ \forall\ i \in \mathbb{Z} \,. \tag{42}$$

Let

$$\mathbf{v} = \phi_i \frac{\partial}{\partial u_i}$$

be a vector field, where we allow $\phi_i = \phi(i, u_i)$ to depend on the discrete index $i \in \mathbb{Z}$. Applying the infinitesimal invariance criterion (41) we obtain the equation

$$\phi(i+2, a(i)u_{i+1} + b(i)u_i) = a(i)\phi(i+1, u_{i+1}) + b(i)\phi(i, u_i) \ , \tag{43}$$

where we replaced u_{i+2} by the right-hand side of (42). Applying the differential operator $\big(1/b(i)\big)\partial_{u_i} - \big(1/a(i)\big)\partial_{u_{i+1}}$ to (43) we obtain the differential–difference equation

$$-\phi'(i+1, u_{i+1}) + \phi'(i, u_i) = 0 \ , \tag{44}$$

where the prime notation means differentiation with respect to the second entry of the function. Differentiating (44) with respect to u_i we obtain

$$\phi''(i, u_i) = 0 \ .$$

Integrating this equation once, we find that

$$\phi'(i, u_i) = \alpha(i) \ , \tag{45}$$

for some arbitrary function $\alpha(i)$. Substituting (45) in (44) yields $\alpha(i+1) = \alpha(i)$. Thus, $\alpha(i) = c$ is constant. Integrating (45), we obtain that

$$\phi(i, u_i) = c\, u_i + \beta(i) \ . \tag{46}$$

Substituting (46) in (43) we conclude that $\beta(i)$ must be a solution of the equation $\beta_{i+2} = a(i)\beta_{i+1} + b(i)\beta_i$. Thus, the Lie algebra of infinitesimal symmetry generators is spanned by

$$\mathbf{v}_1 = u_i \frac{\partial}{\partial u_i}, \qquad \longrightarrow \quad \text{dilations} \ ,$$

$$\mathbf{v}_\beta = \beta(i) \frac{\partial}{\partial u_i}, \qquad \longrightarrow \quad \text{linear superposition of solutions} \ .$$

Example 3.13 As a second example, we consider the autonomous discrete potential Korteweg–de Vries equation (dpKdV)

$$u_{i+1}^{n+1} = u_i^n + \frac{1}{u_{i+1}^n - u_i^{n+1}} \ , \tag{47}$$

which can be found in the work of Hirota [38]. Let

$$\mathbf{v} = \phi_i^n \frac{\partial}{\partial u_i^n} , \quad \phi_i^n = \phi(i, n, u_i^n)$$

be a vector field. Implementing the infinitesimal invariance criterion (41), we obtain the equation

$$\phi_{i+1}^{n+1} = \phi_i^n + \frac{\phi_i^{n+1} - \phi_{i+1}^n}{(u_{i+1}^n - u_i^{n+1})^2} ,$$
$$\text{where } \phi_{i+1}^{n+1} = \phi\left(i+1, n+1, u_i^n + \frac{1}{u_{i+1}^n - u_i^{n+1}}\right) . \tag{48}$$

Applying the operator $\partial_{u_{i+1}^n} + \partial_{u_i^{n+1}}$ yields

$$\phi'(i, n+1, u_i^{n+1}) - \phi'(i+1, n, u_{i+1}^n) = 0 . \tag{49}$$

Differentiating with respect to u_{i+1}^n gives

$$\phi''(i+1, n, u_{i+1}^n) = 0 \quad \text{so that} \quad \phi_i^n = \alpha(i, n) u_i^n + \beta(i, n) .$$

Substituting ϕ_i^n in (49) we obtain the difference equation

$$\alpha(i, n+1) - \alpha(i+1, n) = 0 ,$$

which implies that $\alpha(i, n) = \gamma(i+n)$. Substituting ϕ_i^n in (48) yields the constraints

$$\gamma(i+n+2) = -\gamma(i+n+1) = \gamma(i+n) ,$$
$$\beta(i+1, n+1) = \beta(i, n) , \quad \beta(i+1, n) = \beta(i, n+1) ,$$

which imply that

$$\phi_i^n = c_1(-1)^{i+n} u_i^n + c_2(-1)^{i+n} + c_3 ,$$

where $c_1, c_2, .c_3$ are arbitrary constants. We conclude that the Lie algebra of infinitesimal symmetry generators is spanned by

$$\mathbf{v}_1 = (-1)^{i+n} u_i^n \frac{\partial}{\partial u_i^n} , \quad \mathbf{v}_2 = (-1)^{i+n} \frac{\partial}{\partial u_i^n} , \quad \mathbf{v}_3 = \frac{\partial}{\partial u_i^n} .$$

These vector fields satisfy the commutation relations

$$[\mathbf{v}_1, \mathbf{v}_2] = -\mathbf{v}_3 , \quad [\mathbf{v}_1, \mathbf{v}_3] = -\mathbf{v}_2 , \quad [\mathbf{v}_2, \mathbf{v}_3] = 0 ,$$

which are isomorphic to the commutation relations of the pseudo-Euclidean Lie algebra $\mathfrak{e}(1,1)$ [83].

For more examples, we refer the reader to [41, 44, 56–58].

4 Invariants

Intuitively, an invariant is a quantity that remains unchanged under the action of a group of local transformations. In this section, we review two methods for constructing invariants. The first approach is based on Lie's infinitesimal invariance criterion which leads to systems of first order partial differential equations that can be solved using the method of characteristics. The second approach uses the novel theory of equivariant moving frames. In this framework, invariants are obtained by solving a system of nonlinear algebraic equations. Remarkably, the latter can be solved for a wide variety of group actions.

4.1 Lie's Infinitesimal Approach

As in Sect. 3, we consider the differential and finite difference cases simultaneously by considering an r-parameter local Lie group G acting on $\mathcal{M}$, which can represent either $\mathrm{J}^{(\ell)}$, $\mathcal{J}^{(\ell)}$ or $\mathcal{J}^{[\ell]}$.

Definition 4.1 A function $I\colon \mathcal{M} \to \mathbb{R}$ is said to be a *G-invariant* if

$$I(g \cdot z) = I(z) \quad \text{for all } g \in G \tag{50}$$

where the action is defined. At the infinitesimal level, $I\colon \mathcal{M} \to \mathbb{R}$ is an invariant if

$$\mathbf{v}(I) = 0 \quad \text{for all } \mathbf{v} \in \mathfrak{g}. \tag{51}$$

Remark 4.2 The notion of an invariant is more restrictive than that of an invariant equation. The invariance of an equation only has to hold on its solution space whereas the invariance of a function must hold on its domain of definition.

Finding invariants from the group invariance condition (50) can be difficult as the group action is generally nonlinear. One of the key insights of Sophus Lie was to work with the infinitesimal invariance condition (51) as the latter is a linearized version of the nonlinear problem. Let

$$\mathbf{v}_\kappa = \sum_{a=1}^{d} \zeta_\kappa^a(z) \frac{\partial}{\partial z^a}\,, \quad \kappa = 1, \dots, r = \dim \mathfrak{g}\,, \tag{52}$$

be a basis of the Lie algebra $\mathfrak{g}$ of infinitesimal generators of the Lie group action G. To find the functions $I\colon \mathcal{M} \to \mathbb{R}$ invariant under the group action G, we require that the infinitesimal invariance criterion (51) holds for each basis element (52). This yields the system of first order linear partial differential equations

$$\sum_{a=1}^{d} \zeta_\kappa^a(z) \frac{\partial I}{\partial z^a} = 0 \,, \quad \kappa = 1, \dots, r \,. \tag{53}$$

The latter is solved using the method of characteristics. The corresponding characteristic system of ordinary differential equations is

$$\frac{\mathrm{d}z^1}{\zeta_\kappa^1(z)} = \frac{\mathrm{d}z^2}{\zeta_\kappa^2(z)} = \cdots = \frac{\mathrm{d}z^d}{\zeta_\kappa^d(z)} \,, \quad \kappa = 1, \dots, r \,, \tag{54}$$

and, in the generic case, the system of equations (54) yields a complete set of $\dim \mathcal{M} - r$ functionally independent invariants

$$I^\nu(z) \,, \quad \nu = 1, \dots, \dim \mathcal{M} - r \,.$$

Definition 4.3 A set of invariants $\mathbf{I}_c = \{\dots, I^\nu(z), \dots\}$ is said to be *complete* if any invariant function $I\colon \mathcal{M} \to \mathbb{R}$ can be expressed in terms of those invariants. That is,

$$I(z) = F(\dots, I^\nu(z), \dots) \,.$$

Most textbooks on symmetries and differential equations cover Lie's infinitesimal method of computing differential invariants [11, 12, 43, 68, 71, 76]. Differential invariants are fundamental objects in mathematics and have many applications. They occur in geometry as the curvature of curves, surfaces, and submanifolds [35], they are used in differential equations to reduce the order of ordinary differential equations and find invariant solution of partial differential equations [11, 12, 43, 68, 76], their signature manifold is used to solve local equivalence problems [34, 47, 71, 84], geometric flows of differential invariants are closely related to completely integrable equations [66], and have applications in computer vision [48], climate and turbulence modeling [8], and much more.

In the finite difference situation, since the Lie group G acts trivially on the multi-index N, the components of N will always provide p invariants. Solving the infinitesimal invariance criterion

$$\mathbf{v}_\kappa^{[\ell]}(I) = \sum_K \left[\sum_{i=1}^{p} \xi^i_{\kappa;N+K} \frac{\partial I}{\partial x_{N+K}} + \sum_{\alpha=1}^{q} \phi^\alpha_{\kappa;N+K} \frac{\partial I}{\partial u^\alpha_{N+K}} \right] = 0 \,, \tag{55}$$

where $\kappa = 1, \dots, r$, will, in the generic case, produce $\dim \mathcal{J}^{[\ell]} - p - r$ difference invariants $I^\nu(x_N^{[\ell]}, u_N^{[\ell]})$ independent of the multi-index N.

Example 4.4 To illustrate the application of the infinitesimal invariance criterion (55), we consider the special linear group $SL(2,\mathbb{R})$ acting on $M = \mathbb{R}^2 = \{(x,u)\}$ by the fractional linear action (35) with infinitesimal generators (34). For future reference, we consider the order three discrete jet space $\mathcal{J}^{[3]}$ with coordinates

$$(i, x_{i-1}, u_{i-1}, x_i, u_i, x_{i+1}, u_{i+1}, x_{i+2}, u_{i+2}) \ . \tag{56}$$

To compute a complete set of finite difference invariants on $\mathcal{J}^{[3]}$, we prolong the infinitesimal generators (34) to $\mathcal{J}^{[3]}$:

$$\begin{aligned}
\mathbf{v}_1^{[3]} &= \frac{\partial}{\partial u_{i-1}} + \frac{\partial}{\partial u_i} + \frac{\partial}{\partial u_{i+1}} + \frac{\partial}{\partial u_{i+2}} \ , \\
\mathbf{v}_2^{[3]} &= u_{i-1}\frac{\partial}{\partial u_{i-1}} + u_i\frac{\partial}{\partial u_i} + u_{i+1}\frac{\partial}{\partial u_{i+1}} + u_{i+2}\frac{\partial}{\partial u_{i+2}} \ , \\
\mathbf{v}_3^{[3]} &= u_{i-1}^2\frac{\partial}{\partial u_{i-1}} + u_i^2\frac{\partial}{\partial u_i} + u_{i+1}^2\frac{\partial}{\partial u_{i+1}} + u_{i+2}^2\frac{\partial}{\partial u_{i+2}} \ .
\end{aligned} \tag{57}$$

Omitting the trivial invariant given by the index i, we expect $(\dim \mathcal{J}^{[3]} - 1) - \dim \mathfrak{g} = 8 - 3 = 5$ functionally independent invariants. Clearly, four of them are given by

$$x_{i-1} \ , \quad x_i \ , \quad x_{i+1} \ , \quad x_{i+2} \ . \tag{58}$$

To find the remaining functionally independent invariant $I = I(u_{i-1}, u_i, u_{i+1}, u_{i+2})$, we first solve the differential equation

$$\mathbf{v}_1^{[3]}(I) = \frac{\partial I}{\partial u_{i-1}} + \frac{\partial I}{\partial u_i} + \frac{\partial I}{\partial u_{i+1}} + \frac{\partial I}{\partial u_{i+2}} = 0$$

using the method of characteristics. The corresponding characteristic system of ordinary differential equations is given by

$$\mathrm{d}u_{i-1} = \mathrm{d}u_i = \mathrm{d}u_{i+1} = \mathrm{d}u_{i+2} \ .$$

The three functionally independent solutions are

$$I_{i-1} = u_i - u_{i-1} \ , \quad I_i = u_{i+1} - u_i \ , \quad I_{i+1} = u_{i+2} - u_{i+1} \ . \tag{59}$$

The functions (59) form a complete set of difference invariants for the infinitesimal generator $\mathbf{v}_1$. To proceed further, we notice that any function $I\colon \mathcal{J}^{[3]} \to \mathbb{R}$ invariant under all three infinitesimal generators (57) must necessarily be a function of the invariants (59), that is $I = I(I_{i-1}, I_i, I_{i+1})$. Thus to find the functions that are simultaneously invariant under $\mathbf{v}_1^{[3]}$ and $\mathbf{v}_2^{[3]}$, we must now restrict the vector field $\mathbf{v}_2^{[3]}$ to the variables (59). The result is

$$\mathbf{v}_2^{[3]} = I_{i-1}\frac{\partial}{\partial I_{i-1}} + I_i\frac{\partial}{\partial I_i} + I_{i+1}\frac{\partial}{\partial I_{i+1}} .$$

Thus, the characteristic system associated with the differential equation

$$\mathbf{v}_2^{[3]}(I) = I_{i-1}\frac{\partial I}{\partial I_{i-1}} + I_i\frac{\partial I}{\partial I_i} + I_{i+1}\frac{\partial I}{\partial I_{i+1}} = 0$$

is

$$\frac{dI_{i-1}}{I_{i-1}} = \frac{dI_i}{I_i} = \frac{dI_{i+1}}{I_{i+1}} .$$

The two functionally independent solutions are

$$J_i = \frac{I_{i-1}}{I_i} , \quad J_{i+1} = \frac{I_i}{I_{i+1}} . \tag{60}$$

Therefore, any invariant function I must be expressible in terms of (60). That it, $I = I(J_i, J_{i+1})$. The restriction of the vector field $\mathbf{v}_3^{[3]}$ to the variables (60) yields

$$\mathbf{v}_3^{[3]} = -I_i\left(J_i[J_i+1]\frac{\partial}{\partial J_i} + [1+J_{i+1}]\frac{\partial}{\partial J_{i+1}}\right) .$$

Thus, the equation $\mathbf{v}_3^{[3]}(I) = 0$ becomes

$$J_i[J_i+1]\frac{\partial I}{\partial J_i} + [1+J_{i+1}]\frac{\partial I}{\partial J_{i+1}} = 0 .$$

Solving the characteristic system

$$\frac{\mathrm{d}J_i}{J_i[J_i+1]} = \frac{\mathrm{d}J_{i+1}}{1+J_{i+1}}$$

we find that the cross-ratio

$$R_i = \frac{J_i}{(1+J_i)(1+J_{i+1})} = \frac{(u_i-u_{i-1})(u_{i+2}-u_{i+1})}{(u_{i+1}-u_{i-1})(u_{i+2}-u_i)} \tag{61}$$

is an invariant of the $\mathrm{SL}(2,\mathbb{R})$ product action on $\mathcal{J}^{[3]}$.

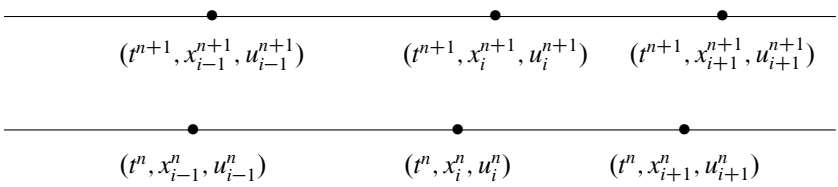
Exercise 4.5 Continuing Exercise 3.8, introduce the discrete points (t_i^n, x_i^n, u_i^n), where $(n,i) \in \mathbb{Z}^2$.

1. Verify that the equation

$$t_{i+1}^n - t_i^n = 0 \,, \tag{62}$$

is invariant. Therefore, Burgers' equation can be invariantly discretized on a mesh with horizontal time layers, the discrete time t^n being only a function of $n \in \mathbb{Z}$.

2. Compute a complete set of difference invariants on the lattice



using Lie's infinitesimal method.

4.2 Moving Frame Approach

The method of equivariant moving frames is a new theoretical formulation of Cartan's method of moving frames [16, 34, 47, 71]. In this novel framework, moving frames are no longer constrained by frame bundles or connections and can thereby be extended to discrete geometry. The theory of equivariant moving frames for local Lie group actions was first presented in [33] and then extended to infinite-dimensional Lie pseudo-group actions in [73, 74]. For a comprehensive introduction we refer the reader to the textbook [64]. In the discrete setting, the theoretical foundations have been expounded in [67, 70].

As in the previous sections, our starting point is an r-dimensional local Lie group of transformations G acting on the d-dimensional manifold $\mathcal{M}$.

Definition 4.6 A *right moving frame* is a G-equivariant map $\rho\colon \mathcal{M} \to G$. The G-equivariance means that

$$\rho(g \cdot z) = \rho(z) g^{-1}.$$

Remark 4.7 It is also possible to consider left moving frames. Given a right moving frame $\rho\colon \mathcal{M} \to G$, a left moving frame $\bar{\rho}\colon \mathcal{M} \to G$ is simply given by group inversion, $\bar{\rho} = \rho^{-1}$. Thus, a left moving frame $\bar{\rho}$ is a G-equivariant map satisfying $\bar{\rho}(g \cdot z) = g \bar{\rho}(z)$.

To guarantee the existence of a moving frame, the group action must satisfy certain regularity assumptions.

Definition 4.8 A Lie group G is said to act *freely* at z if the isotropy group

$$G_z = \{g \in G \mid g \cdot z = z\}$$

is trivial, i.e. $G_z = \{e\}$. The group action is *locally free* at z if the isotropy group is discrete. The action is (locally) free on $\mathcal{M}$ if it is (locally) free at all $z \in \mathcal{M}$.

When the action is (locally) free, the dimension of the group orbits is constant and equal to $r = \dim G$.

Definition 4.9 A Lie group action is said to be *regular* if the orbits form a regular foliation.

The main existence theorem for moving frames is given by the following proposition.

Proposition 4.10 *If the action of G on $\mathcal{M}$ is locally free and regular, then a moving frame locally exists on $\mathcal{M}$.*

Remark 4.11 Let $\mathcal{V}$ be a connected open submanifold of $\mathcal{M}$ where a moving frame exists. By restricting $\mathcal{M}$ to $\mathcal{V}$, we can always assume that a moving frame is globally defined on $\mathcal{M}$.

In practice, the construction of a moving frame is based on the choice of a cross-section $\mathcal{K}$ to the group orbits. For simplicity, we assume that $\mathcal{K}$ is a coordinate cross-section, which means that it is specified by fixing some of the coordinates of $z \in \mathcal{M}$ to constant values:

$$\mathcal{K} = \{z^{a_\kappa} = c^\kappa \mid \kappa = 1, \dots, r = \dim G\} . \tag{63}$$

When the action is free and regular, the right moving frame at z is the unique group element $\rho(z)$ sending z onto the cross-section $\mathcal{K}$, that is $\rho(z)\cdot z \in \mathcal{K}$. The expressions for the right moving frame are obtained by solving the *normalization equations*

$$g \cdot z^{a_\kappa} = c^\kappa , \quad \kappa = 1, \dots, r , \tag{64}$$

for the group parameters $g = \rho(z)$. Given a right moving frame, there is a systematic mechanism for constructing invariants known as the *invariantization* procedure.

Definition 4.12 The *invariantization* of a function $F(z)$ is the invariant

$$\iota(F)(z) = F(\rho(z) \cdot z) . \tag{65}$$

The fact that (65) is an invariant follows from the G-equivariance of the right moving frame:

$$\iota(F)(g \cdot z) = F(\rho(g \cdot z) \cdot g \cdot z) = F(\rho(z) \cdot g^{-1} \cdot g \cdot z) = F(\rho(z) \cdot z) = \iota(F)(z).$$

Geometrically, $\iota(F)$ is the unique invariant that agrees with F on the cross-section $\mathcal{K}$. In particular, the invariantization of an invariant I is the invariant itself, $\iota(I) = I$. Therefore, the invariantization map ι defines a canonical projection (depending upon the moving frame) from the space of functions to the space of invariants.

The invariantization of the components of z is of particular interest. The invariants $\iota(z^a) = \rho(z) \cdot z^a$, $a = 1, \dots, d$, are called *normalized invariants*. By the moving frame construction, the invariantization of the component functions defining the cross-section (63) yields constant invariants, $\iota(z^{a_\kappa}) = c^\kappa$. These are called *phantom invariants*. The following proposition explains why the normalized invariants are important.

Proposition 4.13 *The normalized invariants $\iota(z^a)$, $a = 1, \dots, d$, form a complete set of invariants on $\mathcal{M}$.*

Proposition 4.13 follows from the *replacement principle*. If $I = I(z)$ is an invariant, since $\iota(I) = I$, it follows that

$$I(z) = \iota(I)(z) = I\big(\iota(z)\big) .$$

In other words, the invariant $I(z)$ can be expressed as a function of the normalized invariants by replacing z with the invariants $\iota(z)$.

For an arbitrary manifold $\mathcal{M}$, the group action of G on $\mathcal{M}$, does not have to be free. On the other hand, when $\mathcal{M}$ is either $\mathrm{J}^{[\ell]}$, $\mathcal{J}^{(\ell)}$ or $\mathcal{J}^{[\ell]}$, it is always possible, under some mild assumptions, to choose ℓ large enough so that the prolonged action becomes (locally) free. To state the result precisely, we need the following technical definitions.

Definition 4.14 Let G be a local Lie group of transformations acting on the manifold M. The *isotropy subgroup* of a subset S of M is the subgroup

$$G_S = \{g \in G \mid g \cdot S = S\} .$$

The *global isotropy subgroup* of a subset S of M is the subgroup

$$G_S^\star = \{g \in G \mid g \cdot z = z \text{ for all } z \in S\} .$$

Definition 4.15 A local Lie group of transformations G is said to act *effectively on subsets* if, for any open subset $U \subset M$, $G_U^\star = \{e\}$. The local Lie group acts *locally effectively on subsets* if, for any open subset $U \subset M$, $G_U^\star$ is a discrete subgroup of G.

In the differential case, the following theorem due to Ovsiannikov [76], and corrected by Olver [69], states that if a group acts (locally) effectively on subsets, then its prolonged action will eventually become free.

Proposition 4.16 *If a local Lie group of transformations G acts (locally) effectively on subsets of M, then there exists ℓ_0 such that for all $\ell \geq \ell_0$, the prolonged action of G acts locally freely on an open dense subset $\mathrm{V}^{(\ell)} \subset \mathrm{J}^{(\ell)}$ (or $\mathcal{V}^{(\ell)} \subset \mathcal{J}^{(\ell)}$).*

The discrete version of Proposition 4.16 was proved in [15].

Example 4.17 We now implement the moving frame construction for the projective action (35) on the order three submanifold jet space

$$\mathrm{J}^{(3)} = \{(x, u, u_x, u_{xx}, u_{xxx})\} .$$

We must therefore compute the prolonged action up to the third derivative. Since the independent variable x is an invariant of the action (35), the implicit derivative operator (26) is

$$D_X = D_x = \frac{\partial}{\partial x} + u_x \frac{\partial}{\partial u} + u_{xx} \frac{\partial}{\partial u_x} + u_{xxx} \frac{\partial}{\partial u_{xx}} + \cdots ,$$

and the prolonged action, up to order 3, is

$$\begin{aligned} U_X &= D_X(U) = \frac{u_x}{(cu+d)^2} , \\ U_{XX} &= D_X^2(U) = \frac{u_{xx}}{(cu+d)^2} - \frac{2cu_x^2}{(cu+d)^3} , \\ U_{XXX} &= D_X^3(U) = \frac{u_{xxx}}{(cu+d)^2} - \frac{6cu_xu_{xx}}{(cu+d)^3} + \frac{6c^2u_x^3}{(cu+d)^4} . \end{aligned}$$

Assuming $u_x \neq 0$, we construct a moving frame by choosing the cross-section

$$\mathcal{K} = \{u = 0, u_x = \epsilon = \operatorname{sign}(u_x), u_{xx} = 0\} . \tag{66}$$

Solving the normalization equations

$$\begin{aligned} U = \frac{au+b}{cu+d} = 0 , \quad U_X = \frac{u_x}{(cu+d)^2} = \epsilon , \\ U_{XX} = \frac{u_{xx}}{(cu+d)^2} - \frac{2cu_x^2}{(cu+d)^3} = 0 , \end{aligned}$$

for the group parameters and using the unitary constraint $ad - bc = 1$, we obtain the right moving frame

$$a = \frac{1}{|u_x|^{1/2}} , \quad b = -\frac{u}{|u_x|^{1/2}} , \quad c = \frac{u_{xx}}{2|u_x|^{3/2}} , \quad d = \frac{2u_x^2 - uu_{xx}}{2|u_x|^{3/2}} . \tag{67}$$

Invariantizing ϵu_{xxx}, we obtain the Schwarzian derivative

$$\epsilon\, \iota(u_{xxx}) = \frac{u_x u_{xxx} - (3/2)u_{xx}^2}{u_x^2} .$$

Exercise 4.18 Referring to Exercise 4.5:

1. Find the one-parameter group action induced by each of the infinitesimal generators (37).
2. Construct a moving frame on $\mathrm{J}^{(1)} = \{(t, x, u, u_t, u_x)\}$.
3. Compute the normalized invariant $\iota(u_{xx})$.

Example 4.19 We now reconsider Example 4.4 using the method of moving frames. The product action on $\mathcal{J}^{[3]}$ is

$$X_{i-1} = x_{i-1} , \quad X_i = x_i , \quad X_{i+1} = x_{i+1} , \quad X_{i+2} = x_{i+2} ,$$
$$U_{i-1} = \frac{au_{i-1} + b}{cu_{i-1} + d} , \quad U_i = \frac{au_i + b}{cu_i + d} ,$$
$$U_{i+1} = \frac{au_{i+1} + b}{cu_{i+1} + d} , \quad U_{i+2} = \frac{au_{i+2} + b}{cu_{i+2} + d} .$$

In the following, we let

$$\epsilon_i = \operatorname{sign}\left(\frac{u_{i+1} - u_{i-1}}{(u_i - u_{i-1})(u_{i+1} - u_i)} \right) .$$

Then, a cross-section to the group orbits is given by

$$\mathcal{K} = \{u_{i-1} = \epsilon_i, u_i \to \infty, u_{i+1} = 0\} , \tag{68}$$

where we let u_i tend to infinity. Solving the normalization equations

$$U_{i-1} = \epsilon_i , \quad U_i \to \infty , \quad U_{i+1} = 0 ,$$

we obtain the right moving frame

$$a = -\frac{1}{c(u_{i+1} - u_i)} , \quad b = -\frac{u_{i+1}}{c(u_{i+1} - u_i)} , \quad d = -cu_i ,$$

where

$$c = \pm \sqrt{\left| \frac{u_{i+1} - u_{i-1}}{(u_{i+1} - u_i)(u_i - u_{i-1})} \right|} .$$

Invariantizing $\epsilon_i u_{i+2}$ we obtain the same difference invariant as in (61):

$$\epsilon_i\, \iota(u_{i+2}) = R_i = \frac{(u_{i+2} - u_{i+1})(u_i - u_{i-1})}{(u_{i+2} - u_i)(u_{i+1} - u_{i-1})} .$$

The latter could also be derived from the replacement principle. Invariantizing (61) we find that

$$\begin{aligned} R_i = \iota(R_i) &= \frac{(\iota(u_i) - \iota(u_{i-1}))(\iota(u_{i+2}) - \iota(u_{i+1}))}{(\iota(u_{i+1} - \iota(u_{i-1}))(\iota(u_{i+2}) - \iota(u_i))} \\ &= \frac{(\iota(u_i) - \epsilon_i)\iota(u_{i+2})}{-\epsilon_i(\iota(u_{i+2}) - \iota(u_i))} \xrightarrow[\iota(u_i)\to\infty]{} \epsilon_i\, \iota(u_{i+2}) . \end{aligned}$$

5 Weakly Invariant Equations

As observed in Remark 4.2, the notion of an invariant function is more restrictive than that of an invariant equation. This brings us to distinguish two types of invariant equations.

Definition 5.1 An equation $F(z) = 0$ is said to be *weakly invariant* if it is invariant only on its solution space. That is

$$F(g \cdot z) = 0 \quad \text{provided } F(z) = 0$$

and the action is defined. An equation $F(z) = 0$ is said to be *strongly invariant* if the function $F\colon \mathcal{M} \to \mathbb{R}$ is G-invariant. That is,

$$F(g \cdot z) = F(z) \qquad \text{for all } g \in G$$

where the action is defined.

Remark 5.2 We note that a weakly invariant equation can, sometimes, be made strongly invariant by appropriately multiplying the equation by a certain *relative invariant*. We recall that a relative invariant of weight μ is a function $R(z)$ which satisfies $R(g \cdot z) = \mu(g, z)R(z)$. Indeed, if a weakly invariant equation $F(z) = 0$ is such that $F(g \cdot z) = \mu(g, z)F(z)$, with $\mu(g, z) \neq 0$, then multiplying the equation by a relative invariant $R(z) \neq 0$ of weight $1/\mu$ yields the strongly invariant equation $R(z)F(z) = 0$.

As a simple example, let $\mathcal{M} = \mathcal{J}^{[1]} = \{(i, x_i, x_{i+1}, u_i, u_{i+1})\}$, and consider the product action

$$X_i = \lambda x_i + a , \quad X_{i+1} = \lambda x_{i+1} + a , \quad U_i = \lambda u_i + b , \quad U_{i+1} = \lambda u_{i+1} + b ,$$

where $\lambda > 0$ and $a, b \in \mathbb{R}$. Then the equation

$$u_{i+1} - u_i = 0 \tag{69}$$

is weakly invariant as $g \cdot u_{i+1} - g \cdot u_i = \lambda(u_{i+1} - u_i)$. Dividing Eq. (69) by the relative invariant $h_i = x_{i+1} - x_i$, one obtains the equivalent strongly invariant equation

$$\frac{u_{i+1} - u_i}{x_{i+1} - x_i} = 0.$$

We now explain how to systematically search for weakly invariant equations. As always, we assume that G is an r-dimensional Lie group acting locally on a d-dimensional manifold $\mathcal{M}$.

5.1 Lie's Infinitesimal Approach

A weakly invariant equation is found by searching for a submanifold $\mathcal{S} \subset \mathcal{M}$, defined as the zero locus of an equation $W(z) = 0$, where the isotropy group is nontrivial. To find such a submanifold we consider a basis of infinitesimal generators (52) and introduce the corresponding Lie matrix.

Definition 5.3 The *Lie matrix* is the $r \times d$ matrix whose components are given by the coefficients of the infinitesimal generators (52):

$$\mathbf{L}(z) = \begin{bmatrix} \zeta_1^1(z) & \dots & \zeta_1^d(z) \\ \vdots & & \vdots \\ \zeta_r^1(z) & \dots & \zeta_r^d(z) \end{bmatrix}. \tag{70}$$

Proposition 5.4 *The dimension of the group orbit through $z \in \mathcal{M}$ is equal to the rank of the Lie matrix $\mathbf{L}(z)$.*

Proposition 5.5 *Let $0 \le k \le r$. The set of points*

$$\mathcal{S}_k = \{z \in \mathcal{M} \mid \operatorname{rank} \mathbf{L}(z) = k\}$$

is invariant under the action of G. The number of functionally independent invariants on $\mathcal{S}_k$ is given by the formula

$$\dim \mathcal{M} - \operatorname{rank} \mathbf{L}|_{\mathcal{S}_k} = d - k\,.$$

The sets of points $\mathcal{S}_k$ where the rank of the Lie matrix $\mathbf{L}$ is not maximal, i.e. $\operatorname{rank} \mathbf{L} < r$, are described by equations of the form $W(z) = 0$. By Proposition 5.5, these equations are weakly invariant. Therefore, weakly invariant equations are found by searching for submanifolds where the rank of the Lie matrix is not maximal.

Example 5.6 To illustrate the above considerations, we consider the Lie algebra of vector fields

$$\mathbf{v}_1 = \frac{\partial}{\partial x}\,, \quad \mathbf{v}_2 = \frac{\partial}{\partial u}\,, \quad \mathbf{v}_3 = x\frac{\partial}{\partial x}\,, \quad \mathbf{v}_4 = x\frac{\partial}{\partial u}\,, \quad \mathbf{v}_5 = u\frac{\partial}{\partial u}\,, \tag{71}$$

and search for weakly invariant equations on the discrete jet space

$$\mathcal{J}^{[2]} = \{(i, x_{i-1}, x_i, x_{i+1}, u_{i-1}, u_i, u_{i+1})\}\,. \tag{72}$$

The prolongation of the infinitesimal generators (71) to $\mathcal{J}^{[2]}$ is given by

$$\mathbf{v}_1^{[2]} = \frac{\partial}{\partial x_{i-1}} + \frac{\partial}{\partial x_i} + \frac{\partial}{\partial x_{i+1}}\,, \quad \mathbf{v}_2^{[2]} = \frac{\partial}{\partial u_{i-1}} + \frac{\partial}{\partial u_i} + \frac{\partial}{\partial u_{i+1}}\,,$$

$$\mathbf{v}_3^{[2]} = x_{i-1}\frac{\partial}{\partial x_{i-1}} + x_i\frac{\partial}{\partial x_i} + x_{i+1}\frac{\partial}{\partial x_{i+1}}\,,$$

$$\mathbf{v}_4^{[2]} = x_{i-1}\frac{\partial}{\partial u_{i-1}} + x_i\frac{\partial}{\partial u_i} + x_{i+1}\frac{\partial}{\partial u_{i+1}}\,,$$

$$\mathbf{v}_5^{[2]} = u_{i-1}\frac{\partial}{\partial u_{i-1}} + u_i\frac{\partial}{\partial u_i} + u_{i+1}\frac{\partial}{\partial u_{i+1}}\,,$$

and the corresponding Lie matrix is

$$\mathbf{L} = \begin{bmatrix} 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 \\ x_{i-1} & x_i & x_{i+1} & 0 & 0 & 0 \\ 0 & 0 & 0 & x_{i-1} & x_i & x_{i+1} \\ 0 & 0 & 0 & u_{i-1} & u_i & u_{i+1} \end{bmatrix}.$$

Assuming that $h_i = x_{i+1} - x_i \neq 0$ and $h_{i-1} = x_i - x_{i-1} \neq 0$, the Lie matrix can be row reduced to

$$\mathbf{L} \sim \begin{bmatrix} 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 \\ -h_{i-1} & 0 & h_i & 0 & 0 & 0 \\ 0 & 0 & 0 & -h_{i-1} & 0 & h_i \\ 0 & 0 & 0 & W & 0 & 0 \end{bmatrix},$$

where $W = h_{i-1}(u_{i+1} - u_i) - h_i(u_i - u_{i-1})$. Therefore, when

$$h_{i-1}(u_{i+1} - u_i) - h_i(u_i - u_{i-1}) = 0 \tag{73}$$

the rank of the Lie matrix is not maximal and (73) yields a weakly invariant equation.

5.2 *Moving Frame Approach*

As explained in Sect. 4.2, a moving frame $\rho: \mathcal{M} \to G$ exists provided the group action is free. In terms of the Lie matrix (70), this occurs where the rank of $\mathbf{L}(z) = r = \dim G$ is maximal. Therefore, submanifolds where the rank of the Lie matrix is not maximal occur where a moving frame does not exist. In those situations it is still possible to construct *partial moving frames* [72, 75, 84]. Intuitively, a partial moving frame is the G-equivariant map that one obtains when some of the group parameters cannot be normalized during the normalization procedure. Given a partial moving frame, the invariantization map is still defined as in (65), and a complete set of normalized difference invariants can still be constructed.

In applications, partial moving frames naturally occur as one attempts to solve the normalizing equations (64). The solution to the normalization equations will, in general, require some nondegeneracy conditions to hold and submanifolds where those constraints are not satisfied will determine weakly invariant equations.

Example 5.7 We now reconsider Example 5.6 using the equivariant moving frame method. The group of transformations induced by the infinitesimal generators is given by

$$X = \lambda x + a\,, \quad U = \alpha u + \beta x + b\,,$$

where $\lambda > 0$, $\alpha > 0$, and $a, b, \beta \in \mathbb{R}$. The product action on the discrete jet space (72) is

$$\begin{aligned} X_{i-1} &= \lambda x_{i-1} + a, & U_{i-1} &= \alpha u_{i-1} + \beta x_{i-1} + b\,, \\ X_i &= \lambda x_i + a, & U_i &= \alpha u_i + \beta x_i + b\,, \\ X_{i+1} &= \lambda x_{i+1} + a, & U_{i+1} &= \alpha u_{i+1} + \beta x_{i+1} + b\,. \end{aligned} \tag{74}$$

Starting the normalization process, we first set $X_i = 0$ and $U_i = 0$. Solving the normalization equations

$$0 = X_i = \lambda x_i + a\,, \quad 0 = U_i = \alpha u_i + \beta x_i + b\,,$$

we obtain

$$a = -\lambda x_i\,, \quad b = -\alpha u_i - \beta x_i\,. \tag{75}$$

Introducing the notation

$$h_i = x_{i+1} - x_i\,, \quad h_{i-1} = x_i - x_{i-1}\,, \quad \Delta u_i = u_{i+1} - u_i\,, \quad \Delta u_{i-1} = u_i - u_{i-1}\,,$$

the substitution of the group normalizations (75) into the product action (74) yields

$$\begin{aligned} X_{i-1} &= -\lambda\, h_{i-1}, & U_{i-1} &= -\alpha\, \Delta u_{i-1} - \beta\, h_{i-1}\,, \\ X_{i+1} &= \lambda\, h_i, & U_{i+1} &= \alpha\, \Delta u_i + \beta\, h_i\,. \end{aligned} \tag{76}$$

At this stage, assuming that $h_{i-1} > 0$ (and similarly $h_i > 0$) we can set $X_{i-1} = -1$, which leads to the group normalization

$$\lambda = \frac{1}{h_{i-1}}\,. \tag{77}$$

Substituting (77) into (76) yields the difference invariant

$$H_i = \iota(x_{i+1}) = \frac{h_i}{h_{i-1}}.$$

To normalize the remaining group parameters α and β in

$$\begin{bmatrix} U_{i-1} \\ U_{i+1} \end{bmatrix} = \begin{bmatrix} -\Delta u_{i-1} & -h_{i-1} \\ \Delta u_i & h_i \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix}\,,$$

it is necessary for the coefficient matrix to be invertible. On the other hand, if the matrix is not invertible, that is, if

$$0 = \det \begin{bmatrix} -\Delta u_{i-1} & -h_{i-1} \\ \Delta u_i & h_i \end{bmatrix} = -h_i\, \Delta u_{i-1} + h_{i-1}\, \Delta u_i\,, \tag{78}$$

one can only construct a partial moving frame and (78) is a weakly invariant equation, which is identical to (73). When (78) holds, we can normalize either U_{i+1} or U_{i-1}. Let $U_{i-1} = 0$, then

$$\beta = -\alpha \frac{\Delta u_{i-1}}{h_{i-1}}\,,$$

and one obtains the partial moving frame

$$a = -\frac{x_i}{h_{i-1}}\,, \quad b = \frac{\alpha}{h_{i-1}} \det \begin{bmatrix} u_i & x_i \\ u_{i-1} & x_{i-1} \end{bmatrix}\,, \quad \lambda = \frac{1}{h_{i-1}}\,, \quad \beta = -\alpha \frac{\Delta u_{i-1}}{h_{i-1}}\,.$$

Finally, we note that

$$\iota(u_{i+1}) = \alpha \left[\Delta u_i - \frac{h_i}{h_{i-1}} \Delta u_{i-1} \right] = 0\,,$$

by virtue of (78).

6 Symmetry-Preserving Numerical Schemes

At this point, given a Lie group of local transformations G acting on $\mathcal{M}$, we have everything needed to construct G-invariant equations. As introduced in Sect. 5, a G-invariant equation $F(z) = 0$ will either be weakly invariant or strongly invariant. To obtain strongly invariant equations, the first step consists of computing a complete set of invariants $\mathbf{I}_c$ using either Lie's infinitesimal approach or the moving frame method. Once a complete set of invariants $\mathbf{I}_c$ has been computed, a strongly invariant equation $0 = F(z) = \widetilde{F}(\mathbf{I}_c)$ is simply obtained by combining invariants from $\mathbf{I}_c$. To obtain weakly invariant equations, one simply has to use one of the two procedures outlined in Sect. 5.

When $\mathcal{M} = \mathrm{J}^{(\ell)}$, the above procedure will produce all the differential equations $\Delta\big(x, u^{(\ell)}\big) = 0$ admitting G as a symmetry group. Similarly, when $\mathcal{M} = \mathcal{J}^{(\ell)}$, one obtains all the differential equations $\bar{\Delta}\big(s, x^{(\ell)}, u^{(\ell)}\big) = 0$ invariant under the prolonged action of G. Obtaining these differential equations is referred to as the *inverse problem of group classification*. Given a G-invariant differential equation $\Delta\big(x, u^{(\ell)}\big) = 0$, the procedure can also be used to construct an extended system of equations $\{\bar{\Delta}\big(s, x^{(\ell)}, u^{(\ell)}\big) = 0, \tilde{\Delta}\big(s, x^{(\ell)}, u^{(\ell)}\big) = 0\}$ that is G-compatible with $\Delta\big(x, u^{(\ell)}\big) = 0$.

In the following, we are mainly interested in the case when $\mathcal{M} = \mathcal{J}^{[\ell]}$. Given a differential equation $\Delta\big(x, u^{(\ell)}\big) = 0$ with symmetry group G, we want to construct a system of finite difference equations that approximates the differential equation, specifies constraints on the mesh, and preserves the symmetry group G. This is now obviously done by finding an appropriate collection of strongly invariant and weakly invariant difference equations, which, in the continuous limit, converge to the differential equation. To find an approximation of the differential equation $\Delta\big(x, u^{(\ell)}\big) = 0$, the first step consists of computing a complete set of difference invariants using either Lie's infinitesimal approach or the moving frame method and to consider their Taylor expansion. Then one searches for a combination of these Taylor expansions that will, in the continuous limit, converge to the differential equation, and thereby provide a finite difference approximation of the equation. This step will not always work. It is possible that the difference invariants cannot be combined in such a way to converge to the differential equation in the continuous limit. When this is the case, one should search for a weakly invariant equation $W(x_N^{[\ell]}, u_N^{[\ell]}) = 0$ that converges to $\Delta = 0$. If the later fails, one can try to add more points in the lattice. It is not clear yet if all invariant differential equations admit at least one symmetry-preserving scheme. Differential equations with infinite-dimensional symmetry groups are particularly challenging. To this day, no one has been able to systematically construct symmetry-preserving schemes for such equations.

In parallel, one also searches for a set of strongly and/or weakly invariant difference equations that will constrain the mesh on which the differential equation is approximated. Mesh equations do not always have to be included. If they are avoided, this leads to *invariant meshless discretization schemes* [4], which tend

to be more complicated numerical schemes as they can operate on an arbitrary collection of nodes where the solution is sought numerically. When, included, the mesh equations will influence how the continuous limit should be taken in the above paragraph. The number of equations specifying the mesh is not a priori fixed. The only requirements are that those equations should not impose any constraints on the dependent variables $u_N^{[\ell]}$, that they should be compatible, and have the appropriate continuous limit. The latter can mean different things depending on the point of view used. For example, in [13, 14, 18, 28–30, 56, 61], the discrete indices $N + K$ are assumed to be fixed and in the continuous limit, the points (x_{N+K}, u_{N+K}) converge to (x_N, u_N) for all $K \in \mathbb{Z}^p$. With this perspective, the mesh equations will converge, in the continuous limit, to identities such as $0 = 0$. Alternatively, if one regards the discrete index $N = (n^1, \dots, n^p)$ as sampling the computational variables $s = (s^1, \dots, s^p)$, one can take the limit in the index variables [67, 78, 79]. To this end, we introduce the variation parameters $\epsilon = (\epsilon^1, \dots, \epsilon^p) \in [0, 1]^p$. One can then write the multi-index $N + K$ as

$$N + K = N + \epsilon \cdot K|_{\epsilon=(1,\dots,1)} = (n^1 + \epsilon^1 k^1, \dots, n^p + \epsilon^p k^p)|_{\epsilon=(1,\dots,1)} .$$

Letting $\epsilon \to 0^+$, one has that

$$\lim_{\epsilon \to 0^+} N + \epsilon \cdot K = N .$$

By introducing the variation parameters $\epsilon = (\epsilon^1, \dots, \epsilon^p)$ in the mesh equations and letting $\epsilon \to 0^+$, the latter will now converge to the companion equations (9b).

We now illustrate the above procedure for constructing symmetry-preserving numerical schemes by considering three examples.

Example 6.1 As our first example, we construct a symmetry-preserving scheme for the Schwarzian differential equation (33), whose symmetry group is given by the fractional linear action (35). The difference invariants on the lattice (56) are given by the index i, the discrete x-variables (58), and the cross-ratio (61). These invariants are sufficient to construct a symmetry-preserving scheme of the Schwarzian equation. We begin by specifying the mesh equation, as this step is the easiest. Clearly, we can set

$$x_{i+1} - x_i = h ,$$

where $h > 0$ is a positive constant. From the mesh equation, it follows that

$$x_{i-1} = x_i - h , \quad x_{i+1} = x_i + h , \quad x_{i+2} = x_i + 2h .$$

Therefore, the Taylor expansions of u_{i-1}, u_{i+1}, and u_{i+2} centered at x_i are

$$\begin{aligned} u_{i-1} &= u(x_{i-1}) = u - hu_x + \frac{h^2}{2}u_{xx} - \frac{h^3}{6}u_{xxx} + \mathcal{O}(h^4) \,, \\ u_{i+1} &= u(x_{i+1}) = u + hu_x + \frac{h^2}{2}u_{xx} + \frac{h^3}{6}u_{xxx} + \mathcal{O}(h^4) \,, \\ u_{i+2} &= u(x_{i+2}) = u + 2hu_x + 2h^2u_{xx} + \frac{4h^3}{3}u_{xxx} + \mathcal{O}(h^4) \,, \end{aligned} \tag{79}$$

where the function u and its derivatives are evaluated at x_i. Substituting the Taylor expansions (79) in the difference invariant (61), we obtain

$$R_i = \frac{h^2u_x^2 + h^3u_xu_{xx} + h^4\big((4/3)u_xu_{xxx} - (3/4)u_{xx}^2\big) + \mathcal{O}(h^5)}{4h^2u_x^2 + 4h^3u_xu_{xx} + (10/3)h^4u_xu_{xxx} + \mathcal{O}(h^5)} \,.$$

Therefore,

$$\frac{4 - 1/R_i}{h^2} = \frac{2u_xu_{xxx} - 3u_{xx}^2}{u_x^2} + \mathcal{O}(h)$$

and an invariant approximation of the Schwarzian equation (33) is given by

$$\frac{1}{h^2}\left[2 - \frac{1}{2R_i}\right] = F(x_i) \,. \tag{80}$$

Example 6.2 As a second example, we consider the second order ordinary differential equation

$$u_{xx} = 0 \,. \tag{81}$$

As seen in Exercise 3.6, the infinitesimal symmetry algebra is spanned by the vector fields (32). In the following, we construct a symmetry-preserving scheme of the differential equation (81) invariant under the five-dimensional symmetry subgroup generated by (71) on the discrete jet space $\mathcal{J}^{[2]} = \{(i, x_{i-1}, x_i, x_{i+1}, u_{i-1}, u_i, u_{i+1})\}$. Since $\dim \mathcal{J}^{[2]} - \dim \mathfrak{g} = 7 - 5 = 2$, other than the index i, we expect one more difference invariant. Solving the system of first order partial differential equations

$$\begin{aligned} \mathbf{v}_1^{[2]}(I) &= \frac{\partial I}{\partial x_{i-1}} + \frac{\partial I}{\partial x_i} + \frac{\partial I}{\partial x_{i+1}} = 0 \,, \\ \mathbf{v}_2^{[2]}(I) &= \frac{\partial I}{\partial u_{i-1}} + \frac{\partial I}{\partial u_i} + \frac{\partial I}{\partial u_{i+1}} = 0 \,, \\ \mathbf{v}_3^{[2]}(I) &= x_{i-1}\frac{\partial I}{\partial x_{i-1}} + x_i\frac{\partial I}{\partial x_i} + x_{i+1}\frac{\partial I}{\partial x_{i+1}} = 0 \,, \end{aligned}$$

$$\mathbf{v}_4^{[2]}(I) = x_{i-1}\frac{\partial I}{\partial u_{i-1}} + x_i\frac{\partial I}{\partial u_i} + x_{i+1}\frac{\partial I}{\partial u_{i+1}} = 0\,,$$
$$\mathbf{v}_5^{[2]}(I) = u_{i-1}\frac{\partial I}{\partial u_{i-1}} + u_i\frac{\partial I}{\partial u_i} + u_{i+1}\frac{\partial I}{\partial u_{i+1}} = 0\,,$$

we obtain the invariant

$$H_i = \frac{x_{i+1}-x_i}{x_i-x_{i-1}} = \frac{h_i}{h_{i-1}}\,. \tag{82}$$

Note that this invariant was also found in our construction of a partial moving frame in Example 5.7. Clearly, it is not possible to approximate (81) using only the invariant (82). We therefore search for weakly invariant equations. In Example 5.6 (and Example 5.7) we found that $W = h_{i-1}(u_{i+1}-u_i)-h_i(u_i-u_{i-1}) = 0$ is a weakly invariant equation. Since the product of a weakly invariant equation $W(x_i^{[2]}, u_i^{[2]}) = 0$ by a nonzero difference function $F(i, x_i^{[2]}, u_i^{[2]}) \neq 0$ remains weakly invariant,

$$\frac{2W}{h_ih_{i-1}(h_i+h_{i-1})} = \frac{2}{x_{i+1}-x_{i-1}}\left(\frac{u_{i+1}-u_i}{x_{i+1}-x_i} - \frac{u_i-u_{i-1}}{x_i-x_{i-1}}\right) = 0$$

is weakly invariant equation, and happens to approximate the differential equation $u_{xx} = 0$. As for the mesh equation, we set $H_i = f(i)$, with $f(i) > 0$ for all i, and obtain

$$x_{i+1} - (1+f(i))x_i + f(i)x_{i-1} = 0\,.$$

Exercise 6.3 (This Exercise Was Taken from [81]) The first-order ordinary differential equation

$$u' = A'(x)u + B'(x)\mathrm{e}^{A(x)} \tag{83}$$

is invariant under the infinitesimal symmetry generators

$$\mathbf{v}_1 = \mathrm{e}^{A(x)}\frac{\partial}{\partial u}\,, \quad \mathbf{v}_2 = [u - B(x)\mathrm{e}^{A(x)}]\frac{\partial}{\partial u}\,.$$

Working on the discrete jet space

$$\mathcal{J}^{[1]} = \{(i, x_i, x_{i+1}, u_i, u_{i+1})\}:$$

1. Show that, other than the index i, the only two invariants are x_i and x_{i+1}.
2. Find a weakly invariant difference equation.
3. Write down a symmetry-preserving scheme for (83).

Example 6.4 The standard discretization of the KdV equation on an orthogonal mesh given in (22) is not invariant under the Galilean boosts

$$X = x + vt\,, \quad T = t\,, \quad U = u + v\,, \quad v \in \mathbb{R}\,.$$

Indeed, under this transformation, the second term in (22) is transformed to

$$(u_i^n + v) \cdot \frac{u_{i+1}^n - u_{i-1}^n}{2h}\,,$$

while the other two terms remain unchanged. Thus, the discretization (22) does not preserve all the symmetries of the equation. It is not difficult to see that the discretization (22) is only invariant under shifts and dilations.

We now proceed to the construction of a symmetry-preserving scheme for the KdV equation. Introducing the multi-index $N = (n, i)$, let

$$(t_N, x_N, u_N) = (t_i^n, x_i^n, u_i^n)$$

as in Example 2.17. Recall that the symmetry generators of the KdV equation were found in (31). Clearly, the ratios

$$\frac{t_{i+1}^n - t_i^n}{t_i^{n+1} - t_i^n} \qquad \text{and} \qquad \frac{t_i^{n+1} - t_i^n}{t_i^n - t_i^{n-1}}$$

are invariant under space and time translations, Galilean boosts, and scalings. Therefore, we can use these two invariants to fix invariant constraints on the discretization of the time variable t by setting $\frac{t_{i+1}^n - t_i^n}{t_i^{n+1} - t_i^n} = 0$ and $\frac{t_i^{n+1} - t_i^n}{t_i^n - t_i^{n-1}} = 1$. These two equations are equivalent to

$$t_{i+1}^n - t_i^n = 0\,, \quad t_i^{n+1} - 2t_i^n + t_i^{n-1} = 0\,. \tag{84}$$

The latter imply that a symmetry-preserving scheme for the KdV equation can be formulated on a mesh with flat, equally spaced time layers:

$$t^n = k\,n + t^0\,.$$

From here on, we assume that (84) hold. The prolongation of the vector fields (31) to the points in the stencil depicted in Fig. 1 is given by

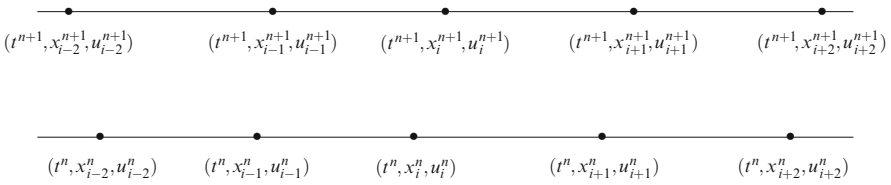


Fig. 1 Stencil for the KdV equation

$$
\begin{aligned}
&\mathbf{v}_1 = \sum_{l=0}^{1} \frac{\partial}{\partial t^{n+l}}\,, \quad \mathbf{v}_2 = \sum_{l=0}^{1}\sum_{j=-2}^{2} \frac{\partial}{\partial x^{n+l}_{i+j}}\,,\\
&\mathbf{v}_3 = \sum_{l=0}^{1}\sum_{j=-2}^{2} t^{n+l}\frac{\partial}{\partial x^{n+l}_{i+j}} + \frac{\partial}{\partial u^{n+l}_{i+j}}, \\
&\mathbf{v}_4 = \sum_{l=0}^{1}\left[3t^{n+l}\frac{\partial}{\partial t^{n+l}} + \sum_{j=-2}^{2} x^{n+l}_{i+j}\frac{\partial}{\partial x^{n+l}_{i+j}} - 2u^{n+l}_{i+j}\frac{\partial}{\partial u^{n+l}_{i+j}}\right].
\end{aligned}
\tag{85}
$$

To simplify the notation, we introduce

$$
\begin{aligned}
&k = t^{n+1} - t^n\,, && h^n_i = x^n_{i+1} - x^n_i\,,\\
&\sigma^n_i = x^{n+1}_i - x^n_i\,, && Du^n_i = \frac{u^n_{i+1} - u^n_i}{h^n_i}\,,
\end{aligned}
\tag{86}
$$

for the spacings and elementary first order discrete x-derivatives. Applying the infinitesimal invariance criterion (53) and solving the corresponding system of first order partial differential equations, we obtain the following 18 functionally independent invariants

$$
\begin{aligned}
&H^{n+l}_{i+j} = \frac{h^{n+l}_{i+j-1}}{h^{n+l}_{i+j}}\,, && l = 0,1, j = -1,0,1\,,\\
&I^n_i = \frac{h^{n+1}_i}{h^n_i}\,, \quad J^n_i = \frac{(h^n_i)^3}{k}\,,\\
&L^n_i = \frac{\sigma^n_i - k\cdot u^n_i}{h^n_i}\,, \quad T^n_i = (u^{n+1}_i - u^n_i)(h^n_i)^2\,,\\
&K^{n+l}_{i+j} = k\cdot Du^{n+l}_{i+j}\,, && l = 0,1, j = -2,-1,0,1\,.
\end{aligned}
\tag{87}
$$

Introducing the invariant quantity

$$Q_i^n = H_{i+1}^n \left(\frac{K_{i+1}^n - K_i^n}{1 + H_{i+1}^n} \right) - \left(\frac{K_i^n - K_{i-1}^n}{1 + H_i^n} \right) ,$$

an invariant numerical scheme for the KdV equation (together with the mesh equations (84)) is given by

$$T_i^n - J_i^n \cdot L_i^n \left(\frac{K_i^n + K_{i-1}^n}{2} \right) + Q_i^n + \frac{Q_{i-1}^n}{(H_i^n)^2} = 0 . \tag{88}$$

Introducing the third order discrete x-derivative

$$D^3 u_i^n = \frac{2}{h_i^n} \left[\left(\frac{Du_{i+1}^n - Du_i^n}{h_{i+1}^n + h_i^n} \right) - \left(\frac{Du_i^n - Du_{i-1}^n}{h_i^n + h_{i-1}^n} \right) \right] , \tag{89}$$

the explicit expression of the invariant scheme (88) is

$$\frac{u_i^{n+1} - u_i^n}{k} + \left(u_i^n - \frac{\sigma_i^n}{k} \right) \frac{Du_i^n + Du_{i-1}^n}{2} + \frac{1}{2} \left[D^3 u_i^n + D^3 u_{i-1}^n \right] = 0 . \tag{90}$$

A more appropriate invariant numerical scheme can be realized on the entire ten point lattice. The latter is given by

$$T_i^n - J_i^n \cdot L_i^n \left(\frac{K_i^n + K_{i-1}^n + K_i^{n+1} + K_{i-1}^{n+1}}{4} \right) + \frac{1}{2} \left[\frac{1}{I_i^n} \left(Q_i^{n+1} + \frac{Q_{i-1}^n}{I_i^n (H_i^{n+1})^2} \right) + Q_i^n + \frac{Q_{i-1}^n}{(H_i^n)^2} \right] = 0 .$$

Explicitly,

$$\frac{u_i^{n+1} - u_i^n}{k} + \left(u_i^n - \frac{\sigma_i^n}{k} \right) \frac{Du_i^n + Du_{i-1}^n + Du_i^{n+1} + Du_{i-1}^{n+1}}{4} + \frac{1}{4} \left[D^3 u_i^{n+1} + D^3 u_{i-1}^{n+1} + D^3 u_i^n + D^3 u_{i-1}^n \right] = 0 . \tag{91}$$

To use the scheme (90) or (91), the *grid velocity*

$$\frac{\sigma_i^n}{k} = \frac{x_i^{n+1} - x_i^n}{k}$$

must be specified in an invariant manner to preserve the symmetries of the KdV equation. One possibility is to set

$$L_i^n = 0 \quad \text{so that} \quad \frac{\sigma_i^n}{k} = u_i^n \,. \tag{92}$$

Together, the Eqs. (84), (90) (or (91)), and (92) provide a numerical approximation of the extended system of differential equations (11), (14), (15) for the KdV equation. The latter scheme can perform poorly as there is no built-in mechanism preventing the clustering of grid points as the numerical integration proceeds. Alternatives to using (92) to obtain the position of the grid points at the next time level will be presented in Sect. 7. Using *adaptive moving mesh methods*, we will construct more reliable invariant numerical schemes.

We conclude this example by discussing the continuous limit of the numerical scheme (90) with mesh equations (84), (92). Let us introduce the variation parameters (ϵ, δ) so that

$$n + l = n + l\epsilon\big|_{\epsilon=1} \qquad \text{and} \qquad i + j = i + j\delta\big|_{\delta=1} \,.$$

In the numerical scheme (90), (84), (92), let

$$u_i^{n+1} - u_i^n = \frac{u_i^{n+\epsilon} - u_i^n}{\epsilon} \,, \quad u_{i+1}^n - u_i^n = \frac{u_{i+\delta}^n - u_i^n}{\delta} \,,$$
$$u_{i+1}^n - 2u_i^n + u_{i-1}^n = \frac{u_{i+\delta}^n - 2u_i^n + u_{i-\delta}^n}{\delta^2} \,,$$
$$u_{i-2}^n - 3u_{i+1}^n + 3u_i^n - u_{i-1}^n = \frac{u_{i+2\delta}^n - 3u_{i+\delta}^n + 3u_i^n - u_{i-\delta}^n}{\delta^3}$$

with $\epsilon = 1$ and $\delta = 1$, and similarly for the differences in t and x. Then, as $\epsilon \to 0$ and $\delta \to 0$,

$$\frac{u_i^{n+\epsilon} - u_i^n}{\epsilon} \to u_\tau \,, \qquad \frac{u_{i+\delta}^n - u_i^n}{\delta} \to u_s \,,$$
$$\frac{u_{i+\delta}^n - 2u_i^n + u_{i-\delta}^n}{\delta^2} \to u_{ss} \,, \qquad \frac{u_{i+2\delta}^n - 3u_{i+\delta}^n + 3u_i^n - u_{i-\delta}^n}{\delta^3} \to u_{sss} \,,$$

and the numerical scheme (90), (84), (92), converges to (15), (11), and (14), respectively.

Alternatively, if one lets $t_{i+j}^{n+l} \to t_i^n$, $x_{i+j}^{n+l} \to x_i^n$, $u_{i+j}^{n+l} \to u_i^n$, without introducing the variation parameters (ϵ, δ), then after multiplying equation (92) by k, the mesh equations (84), (92) converge to the identity $0 = 0$, while (90) converges to the original KdV equation (10).

Exercise 6.5 Using the difference invariants computed in Exercise 4.5 part 2, construct a symmetry-preserving scheme for Burgers' equation (36).

When using the method of equivariant moving frames to construct symmetry-preserving numerical schemes, it is possible to avoid the step where one has to

search for a combination of the difference invariants that will approximate the differential equation $\Delta\big(x, u^{(\ell)}\big) = 0$. In general, for this to be the case, some care needs to be taken when constructing the discrete moving frame $\rho^{[\ell]}\colon \mathcal{J}^{[\ell]} \to G$. The latter has to be *compatible* with a continuous moving frame $\rho^{(\ell)}\colon \mathrm{J}^{(\ell)} \to G$. By this, we mean that the discrete moving frame $\rho^{[\ell]}$ must converge, in the continuous limit, to the moving frame $\rho^{(\ell)}$. If $\mathcal{K}^{[\ell]}$ is the cross-section used to define $\rho^{[\ell]}$ and $\mathcal{K}^{(\ell)}$ is the cross-section defining $\rho^{(\ell)}$, then the moving frame $\rho^{[\ell]}$ will be compatible with $\rho^{(\ell)}$ if, in the coalescing limit, $\mathcal{K}^{[\ell]}$ converges to $\mathcal{K}^{(\ell)}$. As shown in [67], discrete compatible moving frames can be constructed by using the Lagrange interpolation coordinates on $\mathcal{J}^{[\ell]}$, although in applications these can lead to complicated expressions that may limit the scope of the method. It is frequently preferable to fix invariant constraints on the mesh, and then consider finite difference approximations of the derivatives compatible with the mesh. On a nonuniform mesh, these expressions can be obtained by following the procedure of Example 2.11.

Given a compatible moving frame $\rho^{[\ell]}$ an invariant approximation of the differential equation $\Delta\big(x, u^{(\ell)}\big) = 0$ is simply obtained by invariantizing any finite difference approximation $E(N, x_N^{[\ell]}, u_N^{[\ell]}) = 0$, compatible with the mesh. In particular, the equation $E(N, x_N^{[\ell]}, u_N^{[\ell]}) = 0$ does not have to be invariant.

We now illustrate the construction of symmetry-preserving numerical schemes using the method of moving frames.

Example 6.6 As our first example, we revisit Example 6.1 using the moving frame machinery. In Example 4.19, we constructed a discrete moving frame for the symmetry group of the Schwarzian differential equation. This moving frame was constructed using the cross-section (68), which is not compatible with the cross-section (66) used to define a moving frame in the differential case. Indeed, in (66) we have $u = 0$, while in the discrete case we let $u_i \to \infty$. Therefore, one should not expect that the invariantization of the standard scheme

$$\frac{u_{i+2} - 3u_{i+1} + 3u_i - u_{i-1}}{(u_{i+1} - u_i)h^2} - \frac{3}{2}\left(\frac{u_{i+1} - 2u_i + u_{i-1}}{(u_{i+1} - u_i)h}\right)^2 = F(x_i) \tag{93}$$

will provide an invariant approximation of the Schwarzian equation (33). Indeed, the invariantization of (93), yields the inconsistent equation

$$-\frac{9}{h^2} = F(x_i)\ .$$

In this case one has to combine the normalized invariants x_{i-1}, x_i, x_{i+1}, x_{i+2}, and the cross-ratio $\epsilon_i\iota(u_{i+2}) = R_i$ as in Example 6.1 to obtain the invariant numerical scheme (80).

For the invariantization of (93) to give a meaningful invariant discretization, we need to construct a discrete moving frame compatible with (67). Working on the uniform mesh

$$x_{i+1} - x_i = h \,,$$

we introduce the finite difference derivatives

$$Du_i = \frac{u_{i+1} - u_i}{h} \,, \quad D^2u_i = \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} \,,$$
$$D^3u_i = \frac{u_{i+2} - 3u_{i+1} + 3u_i - u_{i-1}}{h^3} \,.$$

To obtain a compatible discrete moving frame, we consider a finite difference approximation of the cross-section (66) used in the differential case. Namely, let

$$\mathcal{K} = \{u_i = 0, Du_i = \epsilon_i, D^2u_i = 0\}$$
$$\text{where } \epsilon_i = \operatorname{sign}(u_{i+1} - u_i)(u_i - u_{i-1})(u_{i+2} - u_{i-1}) \,.$$

The latter is equivalent to

$$\mathcal{K} = \{u_{i-1} = -h\epsilon_i, u_i = 0, u_{i+1} = h\epsilon_i\} \,.$$

Solving the normalization equations

$$-h\epsilon_i = U_{i-1} = \frac{au_{i-1} + b}{cu_{i-1} + b} \,, \quad 0 = U_i = \frac{au_i + b}{cu_i + d} \,,$$
$$h\epsilon_i = U_{i+1} = \frac{au_{i+1} + b}{cu_{i+1} + b} \,,$$

and using the unitary constraint $ad - bc = 1$, we obtain the moving frame

$$a = \frac{D^2u_i}{2c\,Du_i\,Du_{i-1}} \,, \quad b = -\frac{u_iD^2u_i}{2c\,Du_i\,Du_{i-1}} \,,$$
$$d = c \cdot \frac{u_{i+1}\,Du_{i-1} - u_{i-1}\,Du_i}{Du_i - Du_{i-1}} \,,$$

where

$$c^2 = \frac{\epsilon_i(D^2u_i)^2}{2\,Du_i\,Du_{i-1}(Du_i + Du_{i-1})} \,.$$

We note that the right-hand side of the last equality is nonnegative by definition of ϵ_i. Invariantizing the noninvariant scheme (93), we obtain the invariant discretization

$$\frac{(u_{i+2} - u_i)(u_{i+1} - u_{i-1})}{h^3[(u_{i+2} - u_{i-1})Du_i - (u_{i+2} - u_{i+1})Du_{i-1}]} - \frac{2}{h^2} = F(x_i) \,. \tag{94}$$

The latter can be written using cross-ratios in a form similar to the invariant scheme (80). After some simplifications, the invariant scheme (94) is equivalent to

$$\frac{1}{h^2}\left[\frac{1}{\overline{R}_i - R_i} - 2\right] = F(x_i) \ ,$$

where

$$\overline{R}_i = \frac{(u_{i+2} - u_{i-1})(u_{i+1} - u_i)}{(u_{i+2} - u_i)(u_{i+1} - u_{i-1})} \quad \text{and} \quad R_i = \frac{(u_{i+2} - u_{i+1})(u_i - u_{i-1})}{(u_{i+2} - u_i)(u_{i+1} - u_{i-1})} \ .$$

Example 6.7 As our final example, we consider the invariant discretization of the KdV equation. The group action induced by the infinitesimal generators (31) is given by

$$X = \lambda x + vt + a \ , \quad T = \lambda^3 t + b \ , \quad U = \frac{u}{\lambda^2} + v \ , \tag{95}$$

where $a, b, v \in \mathbb{R}$ and $\lambda \in \mathbb{R}^+$. As in Example 6.4, to simplify the computations, we assume that (84) holds. When this is the case, it follows from (18) that

$$u_t \approx \frac{u_i^{n+1} - u_i^n}{k} - \frac{\sigma_i^n}{k} D u_i^n \ , \quad u_x \approx D u_i^n \ ,$$

where we use the notation that was introduced in (86). For better numerical accuracy, we let

$$\begin{aligned} u_t &\approx \Delta_t u_i^n = \frac{u_i^{n+1} - u_i^n}{k} - \frac{\sigma_i^n}{k} \cdot \frac{D u_i^n + D u_{i-1}^n}{2} \ , \\ u_x &\approx \Delta_x u_i^n = \frac{D u_i^n + D u_{i-1}^n}{2} \ . \end{aligned} \tag{96}$$

Also, recalling formula (89), we let

$$u_{xxx} \approx \Delta_x^3 u_i^n = \tfrac{1}{2}[D^3 u_i^n + D^3 u_{i-1}^n] \ . \tag{97}$$

Implementing the discrete moving frame construction, we choose the cross-section

$$\mathcal{K} = \{x_i^n = 0, t^n = 0, u_i^n = 0, \Delta_x u_i^n = 1\} \ ,$$

which is compatible with the cross-section $\{x = 0, t = 0, u = 0, u_x = 1\}$ that one could use to construct a moving frame in the continuous case. Solving the normalization equations

$$\lambda x_i^n + v t^n + a = 0\,, \quad \lambda^3 t^n + b = 0\,, \quad \lambda^{-2} u_i^n + v = 0\,,$$
$$\frac{\lambda^{-2} u_{i+1}^n + v}{\lambda x_{i+1}^n + v t^n + a} + \frac{\lambda^{-2} u_{i-1}^n + v}{\lambda x_{i-1}^n + v t^n + a} = 2\,,$$

for the group parameters a, b, v, λ, we obtain the right moving frame

$$\begin{aligned} a &= -x_i^n (\Delta_x u_i^n)^{1/3} + \frac{t^n u_i^n}{(\Delta_x u_i^n)^{2/3}}\,, & b &= -t^n\, \Delta_x u_i^n\,, \\ v &= -\frac{u_i^n}{(\Delta_x u_i^n)^{2/3}}\,, & \lambda &= (\Delta_x u_i^n)^{1/3}\,. \end{aligned} \tag{98}$$

To obtain an invariant scheme, we approximate the KdV equation using (96) and (97),

$$\Delta_t u_i^n + u_i^n \cdot \Delta_x u_i^n + \Delta_x^3 u_i^n = 0\,. \tag{99}$$

and invariantize the resulting scheme. Since the latter is already invariant, the scheme remains the same. We note that the scheme (99) is the same as (90).

Exercise 6.8 Referring to Exercise 4.5:

1. Construct a discrete moving frame on the stencil

$$\left\{\left(n, i, t^n, t^{n+1}, x_{i-1}^n, x_i^n, x_{i+1}^n, x_{i-1}^{n+1}, x_i^{n+1}, x_{i+1}^{n+1}, u_{i-1}^n, u_i^n, u_{i+1}^n, u_{i-1}^{n+1}, u_i^{n+1}, u_{i+1}^{n+1}\right)\right\}$$

   compatible with the differential moving frame found in Exercise 4.18 part 2.
2. Invariantize the discrete approximation

$$u_{xx} \approx D^2 u_i^n = \frac{2}{h_i^n + h_{i-1}^n}[D u_i^n - D u_{i-1}^n].$$

3. Write a symmetry-preserving scheme for Burgers' equation (36).

7 Numerical Simulations

In this section we present some numerical simulations using the invariant numerical schemes derived in Sect. 6.

7.1 Schwarzian ODE

indexSchwarz' equationWe begin with the Schwarzian ODE (33) with $F(x) = 2$. In other words, we consider the differential equation

$$\frac{u_x\, u_{xxx} - (3/2)u_{xx}^2}{u_x^2} = 2\,. \tag{100}$$

By the Schwarz' Theorem [64], the general solution of (100) is

$$u(x) = \frac{a\sin x + b\cos x}{c\sin x + d\cos x} \quad \text{with } ad - bc \neq 0\,.$$

Choosing $a = d = 1$ and $b = c = 0$, we obtain the particular solution $u(x) = \tan x$. We now aim to obtain this particular solution numerically using the invariant scheme (80) and a standard noninvariant scheme, and compare the results. For the standard method, we choose the explicit fourth order adaptive Runge–Kutta solver `ode45` as provided by MATLAB. On the surface, this appears to be an unfair comparison since the invariant scheme (80) is only first order accurate. However, preserving geometric properties can give a numerical scheme a distinct advantage, even if it is only of relatively low order. This is verified in Fig. 2.

The relative error tolerance controlling the step size in the (noninvariant) adaptive Runge–Kutta method was set to 10^{-12}. Despite this extremely small tolerance, the numerical solution diverges at the point $x = \pi/2$ where the solution has a vertical asymptote. On the other hand, the invariant method, with a step size of $h = 0.01$, is able to integrate beyond this singularity and follows the exact solution $u(x) = \tan x$ very closely. For the conceptually related case where $F(x) = \sin x$ in (33), see [13].

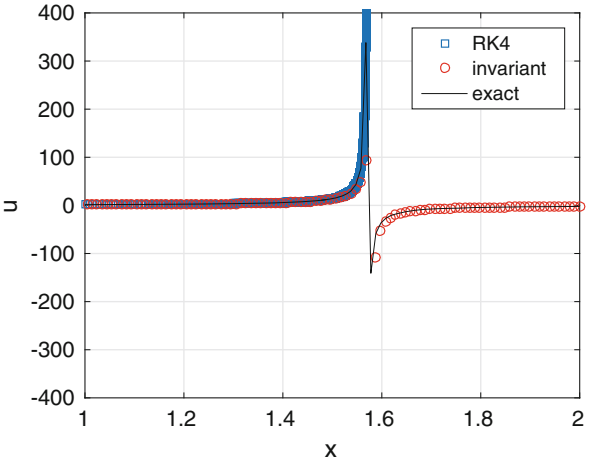


Fig. 2 Numerical integration of the Schwarzian ODE (33) with $F(x) = 2$. *Blue*: Non-invariant fourth order adaptive RK method. *Red*: Invariant first order method. *Black*: Exact solution

7.2 Korteweg–de Vries Equation

As reviewed in the previous sections, the earliest examples of invariant numerical schemes for evolution equations almost exclusively rested on the discretization of their associated Lagrangian form. However, the use of fully Lagrangian techniques for discretizing differential equations is not common due to their tendency to cluster grid points in certain areas of the computational domain and to poorly resolve the remaining parts of the domain. Even more problematic, Lagrangian numerical methods regularly lead to mesh tangling, especially in the case of several space dimensions.

For the KdV equation this basic problem is readily demonstrated using the invariant Lagrangian scheme given by (91) and (92). To do so, we numerically implement this scheme using as initial condition a double soliton solution of the form

$$u(t,x) = \frac{1}{2}c_1 \operatorname{sech}^2\left(\frac{\sqrt{c_1}}{2}(x + a_1 - c_2 t)\right) + \frac{1}{2}c_2 \operatorname{sech}^2\left(\frac{\sqrt{c_2}}{2}(x + a_2 - c_2 t)\right), \tag{101}$$

where $c_1, c_2 \in \mathbb{R}$ are the phase velocities of the individual solitons and $a_1, a_2 \in \mathbb{R}$ are the initial displacements. In our numerical simulations, we set $a_1 = 20$, $a_2 = 5$, $c_1 = 1$, $c_2 = 0.5$, and restricted the computational domain to the interval $[-30, 30]$ discretized with a total of $N = 128$ spatial grid points. The time step k was chosen to be proportional to h^3, $k \propto h^3$, and the final integration time for the Lagrangian experiment was $t = 0.75$. The result of the computation is presented in Fig. 3.

It is visible from the evolution of the mesh points in Fig. 3 (right) that mesh tangling (here: crossing of mesh lines) is about to occur. This leads to numerical

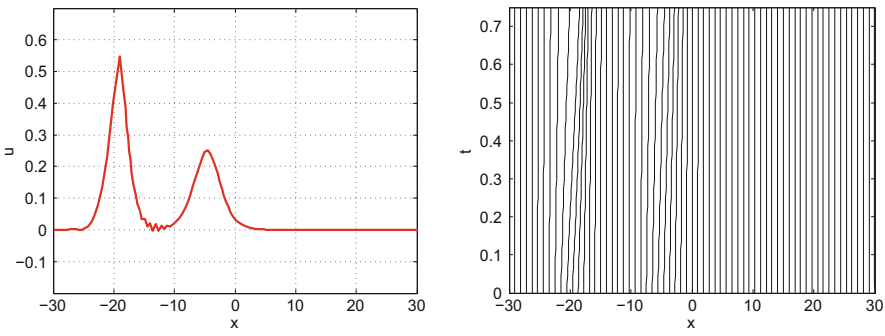


Fig. 3 *Left*: Numerical solution for the KdV equation using the invariant Lagrangian scheme (91) and (92). *Right*: Associated evolution of the mesh points

instability that is visible as high wavenumber oscillations between the two solitons, which sets in almost immediately after the start of the numerical integration. In other words, the invariant Lagrangian scheme is unsuitable for practical applications in virtually all relevant numerical situations, since no inherent control over the evolution of the mesh points is build into the scheme.

It is striking to observe that, despite the well-known shortcomings of Lagrangian numerical schemes, the latter have played a prominent role in the field of symmetry-preserving discretization. This can be explained by the fact that for most papers on the subject, invariant numerical schemes were constructed more as an example highlighting the possibility of deriving symmetry-preserving schemes of differential equations rather than as a tool for practical numerical experiments. Indeed, it is fair to say that even now, the numerical analysis of invariant discretization schemes is still lacking rigor.

In order to make the invariant numerical scheme (91) practical, a different invariant grid equation has to be derived. Possible strategies include the use of *invariant evolution–projection schemes* and *invariant adaptive numerical schemes*.

The invariant evolution–projection scheme conceptually builds upon the invariant Lagrangian scheme. The main idea of this approach is to use the invariant numerical scheme and the invariant mesh equations only over a single time step, and use an interpolation scheme to project the solution of the differential equation defined at the new spatial grid points back to the initial (typically uniform) spatial grid. The entire procedure is invariant if the interpolation scheme used is invariant [5]. The main appeal of this method is that it enables the use of invariant numerical schemes on rectangular meshes.

It is readily verified that classical interpolation methods such as linear, quadratic, cubic or spline interpolations are all invariant under the maximal symmetry group of the KdV equation. The main reason is that all these schemes are polynomials in terms like $(x_{i+1}^{n+1} - x_i^{n+1})$ or $(\hat{x}^{n+1} - x_i^{n+1})/(x_{i+1}^{n+1} - x_i^{n+1})$, where $\hat{x}^{n+1}$ is the interpolation point, which are invariant under spatial and temporal shifts and Galilean boosts. The invariance under scaling transformations follows from the consistency of the interpolation scheme. For example, consider the linear interpolation given by

$$u(\hat{x}_i^{n+1}) = u_i^{n+1} + \frac{u_{i+1}^{n+1} - u_i^{n+1}}{x_{i+1}^{n+1} - x_i^{n+1}}(\hat{x}_i^{n+1} - x_i^{n+1}).$$

Then, under the action of the KdV symmetry group given by (95), the linear interpolation formula remains invariant. In other words, it follows that

$$U(\widehat{X}_i^{n+1}) = U_i^{n+1} + \frac{U_{i+1}^{n+1} - U_i^{n+1}}{X_{i+1}^{n+1} - X_i^{n+1}}(\widehat{X}_i^{n+1} - X_i^{n+1}).$$

For more details and examples, see [5, 6].

In Fig. 4 we present the numerical results for the scheme (91), (92) using the double soliton (101) as initial condition on the interval $[-30, 30]$. As opposed to

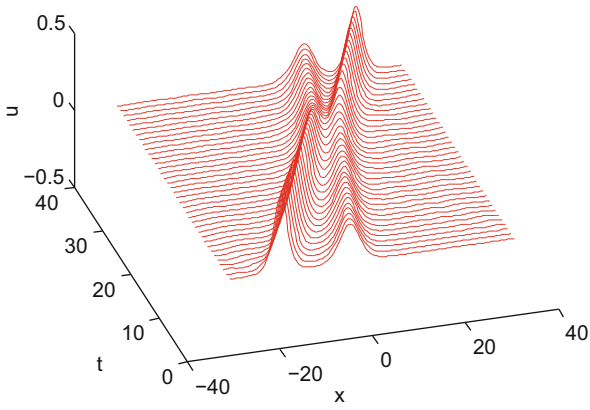


Fig. 4 Numerical solution for the KdV equation using the invariant scheme (91), (92) augmented with a cubic spline interpolation after every step to project the solution back to the original uniform mesh

the previous simulation, we now introduce a cubic spline interpolation at each time integration to project the solution back to the original space grid. The number of discrete spatial points is as before, that is $N = 128$, and the final integration time is $t = 40$. As it can be seen, the two solitons interact with each other and remain unchanged after their collision, which is properly captured by the invariant evolution–projection scheme. We point out though that the scheme is rather dissipative, with the amplitudes of the solitons slowly decreasing over time. While in the present example dissipation can be seen as a disadvantage, this dissipation can be essential in hyperbolic problems that involve shock solutions. For these shock solutions, numerical simulations usually require schemes, such as upwind or Lax–Friedrich and Lax–Wendroff methods, which exhibit artificial dissipation.

A second possibility for completing the invariant numerical scheme (91) without using Lagrangian methods rests on moving mesh methods. Without going into great details, we present here an *invariant r-adaptive scheme* for the KdV equation (for more information, see [9]). In *r*-adaptive numerical schemes a fixed number of grid points is redistributed so that points automatically move to regions where higher resolution is required, for example near shocks. Therefore, *r*-adaptive numerical methods are particularly important for hyperbolic problems. We refer to [39] for a comprehensive review of such methods.

For one-dimensional problems, *r*-adaptive moving meshes on the interval $[a, b]$ are uniquely determined through the *equidistribution principle*, which in differential form reads

$$(\delta(t, x)x_s)_s = 0 \tag{102}$$

with boundary conditions $x(t, 0) = a$ and $x(t, 1) = b$. In (102), the function δ is called the *mesh density function* or *monitor function*. Its role is to control the areas where grid points should concentrate or de-concentrate. It is typically linked to the solution of the physical differential equation. For example, the arc-length type mesh density function is

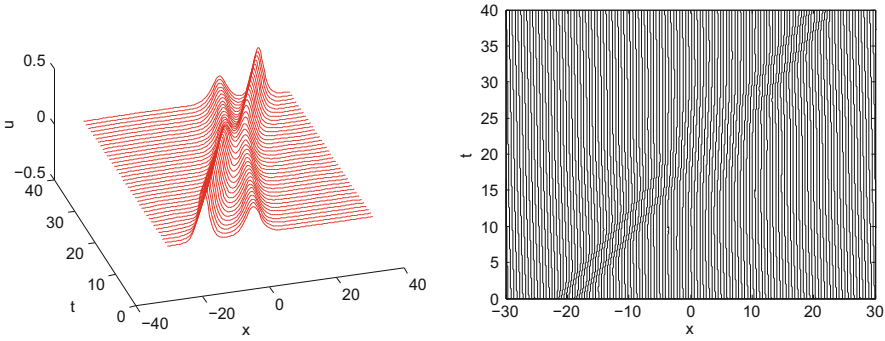


Fig. 5 *Left*: Numerical solution for the KdV equation using the invariant adaptive scheme (91), (104). *Right*: Associated evolution of the mesh points

$$\delta = \sqrt{1 + \alpha u_x^2}\,, \tag{103}$$

where $\alpha \in \mathbb{R}$ is a constant adaptation parameter.

To complete the invariant scheme for the KdV equation, we discretize (102) and (103) using the difference invariants given in (87) or using the invariantization map induced by the discrete moving frame (98). In particular, it turns out that the straightforward discretization

$$\begin{aligned} &\frac{\delta_{i+1}^n + \delta_i^n}{2}(x_{i+1}^{n+1} - x_i^{n+1}) - \frac{\delta_i^n + \delta_{i-1}^n}{2}(x_i^{n+1} - x_{i-1}^{n+1}) = 0\,,\\ &\delta_i^n = \sqrt{1 + \alpha\left(k\frac{u_{i+1}^n - u_i^n}{x_{i+1}^n - x_i^n}\right)^2}\,, \end{aligned} \tag{104}$$

is invariant under the maximal Lie symmetry group of the KdV equation.

In Fig. 5 we present the numerical solution for the KdV equation using the invariant adaptive scheme (91) with (104) and the same double soliton initial condition (101) as in the previous simulation. The final integration time was again chosen to be $t = 40$ and the adaptation parameter was set to $\alpha = 10$.

It is readily seen from Fig. 5 that the invariant adaptive scheme (91), (104) again does not suffer from the shortcomings observed for the Lagrangian scheme (91), (92). In particular, no mesh tangling occurs. The associated adaptive mesh suitably tracks the position of the solitons and remains almost uniform away from the two waves, although the adaptation is relatively weak since the solution does not exhibiting overly steep gradients. An advantage of the invariant r-adaptive scheme over the invariant evolution–projection scheme is that the amplitudes of the solitons are not damped during the adaptation strategy.

In general, using invariant adaptive schemes has the merit of combining a geometric numerical method with a well-proven numerical strategy for dynamically redistributing the points in a mesh. In particular, this technique works for all evolution equations that are invariant under the Galilean group, which are virtually all equations of classical hydrodynamics, including the shallow-water equations, the Euler equations and the Navier–Stokes equations. Since shock waves are physically important solutions in these models, invariant adaptive schemes are of high practical relevance in this field.

7.3 Burgers' Equation

In this section we construct a new numerical scheme for Burgers' equation (36) invariant under the four-parameter symmetry group

$$X = \mathrm{e}^{\epsilon_4} x + \epsilon_3 t + \epsilon_1 \,, \quad T = \mathrm{e}^{2\epsilon_4} t + \epsilon_2 \,, \quad U = \mathrm{e}^{-\epsilon_4} u + \epsilon_3 \,, \qquad \epsilon_1, \epsilon_2, \epsilon_3, \epsilon_4 \in \mathbb{R} \tag{105}$$

generated by the vector fields $\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3, \mathbf{v}_4$ given in (37). We exclude the one-parameter group of transformations generated by $\mathbf{v}_5$ since in numerical simulations the evolution of the time variable t should always be strictly increasing, and allowing the inversion transformations generated by $\mathbf{v}_5$ would enable one to reverse the time direction, which is not desirable from a numerical standpoint.

Remark 7.1 As an exercise, the reader is invited to adapt the constructions below by including the inversion transformations generated by $\mathbf{v}_5$. This has never been attempted and could potentially lead to interesting new results!

Due to the similarities between the symmetry subgroup action (105) and the KdV symmetry group (31), the underlying symmetry-preserving schemes for Burgers' equation are conceptually similar to the invariant schemes constructed before for the KdV equation. Though, one important differences between the two equations is that solutions to Burgers' equation can develop very steep gradients (although remaining smooth for all times provided that $\nu \neq 0$). This is particularly the case if ν approaches zero. Hence, grid adaptation is of practical relevance for this equation.

In [49], an invariantization for the Crank–Nicolson scheme for Burgers' equation was proposed. However, we note that the Crank–Nicolson scheme is implicit and thus in the case where ν is small it might not be the most efficient way of solving Burgers' equation since an explicit scheme should then suffice. In the following, we propose a new scheme which draws some ideas from *high-resolution finite volume methods* [52]. It is well-known that high order schemes, such as the Lax–Wendroff method, lead to oscillations in the numerical solution near shocks, whereas low order schemes, such as the upwind method, develop no such oscillations but exhibit an excessive amount of numerical viscosity. The idea in the high-resolution method

is thus to use a high order method away from the shock and a low resolution method near the shock. The transition between the two regions is accomplished through the use of *flux/slope limiters*.

To formulate an indexinvariant finite volume schemeinvariant finite volume type method for Burgers' equation, we rewrite (36) in the form

$$u_t + \tilde{f}_x = 0\ , \quad \tilde{f} = \tfrac{1}{2}u^2 - \nu u_x\ . \tag{106}$$

We now discretize (106) on a moving mesh, which, as we have previously seen, is enough to guarantee invariance under Galilean transformations. As in Examples 2.8 and 2.10, we introduce the computational variables (τ, s) and let $t = t(\tau) = k\tau + t^0$ and $x = x(\tau, s)$. Then, a suitable conservative form of Burgers' equation in the computational variables (τ, s) is given by

$$(x_s u)_\tau + k\left(\frac{1}{2}u^2 - \nu\frac{u_s}{x_s} - \frac{ux_\tau}{k}\right)_s = (x_s u)_\tau + kf_s = 0\ , \tag{107}$$

see also [39]. We then discretize the flux f in two different ways, once using the second order centered difference method (high resolution) and once using the first order upwind method (low resolution). In doing so, we observe, as in [9], that the invariance under Galilean transformations requires us to discretize (107) in such a way that all spatial derivatives are evaluated using the same finite difference discretizations. With that said, the high order discretization of (107) is $\Delta_\tau (x_s u)^{\text{high}} + k\,\Delta_s f^{\text{high}} = 0$, with

$$\begin{aligned}
\Delta_\tau (x_s u)^{\text{high}} &= (h_i^{n+1} + h_{i-1}^{n+1})u_i^{n+1} - (h_i^n + h_{i-1}^n)u_i^n\ , \\
\Delta_s f^{\text{high}} &= \tfrac{1}{2}\left[(u_{i+1}^n)^2 - (u_{i-1}^n)^2\right] - \nu(Du_i^n - Du_{i-1}^n) \\
&\qquad - \left(\frac{\sigma_{i+1}^n}{k}u_{i+1}^n - \frac{\sigma_{i-1}^n}{k}u_{i-1}^n\right).
\end{aligned}$$

On the other hand, the low order discretization of (107) is $\Delta_\tau (x_s u)^{\text{low}} + k\,\Delta_s f^{\text{low}} = 0$, where

$$\Delta_\tau (x_s u)^{\text{low}} = \begin{cases} h_{i-1}^{n+1}u_i^{n+1} - h_{i-1}^n u_i^n, & u_i^n \geq 0, \\ h_i^{n+1}u_i^{n+1} - h_i^n u_i^n, & u_i^n < 0, \end{cases}$$

and

$$\Delta_s f^{\text{low}} = \begin{cases} \Delta_s f_{\geq}^{\text{low}}, & u_i^n \geq 0, \\ \Delta_s f_{<}^{\text{low}}, & u_i^n < 0, \end{cases}$$

with

$$\Delta_s f^{\text{low}}_{\geq} = \frac{1}{2}\big[(u^n_i)^2 - (u^n_{i-1})^2\big] - \nu(Du^n_{i-1} - Du^n_{i-2}) - \left(\frac{\sigma^n_i}{k}u^n_i - \frac{\sigma^n_{i-1}}{k}u^n_{i-1}\right),$$
$$\Delta_s f^{\text{low}}_{<} = \frac{1}{2}\big[(u^n_{i+1})^2 - (u^n_i)^2\big] - \nu(Du^n_{i+1} - Du^n_i) - \left(\frac{\sigma^n_{i+1}}{k}u^n_{i+1} - \frac{\sigma^n_i}{k}u^n_i\right).$$

The invariant high-resolution method is obtained by dynamically selecting the regions of the domain where the high order and low order methods are used. For this purpose, we introduce the ratio

$$\theta^n_i = \frac{\Delta u^n_{I-1}}{\Delta u^n_{i-1}}\,, \quad \text{where } \Delta u^n_{i-1} = u^n_i - u^n_{i-1}\,,$$

and $I = i - 1$ if $u^n_i \geq 0$ and $I = i + 1$ if $u^n_i < 0$. Geometrically, the quantity θ^n_i measures the smoothness of the solution over the interval $[x_{i-1}, x_i]$. This ratio is, by its definition, invariant under the symmetry subgroup (105), and therefore so is any function of θ^n_i.

We proceed to discretize (107) by considering

$$\Delta_\tau(x_s u) + k\Delta_s f = 0\,, \tag{108}$$

with

$$\Delta_\tau(x_s u) = \Delta_\tau(x_s u)^{\text{low}} - \Phi(\theta^n_{i-1})\big[\Delta_\tau(x_s u)^{\text{low}} - \Delta_\tau(x_s u)^{\text{high}}\big]\,,$$
$$\Delta_s f = \Delta_s f^{\text{low}} - \Phi(\theta^n_{i-1})\big[\Delta_s f^{\text{low}} - \Delta_s f^{\text{high}}\big]\,,$$

and where, for the *flux limiter function* $\Phi(\theta^n_i)$, we choose the so-called minmod-limiter, $\Phi(\theta^n_i) = \max\{0, \min(1, \theta^n_i)\}$. For further discussions on flux limiters, see [52]. To complete the invariant finite volume type scheme for Burgers' equation, we use the same grid adaptation strategy as for the KdV equation to obtain the spatial step size $\sigma^n_i = x^{n+1}_i - x^n_i$ as time evolves.

As a numerical example, we carry out an experiment similar to the one given in [49] for the exact solution

$$u(x) = -\frac{\sinh\big(x/(2\nu)\big)}{\cosh\big(x/(2\nu)\big) + \exp\big(-(c+t)/(4\nu)\big)}\,,$$

where $c \in \mathbb{R}$. We discretize the spatial domain $[-0.5, 0.5]$ with $N = 128$ grid points using Dirichlet boundary conditions, and choose the time step k to be proportional to h^2, $k \propto h^2$. The final integration time is $t = 0.5$ and for numerical purposes $c = 0.25$ and the viscosity was set to $\nu = 0.001$. The adaptation parameter α in the arc-length type mesh density function in (104) was set to $\alpha = 0.5$. The respective numerical results are depicted in Fig. 6.

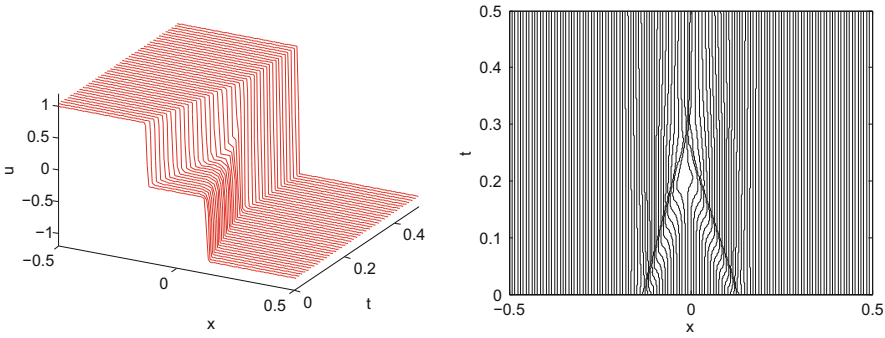


Fig. 6 *Left*: Numerical solution of Burgers' equation using the invariant adaptive scheme (104), (108). *Right*: Corresponding evolution of the mesh points

Unlike in the numerical simulations for the KdV equation presented in Sect. 7.2, Fig. 6 clearly demonstrates the need for an adaptive moving mesh. While this is implied from the structure of the numerical solution, it is remarkable that the requirement for a moving mesh is already encoded in the structure of the symmetry group of Burgers' equation. Hence, numerically preserving symmetries can be seen as a geometrical justification for using *r*-adaptive numerical methods. Moreover, due to the use of a high-resolution finite volume type scheme, no unphysical oscillations around the shock is observed.

8 Conclusion

To recapitulate, let us summarize the algorithm for constructing symmetry-preserving finite difference schemes. Given a differential equation $\Delta\big(x, u^{(\ell)}\big) = 0$:

1. Use the infinitesimal invariance criterion (28) to determine a basis of infinitesimal symmetry generators.
2. Choose a lattice on which the differential equation is to be discretized.
3. When possible, in particular when discretizing a partial differential equation, impose obvious invariant constraints on the mesh. This step is not necessary but if implemented it can, in general, simplify the implementation of the remaining steps.
4. Use either Lie's infinitesimal approach or the moving frame method to compute a complete set of difference invariants, and, if necessary, to find weakly invariant difference equations. When using the moving frame method, one has to exponentiate the infinitesimal generators found in Step 1 to obtain the connected component of the group of local symmetry transformations.
5. Combine the difference invariants and the weakly invariant equations in such a way to obtain an approximation of the differential equation $\Delta\big(x, u^{(\ell)}\big) = 0$ and

(possibly) constraints on the mesh. If using the moving frame method, invariantize a finite difference approximation of the differential equation compatible with the mesh to obtain an invariant approximation of the differential equation.

The basic algorithm for constructing symmetry-preserving numerical schemes is now fairly well-understood. Below are some open problems and comments for the interested reader.

- Many important differential equations in mathematical physics admit an infinite-dimensional symmetry group. Such equations include the Davey–Stewartson equations [20], Liouville's equation, the Kadomtsev–Petviashvili equation [22], the Infeld–Rowland equation [32], the Euler equations [68], and many other equations from fluid dynamics [46]. Implementing the above algorithm for infinite-dimensional symmetry groups remains a challenge. One particularity of these groups is that as new points are added to the stencil, new group parameters appear, which does not occur in the finite-dimensional case. To avoid this difficulty, one possibility is to consider finite-dimensional subgroups of the infinite-dimensional symmetry group and implement the algorithm above [60, 61]. Another possibility, which preserves the infinite-dimensional nature of the group action, is to discretize the Lie pseudo-group action [79].
- In the last 25 years, a great deal of efforts has been devoted to constructing symmetry-preserving finite difference numerical schemes. With the emergence of finite element methods [80], and discrete exterior calculus [1], it would be interesting to extend the above symmetry-preserving algorithm to these settings as well. Further extensions to finite volume and spectral methods should also be considered.
- As with any geometric integrator, one of the motivations for developing symmetry-preserving schemes is to obtain better long term numerical results. As we saw in Sect. 7, and as observed in the literature [13, 14, 18, 50], symmetry-preserving schemes for ordinary differential equations perform extremely well, particularly near singularities. For first order ordinary differential equation, it is even possible to construct symmetry-preserving schemes that will approximate exactly the solution of the original equation [81]. On the other hand, the numerical improvements for partial differential equations are not as clear [4, 9, 21, 49, 61, 78, 79]. In many cases, they tend to be comparable to standard schemes. Now that the theoretical foundations are on firm grounds, one of the main challenges in the field of symmetry-preserving schemes is to investigate the numerical properties of invariant schemes and understand why and when these schemes give better numerical results.
- Most partial differential equations invariantly discretized to date have been evolutionary equations (such as the KdV and Burgers' equations). Much more work, especially from the numerical side, has to be devoted to the invariant discretization of other types of partial differential equations, such as the wave equation, Laplace's equation, and the sine-Gordon equation. In particular, constructing symmetry-preserving schemes compatible with given boundary conditions is an important avenue of research.

- Symmetries are usually not the only geometric properties that a differential equation admits. Other, equally important properties such as a Hamiltonian structure or conservation laws might be present as well. Developing geometric integrators that will preserve more than just one geometric property at the time is an important research direction to pursue.

9 Answers to Selected Exercises

Exercise 4.5, part 2: A complete set of difference invariants is given by the nine invariants

$$I_1 = \frac{h_i^n}{h_{i-1}^n}\,, \quad I_2 = \frac{h_i^{n+1}}{h_{i-1}^{n+1}}\,, \quad I_3 = \frac{h_i^n h_i^{n+1}}{k^n}\,, \quad I_4 = h_i^n h_{i-1}^n (Du_i^n - Du_{i-1}^n)\,,$$

$$I_5 = h_i^{n+1} h_{i-1}^{n+1} (Du_i^{n+1} - Du_{i-1}^{n+1})\,, \quad I_6 = h_i^n \left(\frac{\sigma_i^n}{k^n} - u_i^n\right),$$

$$I_7 = h_i^{n+1} \left(\frac{\sigma_i^n}{k^n} - u_i^{n+1}\right), \quad I_8 = (h_i^n)^2 \left(Du_i^n + \frac{1}{k^n}\right),$$

$$I_9 = (h_i^{n+1})^2 \left(Du_i^{n+1} - \frac{1}{k^n}\right),$$

where

$$h_i^n = x_{i+1}^n - x_i^n\,, \quad k^n = t^{n+1} - t^n, \qquad \sigma_i^n = x_i^{n+1} - x_i^n\,, \quad Du_i^n = \frac{u_{i+1}^n - u_i^n}{h_i^n}\,.$$

Exercise 4.18, part 1: The one-parameter group actions are

$$\begin{aligned}
&\exp[\epsilon_1 \mathbf{v}_1] \cdot (t, x, u) = (x + \epsilon_1, t, u),\\
&\exp[\epsilon_2 \mathbf{v}_2] \cdot (t, x, u) = (x, t + \epsilon_2, u),\\
&\exp[\epsilon_3 \mathbf{v}_3] \cdot (t, x, u) = (x + \epsilon_3 t, t, u + \epsilon_3),\\
&\exp[\epsilon_4 \mathbf{v}_4] \cdot (t, x, u) = (e^{\epsilon_4} x, e^{2\epsilon_4} t, e^{-\epsilon_4} u),\\
&\exp[\epsilon_5 \mathbf{v}_5] \cdot (t, x, u) = \left(\frac{x}{1 - \epsilon_5 t}, \frac{t}{1 - \epsilon_5 t}, (1 - \epsilon_5 t) u + \epsilon_5 x\right).
\end{aligned}$$

Exercise 4.18, part 2: Working on the open dense set $\mathcal{V}^{(1)} = \{(t, x, u, u_t, u_x) \in \mathrm{J}^{(1)} \mid u u_x + u_t \neq 0\}$, the right moving frame corresponding to the cross-section

$$\mathcal{K} = \{t = 0, x = 0, u = 0, u_x = 0, u_t = 1\}$$

is

$$\epsilon_1 = -x\,, \quad \epsilon_2 = -t\,, \quad \epsilon_3 = -u\,, \quad e^{\epsilon_4} = (uu_x + u_t)^{1/3}\,, \quad \epsilon_5 = -u_x\,.$$

Exercise 4.18, part 3: The invariantization of u_{xx} yields the differential invariant

$$\iota(u_{xx}) = \frac{u_{xx}}{uu_x + u_t}\,.$$

Exercise 6.3, part 2: A weakly invariant equation is given by

$$u_{i+1}\mathrm{e}^{-A(x_{i+1})} - u_i\mathrm{e}^{-A(x_i)} - B(x_{i+1}) + B(x_i) = 0\,.$$

Exercise 6.5: Along with the equations (62), we can add the mesh equation $I_6 = 0$ (refer to the solution of Exercise 4.5, part 2). On this mesh, the differential equation can be approximated by

$$-I_7 I_3 = \frac{2\nu I_4 I_1 I_2}{1 + I_1}\,.$$

Explicitly,

$$\frac{h_i^{n+1}h_{i-1}^{n+1}}{h_i^n h_{i-1}^n} \cdot \frac{u_i^{n+1} - u_i^n}{k^n} = \nu D^2 u_i^n\,.$$

Using the mesh equation $\sigma_i^n = k^n u_i^n$, we obtain the explicit scheme

$$(1 + k^n D u_i^n)(1 + k^n D u_{i-1}^n)\left(\frac{u_i^{n+1} - u_i^n}{k^n}\right) = \nu D^2 u_i^n$$

with $t_{i+1}^n = t_i^n$ and $\sigma_i^n = k^n u_i^n$.

Exercise 6.8, part 1: A compatible discrete cross-section is given by

$$\mathcal{K} = \left\{ t^n = 0, x_i^n = 0, u_i^n = 0, \frac{u_{i+1}^n}{x_{i+1}^n} + \frac{u_{i-1}^n}{x_{i-1}^n} = 0, u_i^{n+1} = t^{n+1} \right\}\,.$$

The corresponding discrete moving frame is

$$\epsilon_1 = -x_i^n\,, \quad \epsilon_2 = -t^n\,, \quad \epsilon_3 = -u_i^n\,,$$
$$\mathrm{e}^{\epsilon_4} = [(1 + k^n \Delta_x u_i^n)(\Delta_t u_i^n + u_i^{n+1}\Delta_x u_i^n)]^{1/3}\,, \quad \epsilon_5 = -\Delta_x u_i^n\,,$$

where

$$\Delta_x u_i^n = \frac{Du_i^n + Du_{i-1}^n}{2} \quad \text{and} \quad \Delta_t u_i^n = \frac{u_i^{n+1} - u_i^n}{k^n} - \frac{\sigma_i^n}{k^n} \cdot \Delta_x u_i^n\,.$$

Exercise 6.8, part 2: The invariantization yields the finite difference invariant

$$\iota(D^2u_i^n) = \frac{D^2u_i^n}{(1+k^n\Delta_x u_i^n)(\Delta_t u_i^n + u_i^{n+1}\Delta_x u_i^n)} .$$

Exercise 6.8, part 3: Invariantizing $\Delta_t u_i^n + u_i^n \Delta_x u_i^n = \nu D^2 u_i^n$ we obtain the invariant scheme

$$(1+k^n\Delta_x u_i^n)(\Delta_t u_i^n + u_i^{n+1}\Delta_x u_i^n) = \nu D^2 u_i^n .$$

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References

1. D.N. Arnold, R.S. Falk, R. Winther, Finite element exterior calculus: from Hodge theory to numerical stability. Bull. Am. Math. Soc. (N.S.) **47**(2), 281–354 (2010)
2. M.I. Bakirova, V.A. Dorodnitsyn, An invariant difference model for the equation $u_t = u_{xx} + \delta u \ln u$. Differ. Equ. **30**(10), 1565–1570 (1994)
3. M.I. Bakirova, V.A. Dorodnitsyn, R.V. Kozlov, Symmetry-preserving difference schemes for some heat transfer equations. J. Phys. A **30**(23), 8139–8155 (1997)
4. A. Bihlo, Invariant meshless discretization schemes. J. Phys. A **46**(6), 062001 (2013)
5. A. Bihlo, J.-C. Nave, Invariant discretization schemes using evolution-projection techniques. SIGMA **9**, Paper 052 (2013)
6. A. Bihlo, J.-C. Nave, Convecting reference frames and invariant numerical models. J. Comput. Phys. **272**, 656–663 (2014)
7. A. Bihlo, R.O. Popovych, Invariant discretization schemes for the shallow-water equations. SIAM J. Sci. Comput. **34**(6), B810–B839 (2012)
8. A. Bihlo, E. Dos Santos Cardoso-Bihlo, R.O. Popovych, Invariant parameterization and turbulence modeling on the beta-plane. Phys. D **269**, 48–62 (2014)
9. A. Bihlo, X. Coiteux-Roy, P. Winternitz, The Korteweg–de Vries equation and its symmetry-preserving discretization. J. Phys. A **48**(5), 055201 (2015)
10. A. Bihlo, E. Dos Santos Cardoso-Bihlo, R.O. Popovych, Algebraic method for finding equivalence groups. J. Phys. Conf. Ser. **621**, 012001 (2015)
11. G.W. Bluman, S.C. Anco, *Symmetry and Integration Methods for Differential Equations*. Applied Mathematical Sciences, vol. 154 (Springer, New York, 2002)
12. G.W. Bluman, A.F. Cheviakov, S.C. Anco, *Applications of Symmetry Methods to Partial Differential Equations*. Applied Mathematical Sciences, vol. 168 (Springer, New York, 2010)
13. A. Bourlioux, C. Cyr-Gagnon, P. Winternitz, Difference schemes with point symmetries and their numerical tests. J. Phys. A **39**(22), 6877–6896 (2006)
14. A. Bourlioux, R. Rebelo, P. Winternitz, Symmetry preserving discretization of $\mathrm{sl}(2,\mathbb{R})$ invariant equations. J. Nonlinear Math. Phys. **15**(Suppl. 3), 362–372 (2008)
15. M. Boutin, On orbit dimensions under a simultaneous Lie group action on n copies of a manifold. J. Lie Theory **12**(1), 191–203 (2002)

16. R.L. Bryant, S.S. Chern, R.B. Gardner, H.L. Goldschmidt, P.A. Griffiths, *Exterior Differential Systems*. Mathematical Sciences Research Institute Publications, vol. 18 (Springer, New York, 1991)
17. C. Budd, V. Dorodnitsyn, Symmetry-adapted moving mesh schemes for the nonlinear Schrödinger equation. J. Phys. A **34**(48), 10387–10400 (2001)
18. R. Campoamor-Stursberg, M.A. Rodríguez, P. Winternitz, Symmetry preserving discretization of ordinary differential equations. Large symmetry groups and higher order equations. J. Phys. A **49**(3), 035201 (2016)
19. J. Carminati, K. Vu, Symbolic computation and differential equations: Lie symmetries. J. Symb. Comput. **29**(1), 95–116 (2000)
20. B. Champagne, P. Winternitz, On the infinite-dimensional symmetry group of the Davey–Stewartson equations. J. Math. Phys. **29**(1), 1–8 (1988)
21. M. Chhay, A. Hamdouni, Lie symmetry preservation by finite difference schemes for the Burgers equation. Symmetry **2**(2), 868–883 (2010)
22. D. David, N. Kamran, D. Levi, P. Winternitz, Symmetry reduction for the Kadomtsev–Petviashvili equation using a loop algebra. J. Math. Phys. **27**(5), 1225–1237 (1986)
23. V.A. Dorodnitsyn, Transformation groups in net spaces. J. Sov. Math. **55**(1), 1490–1517 (1991)
24. V. Dorodnitsyn, Noether-type theorems for difference equations. Appl. Numer. Math. **39**(3–4), 307–321 (2001)
25. V. Dorodnitsyn, *Applications of Lie Groups to Difference Equations*. Differential and Integral Equations and Their Applications, vol. 8 (CRC Press, Boca Raton, 2011)
26. V. Dorodnitsyn, R. Kozlov, A heat transfer with a source: the complete set of invariant difference schemes. J. Nonlinear Math. Phys. **10**(1), 16–50 (2003)
27. V. Dorodnitsyn, P. Winternitz, Lie point symmetry preserving discretizations for variable coefficient Korteweg–de Vries equations. Nonlinear Dyn. **22**(1), 49–59 (2000)
28. V. Dorodnitsyn, R. Kozlov, P. Winternitz, Lie group classification of second-order ordinary difference equations. J. Math. Phys. **41**(1), 480–504 (2000)
29. V. Dorodnitsyn, R. Kozlov, P. Winternitz, Symmetries, Lagrangian formalism and integration of second order ordinary difference equations. J. Nonlinear Math. Phys. **10**(Suppl. 2), 41–56 (2003)
30. V. Dorodnitsyn, R. Kozlov, P. Winternitz, Continuous symmetries of Lagrangians and exact solutions of discrete equations. J. Math. Phys. **45**(1), 336–359 (2004)
31. S. Elaydi, *An Introduction to Difference Equations*, 3rd edn. Undergraduate Texts in Mathematics (Springer, New York, 2005)
32. M. Faucher, P. Winternitz, Symmetry analysis of the Infeld–Rowlands equation. Phys. Rev. E (3) **48**(4), 3066–3071 (1993)
33. M. Fels, P.J. Olver, Moving coframes. II. Regularization and theoretical foundations. Acta Appl. Math. **55**(2), 127–208 (1999)
34. R.B. Gardner, *The Method of Equivalence and Its Applications*. CBMS-NSF Regional Conference Series in Applied Mathematics, vol. 58 (SIAM, Philadelphia, 1989)
35. H.W. Guggenheimer, *Differential Geometry*. Dover Books on Advanced Mathematics (Dover, New York, 1977)
36. E. Hairer, C. Lubich, G. Wanner, *Geometric Numerical Integration*, 2nd edn. Springer Series in Computational Mathematics, vol. 31 (Springer, Berlin, 2006)
37. R. Hernández Heredero, D. Levi, P. Winternitz, Symmetry preserving discretization of the Burgers equation, in *SIDE III—Symmetries and Integrability of Difference Equations*, ed. by D. Levi, O. Ragnisco, vol. 25, CRM Proceedings & Lecture Notes (American Mathematical Society, Providence, 2000), pp.197–208
38. R. Hirota, Nonlinear partial difference equations. I. A difference analogue of the Korteweg–de Vries equation. J. Phys. Soc. Jpn. **43**(4), 1424–1433 (1977)
39. W. Huang, R.D. Russell, *Adaptive Moving Mesh Methods*. Applied Mathematical Sciences, vol. 174 (Springer, New York, 2011)
40. P.E. Hydon, Discrete point symmetries of ordinary differential equations. R. Soc. Lond. Proc. Ser. A Math. Phys. Eng. Sci. **454**(1975), 1961–1972 (1998)

41. P.E. Hydon, How to construct the discrete symmetries of partial differential equations. Eur. J. Appl. Math. **11**(5), 515–527 (2000)
42. P.E. Hydon, Symmetries and first integrals of ordinary difference equations. R. Soc. Lond. Proc. Ser. A Math. Phys. Eng. Sci. **456**(2004), 2835–2855 (2000)
43. P.E. Hydon, *Symmetry Methods for Differential Equations*. Cambridge Texts in Applied Mathematics (Cambridge University Press, Cambridge, 2000)
44. P.E. Hydon, *Difference Equations by Differential Equation Methods*. Cambridge Monographs on Applied and Computational Mathematics, vol. 27 (Cambridge University Press, Cambridge, 2014)
45. P.E. Hydon, E.L. Mansfield, Extensions of Noether's second theorem: from continuous to discrete systems. Proc. R. Soc. Lond. Ser. A Math. Phys. Eng. Sci. **467**(2135), 3206–3221 (2011)
46. N.H. Ibragimov, R.N. Ibragimov, *Applications of Lie Group Analysis in Geophysical Fluid Dynamics*. Ser. Complex Nonlinearity Chaos, vol. 2. (World Scientific Publishing, Singapore, 2011)
47. N. Kamran, Contributions to the study of the equivalence problem of Élie Cartan and its applications to partial and ordinary differential equations. Acad. Roy. Belg. Cl. Sci. Mém. Collect. 8^{o} (2) **45**(7) (1989)
48. J.P. Kenney, Evolution of differential invariant signatures and applications to shape recognition. Ph.D. Thesis, University of Minnesota (2009)
49. P. Kim, Invariantization of the Crank–Nicolson method for Burgers' equation. Phys. D **237**(2), 243–254 (2008)
50. P. Kim, P.J. Olver, Geometric integration via multi-space. Regul. Chaotic Dyn. **9**(3), 213–226 (2004)
51. B. Leimkuhler, S. Reich, *Simulating Hamiltonian Dynamics*. Cambridge Monographs on Applied and Computational Mathematics, vol. 14 (Cambridge University Press, Cambridge, 2004)
52. R.J. LeVeque, *Finite Volume Methods for Hyperbolic Problems*. Cambridge Texts in Applied Mathematics (Cambridge University Press, Cambridge, 2002)
53. D. Levi, M.A. Rodríguez, λ-symmetries for discrete equations. J. Phys. A **43**(29), 292001 (2010)
54. D. Levi, R.I. Yamilov, Conditions for the existence of higher symmetries and nonlinear evolutionary equations on the lattice. in *Algebraic Methods in Physics*, ed. by Y. Saint-Aubin, L. Vinet, CRM Series in Mathematical Physics (Springer, New York, 2001), pp. 135–148
55. D. Levi, R.I. Yamilov, The generalized symmetry method for discrete equations. J. Phys. A **42**(45), 454012 (2009)
56. D. Levi, P. Winternitz, Continuous symmetries of difference equations. J. Phys. A **39**(2), R1–R63 (2006)
57. D. Levi, S. Tremblay, P. Winternitz, Lie point symmetries of difference equations and lattices. J. Phys. A **33**(47), 8507–8523 (2000)
58. D. Levi, S. Tremblay, P. Winternitz, Lie symmetries of multidimensional difference equations. J. Phys. A **34**(44), 9507–9524 (2001)
59. D. Levi, M.C. Nucci, M.A. Rodríguez, λ-symmetries for the reduction of continuous and discrete equations. Acta Appl. Math. **122**, 311–321 (2012)
60. D. Levi, L. Martina, P. Winternitz, Lie-point symmetries of the discrete Liouville equation. J. Phys. A **48**(2), 025204 (2015)
61. D. Levi, L. Martina, P. Winternitz, Structure preserving discretizations of the Liouville equation and their numerical tests. SIGMA **11**, Paper 080 (2015)
62. D. Levi, C. Scimiterna, Z. Thomova, P. Winternitz, Contact transformations for difference schemes. J. Phys. A **45**(2), 022001 (2012)
63. H. Levy, F. Lessman, *Finite Difference Equations* (Dover, New York, 2011)
64. E.L. Mansfield, *A Practical Guide to the Invariant Calculus* Cambridge Monographs on Applied and Computational Mathematics, vol. 26 (Cambridge University Press, Cambridge, 2010)

65. E.L. Mansfield, P.E. Hydon, Difference forms. Found. Comput. Math. **8**(4), 427–467 (2008)
66. G. Marí Beffa, P.J. Olver, Poisson structures for geometric curve flows in semi-simple homogeneous spaces. Regul. Chaotic Dyn. **15**(4–5), 532–550 (2010)
67. G. Marí Beffa, E.L. Mansfield, Discrete moving frames on lattice varieties and lattice based multispaces. Found. Comput. Math. (2016). doi:10.1007/s10208-016-9337-5
68. P.J. Olver, *Applications of Lie Groups to Differential Equations*, 2nd edn. Graduate Texts in Mathematics, vol. 107 (Springer, New York, 1993)
69. P.J. Olver, Moving frames and singularities of prolonged group actions. Sel. Math. (N.S.) **6**(1), 41–77 (2000)
70. P.J. Olver, Geometric foundations of numerical algorithms and symmetry. Appl. Algebra Eng. Commun. Comput. **11**(5), 417–436 (2001)
71. P.J. Olver, *Equivalence, Invariants, and Symmetry* (Cambridge University Press, Cambridge, 2009)
72. P.J. Olver, Recursive moving frames. Res. Math. **60**(1–4), 423–452 (2011)
73. P.J., Olver, J. Pohjanpelto, Moving frames for Lie pseudo-groups. Can. J. Math. **60**(6), 1336–1386 (2008)
74. P.J. Olver, J. Pohjanpelto, Differential invariant algebras of Lie pseudo-groups. Adv. Math. **222**(5), 1746–1792 (2009)
75. P.J. Olver, F. Valiquette, Recursive moving frames for Lie pseudo-groups. Preprint, University of Minnesota (2015)
76. L.V. Ovsiannikov, *Group Analysis of Differential Equations* (Academic Press, New York, 1982)
77. G.R.W. Quispel, D.I. McLaren, A new class of energy-preserving numerical integration methods. J. Phys. A **41**(4), 045206, 7 (2008)
78. R. Rebelo, F. Valiquette, Symmetry preserving numerical schemes for partial differential equations and their numerical tests. J. Differ. Equ. Appl. **19**(5), 738–757 (2013)
79. R. Rebelo, F. Valiquette, Invariant discretization of partial differential equations admitting infinite-dimensional symmetry groups. J. Differ. Equ. Appl. **21**(4), 285–318 (2015)
80. J.N. Reddy, *An Introduction to Finite Element Method*. McGraw-Hill Series in Mechanical Engineering, 3rd edn. (McGraw-Hill, New York, 2006)
81. M.A. Rodríguez, P. Winternitz, Lie symmetries and exact solutions of first-order difference schemes. J. Phys. A **37**(23), 6129–6142 (2004)
82. Yu.I. Shokin, *The Method of Differential Approximation*. Springer Series in Computational Physics (Springer, Berlin, 1983)
83. Z. Thomova, P. Winternitz, Maximal abelian subgroups of the isometry and conformal group of Euclidean and Minkowski spaces. J. Phys. A **31**(7), 1831–1858 (1998)
84. F. Valiquette, Solving local equivalence problems with the equivariant moving frame method. SIGMA **9**, Paper 029 (2013)
85. M. Welk, P. Kim, P.J. Olver, Numerical invariantization for morphological PDE schemes, in *Scale Space and Variational Methods in Computer Vision*, ed. by F. Sgallari, A. Murli, N. Paragios. Lecture Notes in Computer Science, vol. 4485 (Springer, New York, 2007), pp. 508–519
86. P. Winternitz, Symmetries of discrete systems, in *Discrete Integrable Systems*, ed. by B. Grammaticos, Y. Kosmann-Schwarzbach, T. Tamizhmani. Lecture Notes in Physics, vol. 644 (Springer, Berlin, 2004), pp. 185–243
87. N.N. Yanenko, Yu.I. Shokin, Group classification of difference schemes for the system of equations of gas dynamics. Trudy Mat. Inst. Steklov. **122**, 85–97 (1973). In Russian
88. G. Zhong, J.E. Marsden, Lie–Poisson Hamilton–Jacobi theory and Lie–Poisson integrators. Phys. Lett. A **133**(3), 134–139 (1988)

Introduction to Cluster Algebras

Max Glick and Dylan Rupel

Abstract These are notes for a series of lectures presented at the ASIDE conference 2016. The definition of a cluster algebra is motivated through several examples, namely Markov triples, the Grassmannians $Gr_2(\mathbb{C}^n)$, and the appearance of double Bruhat cells in the theory of total positivity. Once the definition of cluster algebras is introduced in several stages of increasing generality, proofs of fundamental results are sketched in the rank 2 case. From these foundations we build up the notion of Poisson structures compatible with a cluster algebra structure and indicate how this leads to a quantization of cluster algebras. Finally we give applications of these ideas to integrable systems in the form of Zamolodchikov periodicity and the pentagram map.

1 Introduction

Cluster algebras were introduced by Fomin and Zelevinsky [14] in 2002 as the culmination of their study of total positivity [13] and (dual) canonical bases. The topic of cluster algebras quickly grew into its own as a subject deserving independent study mainly fueled by its emergent close relationship to many areas of mathematics. Here is a partial list of related topics: combinatorics [38], hyperbolic geometry [11, 12, 39], Lie theory [19], Poisson geometry [24], integrable systems [9, 26], representations of associative algebras [5–7, 44–46], mathematical physics [1, 10], and quantum groups [3, 21, 32, 33].

In these notes we will give an introduction to cluster algebras and a couple of the applications mentioned above. These notes are far from exhaustive and

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the references above only touch on the vast literature. Other overviews of cluster algebras can be found in the works [20, 31, 51] which will also provide additional references.

These lecture notes are organized as follows. Section 2 gives several motivating examples from which we will abstract the definition of a cluster algebra. Section 3 contains several variations on the definition of cluster algebras with increasing generality and also the definition of Y-patterns. In Sect. 4, we describe the foundational results in the theory of cluster algebras and sketch, or otherwise indicate the ideas behind, the proofs of these results. Section 5 recalls the theory of Poisson structures compatible with a cluster algebra and describes how this naturally leads to a quantization of cluster algebras. Finally, we conclude with applications of the cluster algebra machinery to problems involving integrable systems in Sect. 6.

2 Motivating Examples

Cluster algebras are certain commutative rings possessing additional structure, including:

- a distinguished collection of generators called *cluster variables*;
- a collection of finite subsets of the set of all cluster variables called *clusters*;
- a *mutation* rule which, given a cluster and one of its variables x, produces another cluster by replacing x with a different cluster variable x' related to x by an *exchange relation*

$$xx' = F,$$

  where F is a binomial in the variables common to the initial and mutated clusters.

Before defining cluster algebras, we describe a few settings illustrating these various components. We leave it to the astute reader to compare these examples with the definitions presented in Sect. 3 and to see how they may be reinterpreted within the cluster algebra framework.

2.1 Markov Triples

A *Markov triple* is a triple (a, b, c) of positive integers satisfying the *Markov equation* $a^2 + b^2 + c^2 = 3abc$; an integer which appears as a term in a Markov triple is called a *Markov number*. The Markov equation is an example of a Diophantine equation and two classical number theoretic problems are to determine the number of solutions and to determine a method for finding all such solutions. We will solve both of these problems for the Markov equation.

Exercise 2.1 Prove that $(1, 1, 1)$ and $(1, 1, 2)$ are (up to reordering) the only Markov triples with repeated values.

Rearranging the Markov equation we see that $c^2 - 3abc + a^2 + b^2 = 0$ and so c is a root of the quadratic $f(x) = x^2 - (3ab)x + (a^2 + b^2)$. But notice that the other root $c' = (a^2 + b^2)/c = 3ab - c$ is a positive integer and so (a, b, c') is again a Markov triple.

Note that there was nothing special about c in the calculation above. Thus given any Markov triple (a, b, c), we may perform three possible exchanges

$$\left(a, b, \frac{a^2 + b^2}{c}\right) \quad \left(a, \frac{a^2 + c^2}{b}, c\right) \quad \left(\frac{b^2 + c^2}{a}, b, c\right)$$

and obtain another Markov triple in each case. The following exercises solve the above two classical problems of Diophantine equations.

Exercise 2.2 (a) Prove that there are infinitely many Markov triples by showing that there is no bound on how large the largest value can be.

(b) Show that all Markov triples may be obtained from the Markov triple $(1, 1, 1)$ by a sequence of exchanges.

2.2 The Grassmannian $Gr_2(\mathbb{C}^n)$

The *Grassmannian* $Gr_k(\mathbb{C}^n)$ is the set of k-dimensional linear subspaces of $\mathbb{C}^n$. A point in the Grassmannian can be described, albeit non-uniquely, as the row span of a full rank matrix $A \in \mathbb{C}^{k\times n}$. The maximal minors of A are called *Plücker coordinates*.

Now, restrict to $k = 2$ and let

$$A = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \end{bmatrix}.$$

The Plücker coordinates are given by $\Delta_{ij} = a_{1i}a_{2j} - a_{1j}a_{2i}$ for $1 \le i < j \le n$. As the matrix A is not uniquely determined by a point in $Gr_2(\mathbb{C}^n)$, the Plücker coordinates are not truly functions on $Gr_2(\mathbb{C}^n)$, but rather they are only well-defined functions up to simultaneous rescaling. That is, the Plücker coordinates determine a closed embedding into the projective space $\mathbb{P}^{\binom{n}{2}-1}$. The following exercise shows that the image of the Plücker embedding lies inside a closed subset of projective space.

Exercise 2.3 Verify that the Δ_{ij} satisfy the so-called *Plücker relations*

$$\Delta_{ik}\Delta_{jl} = \Delta_{ij}\Delta_{kl} + \Delta_{il}\Delta_{jk} \tag{1}$$

for $1 \le i < j < k < l \le n$.

Consider a regular n-gon with vertices labeled $1, 2, \ldots, n$. Let T be a triangulation, i.e., a maximal collection of chords $\overline{ij}$ with $1 \leq i < j \leq n$, no two of which intersect in their interiors. Note that T always consists of $n-3$ diagonals together with the n sides $\overline{12}, \overline{23}, \overline{34}, \ldots, \overline{1n}$. Associate to T the corresponding collection of Plücker coordinates

$$\Delta_T := \{\Delta_{ij} : \overline{ij} \in T\}.$$

Proposition 2.4 *Fix positive reals x_{ij} for all $\overline{ij} \in T$. Then there exists $A \in Gr_2(\mathbb{C}^n)$ such that $\Delta_{ij}(A) = x_{ij}$ for all $\overline{ij} \in T$. Moreover, each $\Delta_{ij}(A)$ with $\overline{ij} \notin T$ can be expressed as a subtraction free rational expression of the x_{ij}.*

For instance, let $n = 4$ and $T = \{\overline{13}, \overline{12}, \overline{23}, \overline{34}, \overline{14}\}$. A possible representing matrix is

$$A = \begin{bmatrix} 1 & \frac{x_{23}}{x_{13}} & 0 & -\frac{x_{34}}{x_{13}} \\ 0 & x_{12} & x_{13} & x_{14} \end{bmatrix}.$$

There is one remaining Plücker coordinate, namely Δ_{24}, and it can be computed from the given ones as

$$\Delta_{24}(A) = \frac{x_{12}x_{34} + x_{14}x_{23}}{x_{13}}$$

which follows from a Plücker relation. This formula can be thought of as a change of coordinates from Δ_T to $\Delta_{T'}$ where $T' = (T \setminus \{\overline{13}\}) \cup \{\overline{24}\}$.

Exercise 2.5 The change of coordinate systems observed above can be understood more classically in terms of the Ptolemy relations for cyclic quadrilaterals. Indeed, consider four distinct points labeled $1, 2, 3, 4$ on a circle in cyclic order and let x_{ij} denote the distance between vertices i and j. Prove that $x_{13}x_{24} = x_{12}x_{34} + x_{14}x_{23}$.

More generally, if T is a triangulation of an n-gon and $\overline{ik} \in T$ is a diagonal (as opposed to a side), then $\overline{ik}$ is part of two triangles of T. Call the third vertices of these two triangles j and l. It follows that $T' = (T \setminus \{\overline{ik}\}) \cup \{\overline{jl}\}$ is again a triangulation. Moreover, it is well known that any two triangulations may be related by a sequence of these flips of diagonals [29]. Performing a sequence of such quadrilateral flips and using a Plücker relation at each step makes it possible to iteratively compute all the rational expressions promised in Proposition 2.4.

2.3 Double Bruhat Cells

An $n \times n$ matrix M is called *totally positive* if the determinant of every square submatrix is a positive real number. In particular, every entry of M is positive and M must be invertible. Write $GL_n^{>0} \subset GL_n$ for the subset of totally positive matrices. To

check that a given matrix $M \in GL_n$ is totally positive one must, a priori, check that all $\binom{2n}{n} - 1$ minors of M are positive. A natural question is whether this verification process can be made more efficient. More precisely, is there a smaller collection of minors one may compute and from the positivity of this subset conclude that every minor is positive, i.e., conclude that $M \in GL_n^{>0}$? We will call such a collection a *total positivity criterion* if it exists.

For small n, such criteria can be found and verified easily. For example, a matrix $M = \left[\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right] \in GL_2$ is totally positive if and only if $a, b, c, ad - bc > 0$ if and only if $b, c, d, ad - bc > 0$.

Exercise 2.6 Find a minimal collection of minors whose positivity guarantees a matrix in GL_3 is totally positive (Hint: any such total positivity criterion consists of 9 minors).

To describe a solution and easily identify total positivity criteria for all general linear groups GL_n, it will be convenient to slightly generalize the notion of total positivity. An $n \times n$ matrix M is called *totally nonnegative* if the determinant of every square submatrix is a nonnegative real number. Write $GL_n^{\geq 0} \subset GL_n$ for the subset of totally nonnegative matrices. Again one may ask: what is a minimal collection of minors needed to check that a matrix is totally nonnegative? Unfortunately, or perhaps fortunately, the total nonnegativity criteria are not uniformly described across all of GL_n. The solution to this problem naturally leads one to study certain subvarieties of GL_n called *double Bruhat cells*, which we now describe.

Let $B_+, B_- \subset GL_n$ denote the subgroups of upper and lower triangular matrices respectively. Identify the symmetric group Σ_n with the subgroup of GL_n consisting of permutation matrices, i.e., matrices having precisely one nonzero entry 1 in each row and column. For example, identify the permutation $(1\ 2) \in \Sigma_2$ (written in cycle notation) with the matrix $\left[\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right]$.

It is well known that GL_n decomposes in two ways (actually many ways) as a union of *Bruhat cells*:

$$GL_n = \bigsqcup_{w \in \Sigma_n} B_+ w B_+ = \bigsqcup_{w \in \Sigma_n} B_- w B_- \ .$$

To understand total nonnegativity criteria for GL_n, we will consider the *double Bruhat cells* $GL_n^{u,v} = B_+ u B_+ \cap B_- v B_-$ for $u, v \in \Sigma_n$.

Exercise 2.7 Find all four double Bruhat cells in GL_2 and verify that they partition the space. If you are brave, find all double Bruhat cells in GL_3 and verify that they partition the space.

For $I, J \subset [1, n]$ with $|I| = |J|$, denote by $\Delta_{I,J}$ the function on GL_n which returns the determinant of the submatrix on row set I and column set J.

Example 2.8 Let $w_0 = (1\ n)(2\ n-1)\cdots(\lfloor n/2 \rfloor\ \lceil n/2 \rceil)$ denote the longest permutation in Σ_n. The double Bruhat cell $GL_n^{w_0,w_0}$ is given as follows:

$$GL_n^{w_0,w_0} = \{M \in GL_n : \Delta_{[1,i],[n+1-i,n]}(M) \neq 0, \Delta_{[n+1-i,n],[1,i]}(M) \neq 0 \text{ for all } i\} .$$

It turns out that each double Bruhat cell admits its own collection of total positivity criteria, i.e., for each $u, v \in \Sigma_n$ there exists a minimal collection of minors whose positivity identifies the subset $GL_n^{u,v} \cap GL_n^{\geq 0}$ inside the double Bruhat cell $GL_n^{u,v}$. Some of these total nonnegativity criteria in $GL_n^{u,v}$ can be conveniently described using double wiring diagrams. Write $s_i = (i\ i+1) \in \Sigma_n$ for the simple transposition interchanging i and $i+1$. A *reduced word* for $w \in \Sigma_n$ is a minimal sequence $(i_1, \ldots, i_r)$ so that $w = s_{i_1} \cdots s_{i_r}$, where $\ell(w) := r$ is called the *length* of w. A reduced word $(i_1, \ldots, i_r)$ is naturally encoded in a *wiring diagram*, i.e., a collection of n strands with a crossing between the ith and $(i+1)$th strands each time i appears in the reduced word, see Fig. 1.

Given $(u, v) \in \Sigma_n^2$, a double reduced word for (u, v) is an arbitrary shuffle of a reduced word for u and a reduced word for v, where terms in the reduced word for v are taken from the set $\{-1, \ldots, -(n-1)\}$ for clarity. For example, taking $u = (1\ 3\ 2), v = (1\ 3) \in \Sigma_3$, one double reduced word for (u, v) is $(-1, 2, -2, 1, -1)$. Given a double reduced word $(i_1, \ldots, i_r)$, build a double wiring diagram by superposing wiring diagrams associated to the reduced word for u and the reduced word for v with crossings ordered according to the double reduced word (see Fig. 2).

In a double wiring diagram, we label the strands in u's wiring diagram on the right by 1 through n starting from the bottom and label the strands in v's wiring

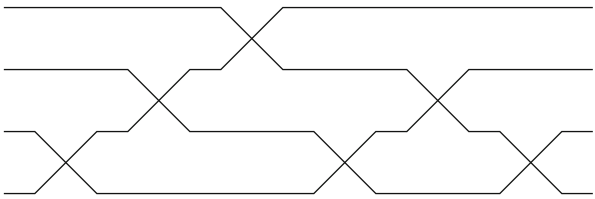
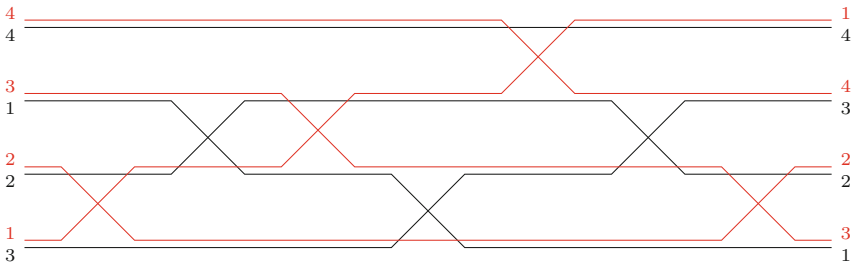


Fig. 1 A wiring diagram for the reduced word $(1, 2, 3, 1, 2, 1) \in \Sigma_4$



$$\Delta_{1,3}, \Delta_{2,3}, \Delta_{2,1}, \Delta_{3,1}, \Delta_{12,23}, \Delta_{12,13}, \Delta_{23,13}, \Delta_{23,12}, \Delta_{123,123}, \Delta_{234,123}, \Delta_{1234,1234}$$

Fig. 2 A double wiring diagram for the double reduced word $(-1, 2, -2, 1, -3, 2, -1) \in \Sigma_4$ and the collection of chamber minors determined by this double wiring diagram

diagram similarly on the left. In this way, each chamber of the double wiring diagram determines a minor with row set given by the labels of strands in v's wiring diagram lying below the chamber and column set given by the labels of strands in u's wiring diagram lying below the chamber (see Fig. 2). Now we may describe a collection of total positivity criteria for $GL_n^{u,v}$.

Theorem 2.9 ([13]) *Each double wiring diagram for (u, v) determines a total positivity criterion for $GL_n^{u,v}$, i.e., an element of $GL_n^{u,v}$ lies in $GL_n^{\geq 0}$ if and only if all $n + \ell(u) + \ell(v)$ chamber minors determined by the double wiring diagram are positive.*

The totally positive matrices are exactly the elements of $GL_n^{w_0,w_0} \cap GL_n^{\geq 0}$. Thus Theorem 2.9 provides many total positivity criteria for GL_n.

Exercise 2.10 Use double wiring diagrams to find a total positivity criterion for GL_3. Does the total positivity criterion you found in Exercise 2.6 come from a double wiring diagram?

To finish the section and connect to the theory of cluster algebras to be presented in the next section we make the following observation. Suppose a double reduced word for (u, v) contains neighboring letters, one belonging to a reduced word for u and one belonging to a reduced word for v. In Fig. 3, we show the local effect on a double wiring diagram when these letters are interchanged.

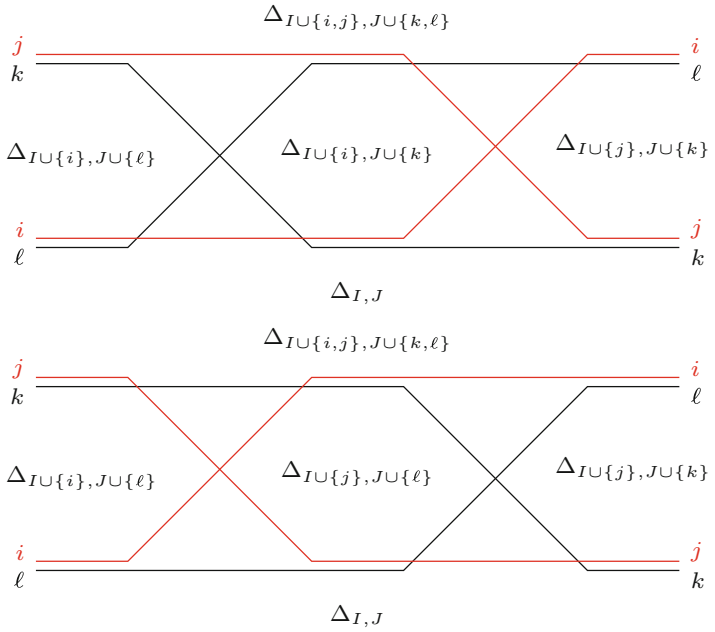


Fig. 3 Chamber minors associated to a simple transposition of opposite letters in a double reduced word

Observe that under such an exchange we have the following exchange relation analogous to (1):

$$\Delta_{I\cup\{i\},J\cup\{k\}}\Delta_{I\cup\{j\},J\cup\{\ell\}} \;=\; \Delta_{I,J}\Delta_{I\cup\{i,j\},J\cup\{k,\ell\}} \;+\; \Delta_{I\cup\{i\},J\cup\{\ell\}}\Delta_{I\cup\{j\},J\cup\{k\}}. \tag{2}$$

Moreover, observe that any two collections of chamber minors for double reduced words of (u, v) can be obtained from each other by a sequence of these exchanges.

Exercise 2.11 Prove (2).

Exercise 2.12 Another local transformation of a double wiring diagram is given by braid moves, either within u or within v. As an example, suppose a doubled word for u, v begins $1, 2, 1$ (i.e., u begins $1, 2, 1$ and these all occur before the first letter of v in the doubled word). Consider the double wiring diagrams both for this word and the one obtained by replacing the first three letters with $2, 1, 2$. Show that the two corresponding collections of chamber minors differ in one element. Find and prove an exchange relation that describes this transformation.

3 A Unifying Concept: Cluster Algebras

We now define cluster algebras of geometric type and Y-patterns, with a focus on the underlying dynamics of seed mutations. All definitions are due to Fomin and Zelevinsky and are drawn from [14] and [17].

3.1 Basic Definitions

Each cluster algebra is defined recursively from some initial data called a seed. A seed consists of a cluster, which was informally described at the beginning of Sect. 2, together with some combinatorial data that encode the mutations that can be performed.

Definition 3.1 Let $\mathcal{F}$ be a purely transcendental field extension of $\mathbb{C}$. A *seed* is a pair $(\mathbf{x}, B)$ where $\mathbf{x} = (x_1, \ldots, x_n)$ is an n-tuple of elements forming a transcendence basis of $\mathcal{F}$ over $\mathbb{C}$ and B is a skew-symmetric integer $n \times n$ matrix. The collection $\mathbf{x}$ is called the *cluster* and the matrix B is called the *exchange matrix*.

The following employs the notation $[a]_+ = \max(a, 0)$.

Definition 3.2 Given a seed $(\mathbf{x}, B)$ and an integer $k = 1, 2, \ldots, n$ the *seed mutation* μ_k in direction k produces a new seed $\mu_k(\mathbf{x}, B) = (\mathbf{x}', B')$ where $\mathbf{x}' = (x_1, \ldots, x_{k-1}, x_k', x_{k+1}, \ldots, x_n)$ with

$$x'_k = \frac{\prod_{b_{ik}>0} x_i^{b_{ik}} + \prod_{b_{ik}<0} x_i^{-b_{ik}}}{x_k} \tag{3}$$

and B' is defined by

$$b'_{ij} = \begin{cases} -b_{ij} & \text{if } i = k \text{ or } j = k; \\ b_{ij} + [b_{ik}]_+[b_{kj}]_+ - [-b_{ik}]_+[-b_{kj}]_+ & \text{otherwise.} \end{cases} \tag{4}$$

In words, the mutation μ_k has the following effects:

1. x_k changes to x'_k satisfying $x_k x'_k =$ (binomial in the other x_i);
2. the entries b_{ij} of B away from row and column k increase (resp. decrease) by $b_{ik}b_{kj}$ if b_{ik} and b_{kj} are both positive (resp. both negative);
3. the entries of the kth row and the kth column of B are negated.

Lemma 3.3 *Let* $(\mathbf{x}, B)$ *be a seed in* $\mathcal{F}$. *For* $k = 1, \ldots, n$, *the following hold*:

1. $\mu_k(\mathbf{x}, B)$ *is also a seed in* $\mathcal{F}$;
2. *the seed mutation* μ_k *is involutive*, *i.e.*, $\mu_k\big(\mu_k(\mathbf{x}, B)\big) = (\mathbf{x}, B)$.

Definition 3.4 Fix an ambient field $\mathcal{F}$ and an initial seed $(\mathbf{x}, B)$. The entries of the clusters of all seeds reachable from this one by a sequence of mutations are called the *cluster variables*. The *cluster algebra* associated with the initial seed is the subalgebra $\mathcal{A} := \mathcal{A}(\mathbf{x}, B)$ of $\mathcal{F}$ generated by the set of all cluster variables.

Example 3.5 Let $\mathbf{x} = (x_1, x_2)$ be the initial cluster with initial exchange matrix

$$B = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}.$$

Then $\mu_1(\mathbf{x}, B) = \big((x'_1, x_2), -B\big)$ where

$$x'_1 = \frac{x_2 + 1}{x_1}.$$

It is convenient to denote the new cluster variable $x'_1 = x_3$. Next $\mu_2((x_3, x_2), -B) = ((x_3, x_4), B)$ where

$$x_4 = \frac{x_3 + 1}{x_2} = \frac{(x_2 + 1)/x_1 + 1}{x_2} = \frac{x_1 + x_2 + 1}{x_1 x_2}$$

and $\mu_2((x_3, x_4), B) = ((x_5, x_4), -B)$ where

$$x_5 = \frac{x_4 + 1}{x_3} = \frac{(x_1 + x_2 + 1)/(x_1 x_2) + 1}{(x_2 + 1)/x_1} = \frac{x_1 + 1}{x_2}.$$

The mutation pattern seems clear, but remarkably the next variable $x_6 = (1 + x_5)/x_4$ equals the first variable x_1. In fact, the only distinct cluster variables that can be obtained are x_1 through x_5, so

$$\mathcal{A}(\mathbf{x}, B) = \mathbb{C}\left[x_1, x_2, \frac{x_2+1}{x_1}, \frac{x_1+x_2+1}{x_1x_2}, \frac{x_1+1}{x_2}\right] \subseteq \mathbb{C}[x_1^{\pm 1}, x_2^{\pm 1}].$$

Note the generating set is not minimal, in fact, any four of the given elements generate $\mathcal{A}(\mathbf{x}, B)$.

In the preceding example, there were only finitely many cluster variables. As we will see, this is typically not the case. However, a more subtle feature does hold in general, namely that each of the cluster variables is a Laurent polynomial in the variables of the initial seed.

Theorem 3.6 *For any initial seed* $(\mathbf{x}, B)$ *with* $\mathbf{x} = (x_1, \ldots, x_n)$, *the associated cluster algebra lies in the Laurent polynomial ring*

$$\mathcal{A}(\mathbf{x}, B) \subseteq \mathbb{C}[x_1, x_1^{-1}, \ldots, x_n, x_n^{-1}].$$

In particular, *every cluster variable can be expressed as a Laurent polynomial in* $x_1, \ldots, x_n$.

Section 4 will go into more detail on this result, called the Laurent phenomenon, as well as several more main theorems on cluster algebras.

3.2 Increased Generality

We generalize the previous definitions in two ways, first by allowing more general exchange matrices and then by allowing for certain coefficients in the exchange relations.

Definition 3.7 An $n \times n$ integer matrix B is *skew-symmetrizable* if there is a diagonal matrix D with positive integer diagonal entries such that DB is skew-symmetric.

As an example, a 2×2 matrix B is skew-symmetrizable if and only if

$$B = \begin{bmatrix} 0 & b \\ -c & 0 \end{bmatrix} \quad \text{or} \quad B = \begin{bmatrix} 0 & -b \\ c & 0 \end{bmatrix}$$

$=$ for positive integers b and c. In either case, a possible symmetrizing matrix is

$$D = \begin{bmatrix} c & 0 \\ 0 & b \end{bmatrix}.$$

The *rank* of a cluster algebra is the number n of elements in each cluster, so the exchange matrices B just described give rise to all possible rank 2 cluster algebras.

The second generalization is to allow so-called *frozen variables* that never mutate, but which play a part in the exchange relations for the cluster variables. An *extended cluster*, by convention, is typically written $\mathbf{x} = (x_1, \ldots, x_n, x_{n+1}, \ldots x_m)$ where $x_1, \ldots, x_n$ are the cluster variable and $x_{n+1}, \ldots, x_m$ are the frozen variables. An *extended exchange matrix* is an $m \times n$ integer matrix $\widetilde{B}$ with the property that its upper $n \times n$ submatrix is skew-symmetrizable.

Definition 3.8 Fix a seed $(\mathbf{x}, \widetilde{B})$ with $\mathbf{x} = (x_1, \ldots, x_m)$ an extended cluster and $\widetilde{B}$ an extended exchange matrix. For an integer $k = 1, 2, \ldots, n$, the *seed mutation* μ_k in direction k produces a new seed $\mu_k(\mathbf{x}, \widetilde{B}) = (\mathbf{x}', \widetilde{B}')$ with $\mathbf{x}' = (x_1, \ldots, x_{k-1}, x_k', x_{k+1}, \ldots, x_m)$. The formulas for x_k' and the entries $\widetilde{B}'_{ij}$ of B' are the same as in (3) and (4), where the products in (3) now range from 1 to m instead of from 1 to n.

Lemma 3.9 *Lemma 3.3 holds in this generalized setting. Moreover, the skew-symmetrizing matrix D is unchanged by mutation.*

Given a seed $(\mathbf{x}, \widetilde{B})$ as above, the corresponding cluster algebra $\mathcal{A}(\mathbf{x}, \widetilde{B})$ is defined to be the subalgebra of $\mathbb{C}(x_1, \ldots, x_m)$ generated by all cluster variables reachable from this seed together with the frozen variables (which appear in every seed). Cluster algebras at this level of generality are referred to as cluster algebras of *geometric type*. In comparison, the earlier definition given was of *skew-symmetric* cluster algebras with *trivial coefficients*.

Example 3.10 Consider a rank 2 cluster algebras with trivial coefficients (so $n = m = 2$). The initial exchange matrix can be taken to be

$$B = \begin{bmatrix} 0 & b \\ -c & 0 \end{bmatrix}.$$

with b, c positive integers. Then $\mu_1(B) = \mu_2(B) = -B$ and $\mu_1(-B) = \mu_2(-B) = B$, so as in Example 3.5 (the case where $b = c = 1$) the cluster variables can be identified as $\{x_i : i \in \mathbb{Z}\}$ (possibly with redundant labels) and the mutations given by

$$\cdots \overset{\mu_1}{\longleftrightarrow} \big((x_1, x_0), -B\big) \overset{\mu_2}{\longleftrightarrow} \big((x_1, x_2), B\big)$$
$$\overset{\mu_1}{\longleftrightarrow} \big((x_3, x_2), -B\big) \overset{\mu_2}{\longleftrightarrow} \big((x_3, x_4), B\big) \overset{\mu_1}{\longleftrightarrow} \cdots$$

The exchange relations are

$$x_{k-1}x_{k+1} = \begin{cases} x_k^b + 1 & \text{if } k \text{ is odd;} \\ x_k^c + 1 & \text{if } k \text{ is even.} \end{cases}$$

Exercise 3.11 1. Compute all cluster variables and coefficient variables for cluster algebras associated to $B = \left[\begin{smallmatrix} 0 & b \\ -c & 0 \end{smallmatrix}\right]$ with $b, c \in \mathbb{Z}_{>0}$ and $bc \leq 3$.
2. Justify why attempting such a calculation is futile for $bc \geq 4$. Hint: consider the degrees appearing in the denominators of the cluster variables.

Exercise 3.12 Prove the Laurent phenomenon for rank 2 cluster algebras. Hint: start by showing that $x_4 \in \mathbb{Z}[x_0, x_1, x_2, x_3]$ by considering the monomial $x_0 x_3^b$.

Example 3.13 Let $n = 3$ and $m = 9$. Denote the cluster

$$\mathbf{x} = (\Delta_{13}, \Delta_{14}, \Delta_{15}, \Delta_{12}, \Delta_{23}, \Delta_{34}, \Delta_{45}, \Delta_{56}, \Delta_{16})$$

where the last $m - n = 6$ variables are frozen. Let

$$\widetilde{B} = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \\ -1 & 0 & 0 \\ 1 & -1 & 0 \\ 0 & 1 & -1 \\ 0 & 0 & 1 \\ 0 & 0 & -1 \end{bmatrix}.$$

Let $\mathcal{A} = \mathcal{A}(\mathbf{x}, \widetilde{B})$. Interpreting the initial variables as the indicated Plücker coordinates on $Gr_{2,6}$ we obtain a cluster algebra in the ring of rational functions on $Gr_{2,6}$.

Exercise 3.14 Prove the following statements about the cluster algebra $\mathcal{A}$ just defined:

- The cluster variables of $\mathcal{A}$ are precisely the Plücker coordinates Δ_{ij} with $1 \leq i < j \leq n$.
- The clusters of $\mathcal{A}$ are precisely the collections Δ_T (see Sect. 2.2) for T a triangulation of a hexagon.

For instance, the new cluster variable produced by applying the mutation μ_1 to the initial seed is

$$\frac{\Delta_{12}\Delta_{34} + \Delta_{14}\Delta_{23}}{\Delta_{13}}$$

which equals Δ_{24}.

There is an alternate formulation of cluster algebras of geometric type which focuses on the roles played by the frozen variables $x_{n+1}, \ldots, x_m$ in the exchange relations, rather than on the variables themselves. Let $(\mathbf{x}, \widetilde{B})$ be an extended seed. For $k = 1, \ldots, n$ let

$$y_k = \prod_{i=n+1}^{m} x_i^{b_{ik}}.$$

Define an operation $\oplus$ (called *auxiliary addition*) on Laurent monomials by

$$\prod_{i=n+1}^{m} x_i^{e_i} \oplus \prod_{i=n+1}^{m} x_i^{f_i} = \prod_{i=n+1}^{m} x_i^{\min(e_i, f_i)}.$$

Using this operation, we can extract positive and negative exponents as follows

$$\frac{y_k}{1 \oplus y_k} = \prod_{\substack{i=n+1,\ldots,m \\ b_{ik}>0}} x_i^{b_{ik}} \qquad \frac{1}{1 \oplus y_k} = \prod_{\substack{i=n+1,\ldots,m \\ b_{ik}<0}} x_i^{-b_{ik}}.$$

The change in going from the original exchange relation (3) to the one in geometric type can then be summarized by saying that the two terms of the binomial are enriched with coefficients $y_k/(1 \oplus y_k)$ and $1/(1 \oplus y_k)$. We now write

$$x_k' = \frac{y_k \prod_{b_{ik}>0} x_i^{b_{ik}} + \prod_{b_{ik}<0} x_i^{-b_{ik}}}{(1 \oplus y_k) x_k}$$

where the products range over i from 1 to n.

3.3 Y-Patterns

There is an alternate version of seeds and mutations, closely related to the previous one, which itself arises in many applications. The resulting structures are called *Y-patterns*.

Definition 3.15 A *Y-seed* is a pair $(\mathbf{y}, B)$ consisting of an n-tuple $\mathbf{y} = (y_1, \ldots, y_n)$ and an $n \times n$ skew-symmetric matrix B. For $k = 1, \ldots, n$, the *Y-seed mutation* μ_k is defined by

$$\mu_k\big((y_1, \ldots, y_n), B\big) = \big((y_1', \ldots, y_n'), B'\big)$$

for B' as defined in (4) and

$$y_j' = \begin{cases} y_k^{-1} & \text{if } j = k; \\ y_j y_k^{[-b_{jk}]_+} (1 + y_k)^{b_{jk}} & \text{if } j \neq k. \end{cases} \tag{5}$$

In words, the Y-seed mutation μ_k has the following effects:

1. For each $j \neq k$, y_j is multiplied by $(1 + y_k)^{b_{jk}}$ if $b_{jk} > 0$ and by $(1 + y_k^{-1})^{b_{jk}}$ if $b_{jk} < 0$,
2. y_k is inverted,
3. B is changed in the same way as for ordinary seed mutations.

The Y-dynamics also go by the name *coefficient dynamics* because the coefficients in a geometric type cluster algebra evolve in this manner with respect to auxiliary addition $\oplus$ and ordinary multiplication of Laurent monomials.

Another connection between cluster algebra and Y-pattern dynamics comes by way of a certain Laurent monomial change of variables. Let $\widetilde{B}$ be an $m \times n$ extended exchange matrix with B its upper $n \times n$ submatrix. Given a seed $\big((x_1, \ldots, x_m), \widetilde{B}\big)$, define an associated Y-seed $\big((\hat{y}_1, \ldots, \hat{y}_n), B\big)$ by

$$\hat{y}_j = \prod_{i=1}^{m} x_i^{b_{ij}} .$$

Proposition 3.16 *Fix $k = 1, \ldots, n$ and suppose $\mu_k(\mathbf{x}, \widetilde{B}) = (\mathbf{x}', \widetilde{B}')$. Define $(\hat{y}_1, \ldots, \hat{y}_n)$ from $(\mathbf{x}, \widetilde{B})$ and $(\hat{y}'_1, \ldots, \hat{y}'_n)$ from $(\mathbf{x}', \widetilde{B}')$ as above. Then*

$$\mu_k\big((\hat{y}_1, \ldots, \hat{y}_n), B\big) = \big((\hat{y}'_1, \ldots, \hat{y}'_n), B'\big) .$$

Exercise 3.17 Prove Proposition 3.16.

4 Foundational Results

As mentioned in the introduction cluster algebras have found applications in a surprising array of mathematical disciplines. Much of their ubiquity comes from a number of remarkable theorems which we now explain.

The first of these results is the aforementioned Laurent phenomenon (Theorem 3.6). The Laurent property originates from the study of several classical recurrences that seem as though they should produce rational numbers, but turn out to give only integers under certain initial conditions [15]. As with several of the results in this section, we give a complete proof in the case of rank 2 cluster algebras.

Recalling Example 3.10, consider the rank 2 cluster algebra with initial exchange matrix $B = \left[\begin{smallmatrix} 0 & b \\ -c & 0 \end{smallmatrix}\right]$ and cluster variables x_k, $k \in \mathbb{Z}$ which satisfy the recursion

$$x_{k-1}x_{k+1} = \begin{cases} x_k^b + 1 & \text{if } k \text{ is odd;} \\ x_k^c + 1 & \text{if } k \text{ is even.} \end{cases}$$

Theorem 4.1 *For any $m \in \mathbb{Z}$, each x_k is an element of $\mathbb{Z}[x_{m-1}, x_m, x_{m+1}, x_{m+2}]$.*

Remark 4.2 The ring $\mathbb{Z}[x_{m-1}, x_m, x_{m+1}, x_{m+2}]$ is called the *lower bound* of $\mathcal{A}(\mathbf{x}, B)$ at the cluster $\{x_m, x_{m+1}\}$. We will give more details below and see that this result is a special case of Theorem 4.22.

Proof Assume without loss of generality that m is odd (otherwise interchange b and c in the calculation below). Then we may compute

$$\begin{aligned} x_{m-1}x_{m+2}^b &= \frac{x_m^b + 1}{x_{m+1}} x_{m+2}^b \\ &= \frac{x_m^b x_{m+2}^b - 1}{x_{m+1}} + \frac{x_{m+2}^b + 1}{x_{m+1}} \\ &= \frac{(x_{m+1}^c + 1)^b - 1}{x_{m+1}} + x_{m+3} \, . \end{aligned}$$

In particular, we see that $x_{m+3} \in \mathbb{Z}[x_{m-1}, x_m, x_{m+1}, x_{m+2}]$. A similar calculation shows $x_{m-2} \in \mathbb{Z}[x_{m-1}, x_m, x_{m+1}, x_{m+2}]$ and a simple induction argument of "shifting the viewing window" establishes the result. □

Having shown x_k to be a polynomial in $x_{m-1}, x_m, x_{m+1}, x_{m+2}$, each of which is directly seen to be a Laurent polynomial in x_m, x_{m+1}, the rank 2 Laurent phenomenon follows. As such, the above is a solution to Exercise 3.12. With more work one may establish the following result which can be leveraged to prove the Laurent phenomenon in general.

Theorem 4.3 *Assume $b, c \neq 0$. For any $m \in \mathbb{Z}$, the cluster algebra $\mathcal{A}(\mathbf{x}, B)$ is equal to $\bigcap_{k\in\mathbb{Z}} \mathbb{Z}[x_k^{\pm 1}, x_{k+1}^{\pm 1}] = \bigcap_{k=m-1}^{m+1} \mathbb{Z}[x_k^{\pm 1}, x_{k+1}^{\pm 1}]$.*

The proof of this result is somewhat technical and seems unlikely to be very informative so we will omit the details.

Remark 4.4 If one allows extended exchange matrices and imposes an additional coprimality assumption (see Def. 4.17), then the condition $b, c \neq 0$ may be dropped. The ring $\bigcap_{k=m-1}^{m+1} \mathbb{Z}[x_k^{\pm 1}, x_{k+1}^{\pm 1}]$ is called the *upper bound* of $\mathcal{A}(\mathbf{x}, B)$ at the cluster $\{x_m.x_{m+1}\}$ and the ring $\bigcap_{k\in\mathbb{Z}} \mathbb{Z}[x_k^{\pm 1}, x_{k+1}^{\pm 1}]$ is called the *upper cluster algebra*. We will give more details below at which point this result will be a special case of Theorems 4.22 and 4.20.

The next result is the classification of cluster algebras of *finite type*, i.e. those that have only finitely many cluster variables. As we have seen in Sects. 2.2 and 2.3, cluster algebras have roots in classical Lie theory. A large number of objects in this realm are classified by Dynkin diagrams and finite type cluster algebras are no exception. Given an extended exchange matrix $\widetilde{B}$ with principal square submatrix $B = (b_{ij})_{i,j=1}^n$, write $A := A_{\widetilde{B}} = (a_{ij})_{i,j=1}^n$ for the *Cartan companion* of $\widetilde{B}$ given by

$$a_{ij} = \begin{cases} 2 & \text{if } i = j; \\ -|b_{ij}| & \text{otherwise.} \end{cases}$$

Note that the Cartan companion only depends on the principal part of $\widetilde{B}$.

Theorem 4.5 ([16]) *A cluster algebra $\mathcal{A}(\mathbf{x}, \widetilde{B})$ is of finite type if and only if there exists an extended exchange matrix mutation equivalent to $\widetilde{B}$ whose Cartan companion is a finite-type Cartan matrix.*

Example 4.6 The irreducible finite type 2×2 Cartan matrices are (up to transposition) given by

$$A_2 : \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix}, \quad B_2 : \begin{bmatrix} 2 & -2 \\ -1 & 2 \end{bmatrix}, \quad G_2 : \begin{bmatrix} 2 & -3 \\ -1 & 2 \end{bmatrix},$$

or put another way, they are the matrices $\left[\begin{smallmatrix} 2 & -b \\ -c & 2 \end{smallmatrix}\right]$ with $bc \leq 3$. This is precisely the Cartan counterpart A_B of the exchange matrix $B = \left[\begin{smallmatrix} 0 & b \\ -c & 0 \end{smallmatrix}\right]$. Therefore, the rank 2 cluster algebra with this exchange matrix, or any cluster algebra obtained from it by adding coefficients, has finite type if and only if $bc \leq 3$. This was the content of Exercise 3.11.

We now provide an outline to the solution of Exercise 3.11. Let $B = \left[\begin{smallmatrix} 0 & b \\ -c & 0 \end{smallmatrix}\right]$ and let $x_k, k \in \mathbb{Z}$ be the cluster variables of this cluster algebra. We need some more notation. For $k \neq 1, 2$, let $d^{(k)} = (d_1^{(k)}, d_2^{(k)})$ denote the exponents of the monomial $x_1^{d_1^{(k)}} x_2^{d_2^{(k)}}$ appearing in the denominator of x_k when expressed as a Laurent polynomial in x_1, x_2. Let $U_\ell(t)$ denote the (normalized) Chebyshev polynomial (of the second kind) defined recursively by

$$U_{\ell+1}(t) = tU_\ell(t) - U_{\ell-1}(t), \quad U_1(t) = 1, \quad U_0(t) = 0,$$

and for $j \in \{1, 2\}$ define

$$u_{\ell,j} = \begin{cases} U_\ell(\sqrt{bc}) & \text{if } \ell \text{ is odd;} \\ \sqrt{b/c}\, U_\ell(\sqrt{bc}) & \text{if } \ell \text{ is even and } j = 1; \\ \sqrt{c/b}\, U_\ell(\sqrt{bc}) & \text{if } \ell \text{ is even and } j = 2. \end{cases}$$

Note that $U_\ell(t)$ is an odd (resp. even) function when ℓ is even (resp. odd), so each $u_{\ell,j}$ is a polynomial in b and c. Moreover, one may easily show that each $u_{\ell,j}$, $\ell \geq 1$ is a positive integer when $bc \geq 4$.

The rank 2 finite type classification now boils down to verifying the following:

- The denominator vector of x_k for $k \in \mathbb{Z} \setminus \{1, 2\}$ is

$$d^{(k)} = \begin{cases} (u_{k-2,1}, u_{k-3,2}) & \text{if } k \geq 3; \\ (u_{-k,1}, u_{-k+1,2}) & \text{if } k \leq 0. \end{cases} \tag{6}$$

- $U_n\big(2\cos(\theta)\big) = \sin(n\theta)/\sin(\theta)$ from which it follows that there are infinitely many $d^{(k)}$ if and only if $bc \geq 4$. In particular, there are infinitely many cluster variables if $bc \geq 4$.
- By explicit calculation, there are only finitely many cluster variables in each case where $bc \leq 3$.

More generally, if $\widetilde{B}$ is any $m \times n$ extended exchange matrix and $|b_{ij}b_{ji}| \geq 4$ for some $i, j = 1, \ldots, n$, then iteratively mutating at i and j alone will produce infinitely many cluster variables. Call an extended exchange matrix $\widetilde{B} = (b_{ij})$ 2-*finite* if every matrix $\widetilde{B}' = (b'_{ij})$ mutation equivalent to $\widetilde{B}$ satisfies the condition $|b'_{ij}b'_{ji}| \leq 3$ for all i, j. By the above reasoning, 2-finiteness is a necessary condition for a cluster algebra to be of finite type. It is quite remarkable that it is sufficient as well.

Theorem 4.7 ([16]) *A cluster algebra $\mathcal{A}(\mathbf{x}, \widetilde{B})$ is of finite type if and only if $\widetilde{B}$ is 2-finite.*

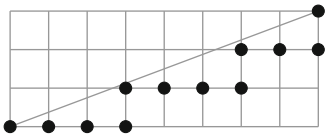
The next result gives the positivity of the initial cluster Laurent expansions of all cluster variables. This result was conjectured with the introduction of cluster algebras [14] and remained open for more than ten years.

Theorem 4.8 ([28, 37]) *Let $\mathcal{A}(\mathbf{x}, \widetilde{B})$ be a cluster algebra. Any cluster variable of $\mathcal{A}(\mathbf{x}, \widetilde{B})$ is an element of $\mathbb{Z}_{\geq 0}[x_1^{\pm 1}, \ldots, x_m^{\pm 1}]$.*

The proof in skew-symmetric types builds on a concrete combinatorial construction of cluster variables in rank 2 [35, 36]. For the more general skew-symmetrizable cluster algebras the proof was given in [28] using the theory of scattering diagrams built on connections to mirror symmetry. We describe the combinatorial approach to the skew-symmetric case here, but first we need more notation.

For $k \in \mathbb{Z} \setminus \{1, 2\}$, denote by R_k the rectangle in $\mathbb{Z}^2$ with corner vertices $(0, 0)$ and $d^{(k)}$ from (6). Write D_k for the maximal Dyck path in R_k beginning at $(0, 0)$, taking East and North steps to end at the upper right corner of R_k while never passing above the main diagonal, and such that the area below D_k inside R_k is maximized.

Example 4.9 For $b = c = 3$, the maximal Dyck path D_5 is

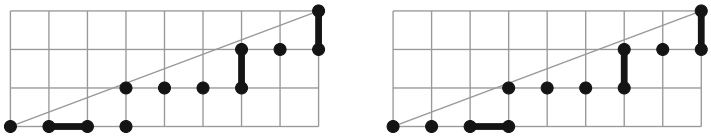


For edges $e, e' \in D_k$, write $e < e'$ if e precedes e' along D_k, in other words if e is closer to $(0,0)$. In this case write ee' for the subpath of D_k beginning with the edge e and ending with the edge e'. Write $(ee')_H$ and $(ee')_V$ for the sets of horizontal and vertical edges in the path ee' respectively. Let $H, V \subset D_k$ denote the sets of horizontal and vertical edges of D_k.

Call subsets $S_H \subset H$ and $S_V \subset V$ compatible if for each $h \in S_H$ and $v \in S_V$ with $h < v$, there exists $e \in hv$ so that one of the following holds:

- $e \neq v$ and $|(he)_V| = c|(he)_H \cap S_H|$;
- $e \neq h$ and $|(ev)_H| = b|(ev)_V \cap S_V|$.

Example 4.10 For $b = c = 3$, the picture below on the left shows a compatible collection of edges of D_5 while the collection on the right is not compatible.



Exercise 4.11 Find all other compatible collections for D_5 in the case $b = c = 3$.

Theorem 4.12 ([35]) *For $k \in \mathbb{Z} \setminus \{1,2\}$, the cluster variable x_k is given by*

$$x_k = \sum_{(S_H, S_V)} x_1^{-d_1^{(k)} + b|S_V|} x_2^{-d_2^{(k)} + c|S_H|},$$

where the sum ranges over all compatible collections of edges in the maximal Dyck path D_k. In particular, each cluster variable is contained in $\mathbb{Z}_{\geq 0}[x_1^{\pm 1}, x_2^{\pm 1}]$.

Remark 4.13 The idea of obtaining positivity for arbitrary cluster algebras goes as follows (see [37]): any sequence of mutations can be viewed as a collection of rank 2 mutation sequences, so iteratively applying Theorem 4.12 will (after a considerable amount of work) lead to a proof of positivity in general.

One motivation for the discovery of the cluster algebra formalism was the desire to find a combinatorial construction of dual canonical basis elements for (quantum) algebraic groups. The dual canonical basis of a semisimple algebraic group induces bases on the coordinate rings of any of its subvarieties. As we saw in Example 2.3 there appears to be some kind of cluster algebra structure on the double Bruhat cells of a semisimple algebraic group, which one can hope will shed some light on the dual canonical basis. In most cases the double Bruhat cell does not actually admit a cluster algebra structure but does admit a closely related structure.

Definition 4.14 Let $(\mathbf{x}, \widetilde{B})$ denote an extended seed. Define the *upper cluster algebra* $\overline{\mathcal{A}}(\mathbf{x}, \widetilde{B})$ as the intersection of all Laurent rings associated to extended seeds mutation equivalent to $(\mathbf{x}, \widetilde{B})$.

Remark 4.15 The upper cluster algebra is exactly the collection of all rational functions in $\{x_1, \ldots, x_m\}$ which are expressed as Laurent polynomials in terms of any cluster. Thus the Laurent phenomenon Theorem 3.6 establishes the inclusion $\mathcal{A}(\mathbf{x}, \widetilde{B}) \subset \bar{\mathcal{A}}(\mathbf{x}, \widetilde{B})$, hence the name "upper" cluster algebra.

Theorem 4.16 ([2]) *The coordinate ring of any double Bruhat cell $GL_n^{u,v}$ is an upper cluster algebra such that each collection of chamber minors determines a cluster.*

In some special cases, the cluster algebra coincides with its upper cluster algebra. First we describe a necessary intermediate concept.

Definition 4.17 Let $(\mathbf{x}, \widetilde{B})$ be an extended seed and denote by $P_k := x_k x_k'$ the binomial on the right hand side of the exchange relation (3). We say that $(\mathbf{x}, \widetilde{B})$ is *coprime* if the binomials P_k are pairwise relatively prime.

The *upper bound* $\mathcal{U}(\mathbf{x}', \widetilde{B})$ for $\mathcal{A}(\mathbf{x}, \widetilde{B})$ at a seed $(\mathbf{x}', \widetilde{B}')$ mutation equivalent to $(\mathbf{x}, \widetilde{B})$ is the intersection of the Laurent ring generated by variables in $\mathbf{x}'$ with all Laurent rings associated to seeds which can be obtained from $(\mathbf{x}', \widetilde{B}')$ by a single mutation.

Theorem 4.18 ([2]) *If $(\mathbf{x}, \widetilde{B})$ and $(\mathbf{x}', \widetilde{B}')$ are mutation equivalent coprime seeds, then their upper bounds $\mathcal{U}(\mathbf{x}, \widetilde{B})$ and $\mathcal{U}(\mathbf{x}', \widetilde{B})$ coincide. In particular, if every seed mutation equivalent to an extended seed $(\mathbf{x}, \widetilde{B})$ is coprime, then $\bar{\mathcal{A}}(\mathbf{x}, \widetilde{B}) = \mathcal{U}(\mathbf{x}', \widetilde{B}')$ for any seed mutation equivalent to $(\mathbf{x}, \widetilde{B})$.*

Definition 4.19 An exchange matrix $B = (b_{ij})$ is called *acyclic* if there exists a permutation σ so that $b_{\sigma i \sigma j} \leq 0$ for $i < j$.

This terminology can be easily understood in the case of a skew-symmetric exchange matrix; the matrix is acyclic exactly when its associated quiver (see Sect. 6) has no oriented cycles.

Theorem 4.20 ([2]) *Let $\mathcal{A}(\mathbf{x}, \widetilde{B})$ be a cluster algebra where $\widetilde{B}$ is coprime and has acyclic principal part. Then the cluster algebra $\mathcal{A}(\mathbf{x}, \widetilde{B})$ coincides with its upper bound $\mathcal{U}(\mathbf{x}, \widetilde{B})$.*

Acyclicity also guarantees the existence of easily identifiable bases of a cluster algebra. These are best understood by identifying the cluster algebra with another related algebra, its lower bound.

Definition 4.21 Let $(\mathbf{x}, \widetilde{B})$ be an extended seed and write x_k' for the variable obtained by mutation in direction k. The *lower bound* of $\mathcal{A}(\mathbf{x}, \widetilde{B})$ at $(\mathbf{x}, \widetilde{B})$ is the subalgebra $\mathcal{L}(\mathbf{x}, \widetilde{B}) = \mathbb{C}[x_1, x_1', \ldots, x_n, x_n', x_{n+1}, \ldots, x_m]$.

Theorem 4.22 ([2]) *Let $\mathcal{A}(\mathbf{x}, \widetilde{B})$ be a cluster algebra where $\widetilde{B}$ is coprime and has acyclic principal part. Then the cluster algebra $\mathcal{A}(\mathbf{x}, \widetilde{B})$ coincides with its lower bound $\mathcal{L}(\mathbf{x}, \widetilde{B})$. Moreover, the collection of all* standard monomials *in the variables $x_1, x_1', \ldots, x_n, x_n', x_{n+1}, \ldots, x_m$, i.e., those which do not contain both x_k and x_k' for any k, forms a basis of the cluster algebra $\mathcal{A}(\mathbf{x}, \widetilde{B})$.*

Example 4.23 Acyclic cluster algebras are particularly nice but should not be taken as the general case: there exist cluster algebras where anything that can go wrong seems to go wrong. The primary example of this is the *Markov cluster algebra* with exchange matrix

$$B = \begin{bmatrix} 0 & 2 & -2 \\ -2 & 0 & 2 \\ 2 & -2 & 0 \end{bmatrix}.$$

Comparing with Example 2.1 we see that the Markov cluster algebra has infinitely many cluster variables. In this case, the following undesirable properties all hold:

- the standard monomials are linearly dependent;
- the Markov cluster algebra is not finitely generated and not Noetherian;
- the Markov cluster algebra (over $\mathbb{C}$) contains non-prime cluster variables;
- the Markov cluster algebra does not equal its upper cluster algebra.

5 Compatible Poisson Structures and Quantization

Many natural examples of cluster algebras carry the following additional structure.

Definition 5.1 A *Poisson algebra* $(A, \{\cdot,\cdot\})$ is an associative algebra A equipped with an additional skew-symmetric bilinear operation, called the Poisson bracket (written as $\{x, y\}$ for $x, y \in A$), for which the following holds:

- given any $x \in A$, the endomorphism $\{x, \cdot\}: A \to A$, $y \mapsto \{x, y\}$ is a derivation with respect to both binary operations on A, i.e., for $x, y, z \in A$ we have

(Leibnitz rule) $$\{x, yz\} = \{x, y\}z + y\{x, z\}$$

(Jacobi identity) $$\{x, \{y, z\}\} = \{\{x, y\}, z\} + \{y, \{x, z\}\}.$$

In the case of cluster algebras, the Poisson brackets take an especially simple form when applied to cluster variables.

Definition 5.2 Let $\mathcal{A}$ be a cluster algebra. A Poisson bracket $\{\cdot,\cdot\}$ on $\mathcal{A}$ is compatible with the cluster algebra structure if every cluster $\mathbf{x}$ of $\mathcal{A}$ is *log-canonical* with respect to $\{\cdot,\cdot\}$, that is there exists a skew-symmetric matrix $\Omega_{\mathbf{x}} = (\Omega_{ij})$ so that $\{x_i, x_j\} = \Omega_{ij} x_i x_j$ for all i, j.

The existence of a compatible Poisson structure is quite restrictive and requires a particular relationship between the matrix $\Omega_{\mathbf{x}}$ and the exchange matrix of a seed with cluster $\mathbf{x}$.

Lemma 5.3 *Let $\mathcal{A}(\mathbf{x}, \widetilde{B})$ be a cluster algebra, where $\widetilde{B}$ is $(m+n) \times n$, with compatible Poisson structure $\{\cdot,\cdot\}$. Then writing $\Omega_{\mathbf{x}}$ for the $(m+n)\times(m+n)$ matrix of Poisson bracket coefficients, we have $\widetilde{B}^T \Omega_{\mathbf{x}} = [D\,\mathbf{0}]$, where D is a diagonal matrix which skew-symmetrizes B.*

Exercise 5.4 Prove Lemma 5.3 using the condition that each neighboring cluster to $\mathbf{x}$ should also be log-canonical.

In fact, these conditions can only hold in the following situation, in which case all possible compatible Poisson structures can be easily understood.

Theorem 5.5 ([24]) *If an extended exchange matrix $\tilde{B}$ has full rank then a compatible Poisson structure exists for the associated cluster algebra. Moreover, the collection of all such Poisson structures is parametrized by an affine space of dimension $\rho(B) + \binom{m}{2}$, where $\rho(B)$ denotes the number of connected components of the quiver associated to the principal submatrix B of $\tilde{B}$.*

The primary motivating example for compatible Poisson structures comes in the form of the double Bruhat cells of Sect. 2.3. To introduce the relevant Poisson structure and place the double Bruhat cells in the proper context we need to introduce more notation.

A smooth manifold M together with a Poisson structure on its algebra $\mathcal{O}(M)$ of regular functions is called a *Poisson manifold*. The best understood examples of such structures comes from the theory of symplectic geometry.

Example 5.6 A symplectic manifold (M, ω) is a smooth even-dimensional manifold M^{2n} together with a 2-form $\omega \in H^2(M)$ that is non-degenerate, i.e., $\omega^n \neq 0$ is a volume form. The symplectic structure ω provides a natural association of a vector field ξ_f to a function $f \in \mathcal{O}(M)$ via the contraction formula $\iota_{\xi_f}\omega = -df$. The algebra of smooth functions on the symplectic manifold M is then naturally a Poisson algebra via $\{f, g\} = \omega(\xi_f, \xi_g)$ for $f, g \in \mathcal{O}(M)$.

A smooth map $\varphi\colon M \to N$ between Poisson manifolds is a *Poisson morphism* if it induces a Poisson morphism $\varphi^*\colon \mathcal{O}(N) \to \mathcal{O}(M)$ on their algebras of smooth functions, i.e., if $\{f\circ\varphi, g\circ\varphi\}_M = \{f, g\}_N \circ \varphi$ for all $f, g \in \mathcal{O}(N)$. Given two Poisson manifolds M and N, there is a natural Poisson structure on $M \times N$ given by

$$\{f, g\}(x, y) = \{f(\cdot, y), g(\cdot, y)\}_M(x) + \{f(x, \cdot), g(x, \cdot)\}_N(y)$$

for $f, g \in \mathcal{O}(M \times N)$.

Example 5.7 The general linear group GL_n is a Poisson manifold where the Poisson bracket on matrix entries is given by

$$\{x_{ij}, x_{k\ell}\} = \tfrac{1}{2}\big(\operatorname{sign}(k-i) + \operatorname{sign}(\ell - j)\big)x_{i\ell}x_{kj}\ . \tag{7}$$

In fact, GL_n has the structure of a Poisson-Lie group, that is the multiplication map $GL_n \times GL_n \to GL_n$ is a Poisson morphism when $GL_n \times GL_n$ is given the product Poisson structure.

With this we may describe the Poisson structure on the double Bruhat cells.

Theorem 5.8 ([25]) *The cluster algebra structure on $GL_n^{u,v}$ from Theorem 4.16 is compatible with the restriction of the Poisson structure from GL_n.*

The double Bruhat cells actually have a much closer connection to the Poisson geometry of GL_n. To describe it we need to introduce a few additional concepts.

The existence of a Poisson structure on a manifold allows one to construct vector fields associated to functions in a similar manner to the symplectic case.

Lemma 5.9 *Let $(M, \{\cdot,\cdot\})$ be a Poisson manifold. For any $h \in \mathcal{O}(M)$, there exists a vector field ξ_h on M such that for any $f \in \mathcal{O}(M)$ we have $\xi_h(f) = \{f, h\}$.*

The vector field ξ_h from Lemma 5.9 is simply the vector field canonically associated to the derivation $\{\cdot, h\}$ and is called a *Hamiltonian vector field*. Flowing along Hamiltonian vector fields defines an equivalence relation on a Poisson manifold as follows:

> $p \sim q$ if there exists a piecewise smooth curve connecting p and q where each smooth segment is the trajectory of a Hamiltonian vector field.

The equivalence class M_p containing $p \in M$ is a connected submanifold of M and by definition its tangent space $T_q M_p \subset T_q M$ is spanned by Hamiltonian tangent vectors. We may view M_p as a symplectic manifold whose 2-form is given by $\omega(\xi_f, \xi_g) = \{f, g\}$ and thus M_p is called the *symplectic leaf* of M through p.

Example 5.10 The symplectic leaves of GL_n have been explicitly computed (e.g., see [34] and references therein). In particular, it is known that each double Bruhat cell in GL_n is foliated by symplectic leaves of GL_n. As an example (c.f. Example 2.8) the following set is a symplectic leaf living in $GL_n^{w_0,w_0}$:

$$\{M \in GL_n : \Delta_{[1,i],[n+1-i,n]}(M) = \Delta_{[i+1,n],[1,n-i]}(M) \neq 0 \text{ for all } i\}.$$

Exercise 5.11 Find a matrix $M \in GL_2$ so that the symplectic leaf above is the symplectic leaf of GL_2 through M. Do the same for GL_3.

A final reason to care about Poisson structures on a cluster algebra is that they provide a canonical quantization of the cluster algebra structure. Rather than giving precise definitions, we indicate here the intuition motivating the definition and refer the reader to [4] for more details.

Given a cluster algebra $\mathcal{A}(\mathbf{x}, \widetilde{B})$ of full rank, any choice of compatible Poisson structure gives rise to a canonical quantization of $\mathcal{A}(\mathbf{x}, \widetilde{B})$ by the following procedure, where v denotes a formal variable:

- Each cluster should be replaced by a collection of quasi-commuting elements $\{X_1, \ldots, X_m\}$ satisfying $X_i X_j = v^{2\Lambda(\varepsilon_j, \varepsilon_i)} X_j X_i$ for a skew-symmetric bilinear form

$\Lambda : \mathbb{Z}^m \times \mathbb{Z}^m \to \mathbb{Z}$, where ε_i denotes the ith standard basis vector of $\mathbb{Z}^m$. That is, this *quantum cluster* generates a *quantum torus* $\mathcal{T} = \mathbb{Z}[v^{\pm 1}]\langle X_1^{\pm 1}, \ldots, X_m^{\pm 1}\rangle$ with a $\mathbb{Z}[v^{\pm 1}]$-basis

$$\left\{ X^{\mathbf{a}} := v^{\sum_{i<j} a_i a_j \Lambda(\varepsilon_i, \varepsilon_j)} X_1^{a_1} \cdots X_m^{a_m} \;\middle|\; \mathbf{a} = (a_1, \ldots, a_m) \in \mathbb{Z}^m \right\} .$$

- Each quantum cluster obtained by mutation from this one should again generate a quantum torus. This forces a compatibility condition on the exchange matrix $\widetilde{B}$ and the commutation matrix Λ (by a slight abuse of notation we freely identify the bilinear form Λ with a skew-symmetric matrix), that is

$$\Lambda(\mathbf{b}_k, \varepsilon_\ell) = 0 \quad \text{if } k \neq \ell \,, \tag{8}$$

  where $\mathbf{b}_k$ denotes the kth column of $\widetilde{B}$ thought of as an element of $\mathbb{Z}^m$.
- The above conditions still leave a great deal of freedom. To restrict further, notice that the quasi-commutation relation above can be rewritten as $v^{\Lambda(\varepsilon_i, \varepsilon_j)} X_i X_j = v^{\Lambda(\varepsilon_j, \varepsilon_i)} X_j X_i$, in particular this implies that $\mathcal{T}$ admits an anti-automorphism $X \mapsto \overline{X}$ which fixes each X_i and sends v to v^{-1} (recall that Λ was assumed skew-symmetric). Since each initial cluster variable was *bar-invariant*, the same should be true of all cluster variables since a cluster algebra is independent of the choice of initial cluster. This uniquely determines how to incorporate powers of v into the exchange relations (3); more precisely, the new variable obtained by mutation in direction k must be

$$X_k' = X^{-\varepsilon_k + \sum_{b_{ik}>0} b_{ik}\varepsilon_i} + X^{-\varepsilon_k - \sum_{b_{ik}<0} b_{ik}\varepsilon_i} .$$

Exercise 5.12 Verify the compatibility condition (8) and show that it is the same as the compatibility condition from Lemma 5.3.

6 Applications to Integrable Systems

We now explore connections between cluster algebras and discrete integrable systems. In this context, it is common to represent the exchange matrix as a quiver.

Definition 6.1 A *quiver* is a directed graph without loops (arrows from a vertex to itself) and without oriented 2-cycles.

A skew-symmetric $n \times n$ exchange matrix B can be encoded as a quiver Q on vertex set $\{1, 2, \ldots, n\}$. More precisely, if i, j are such that $b_{ij} > 0$ then Q has b_{ij} arrows from i to j (and none from j to i). Matrix mutation on B induces so-called *quiver mutation* on Q.

Definition 6.2 Given some $k = 1, 2, \ldots, n$, the *quiver mutation* μ_k gives rise to $Q' = \mu_k(Q)$ by applying the following steps to Q:

1. for each pair of vertices i, j and arrows $i \to k$ and $k \to j$, add an arrow $i \to j$,
2. reverse all arrows $i \to k$ and $k \to j$,
3. erase in turn pairs of arrows $i \to j$ and $j \to i$ to eliminate any 2-cycles.

Given a quiver Q and a sequence $k_1, k_2, \ldots, k_l$ of its vertices (possibly with repeats), one can consider the dynamical system obtained by repeated applications of the composite mutation $\mu_{k_l} \circ \cdots \circ \mu_{k_2} \circ \mu_{k_1}$ starting from an initial seed $(\mathbf{x}, Q)$ or Y-seed $(\mathbf{y}, Q)$. In the special case when the final quiver after one application equals the initial one, i.e.

$$\mu_{k_l} \circ \cdots \circ \mu_{k_2} \circ \mu_{k_1}(Q) = Q,$$

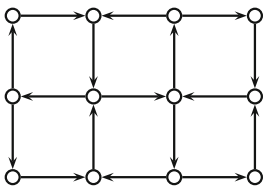
the system amounts to iterating a fixed birational transformation. It is natural to investigate these mappings for properties such as periodicity and integrability.

We focus on two (families of) quivers, one giving rise to the Y-system of type $A \times A$ and the other corresponding to the pentagram map. Some of the many other systems that have been investigated from a cluster algebra point of view are Q-systems [9], T-systems [8], Somos sequences [30], and mutations in box products of quivers [43]. A systematic study of quivers that return to (isomorphic copies of) themselves under mutation was undertaken in [18]. We also refer the reader to [22, 40], where periodicities of cluster algebra mutations are used to derive dilogarithm identities.

For the remainder of this section, all mutations are understood to be of Y-pattern type.

6.1 Zamolodchikov Periodicity

Fix positive integers r and s and consider the quiver Q on vertex set $\{1, \ldots, r\} \times \{1, \ldots, s\}$ as illustrated in the case $r = 4$, $s = 3$ by



Let μ_{even} be the compound mutation given by applying each $\mu_{i,j}$ with $i + j$ even in turn. As no arrows connect these even vertices, it follows that these mutations commute and so the order does not matter. Define μ_{odd} similarly as the compound mutation at all odd vertices.

Exercise 6.3 Let $Y = (Y_{i,j})_{i=1,\ldots,r;j=1,\ldots,s}$. Then $\mu_{\text{even}}(Y, Q) = (Y', -Q)$ where

$$Y'_{i,j} = \begin{cases} Y_{i,j}^{-1} & \text{if } i+j \text{ even} \\ Y_{i,j} \frac{\prod_{|i-i'|=1}(1+Y_{i',j})}{\prod_{|j-j'|=1}(1+Y_{i,j'}^{-1})} & \text{if } i+j \text{ odd} \end{cases} \tag{9}$$

and $-Q$ denotes Q with all its arrows reversed.

Now begin with the Y-seed (Y_0, Q) and let

$$\begin{aligned} (Y_1, -Q) &= \mu_{\text{even}}(Y_0, Q) \\ (Y_2, Q) &= \mu_{\text{odd}}(Y_1, -Q) \\ (Y_3, -Q) &= \mu_{\text{even}}(Y_2, Q) \\ &\vdots \end{aligned}$$

where $Y_t = (Y_{ijt})_{i=1,\ldots,r;j=1,\ldots,s}$. It follows from the above that

$$Y_{i,j,t+1} = \begin{cases} Y_{i,j,t}^{-1} & \text{if } i+j+t \text{ even} \\ Y_{i,j,t} \frac{\prod_{|i-i'|=1}(1+Y_{i',j,t})}{\prod_{|j-j'|=1}(1+Y_{i,j',t}^{-1})} & \text{if } i+j+t \text{ odd} \end{cases}$$

It is convenient to consider only the $Y_{i,j,t}$ with $i+j+t$ even, which satisfy their own recurrence

$$Y_{i,j,t-1} Y_{i,j,t+1} = \frac{\prod_{|i-i'|=1}(1 + Y_{i',j,t})}{\prod_{|j-j'|=1}(1 + Y_{i,j',t}^{-1})} \tag{10}$$

for all $i+j+t$ odd. This recurrence is called the type $A_r \times A_s$ Y-system, a special case of a family of systems conjectured by Zamolodchikov to be periodic. The proof, in this case, is due to Volkov [50].

Theorem 6.4 *The Y-system (10) on variables $Y_{i,j,t}$ with $i+j+t$ odd, $i = 1, \ldots, r$, and $j = 1, \ldots, s$ has period $2(r+s+2)$ in the t-direction, that is*

$$Y_{i,j,t+2(r+s+2)} = Y_{i,j,t} \ .$$

Returning to the Y-pattern point of view, the initial seed (Y_0, Q) consists of the $Y_{i,j,0}$ for $i+j$ even and the $Y_{i,j,-1}^{-1}$ for $i+j$ odd. The seed $(Y_2, Q) = \mu_{\text{odd}}\big(\mu_{\text{even}}(Y_0, Q)\big)$ consists of the $Y_{i,j,2}$ for $i+j$ even and the $Y_{i,j,1}^{-1}$ for $i+j$ odd. The periodicity theorem, then, asserts that the rational map $\mu_{\text{odd}} \circ \mu_{\text{even}}$ has order $r+s+2$.

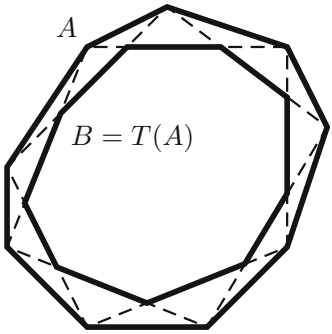


Fig. 4 An application of the pentagram map

6.2 The Pentagram Map

The pentagram map is a discrete dynamical system defined on the space of polygons in the projective plane. Figure 4 shows a polygon A and the corresponding output $B = T(A)$, with T being the notation for the pentagram map. Each vertex of B lies at the intersection of two consecutive "shortest" diagonals of A.

The pentagram map was introduced by Schwartz [47] and extensively studied by Ovsienko et al. [41, 42]. In particular, they demonstrated that the pentagram map is a completely integrable system. Another take on integrability was provided by Soloviev [49]. In the same span of time, Glick [26] described the pentagram map as mutations in a Y-pattern, building on work of Schwartz [48] who had found a lift to the octahedron recurrence. Finally, Gekhtman et al. [23] gave a uniform treatment of integrability and the cluster algebra structure of the pentagram map, and generalizations thereof, in terms of weighted networks on tori. A similar framework is provided by the cluster integrable systems of Goncharov and Kenyon [27], albeit without any explicit mention of the pentagram map.

The connection between the pentagram map and Y-patterns comes by way of certain geometrically defined coordinates on the space of polygons. The *cross-ratio* of four real numbers x_1, x_2, x_3, x_4 is

$$\chi(x_1, x_2, x_3, x_4) = \frac{(x_1 - x_2)(x_3 - x_4)}{(x_1 - x_3)(x_2 - x_4)}.$$

The cross-ratio is invariant under projective transformations, that is

$$\chi\big(f(x_1), f(x_2), f(x_3), f(x_4)\big) = \chi(x_1, x_2, x_3, x_4)$$

for any fractional linear map $f(x) = (ax + b)/(cx + d)$. For this reason, there is a well-defined notion in the plane of the cross-ratio of four collinear points or of four concurrent lines.

Given an n-gon A, label its sides and vertices consecutively with the integers $\{1, 2, \ldots, 2n\}$. Such a labeling induces a canonical labeling on $T(A)$ as is illustrated

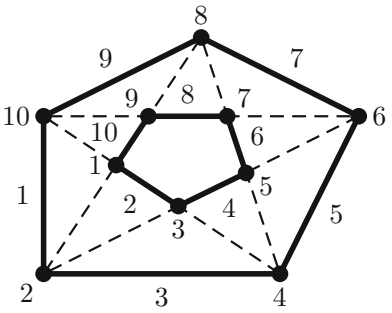


Fig. 5 Possible labelings of two polygons related by the pentagram map

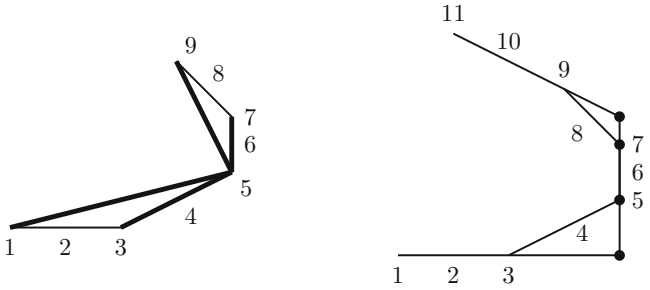


Fig. 6 The cross-ratios corresponding to the two types of y-parameters. On the left, $-(y_5)^{-1}$ is the cross-ratio of the lines $\langle 5, 1\rangle$, 4, 6, and $\langle 5, 9\rangle$. On the right, $-y_6$ is the cross-ratio of the points $6 \cap 2$, 5, 7, and $6 \cap 10$

in Fig. 5. Note that the parities of the vertex labels and of the edge labels are interchanged by T. In what follows, let $\langle i, j\rangle$ denote the line between two points labeled i and j and let $k \cap l$ denote the point of intersection of two lines labeled k and l.

Definition 6.5 The *y-parameters* of a polygon A are real numbers $y_1(A), \ldots, y_{2n}(A)$ defined by

$$y_i(A) = \begin{cases} -\big(\chi(\langle i, (i-4)\rangle, i-1, i+1, \langle i, (i+4)\rangle)\big)^{-1} & \text{if } i \text{ is a vertex of } A \\ -\chi\big(i \cap (i-4), i-1, i+1, i \cap (i+4)\big) & \text{if } i \text{ is a side of } A \end{cases}$$

This definition is illustrated in Fig. 6.

Proposition 6.6 *Let A be an n-gon with y-parameters $y_i = y_i(A)$. Let $B = T(A)$ and denote its y-parameters $y'_i = y_i(B)$. Then*

$$y'_i = \begin{cases} y_i^{-1} & \text{if } i \text{ is a side of } B \\ y_i \frac{(1+y_{i-1})(1+y_{i+1})}{(1+y_{i-3}^{-1})(1+y_{i+3}^{-1})} & \text{if } i \text{ is a vertex of } B \end{cases} \tag{11}$$

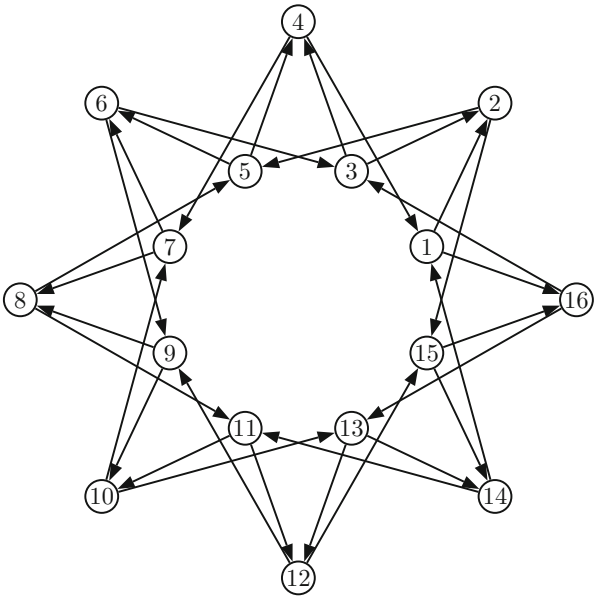


Fig. 7 The quiver related to the action of the pentagram map on octagons

In this equation, all indices are considered modulo $2n$.

The formula (11) bears a distinct resemblance to (9), so it is plausible that it can also be described by Y-pattern mutations for an appropriate quiver. The desired quiver Q_n has vertex set $\{1, 2, \ldots, 2n\}$ and arrows $j \to (j \pm 1)$ and $j \leftarrow (j \pm 3)$ for each odd j, with vertices considered modulo $2n$. The quiver Q_8 is shown in Fig. 7. Similar to before, define compound mutations

$$\mu_{\text{odd}} = \mu_{2n-1} \circ \cdots \circ \mu_3 \circ \mu_1,$$
$$\mu_{\text{even}} = \mu_{2n} \circ \cdots \circ \mu_4 \circ \mu_2.$$

Theorem 6.7 ([26]) *Let A be an n-gon with y-parameters $y_1, \ldots, y_{2n}$ and let k be a positive integer. Beginning from the Y-seed $\big((y_1, \ldots, y_{2n}), Q_n\big)$, apply k compound mutations alternating between μ_{even} and μ_{odd}. The result will have the form $\big((y'_1, \ldots, y'_{2n}), (-1)^k Q_n\big)$ where*

$$y'_i = y_i\big(T^k(A)\big)\ .$$

Remark 6.8 It is natural to ask what values the n-tuple $\big(y_1(A), \ldots, y_{2n}(A)\big)$ can take, and also to what extent this data suffices to reconstruct A. These questions are easier to answer after extending to a larger family of objects called twisted polygons. In this setting, the y_i satisfy a single relation $y_1 \cdots y_{2n} = 1$. Moreover,

the y_i determine a twisted polygon uniquely up to projective equivalence and a one-parameter rescaling operation due to Schwartz [48]. The Y-pattern dynamics described in Theorem 6.7, then, characterize the dynamics of the pentagram map on the space of twisted polygons modulo these equivalences.

We now give a somewhat informal presentation of integrability of the pentagram map from the cluster algebra perspective. The first ingredient is a compatible Poisson structure, which can be obtained directly from the Y-pattern analogue of Theorem 5.5.

Proposition 6.9 ([23, 41]) *Define a Poisson bracket by $\{y_i, y_j\} = b_{ij} y_i y_j$ where B is the exchange matrix associated to the pentagram quiver Q_n. Then this bracket is preserved by the pentagram map, i.e.,*

$$\{f, g\} \circ T = \{f \circ T, g \circ T\}$$

for all functions f and g of the y-parameters.

Some more work is needed to get at the conserved quantities. We follow the approach of [27]. The quiver Q_n can be lifted to an infinite doubly periodic quiver in the plane as in Fig. 8. This lift represents an embedding of Q_n on a torus. Let $G = (V, E)$ be the dual graph on the torus with $V = \{1, 2, \ldots, 2n\}$ where $i \in V$ corresponds to the face of the quiver with vertices $i \pm 2, i \pm 1$. Coincidentally, G is identical to Q_n except without orientations, so $\overline{ij} \in E$ if and only if $i - j \equiv \pm 1, \pm 3 \pmod{2n}$. Figure 9 shows the graph G on the torus in the case $n = 4$, with the vertices $1, 2, \ldots, 8$ appearing in order from left to right.

Assign edge weights to G as follows: each "horizontal" edge $\overline{i(i+1)}$ gets weight 1 and each "vertical edge" $\overline{(i-2)(i+1)}$ gets weight $(-1)^i x_i$. The x_i represent the *corner invariants* [48] of a polygon, certain coordinates related to the y-parameters by

$$y_i = \begin{cases} -(x_i x_{i+1})^{-1} & \text{if } i \text{ is a vertex of } A; \\ -x_i x_{i+1} & \text{if } i \text{ is a side of } A. \end{cases}$$

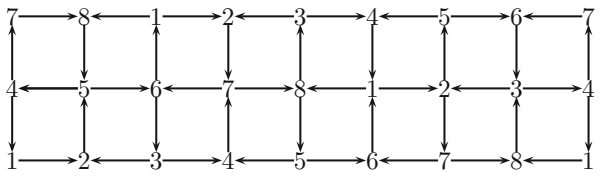


Fig. 8 A lift of Q_4 to a doubly periodic quiver in the plane

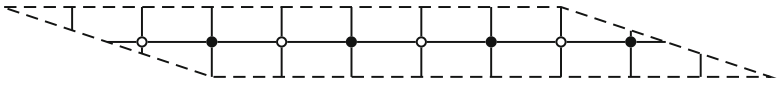


Fig. 9 A bipartite graph on the torus dual to the quiver Q_4

A *perfect matching* of G is a collection M of its edges such that each $i \in V$ is an endpoint of exactly one $e \in M$. The *weight* of M, denoted $wt(M)$, is the product of the weights of its edges. For instance,

$$M = \{\overline{12}, \overline{36}, \overline{47}, \overline{58}\}$$

is a perfect matching of G_4 and its weight is $(1)(-x_5)(x_6)(-x_7) = x_5x_6x_7$. The conserved quantities of the pentagram map are sums of weights of perfect matchings, refined by a notion of homology class of a matching defined in [27].

Proposition 6.10 *For any homology class, the sum*

$$\sum_M wt(M)$$

over perfect matchings M of G_n in that class is a conserved quantity of the pentagram map acting on n-gons.

In the case of the graph G_4 pictured in Fig. 9, there are 22 perfect matchings which represent 8 different homology classes. Table 1 gives the 8 corresponding conserved quantities for the pentagram map. The first 2 are trivial but the remaining 6 are (up to a sign) the original conserved quantities discovered by Schwartz [48] by different means.

The invariant Poisson bracket from Proposition 6.9 and the conserved quantities from Proposition 6.10 are the main ingredients for complete integrability, but there are several more conditions that they need to satisfy. We conclude by listing these properties, proofs for which can be found in [23, 41] and [27].

- The conserved quantities are algebraically independent.
- The conserved quantities Poisson commute, i.e., the bracket of any two of them equals zero.

Table 1 Conserved quantities for the pentagram map acting on twisted quadrilaterals

Name	Formula	Representative matching
n.a.	1	$\{\overline{12}, \overline{34}, \overline{56}, \overline{78}\}$
n.a.	1	$\{\overline{23}, \overline{45}, \overline{67}, \overline{18}\}$
O_1	$-x_1 - x_3 - x_5 - x_7 + x_1x_2x_3 + x_3x_4x_5$ $+x_5x_6x_7 + x_1x_7x_8$	$\{\overline{27}, \overline{34}, \overline{56}, \overline{18}\}$
E_1	$x_2 + x_4 + x_6 + x_8 - x_2x_3x_4 - x_4x_5x_6$ $-x_6x_7x_8 - x_1x_2x_8$	$\{\overline{38}, \overline{12}, \overline{45}, \overline{67}\}$
O_2	$x_1x_5 + x_3x_7$	$\{\overline{27}, \overline{36}, \overline{45}, \overline{18}\}$
E_2	$x_2x_6 + x_4x_8$	$\{\overline{38}, \overline{47}, \overline{12}, \overline{56}\}$
O_4	$x_1x_3x_5x_7$	$\{\overline{14}, \overline{36}, \overline{58}, \overline{27}\}$
E_4	$x_2x_4x_6x_8$	$\{\overline{16}, \overline{38}, \overline{25}, \overline{47}\}$

The matching M is such that $wt(M)$ is the first term appearing in the corresponding formula

- The number of Casimirs plus twice the number of other conserved quantities equals the dimension of the system.

In the last item, the term *Casimir* refers to a function that Poisson commutes with all other functions. In the case summarized in Table 1, the 4 functions O_2, E_2, O_4, E_4 are Casimirs while the other two conserved quantities O_1 and E_1 are not. The calculation checks out as $4 + 2(2) = 8$ is the dimension of the space of twisted quadrilaterals.

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References

1. N. Arkani-Hamed, J.L. Bourjaily, F. Cachazo, A.B. Goncharov, A. Postnikov, J. Trnka, Scattering amplitudes and the positive Grassmannian. arXiv:1212.5605
2. A. Berenstein, S. Fomin, A. Zelevinsky, Cluster algebras. III. Upper bounds and double Bruhat cells. Duke Math. J. **126**(1), 1–52 (2005)
3. A. Berenstein, D. Rupel, Quantum cluster characters of Hall algebras. Sel. Math. N. Ser. **21**(4), 1121–1176 (2015)
4. A. Berenstein, A. Zelevinsky, Quantum cluster algebras. Adv. Math. **195**(2), 405–455 (2005)
5. A.B. Buan, R. Marsh, M. Reineke, I. Reiten, G. Todorov, Tilting theory and cluster combinatorics. Adv. Math. **204**(2), 572–618 (2006)
6. P. Caldero, F. Chapoton, Cluster algebras as Hall algebras of quiver representations. Comment. Math. Helv. **81**(3), 595–616 (2006)
7. P. Caldero, B. Keller, From triangulated categories to cluster algebras. II. Ann. Sci. École Norm. Sup. (4) **39**(6), 983–1009 (2006)
8. P. Di Francesco, R. Kedem, Positivity of the T-system cluster algebra. Electron. J. Comb. **16**(1), 140 (2009)
9. P. Di Francesco, R. Kedem, Q-systems, heaps, paths and cluster positivity. Commun. Math. Phys. **293**(3), 727–802 (2010)
10. R. Eager, S. Franco, Colored BPS pyramid partition functions, quivers and cluster transformations. J. High Energy Phys. **2012**(9), 038 (2012)
11. V. Fock, A. Goncharov, Moduli spaces of local systems and higher Teichmüller theory. Publ. Math. Inst. Hautes Études Sci. **103**, 1–211 (2006)
12. S. Fomin, M. Shapiro, D. Thurston, Cluster algebras and triangulated surfaces. I. Cluster complexes. Acta Math. **201**(1), 83–146 (2008)
13. S. Fomin, A. Zelevinsky, Double Bruhat cells and total positivity. J. Am. Math. Soc. **12**(2), 335–380 (1999)
14. S. Fomin, A. Zelevinsky, Cluster algebras. I. Foundations. J. Am. Math. Soc. **15**(2), 497–529 (electronic) (2002)
15. S. Fomin, A. Zelevinsky, The Laurent phenomenon. Adv. Appl. Math. **28**(2), 119–144 (2002)
16. S. Fomin, A. Zelevinsky, Cluster algebras. II. Finite type classification. Invent. Math. **154**(1), 63–121 (2003)
17. S. Fomin, A. Zelevinsky, Cluster algebras. IV. Coefficients. Compos. Math. **143**(1), 112–164 (2007)
18. A.P. Fordy, R.J. Marsh, Cluster mutation-periodic quivers and associated Laurent sequences. J. Algebraic Comb. **34**(1), 19–66 (2011)

19. C. Geiß, B. Leclerc, J. Schröer, Rigid modules over preprojective algebras. Invent. Math. **165**(3), 589–632 (2006)
20. C. Geiß, B. Leclerc, J. Schröer, Cluster algebras in algebraic Lie theory. Transform. Groups **18**(1), 149–178 (2013)
21. C. Geiß, B. Leclerc, J. Schröer, Cluster structures on quantum coordinate rings. Sel. Math. N. Ser. **19**(2), 337–397 (2013)
22. M. Gekhtman, T. Nakanishi, D. Rupel, Hamiltonian and Lagrangian formalisms of mutations in cluster algebras and application to dilogarithm identities. arXiv:16118.02813
23. M. Gekhtman, M. Shapiro, S. Tabachnikov, A. Vainshtein, Higher pentagram maps, weighted directed networks, and cluster dynamics. Electron. Res. Announc. Math. Sci. **19**, 1–17 (2012)
24. M. Gekhtman, M. Shapiro, A. Vainshtein, Cluster algebras and Poisson geometry. Mosc. Math. J. **3**(3), 899–934 (2003)
25. M. Gekhtman, M. Shapiro, A. Vainshtein, *Cluster Algebras and Poisson Geometry*. Mathematical Surveys and Monographs, vol. 167 (American Mathematical Society, Providence, 2010)
26. M. Glick, The pentagram map and *Y*-patterns. Adv. Math. **227**(2), 1019–1045 (2011)
27. A.B. Goncharov, R. Kenyon, Dimers and cluster integrable systems. Ann. Sci. Éc. Norm. Supér. (4) **46**(5), 747–813 (2013)
28. M. Gross, P. Hacking, S. Keel, M. Kontsevich, Canonical bases for cluster algebras. arXiv:1411.1394
29. A. Hatcher, On triangulations of surfaces. Topol. Appl. **40**(2), 189–194 (1991)
30. A.N.W. Hone, Sigma function solution of the initial value problem for Somos 5 sequences. Trans. Am. Math. Soc. **359**(10), 5019–5034 (2007)
31. B. Keller, Categorification of acyclic cluster algebras: an introduction. arXiv:0801.3103
32. Y. Kimura, Quantum unipotent subgroup and dual canonical basis. Kyoto J. Math. **52**(2), 277–331 (2012)
33. Y. Kimura, F. Qin, Graded quiver varieties, quantum cluster algebras and dual canonical basis. Adv. Math. **262**, 261–312 (2014)
34. M. Kogan, A. Zelevinsky, On symplectic leaves and integrable systems in standard complex semisimple Poisson–Lie groups. Int. Math. Res. Not. **2002**(32), 1685–1702 (2002)
35. K. Lee, L. Li, A. Zelevinsky, Greedy elements in rank 2 cluster algebras. Sel. Math. N. Ser. **20**(1), 57–82 (2014)
36. K. Lee, R. Schiffler, A combinatorial formula for rank 2 cluster variables. J. Algebraic Comb. **37**(1), 67–85 (2013)
37. K. Lee, R. Schiffler, Positivity for cluster algebras. Ann. Math. (2) **182**(1), 73–125 (2015)
38. G. Musiker, J. Propp, Combinatorial interpretations for rank-two cluster algebras of affine type. Electron. J. Comb. **14**(1), 15 (2007)
39. G. Musiker, R. Schiffler, L. Williams, Bases for cluster algebras from surfaces. Compos. Math. **149**(2), 217–263 (2013)
40. T. Nakanishi, Periodicities in cluster algebras and dilogarithm identities. in *Representations of Algebras and Related Topics*, ed. by A. Skowroński, K. Yamagata, EMS Series of Congress Reports (European Mathematical Society, Zürich, 2011), pp. 407–443
41. V. Ovsienko, R. Schwartz, S. Tabachnikov, The pentagram map: a discrete integrable system. Commun. Math. Phys. **299**(2), 409–446 (2010)
42. V. Ovsienko, R.E. Schwartz, S. Tabachnikov, Liouville–Arnold integrability of the pentagram map on closed polygons. Duke Math. J. **162**(12), 2149–2196 (2013)
43. P. Pylyavskyy, Zamolodchikov integrability via rings of invariants. arXiv:1506.05378
44. F. Qin, Quantum cluster variables via Serre polynomials. J. Reine Angew. Math. **668**, 149–190 (2012)
45. D. Rupel, On a quantum analog of the Caldero–Chapoton formula. Int. Math. Res. Not. **2011**(14), 3207–3236 (2011)
46. D. Rupel, Quantum cluster characters for valued quivers. Trans. Am. Math. Soc. **367**(10), 7061–7102 (2015)
47. R. Schwartz, The pentagram map. Exp. Math. **1**(1), 71–81 (1992)

48. R.E. Schwartz, Discrete monodromy, pentagrams, and the method of condensation. J. Fixed Point Theory Appl. **3**(2), 379–409 (2008)
49. F. Soloviev, Integrability of the pentagram map. Duke Math. J. **162**(15), 2815–2853 (2013)
50. A.Y. Volkov, On the periodicity conjecture for Y-systems. Commun. Math. Phys. **276**(2), 509–517 (2007)
51. L. Williams, Cluster algebras: an introduction. arXiv:1212.6263

An Introduction to Difference Galois Theory

Julien Roques

Abstract This article comes from notes written for my lectures at the summer school "Abecedarian of SIDE" held at the CRM (Montréal) in June 2016. They are intended to give a short introduction to difference Galois theory, leaving aside the technicalities.

1 Introduction

This article comes from notes written for my lectures at the summer school "Abecedarian of SIDE" held at the CRM (Montréal) in June 2016. They are intended to give a short introduction to difference Galois theory, leaving aside the technicalities. There already exist several nice introductory papers/surveys about differential Galois theory, e.g., [6, 7, 22, 32, 33], and (parameterized) difference Galois theory, e.g., [10, 18]. For complete proofs and further results concerning difference Galois theory, we refer the reader to van der Put and Singer's [23].

2 First Steps: From Classical Galois Theory to Difference Galois Theory

2.1 The Classical Galois Groups

The Galois group over $\mathbb{Q}$ of a polynomial $P(X) \in \mathbb{Q}[X]$ can be defined as follows. We start with the base field $\mathbb{Q}$. We then consider a splitting field K of $P(X)$ over $\mathbb{Q}$, i.e., a minimal field extension of $\mathbb{Q}$ over which $P(X)$ decomposes as a product a polynomials of degree 1. Then, the Galois group of $P(X)$ over $\mathbb{Q}$ is made of the field automorphisms σ of K such that $\sigma_{|\mathbb{Q}} = \mathrm{Id}_{\mathbb{Q}}$.

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Exercise 2.1 Recall why we can describe the elements of this Galois group as the permutations of the roots of $P(X)$ preserving the algebraic relations with coefficients in $\mathbb{Q}$ among these roots. This was Galois's original approach.

2.2 The Differential Galois Groups

This construction can be extended to linear differential equations with coefficients in $\mathbb{C}(z)$ as follows. Instead of a polynomial $P(X)$ with coefficients in $\mathbb{Q}$, we consider a linear differential system

$$Y'(z) = A(z)Y(z) \quad \text{with } A(z) \in \mathrm{M}_n\big(\mathbb{C}(z)\big) .$$

The base field $\mathbb{Q}$ of Sect. 2.1 above is now replaced by the field $\mathbb{C}(z)$ or, better, by the field $\mathbb{C}(z)$ endowed with the derivation $\mathrm{d}/\mathrm{d}z\colon \mathbb{C}(z) \to \mathbb{C}(z)$. Consider some complex number z_0 which is not a pole of $A(z)$. According to Cauchy's theorem, there exists $\mathfrak{Y}(z) \in \mathrm{GL}_n(\mathbb{C}\{z - z_0\})$ such that

$$\mathfrak{Y}'(z) = A(z)\mathfrak{Y}(z)$$

(we have denoted by $\mathbb{C}\{z - z_0\}$ the ring of analytic functions near z_0). The analogue of the splitting field of the polynomial $P(X)$ over $\mathbb{Q}$ is the field extension

$$K = \mathbb{C}(z)\big(\mathfrak{Y}(z)\big)$$

of $\mathbb{C}(z)$ generated by the entries of $\mathfrak{Y}(z)$. Note that K is stable by the usual derivation $\mathrm{d}/\mathrm{d}z$, which is an extension of the derivation $\mathrm{d}/\mathrm{d}z$ attached to the base field $\mathbb{C}(z)$. The field K endowed with the derivation $\mathrm{d}/\mathrm{d}z\colon K \to K$ is called a Picard–Vessiot field for $Y'(z) = A(z)Y(z)$ over $\mathbb{C}(z)$. The corresponding differential Galois group of $Y'(z) = A(z)Y(z)$ over $\mathbb{C}(z)$ is then made of the field automorphisms σ of K such that

$$\sigma_{|\mathbb{C}(z)} = \mathrm{Id}_{\mathbb{C}(z)} \quad \text{and} \quad \sigma \circ \mathrm{d}/\mathrm{d}z = \mathrm{d}/\mathrm{d}z \circ \sigma .$$

In particular, these conditions ensure that any element of the differential Galois group transforms any solution of $Y'(z) = A(z)Y(z)$ with coefficients in K into another solution: for any element σ of the differential Galois group and for all $F \in M_{n,1}(K)$ such that $F'(z) = A(z)F(z)$, we have $\sigma(F)'(z) = A(z)\sigma(F)(z)$.

Exercise 2.2 Let σ be a field automorphism of K such that $\sigma_{|\mathbb{C}(z)} = \mathrm{Id}_{\mathbb{C}(z)}$. Prove that the following properties are equivalent:

- σ transforms any solution of $Y'(z) = A(z)Y(z)$ with coefficients in K into another solution;
- $\sigma \circ \mathrm{d}/\mathrm{d}z = \mathrm{d}/\mathrm{d}z \circ \sigma$.

2.3 Toward Difference Galois Groups

Can we extend the construction of Sect. 2.2 to other linear functional equations? Let us consider this question for very simple difference systems of rank one of the form

$$y(z+1) = a(z)y(z) \quad \text{with } a(z) \in \mathbb{C}(z)^{\times} .$$

The base field is still $\mathbb{C}(z)$, but the role played by the derivation $\mathrm{d}/\mathrm{d}z$ in Sect. 2.2 is now played by the field automorphism τ of $\mathbb{C}(z)$ defined by $\tau{:}f(z) \mapsto f(z+1)$. Inspired by Sect. 2.2, it seems natural to look for a field extension K of $\mathbb{C}(z)$ such that:

1. K can be endowed with a field automorphism extending τ, still denoted by τ;
2. there exists $\mathfrak{y} \in K^{\times}$ such that

$$\tau(\mathfrak{y}) = a(z)\mathfrak{y};$$

3. K is minimal for the above properties, i.e.,

$$K = \mathbb{C}(z)(\mathfrak{y});$$

and, then, to define the difference Galois group of $y(z+1) = a(z)y(z)$ over $\mathbb{C}(z)$ as the group made of the field automorphisms σ of K such that

$$\sigma_{|\mathbb{C}(z)} = \mathrm{Id}_{\mathbb{C}(z)} \quad \text{and} \quad \sigma \circ \tau = \tau \circ \sigma .$$

Let us first study the case $a(z) = 1$, i.e., the equation

$$y(z+1) = y(z) .$$

Note that

$$\mathfrak{y}(z) = 1 \quad \text{and} \quad K = \mathbb{C}(z)\big(\mathfrak{y}(z)\big) = \mathbb{C}(z)$$

endowed with $\tau{:}f(z) \mapsto f(z+1)$ have the required properties. It is easily seen that the corresponding difference Galois group is trivial, i.e., reduced to $\{\mathrm{Id}_{\mathbb{C}(z)}\}$. This is consistent with the fact that the equation $y(z+1) = y(z)$ is the simplest possible ("trivial").

However, the choice $\mathfrak{y}(z) = 1$ may seem somewhat arbitrary. For instance, one could have chosen $\mathfrak{y}(z) = \sin(2\pi z)$ instead of 1 and $K = \mathbb{C}(z)\big(\mathfrak{y}(z)\big)$ endowed with $\tau{:}f(z) \mapsto f(z+1)$. The corresponding difference Galois group contains a subgroup isomorphic to $\mathrm{PGL}_2(\mathbb{C})$ (i.e., the automorphisms of K defined by $r\big(z, \mathfrak{y}(z)\big) \mapsto r\big(z, (a\mathfrak{y}(z)+b)/(c\mathfrak{y}(z)+d)\big)$ with $a, b, c, d \in \mathbb{C}$ such that $ad-bc \neq 0$). This is not reasonable and not consistent with what precedes. Actually, the problem is that, in the process of going from $\mathbb{C}(z)$ to K by adjoining $\mathfrak{y} = \sin(2\pi z)$, we

have introduced new constants i.e., elements of K fixed by τ which do not belong to the base field $\mathbb{C}(z)$ (or, equivalently, to $\mathbb{C}$). This leads us to require the further condition that

4. $K^\tau := \{f \in K \mid \tau(f) = f\}$ must be equal to $\mathbb{C}$.

This condition excludes the choice $\mathfrak{y}(z) = \sin(2\pi z)$.

Let us now consider the case $a(z) = -1$, i.e., the equation

$$y(z+1) = -y(z)\ .$$

We claim that, in this case, it is impossible to find a field K satisfying to the conditions 1 to 4 above. Indeed, assume at the contrary that such a field K exists. Then, $\mathfrak{y}^2$ is fixed by τ and hence belongs to $\mathbb{C}$. Therefore, $\mathfrak{y}$ belongs to $\mathbb{C}$. This is a contradiction: the equation $\tau(\mathfrak{y}) = -\mathfrak{y}$ does not have any solution in $\mathbb{C}(z)$.

Actually, we will have to work with rings and to accept zero divisors. More precisely, the basic objects will be rings endowed with an automorphism: these will be called difference rings. In the present case, we will see that a correct analogue of the splitting field is given by the quotient ring $\mathbb{C}(z)[X, X^{-1}]/(X^2 - 1)$ endowed with its unique ring automorphism ϕ such that $\phi_{|\mathbb{C}(z)} = \tau$ and $\phi(\overline{X}) = -\overline{X}$.

2.4 Organization of the Lecture Notes

Section 4 is devoted to the difference rings. The analogue(s) for difference equations of the splitting fields of Sect. 2.1, called Picard–Vessiot rings and total Picard–Vessiot rings, are defined and studied in Sect. 5. The difference Galois groups are introduced in Sect. 6, where their first properties are studied. This study is pursued in Sect. 7 (where we describe the algebraic relations among the solutions of difference equations in terms of the difference Galois groups) and in Sect. 8 (devoted to the Galois correspondence). In Sect. 9, we focus our attention on regular q-difference systems. In Sect. 9.2, we introduce Birkhoff's connection matrices and explain their Galoisian meaning. In Sect. 9.3, we consider the q-difference equations as deformations of differential systems and explain in which sense the connection matrices deform the monodromy representations attached to differential equations. Section 10 is concerned with the explicit calculation of difference Galois groups (mainly references). Section 11 is a brief introduction to parameterized difference Galois theory.

3 A Table of Analogies

The following table summarizes some analogies between the classical Galois theory and difference Galois theory. The concepts in the right-hand column will be introduced in the next sections.

Galois theory	Difference Galois theory
Polynomial equations	Difference equations
Rings	Difference rings
Fields	Difference fields
Splitting fields	Picard–Vessiot rings and total Picard–Vessiot rings
Galois groups	Difference Galois groups
Finite groups	Linear algebraic groups

4 Difference Rings and Difference Fields

Definition 4.1 A difference ring is a couple (R, ϕ) where R is a ring and ϕ is a ring automorphism of R. If R is a field, then (R, ϕ) is called a difference field.

Example 4.2 The couple (R, ϕ) is a difference ring in the following cases:

1. any ring R and $\phi = \mathrm{Id}_R$;
2. $R = \mathbb{C}(z)$ and $\phi: f(z) \mapsto f(qz)$ where $q \in \mathbb{C}^\times$;
3. $R = \mathbb{C}(z)$ and $\phi: f(z) \mapsto f(z + h)$ where $h \in \mathbb{C}$;
4. $R = \bigcup_{j \geq 0} \mathbb{C}(z^{p^{-j}})$ and $\phi: f(z) \mapsto f(z^p)$ where p is a positive integer. Note that $\mathbb{C}(z)$ endowed with $\phi: f(z) \mapsto f(z^p)$ is not a difference field because ϕ is not surjective.
5. $R = \mathbb{C}^{\mathbb{Z}}$ and $\phi: (x_n)_{n \in \mathbb{Z}} \mapsto (x_{n+1})_{n \in \mathbb{Z}}$.

Definition 4.3 Let (R, ϕ) be a difference ring. An ideal I of R such that $\phi(I) \subset I$ is called a difference ideal of (R, ϕ). We say that (R, ϕ) is a simple difference ring if its difference ideals are $\{0\}$ and R.

Exercise 4.4 Let (R, ϕ) be a difference ring. Let I be a maximal difference ideal of (R, ϕ), i.e., a proper difference ideal of (R, ϕ) which is maximal among the difference ideals of (R, ϕ) (be careful, I is not necessarily a maximal ideal). Prove that $\phi(I) = I$.

Exercise 4.5 Let I be a difference ideal of the difference ring (R, ϕ). Then, ϕ induces a ring endomorphism $\overline{\phi}$ of R/I.

Prove that $(R/I, \overline{\phi})$ is a difference ring if and only if $\phi(I) = I$.

Exercise 4.6 Let (R, ϕ) be a difference ring.

1. Prove that if R is a Noetherian ring and if I is a difference ideal of (R, ϕ) then $\phi(I) = I$.
2. Give an example of difference ring (R, ϕ) such that $\phi(I) \subsetneq I$.

Example 4.7 1. Any difference field is a simple difference ring.

2. Consider the difference ring (R, ϕ) where $R = \mathbb{C}(z)[y, y^{-1}]$ is the ring of Laurent polynomials with coefficients in $\mathbb{C}(z)$ and ϕ is the ring automorphism of R defined by $\phi\big(f(z, y)\big) = f(z + 1, zy)$. We claim that (R, ϕ) is a simple difference ring. Indeed, let I be a nonzero difference ideal of (R, ϕ). Note that R is a principal

ideal domain (in particular, it is Noetherian, so $\phi(I) = I$ according to Exercise 4.6). Let $P(z, y) \in R \setminus \{0\}$ be such that $I = \big(P(z, y)\big)$. We have $\phi(I) = \big(P(z+1, zy)\big)$. Since $\phi(I) = I$, we get $P(z+1, zy) = c(z)y^i P(z, y)$ for some $c(z) \in \mathbb{C}(z)^\times$ and $i \in \mathbb{Z}$. It follows easily that $P(z, y)$ is a monomial in y. So $P(z, y) \in R^\times$ and, hence, $I = R$.

3. The difference ring (R, ϕ) where $R = \mathbb{C}(z)[y]$ is the ring of polynomials with coefficients in $\mathbb{C}(z)$ and ϕ is the ring automorphism of R given by $\phi\big(f(z, y)\big) = f(z+1, zy)$ is not a simple difference ring. Indeed, (y) is a proper nontrivial difference ideal.

Definition 4.8 A morphism (resp. isomorphism) from the difference ring (R, ϕ) to the difference ring $(\widetilde{R}, \tilde{\phi})$ is a ring morphism (resp. isomorphism) $\varphi: R \to \widetilde{R}$ such that $\varphi \circ \phi = \tilde{\phi} \circ \varphi$.

Exercise 4.9 Prove that, for difference rings, "being isomorphic" is an equivalence relation.

Exercise 4.10 We have already seen that $\mathbb{C}(z)$ endowed with the ring automorphism $\sigma_q: f(z) \mapsto f(qz)$ $(q \in \mathbb{C}^\times)$ or $\tau_h: f(z) \mapsto f(z+h)$ $(h \in \mathbb{C})$ is a difference field. Prove that, up to isomorphism, these are the only difference fields of the form $(\mathbb{C}(z), \phi)$ such that $\phi_{|\mathbb{C}} = \mathrm{Id}_{\mathbb{C}}$. **Hint.** We recall that, as any field automorphism of $\mathbb{C}(z)$ over $\mathbb{C}$, ϕ is of the form $f(z) \mapsto f\big((az+b)/(cz+d)\big)$ for some $a, b, c, d \in \mathbb{C}$ such that $ad - bc \neq 0$. If it is not equal to the identity, the automorphism $z \mapsto (az+b)/(cz+d)$ of $\mathbb{P}^1(\mathbb{C})$ has one or two fixed points and is conjugate to some $z \mapsto z + h$ if it has one fixed point and conjugate to some $z \mapsto qz$ if it has two fixed points.

Definition 4.11 A difference ring $(\widetilde{R}, \tilde{\phi})$ is a difference ring extension of a difference ring (R, ϕ) if $\widetilde{R}$ is a ring extension of R and if $\tilde{\phi}_{|R} = \phi$; in this case, we will often denote $\tilde{\phi}$ by ϕ.

A difference ring (R, ϕ) is a difference subring of a difference ring $(\widetilde{R}, \tilde{\phi})$ if $(\widetilde{R}, \tilde{\phi})$ is a difference ring extension of (R, ϕ).

Two difference ring extensions $(\widetilde{R}_1, \tilde{\phi}_1)$ and $(\widetilde{R}_2, \tilde{\phi}_2)$ of a difference ring (R, ϕ) are isomorphic over (R, ϕ) if there exists a difference ring isomorphism φ from $(\widetilde{R}_1, \tilde{\phi}_1)$ to $(\widetilde{R}_2, \tilde{\phi}_2)$ such that $\varphi_{|R} = \mathrm{Id}_R$.

Definition 4.12 The ring of constants R^ϕ of the difference ring (R, ϕ) is defined by

$$R^\phi := \{f \in R \mid \phi(f) = f\} .$$

Exercise 4.13 Let (R, ϕ) be a difference ring.

1. Prove that the ring of constants R^ϕ is a ring (!).
2. Prove that if R is a field then R^ϕ is a field.

Exercise 4.14 Let (k', ϕ) be a difference field extension of a difference field (k, ϕ).

1. Prove that if k' is an algebraic extension of k, then k'^{ϕ} is an algebraic extension of k^{ϕ}. In particular, if k' is an algebraic extension of k and if k^{ϕ} is algebraically closed, then $k'^{\phi} = k^{\phi}$.
2. Prove that if k is algebraically closed, then k^{ϕ} is not necessary algebraically closed.

Exercise 4.15 Let (k, ϕ) be a difference field. Prove that ϕ can be extended into a ring automorphism of $\bar{k}$, the algebraic closure of k. In other words, $\bar{k}$ can be endowed with a structure of difference field extension of (k, ϕ).

In what follows, we will frequently denote the difference ring (R, ϕ) by R.

5 Picard–Vessiot Theory

Let (k, ϕ) be a difference field and denote by $C := k^{\phi}$ its field of constants.

5.1 Picard–Vessiot Rings

Consider a difference system

$$\phi(Y) = AY \quad \text{with } A \in \mathrm{GL}_n(k) \,. \tag{1}$$

Definition 5.1 A Picard–Vessiot ring for (1) over (k, ϕ) is a difference ring extension R of (k, ϕ) such that

1. there exists $\mathfrak{Y} \in \mathrm{GL}_n(R)$ such that $\phi(\mathfrak{Y}) = A\mathfrak{Y}$ (such a $\mathfrak{Y}$ is called a fundamental matrix of solutions of (1));
2. R is generated, as a k-algebra, by the entries of $\mathfrak{Y}$ and $\det(\mathfrak{Y})^{-1}$;
3. R is a simple difference ring.

The Picard–Vessiot rings will play the same role as the splitting fields in classical Galois theory.

We shall now address the following questions:

1. Do Picard–Vessiot rings exist?
2. Are Picard–Vessiot extensions unique?

The answer to the first question is given by the following result.

Proposition 5.2 ([23, Sect. 1.1]) *There exists a Picard–Vessiot ring for* (1) *over* (k, ϕ).

Proof We shall first construct a difference ring extension of (k, ϕ) satisfying to conditions 1 and 2 of Definition 5.1. We let $X = (X_{i,j})_{1 \le i,j \le n}$ be a matrix of indeterminates and we consider the ring $k[X, \det(X)^{-1}]$ of polynomials with coefficients in k, in n^2 indeterminates, and localized at $\det(X)$. We consider the

unique difference ring extension $(k[X, \det(X)^{-1}], \psi)$ of (k, ϕ) defined by $\psi(X) = AX$. The first two conditions of Definition 5.1 are satisfied by $(k[X, \det(X)^{-1}], \psi)$, but not necessarily the last one.

Example 5.3 1. Consider the case $k = \mathbb{C}(z)$, $\phi: f(z) \mapsto f(qz)$, $q \in \mathbb{C}^\times$, and $A(z) = -1 \in \mathrm{GL}_1(\mathbb{C})$. Then, the difference ring $(k[X, \det(X)^{-1}] = k[X, X^{-1}], \psi)$ is not simple. For instance, $(X^2 - 1)$ is a proper nontrivial difference ideal.

2. Consider the case $k = \mathbb{C}(z)$, $\phi: f(z) \mapsto f(qz)$, $q \in \mathbb{C}^\times$, and $A(z) = q^{1/2} \in \mathrm{GL}_1(\mathbb{C})$. Then, the difference ring $(k[X, \det(X)^{-1}] = k[X, X^{-1}], \psi)$ is not simple. For instance, $(X^2 - z)$ is a proper nontrivial difference ideal.

3. Consider the case $k = \mathbb{C}(z)$, $\phi: f(z) \mapsto f(qz)$, $q \in \mathbb{C}^\times$, and $A(z) = z \in \mathrm{GL}_1(\mathbb{C})$. Then, the difference ring $(k[X, \det(X)^{-1}] = k[X, X^{-1}], \psi)$ is simple. Indeed, let I be a nonzero difference ideal. Let $P(z, X) \in k[X, \det(X)^{-1}]$ be such that $I = \big(P(z, X)\big)$. Since $\big(P(qz, zX)\big) = \psi(I) = I = \big(P(X)\big)$, there exists $c(z) \in k^\times$ and $i \in \mathbb{Z}$ such that $P(qz, zX) = c(z)X^i P(z, X)$. So, $i = 0$ and it is easily seen that $P(z, X)$ is a monomial in X and, hence, is invertible in $k[X, \det(X)^{-1}]$. Thus, $I = k[X, \det(X)^{-1}]$.

In order to remedy this problem, we consider a maximal difference ideal I of R, i.e., a proper difference ideal of R which is maximal among the difference ideals of R (be careful, I is not necessarily a maximal ideal) and we consider the difference ring extension

$$(R, \phi) = (k[X, \det(X)^{-1}]/I, \bar{\psi})$$

of (k, ϕ) where $\phi = \bar{\psi}: R \to R$ is the ring automorphism induced by ψ (see Exercises 4.4 and 4.5). It is clear that the first two conditions of Definition 5.1 are satisfied by (R, ϕ). Moreover, the 1–1 correspondence between the difference ideals of $k[X, \det(X)^{-1}]/I$ and the difference ideals of $k[X, \det(X)^{-1}]$ containing I (see Exercise 4.5) shows that (R, ϕ) is a simple difference ring. This concludes the proof of the existence of the Picard–Vessiot rings.

Example 5.4 1. We come back to the case $k = \mathbb{C}(z)$, $\phi: f(z) \mapsto f(qz)$, $q \in \mathbb{C}^\times$, $A(z) = -1 \in \mathrm{GL}_1(\mathbb{C})$. Then, $(X^2 - 1)$ is a maximal difference ideal of $(k[X, X^{-1}], \psi)$. Indeed, the proper ideals of $k[X, X^{-1}]$ containing (X^2-1) are $(X-1)$ and $(X+1)$ and none of them is stable by ϕ. Therefore, a Picard–Vessiot ring is given by $(k[X, X^{-1}]/(X^2 - 1), \bar{\psi})$.

2. We come back to the case $k = \mathbb{C}(z)$, $\phi: f(z) \mapsto f(qz)$, $q \in \mathbb{C}^\times$, $A(z) = q^{1/2} \in \mathrm{GL}_1(\mathbb{C})$. Then, $(X^2 - z)$ is a maximal ideal of $k[X, X^{-1}]$ (because $X^2 - z$ is irreducible) and, hence, a maximal difference ideal of $(k[X, X^{-1}], \psi)$. Therefore, a Picard–Vessiot ring is given by $(k[X, X^{-1}]/(X^2 - z), \bar{\psi})$, which is isomorphic over (k, ϕ) to $k[z^{1/2}, z^{-1/2}]$ endowed with the automorphism $f(z^{1/2}) \mapsto f(q^{1/2}z^{1/2})$.

3. We come back to the case $k = \mathbb{C}(z)$, $\phi: f(z) \mapsto f(qz)$, $q \in \mathbb{C}^\times$, $A(z) = z \in \mathrm{GL}_1(\mathbb{C})$. Then, a Picard–Vessiot ring is given by $(k[X, X^{-1}], \psi)$. □

Note the following fundamental property of the Picard–Vessiot rings:

Proposition 5.5 ([23, Lemma 1.18]) *Assume that the characteristic of k is 0 and that C is algebraically closed. Then, for any Picard–Vessiot ring R for (1) over (k, ϕ), we have*

$$R^{\phi} = C .$$

This is consistent with the discussion of Sect. 2. We will see later, in Proposition 5.14, another characterization of the Picard–Vessiot rings very close to the spirit of the discussion of Sect. 2.

Our question concerning uniqueness is answered by the following result.

Theorem 5.6 ([23, Proposition 1.19]) *Assume that the characteristic of k is 0 and that C is algebraically closed. Then, any two Picard–Vessiot rings for (1) over (k, ϕ) are isomorphic over the difference ring (k, ϕ).*

Remark 5.7 If C is not algebraically closed, then the previous two results may fail. Indeed, let us come back to the case $k = \mathbb{C}(z)$, $\phi: f(z) \mapsto f(qz)$, $A(z) = -1 \in \mathrm{GL}_1(\mathbb{C})$ in the special case $q = -1$. Then $\mathbb{C}(z)^{\phi} = \mathbb{C}(z^2)$ is not algebraically closed. The proof of Theorem 5.2 yields the Picard–Vessiot ring $(R, \phi) = (\mathbb{C}(z)[X, X^{-1}]/(X^2 - 1), \phi)$ where ϕ is determined by $\phi(\overline{X}) = -\overline{X}$. This difference ring has new constants with respect to the base difference field (k, ϕ), e.g., $\overline{zX}$ belongs to R^{ϕ} but not to $k^{\phi} = \mathbb{C}(z)^{\phi} = \mathbb{C}(z^2)$. On the other hand, $\mathbb{C}(z)$ endowed with ϕ is itself is a Picard–Vessiot ring for $\phi(y) = -y$ over k (because z is a fundamental matrix of solutions of $\phi(y) = -y$). The two difference rings R and k are not isomorphic.

Hypothesis 5.8 From now on, we assume that the characteristic of k is 0 and that C is algebraically closed.

We shall now study the structure of the Picard–Vessiot rings in more details. We start with an example.

Example 5.9 We pursue the study of the example $k = \mathbb{C}(z)$, $\phi: f(z) \mapsto f(qz)$, $q \in \mathbb{C}^{\times}$, and $A(z) = -1 \in \mathrm{GL}_1(\mathbb{C})$. A Picard–Vessiot ring is given by the unique difference ring extension $(R, \phi) = (k[X, X^{-1}]/(X^2 - 1), \phi)$ of (k, ϕ) such that $\phi(\overline{X}) = -\overline{X}$. Note that R is not a domain, so that the Picard–Vessiot rings are not integral domains in general (in particular, it is in general impossible to realize the Picard–Vessiot rings as subrings of some field of meromorphic functions). Letting $R'_0 = k[X, X^{-1}]/(X-1)$ and $R'_1 = k[X, X^{-1}]/(X+1)$, the Chinese reminder theorem ensures that

$$\begin{aligned} f: R &\to R'_0 \oplus R'_1 = R' \\ \overline{P} &\mapsto (\widehat{P}, \widetilde{P}) \end{aligned}$$

is a ring isomorphism. This is even a difference ring isomorphism if R' is endowed with the automorphism

$$\phi' = f \circ \phi \circ f^{-1} .$$

We let $e'_0 = (\hat{1}, \tilde{0}) = f\big((X+1)/2\big) \in R'_0 \oplus R'_1$ and $e'_1 = (\hat{0}, \tilde{1}) = f\big((-X+1)/2\big) \in R'_0 \oplus R'_1$. We have

$$R'_0 = R'e'_0 \quad \text{and} \quad R'_1 = R'e'_1.$$

Moreover, we have

$$\phi'(e'_0) = f \circ \phi \circ f^{-1}(e'_0) = f\left(\phi\left(\frac{X+1}{2}\right)\right) = f\left(\frac{-X+1}{2}\right) = e'_1$$

and

$$\phi'(e'_1) = f \circ \phi \circ f^{-1}(e'_1) = f\left(\phi\left(\frac{-X+1}{2}\right)\right) = f\left(\frac{X+1}{2}\right) = e'_0 .$$

So, letting $R_0 = f^{-1}(R'_0)$, $e_0 = f^{-1}(e'_0)$ and $R_1 = f^{-1}(R'_1)$, $e_1 = f^{-1}(e'_1)$, we have decomposed R as a direct product of rings

$$R = R_0 \oplus R_1 \quad \text{with} \quad \breve{a}R_i = Re_i$$

where

- e_0 and e_1 are idempotent elements of R,
- R_0 and R_1 are integral domains,
- $\phi(e_0) = e_1$ and $\phi(e_1) = e_0$, hence, $\phi(R_0) = R_1$ and $\phi(R_1) = R_0$.

Remark 5.10 In the case $k = \mathbb{C}(z)$, $\phi: f(z) \mapsto f(qz)$, $q \in \mathbb{C}^\times$, $A(z) = q^{1/2}$ or $z \in \mathrm{GL}_1(\mathbb{C})$, the Picard–Vessiot rings described in Example 5.4 are integral domains.

Actually, the property discovered in the previous example is a special case of a general fact.

Theorem 5.11 ([23, Corollary 1.16]) *We can decompose R as a direct product of rings*

$$R = \bigoplus_{x \in X} R_x \quad \textit{with } R_x = Re_x$$

where

- *$X = \mathbb{Z}/t\mathbb{Z}$ for some integer $t \geq 1$,*
- *for all $x \in X$, e_x is an idempotent element of R (and, hence, $e_x = 1_{R_x}$),*
- *for all $x \in X$, R_x is an integral domain,*
- *for all $x \in X$, $\phi(e_x) = e_{x+1_x}$ and, hence, $\phi(R_x) = R_{x+1_x}$.*

5.2 Total Picard–Vessiot Rings

We maintain the notations and hypotheses of the previous section. In particular, we assume that k has characteristic 0 and that C is algebraically closed. We let R be a Picard–Vessiot ring over k attached to the system (1). Since R is not necessary an integral domain, we cannot consider its field of fractions in general. But, we can consider its total ring of fractions K, i.e.,

$$K = S^{-1}R$$

where S is the multiplicative subset of R made of the nonzero divisors (if R is an integral domain, then K is nothing but the field of fractions of R). Recall that

$$S^{-1}R = R \times R/\sim$$

where $\sim$ is the equivalence relation on $R \times R$ defined by

$$(r, s) \sim (r', s') \iff \exists t \in S, t(rs' - r's) = 0 .$$

The equivalence class of (r, s) will be denoted by r/s. There is a natural ring structure on $S^{-1}R$ given by

$$r/s + r'/s' = (rs' + r's)/(ss') \quad \text{and} \quad (r/s)(r'/s') = (rr')/(ss') .$$

Moreover, $\phi: R \to R$ admits a unique extension into a ring automorphism $\phi: K \to K$, and it is given by

$$\phi(r/s) = \phi(r)/\phi(s).$$

Definition 5.12 In this way, K is a difference ring extension of R, called the total Picard–Vessiot ring of (1) over (k, ϕ).

In the process of taking the total quotient ring, we have not increased the ring of constants:

Proposition 5.13 *We have $K^\phi = C$.*

Proof Indeed, consider $r/s \in K^\phi$. Then, $I = \{a \in R \mid ar/s \in R\}$ is a difference ideal of R containing s, so $I = R$. In particular, $1 \in I$ and hence $r/s \in R$. Therefore, $K^\phi = R^\phi = C$. □

We consider a decomposition of R as given by Theorem 5.11:

$$R = \bigoplus_{x \in X} R_x.$$

It is easily seen that K can be identified with the direct product of fields

$$K = \bigoplus_{x \in X} K_x$$

where K_x is the field of fractions of R_x.

Collecting the previous results, we obtain the direct implication of the following result, which gives a new characterization of the Picard–Vessiot rings; for the proof of the other implication, we refer to [23, Corollary 1.24].

Proposition 5.14 ([23, Corollary 1.24]) *Let R be a difference ring extension of (k, ϕ). Then, R is a Picard–Vessiot ring for (1) if and only if the following properties hold*:

1. *R has no nilpotent element*;
2. *the ring of constants of the total quotient ring of R (i.e., of the associated total Picard–Vessiot ring) is C*;
3. *there exists $\mathfrak{Y} \in \mathrm{GL}_n(R)$ such that $\phi(\mathfrak{Y}) = A\mathfrak{Y}$*
4. *R is minimal with respect to the above properties.*

Remark 5.15 In the previous result, it is important to consider the ring of constants of the total Picard–Vessiot ring associated to R, and not only of the Picard–Vessiot ring R; see [23, Example 1.25].

6 Difference Galois Groups

Let (k, ϕ) be a difference field. We assume that k is of characteristic 0 and that the field of constants $C := k^\phi$ is algebraically closed.

Consider a difference system

$$\phi(Y) = AY \quad \text{with } A \in \mathrm{GL}_n(k)\ . \tag{2}$$

We let R be a Picard–Vessiot ring for this system over k, and we denote by K the corresponding total Picard–Vessiot ring.

Definition 6.1 The corresponding difference Galois group $\mathrm{Gal}^\phi(R/k)$ over (k, ϕ) of (2) is the group of the k-linear ring automorphisms of R commuting with ϕ:

$$\mathrm{Gal}^\phi(R/k) := \{\sigma \in \mathrm{Aut}(R/k) \mid \phi \circ \sigma = \sigma \circ \phi\}\ .$$

Example 6.2 1. We come back to the case $k = \mathbb{C}(z)$, $\phi : f(z) \mapsto f(qz)$, $q \in \mathbb{C}^\times$ not a root of the unity, $A(z) = -1 \in \mathrm{GL}_1(\mathbb{C})$. We recall that a Picard–Vessiot ring is given by $(R, \phi) = (k[X, X^{-1}]/(X^2 - 1), \phi)$ where ϕ is determined by $\phi(\overline{X}) = -\overline{X}$. Let $\sigma \in \mathrm{Gal}^\phi(R/k)$. Then, we have $\phi\big(\sigma(\overline{X})\big) = \sigma\big(\phi(\overline{X})\big) = \sigma(-\overline{X}) = -\sigma(\overline{X})$. Therefore, there exists $c \in k^\phi = \mathbb{C}$ such that $\sigma(\overline{X}) = c\overline{X}$. Moreover, we have $\overline{X}^2 = 1 \in k$ so $\sigma(\overline{X})^2 = \sigma(\overline{X}^2) = \sigma(1) = 1$, i.e., $c^2\overline{X}^2 = c^2 = 1$ and, hence, $c = \pm 1$.

It follows that $\mathrm{Gal}^{\phi}(R/k) \subset \{\mathrm{Id}_R, \sigma\}$ where σ is the unique automorphism of R/k such that $\sigma(\overline{X}) = -\overline{X}$. It is easily seen that this inclusion is actually an equality.
2. We come back to the case $k = \mathbb{C}(z)$, $\phi{:}f(z) \mapsto f(qz)$, $q \in \mathbb{C}^{\times}$ not a root of the unity, $A(z) = q^{1/2} \in \mathrm{GL}_1(\mathbb{C})$. We recall that a Picard–Vessiot ring is given by $R = k[z^{1/2}, z^{-1/2}]$ endowed with the automorphism $f(z^{1/2}) \mapsto f(q^{1/2}z^{1/2})$. Arguing as in the previous example, one can prove that $\mathrm{Gal}^{\phi}(R/k) = \{\mathrm{Id}_R, \sigma\}$ where σ is the unique automorphism of R/k such that $\sigma(z^{1/2}) = -z^{1/2}$.
3. We come back to the case $k = \mathbb{C}(z)$, $\phi{:}f(z) \mapsto f(qz)$, $q \in \mathbb{C}^{\times}$ not a root of the unity, $A(z) = z \in \mathrm{GL}_1(\mathbb{C})$. Then, a Picard–Vessiot ring is given by $(R, \phi) = (k[X, X^{-1}], \phi)$, where ϕ is determined by $\phi(X) = zX$. Then, we have $\mathrm{Gal}^{\phi}(R/k) = \{\sigma_c \mid c \in \mathbb{C}^{\times}\}$ where σ_c is the unique automorphism of R/k such that $\sigma(X) = cX$.

Exercise 6.3 Set

$$\mathrm{Gal}^{\phi}(K/k) := \{\sigma \in \mathrm{Aut}(K/k) \mid \phi \circ \sigma = \sigma \circ \phi\}.$$

Prove that the map

$$\begin{aligned} \mathrm{Gal}^{\phi}(K/k) &\to \mathrm{Gal}^{\phi}(R/k) \\ \sigma &\mapsto \sigma_{|R} \end{aligned}$$

is well-defined (i.e., takes its values in $\mathrm{Gal}^{\phi}(R/k)$) and gives a group isomorphism between $\mathrm{Gal}^{\phi}(K/k)$ and $\mathrm{Gal}^{\phi}(R/k)$.

Exercise 6.4 What happens if we choose another Picard–Vessiot ring?

One can identify $\mathrm{Gal}^{\phi}(R/k)$ with a subgroup of $\mathrm{GL}_n(C)$ as follows (this is analogous to the identification of the Galois group of an algebraic equation to a group of permutations of its roots). Let $\mathcal{Y} \in \mathrm{GL}_n(R)$ be a fundamental matrix of solutions of (2). For any $\sigma \in \mathrm{Gal}^{\phi}(R/k)$, there exists a unique $C(\sigma) \in \mathrm{GL}_n(C)$ such that

$$\sigma(\mathcal{Y}) = \mathcal{Y}C(\sigma)\ .$$

Indeed, we have $\phi(\mathcal{Y}) = A\mathcal{Y}$ so $\sigma\big(\phi(\mathcal{Y})\big) = \sigma(A\mathcal{Y})$ and, hence, $\phi\big(\sigma(\mathcal{Y})\big) = A\sigma(\mathcal{Y})$. It follows that $\mathcal{Y}^{-1}\sigma(\mathcal{Y})$ is left invariant by ϕ and, hence, has coefficients in C. Moreover, $\det\big(\mathcal{Y}^{-1}\sigma(\mathcal{Y})\big) = \det(\mathcal{Y})^{-1}\sigma\big(\det(\mathcal{Y})\big) \in R^{\times}$. Therefore, $\mathcal{Y}^{-1}\sigma(\mathcal{Y})$ belongs to $M_n(C) \cap \mathrm{GL}_n(R) = \mathrm{GL}_n(C)$, as expected.

The proof of the following result is left as an exercise.

Proposition 6.5 *The map*

$$\begin{aligned} \rho_{\mathrm{gal}}\colon \mathrm{Gal}^{\phi}(R/k) &\to \mathrm{GL}_n(C) \\ \sigma &\mapsto C(\sigma) \end{aligned}$$

is faithful linear representation of $\mathrm{Gal}^{\phi}(R/k)$ (*i.e., an injective group morphism*). *Its image is denoted by* G_{gal}.

Exercise 6.6 What happens to ρ_{gal} if we choose another fundamental matrix of solutions $\mathfrak{Y} \in \mathrm{GL}_n(R)$?

Example 6.7 For the cases 1 to 3 considered in Example 6.2, we have $G_{\mathrm{gal}} = \{\pm 1\}, \{\pm 1\}$ and $\mathbb{C}^\times$ for the choices $\mathfrak{y} = \overline{X}, z^{1/2}$ and X respectively.

We now come to a crucial property of the difference Galois groups.

Theorem 6.8 ([23, Theorem 1.13]) *The image G_{gal} of ρ_{gal} is an* algebraic *subgroup of* $\mathrm{GL}_n(C)$.

Recall that this means that G_{gal} is

- a subgroup of $\mathrm{GL}_n(C)$ and
- the zero-locus of a set of polynomials in $C[(X_{i,j})_{1\leq i,j\leq n}, \det X^{-1}]$.

7 Galois Groups and Algebraic Relations

We let (k, ϕ) be a difference field. We assume that k is of characteristic 0 and that the field of constants $C := k^\phi$ is algebraically closed.

Consider a difference system

$$\phi(Y) = AY \quad \text{with } A \in \mathrm{GL}_n(k)\ . \tag{3}$$

We let R be a Picard–Vessiot ring for this system over k. Let $\mathfrak{y} \in \mathrm{GL}_n(R)$ be a fundamental matrix of solutions of (3). We denote by

$$\begin{aligned} \rho_{\mathrm{gal}}\colon \mathrm{Gal}^\phi(R/k) &\to \mathrm{GL}_n(C) \\ \sigma &\mapsto C(\sigma) \end{aligned}$$

the faithful linear representation attached to $\mathfrak{y}$ as in Sect. 6, so that, for all $\sigma \in \mathrm{Gal}^\phi(R/k)$, $\sigma(\mathfrak{Y}) = \mathfrak{Y}C(\sigma)$. We set

$$G_{\mathrm{gal}} = \mathrm{Im}(\rho_{\mathrm{gal}})\ .$$

The aim of this section is to give a precise meaning to the following assertion:

> "the difference Galois group $\mathrm{Gal}(R/k)$ measures the algebraic relations among the solutions of the difference system (3)."

We let I be the ideal of the algebraic relations in $k[X, \det(X)^{-1}]$ among the entries of $\mathfrak{y}$, i.e., I is the kernel of the unique k-algebra morphism $\varphi\colon k[X, \det(X)^{-1}] \to R$ such that $\varphi(X) = \mathfrak{y}$. So, I is a maximal difference ideal of $k[X, \det(X)^{-1}]$. We will use the following exercise in what follows.

Exercise 7.1 Prove that I is a radical ideal.

7.1 The Case When k Is Algebraically Closed

We shall first assume that k is algebraically closed.

We let V be the k-algebraic subset of $\mathrm{GL}_n(k)$ defined by I, i.e.,

$$V = \{v \in \mathrm{GL}_n(k) \mid \forall P(X) \in I, P(v) = 0\} .$$

We have a natural map

$$\begin{aligned} V \times G_{\mathrm{gal}} &\to V \\ (v, M) &\mapsto vM . \end{aligned}$$

Indeed, for any $\big(v, M = C(\sigma)\big) \in V \times G_{\mathrm{gal}}$, we have, for all $P \in I$, $P(v) = 0$ so $P\big(vC(\sigma)\big) = P\big(\sigma(v)\big) = \sigma\big(P(v)\big) = 0$ so $vC(\sigma) \in V$. One deduces easily that we have the natural map

$$\begin{aligned} V \times G_{\mathrm{gal}}(k) &\to V \\ (v, M) &\mapsto vM \end{aligned}$$

where $G_{\mathrm{gal}}(k)$ is the C-algebraic subgroup of $\mathrm{GL}_n(k)$ defined by the equations of G_{gal} seen as an algebraic subgroup of $\mathrm{GL}_n(C)$. This group action is actually transitive:

Theorem 7.2 ([23, Theorem 1.13]) *For all $v, w \in V$, there exists a unique $M \in G_{\mathrm{gal}}(k)$ such that*

$$w = vM .$$

We denote by J_c the ideal of $C[X, \det(X)^{-1}]$ defining G_{gal}, i.e.,

$$J_c = \{P(X) \in C[X, \det(X)^{-1}] \mid \forall M \in G_{\mathrm{gal}}, P(M) = 0\} .$$

We denote by J_k the ideal of $k[X, \det(X)^{-1}]$ defining $G_{\mathrm{gal}}(k)$, i.e.,

$$J_k = \{P(X) \in k[X, \det(X)^{-1}] \mid \forall M \in G_{\mathrm{gal}}(k), P(M) = 0\} .$$

We have

$$J_k = kJ_c .$$

Consider $v \in V$ (V is nonempty). Theorem 7.2 ensures that

$$V = vG_{\mathrm{gal}}(k) .$$

This yields the following description of the algebraic relations with coefficients in k among the entries of $\mathfrak{y}$ in terms of the algebraic equations defining the algebraic group G_{gal}:

Proposition 7.3 *We have*

$$I = \{P(v^{-1}X) \mid P(X) \in J_k\} = \{P(v^{-1}X) \mid P(X) \in kJ_c\}\ .$$

Example 7.4 For instance, if

$$G_{\mathrm{gal}} = \{M \in \mathrm{GL}_n(C) \mid (\det M)^m = 1\}$$

for some positive integer m, then

$$I = \left((\det X)^m - \lambda\right)$$

for some $\lambda = \det(v)^m \in k^\times$.

Exercise 7.5 Another way to state this is that the k-algebras $C[G_{\mathrm{gal}}] \otimes_c k$ and R are isomorphic. Prove this and give an isomorphism.

7.2 The General Case

We no longer assume that k is algebraically closed. Then, the previous results are false in general, as shown by the following example.

Example 7.6 Consider the case $k = \mathbb{C}(z)$, $\phi = \sigma_q$, $q \in \mathbb{C}^\times$ not a root of the unity, $\phi(y) = q^{1/2}y$. A Picard–Vessiot ring is given by $R = k[z^{1/2}, z^{-1/2}]$ with $\phi(z^{1/2}) = q^{1/2}z^{1/2}$. A fundamental solution is given by $\mathfrak{y} = z^{1/2} \in \mathrm{GL}_1(R)$. The Galois group is $G_{\mathrm{gal}} = \{\pm 1\} \subset \mathrm{GL}_1(\mathbb{C})$ so that $C[G_{\mathrm{gal}}] = C[X, X^{-1}]/(X^2 - 1)$. Then, R and $C[G_{\mathrm{gal}}] \otimes_c k$ are not isomorphic since the former is an integral domain, but not the latter. However, these rings become isomorphic if we tensor with $\bar{k}$ over k.

Actually, we have the following result:

Proposition 7.7 ([23, Theorem 1.13]) *We have*

$$\bar{k}I = \{P(v^{-1}X) \mid P \in \bar{k}J_c\}\ .$$

Exercise 7.8 Another way to state this is that the rings $C[G_{\mathrm{gal}}] \otimes_c \bar{k}$ and $R \otimes_k \bar{k}$ are isomorphic. Prove this and give an isomorphism.

Remark 7.9 Actually, what precedes can be (and must be) rephrased in terms of torsors.

In some circumstances, we do not need to go to $\bar{k}$. For instance, if G_{gal} is connected and k is a $\mathcal{C}^1$-field, then Proposition 7.3 is true even if k is not algebraically closed. (The $G_{\mathrm{gal}} \otimes k$-torsors are trivial in this case.)

8 Galois Correspondence

Let (k, ϕ) be a difference field. We assume that k is of characteristic 0 and that the field of constants $C := k^\phi$ is algebraically closed.

Consider a difference system

$$\phi(Y) = AY \quad \text{with } A \in \mathrm{GL}_n(k) \,. \tag{4}$$

Let R be a Picard–Vessiot ring for this system over k and denote by K the corresponding total Picard–Vessiot ring. We consider its difference Galois group $\mathrm{Gal}^\phi(R/k) = \mathrm{Gal}^\phi(K/k)$ (see Exercise 6.3 for the identification between the two groups), endowed with its structure of linear algebraic group.

There is a Galois correspondence in difference Galois theory. Note that the total Picard–Vessiot rings are used instead of the Picard–Vessiot rings themselves.

Theorem 8.1 ([23, Theorem 1.29]) *Let $\mathcal{F}$ be the set of difference subrings F of K such that $k \subset F$ and such that every nonzero divisor of F is actually a unit of F. Let $\mathcal{G}$ be the set of algebraic subgroups of* $\mathrm{Gal}^\phi(K/k)$. *Then,*

- *for any $F \in \mathcal{F}$, the set $G(K/F)$ of elements of* $\mathrm{Gal}^\phi(K/k)$ *which fix F pointwise is an algebraic subgroup of* $\mathrm{Gal}^\phi(K/k)$;
- *for any algebraic subgroup H of* $\mathrm{Gal}^\phi(K/k)$, $K^H := \{f \in K \mid \forall \sigma \in H, \sigma(f) = f\}$ *belongs to $\mathcal{F}$;*
- *the maps $\mathcal{F} \to \mathcal{G}$, $F \mapsto G(K/F)$ and $\mathcal{G} \to \mathcal{F}$, $H \mapsto K^H$ are each other's inverses.*

Remark 8.2 Note that, if R is an integral domain, then Theorem 8.1 gives a correspondence between the difference subfields of K containing k, on the one hand, and the algebraic subgroups of $\mathrm{Gal}^\phi(K/k)$, on the other hand.

In particular, for any subgroup H of $\mathrm{Gal}^\phi(K/k)$, if $K^H = k$, then H is Zariski-dense in $\mathrm{Gal}^\phi(K/k)$. We will use this fact in Sect. 9.

We also have the following property: if H is a normal algebraic subgroup of $\mathrm{Gal}^\phi(K/k)$, then the restriction morphism $\mathrm{Gal}^\phi(K/k) \to \mathrm{Gal}^\phi(K^H/k)$ induces an isomorphism $\mathrm{Gal}^\phi(K/k)/H \cong \mathrm{Gal}^\phi(K^H/k)$.

9 Galoisian Ambiguities Coming from Analysis for Regular q-Difference Equations

In this section, we study the Galois groups of the regular q-difference equations and their relationship with transcendental invariants introduced by Birkhoff, namely the connection matrices. The main references are Etingof's [15] and Sauloy's [30].

We shall first recall some classical facts concerning the monodromy of linear differential equations.

9.1 Monodromy and Differential Galois Groups

Consider a linear differential system

$$Y'(z) = A(z)Y(z) \quad \text{with } A(z) \in \mathrm{M}_n\big(\mathbb{C}(z)\big)\ . \tag{5}$$

Its set of singularities on $\mathbb{P}^1(\mathbb{C})$ is denoted by S.

We shall first recall the definition of the monodromy representation attached to this differential system. Let $z_0 \in \mathbb{P}^1(\mathbb{C}) \setminus S$. According to Cauchy's theorem, there exists $\mathfrak{Y}(z) \in \mathrm{GL}_n(\mathcal{O}_{\mathbb{P}^1(\mathbb{C}),z_0})$ such that

$$\mathfrak{Y}'(z) = A(z)\mathfrak{Y}(z)$$

(we have denoted by $\mathcal{O}_{\mathbb{P}^1(\mathbb{C})}$ the sheaf of analytic functions over $\mathbb{P}^1(\mathbb{C})$ and by $\mathcal{O}_{\mathbb{P}^1(\mathbb{C}),z_0}$ its stalk at z_0). Let

$$\gamma\colon [0,1] \to \mathbb{P}^1(\mathbb{C}) \setminus S$$

be a continuous path such that $\gamma(0) = \gamma(1) = z_0$. It turns out that $\mathfrak{Y}(z)$ can be analytically continued along γ.

Exercise 9.1 Prove this!

After analytic continuation along γ, we get a new solution $\gamma\mathfrak{Y}(z) \in \mathrm{GL}_n(\mathcal{O}_{\mathbb{P}^1(\mathbb{C}),z_0})$ of $Y'(z) = A(z)Y(z)$. Therefore, there exists $M(\gamma) \in \mathrm{GL}_n(\mathbb{C})$ such that

$$\gamma\mathfrak{Y}(z) = \mathfrak{Y}(z)M(\gamma)\ .$$

This matrix $M(\gamma)$ is called the monodromy matrix along γ of the differential equation (5). This matrix only depends on the homotopy class of γ in $\mathbb{P}^1(\mathbb{C}) \setminus S$. Therefore, we have a map

$$\rho_{\text{mono}}\colon \pi_1(\mathbb{P}^1(\mathbb{C}) \setminus S, z_0) \to \mathrm{GL}_n(\mathbb{C})$$
$$[\gamma] \mapsto M([\gamma]) := M(\gamma) .$$

This is a group morphism.

Definition 9.2 The map ρ_{mono} is a linear representation of $\pi_1(\mathbb{P}^1(\mathbb{C}) \setminus S, z_0)$ called the monodromy representation.

Its image is called the monodromy group and denoted by G_{mono}.

Exercise 9.3 We emphasize that the monodromy representation and group depends on the choice of $\mathfrak{Y}(z)$ and z_0. Study the dependence of the monodromy representation and group on z_0 and $\mathfrak{Y}(z)$.

On the other hand, we recall (see Sect. 2.2) that the differential Galois group of the differential system (5) can be described as

$$\mathrm{Gal}^{\mathrm{d}/\mathrm{d}z}\big(K/\mathbb{C}(z)\big) = \big\{\sigma \in \mathrm{Aut}\big(K/\mathbb{C}(z)\big) \;\big|\; \sigma \circ \mathrm{d}/\mathrm{d}z = \mathrm{d}/\mathrm{d}z \circ \sigma\big\}$$

where

$$K = \mathbb{C}(z)\big(\mathfrak{Y}(z)\big)$$

is the field generated over $\mathbb{C}(z)$ by the entries of $\mathfrak{Y}(z)$. We can realize $\mathrm{Gal}^{\mathrm{d}/\mathrm{d}z}\big(K/\mathbb{C}(z)\big)$ as an algebraic subgroup G_{gal} of $\mathrm{GL}_n(\mathbb{C})$ as follows (this is similar to what we did in Sect. 6). For any $\sigma \in \mathrm{Gal}^{\mathrm{d}/\mathrm{d}z}\big(K/\mathbb{C}(z)\big)$, there exists a unique $C(\sigma) \in \mathrm{GL}_n(C)$ such that

$$\sigma(U) = UC(\sigma) .$$

Then,

$$\rho_{\text{gal}}\colon \mathrm{Gal}^{\mathrm{d}/\mathrm{d}z}\big(K/\mathbb{C}(z)\big) \to \mathrm{GL}_n(C)$$
$$\sigma \mapsto C(\sigma)$$

is faithful linear representation of $\mathrm{Gal}^{\mathrm{d}/\mathrm{d}z}\big(K/\mathbb{C}(z)\big)$ and its image, denoted by G_{gal}, is an algebraic subgroup of $\mathrm{GL}_n(\mathbb{C})$.

We shall now prove that the monodromy is Galoisian. Indeed, any element of K can be continued meromorphically along any continuous path $\gamma\colon [0, 1] \to \mathbb{P}^1(\mathbb{C}) \setminus S$ such that $\gamma(0) = \gamma(1) = z_0$ (because the entries of $\mathfrak{Y}(z)$ can be analytically continued along any such path). This induces an element σ_γ of $\mathrm{Gal}^{\mathrm{d}/\mathrm{d}z}\big(K/\mathbb{C}(z)\big)$ such that

$$C(\sigma_\gamma) = M(\gamma) .$$

Therefore, we have proved the following result.

Proposition 9.4 *We have*

$$G_{\text{mono}} \subset G_{\text{gal}} .$$

In case the system is regular singular,[1] the differential Galois group is "what algebra see of analysis":

Theorem 9.5 (Schlesinger; [24, Theorem 5.8]) *Assume that the differential system* (5) *is regular singular. Then, the monodromy group* G_{mono} *is Zariski-dense in the Galois group* G_{gal}.

Remark 9.6 If the system is irregular, then this result may be false. The typical counter-example is $y'(z) = y(z)$. There is an extension of this result to arbitrary linear differential equations due to Ramis.

9.2 Birkhoff Connection Matrices and Difference Galois Groups

Let q be a nonzero complex number such that $|q| < 1$. We consider the difference field $(\mathbb{C}(z), \sigma_q)$ where $\sigma_q : f(z) \mapsto f(qz)$ and a q-difference system

$$\sigma_q Y = AY \quad \text{with } A \in \mathrm{GL}_n\big(\mathbb{C}(z)\big) . \tag{6}$$

Note that $\mathbb{C}(z)$ is of characteristic 0 and that the field of constants $\mathbb{C}(z)^{\sigma_q} = \mathbb{C}$ is algebraically closed. Thus, we can apply most of the results of the previous sections.

In this section, we assume that the following hypothesis is satisfied:

Hypothesis 9.7 The q-difference system (6) is regular at 0 and ∞, i.e., $A(z)$ is analytic at 0 and ∞ and

$$A(0) = A(\infty) = I_n .$$

Our first task is to construct fundamental matrices of solutions attached to 0 and ∞.

The infinite product

$$\mathfrak{Y}_0(z) = A(z)^{-1} A(qz)^{-1} A(q^2 z)^{-1} \cdots$$

defines an element of $\mathrm{GL}_n(\mathcal{O}_{\mathbb{P}^1(\mathbb{C}),0})$ such that

$$\mathfrak{Y}_0(qz) = A(z)\mathfrak{Y}_0(z) \quad \text{and} \quad \mathfrak{Y}_0(0) = I_n .$$

[1] This means that, for any $s \in S$, the growth of the entries of $\mathfrak{y}(z)$ as z tends to s along any sector of finite aperture and centered at s is at most polynomial.

This functional equation shows that $\mathfrak{Y}_0(z)$ can be extended into a meromorphic function over $\mathbb{C}$:

$$\mathfrak{Y}_0(z) \in \mathrm{GL}_n\big(\mathcal{M}(\mathbb{C})\big) .$$

We let

$$R_0 = \mathbb{C}(z)\Big[\mathfrak{Y}_0(z), \Big(\det\big(\mathfrak{Y}_0(z)\big)\Big)^{-1}\Big]$$

be the $\mathbb{C}(z)$-algebra generated by the entries of $\mathfrak{Y}_0(z)$ and the inverse of its determinant. This ring has a natural structure of difference ring extension of $(\mathbb{C}(z), \sigma_q)$. It is an integral domain, therefore its total Picard–Vessiot ring K_0 is nothing but the field of fractions of R_0:

$$K_0 = \mathbb{C}(z)\big(\mathfrak{Y}_0(z)\big) .$$

Proposition 9.8 ([15, Sect. 3]) *The difference ring R_0 is a Picard–Vessiot ring for the q-difference system (6) over $\mathbb{C}(z)$. Hence, the difference field K_0 is a total Picard–Vessiot ring for this system over $\mathbb{C}(z)$.*

Proof We use the characterization of the Picard–Vessiot rings given by Proposition 5.14. The only nontrivial point is that $K_0^{\sigma_q} = \mathbb{C}$. Let $f(z)$ be an element of $K_0^{\sigma_q}$. Then, $f(z)$ is meromorphic over $\mathbb{C}$ and satisfies $f(qz) = f(z)$. This implies that $f(z)$ is analytic over $\mathbb{C}^\times$. (Indeed, otherwise, $f(z)$ would have a pole $z_0 \in \mathbb{C}^\times$. Since $f(qz) = f(z)$, any element of $\{q^k z_0 \mid k \geq 0\}$ would be a pole of f as well. But this set accumulates at 0. This would be in contradiction with the fact that $f(z)$ is meromorphic at 0). Therefore, $f(z)$ induces an analytic function over the compact Riemann surface $\mathbb{C}^\times/q^{\mathbb{Z}}$. Such a function is necessarily constant. It follows that $f(z)$ itself is constant over $\mathbb{C}^\times$ and, hence, over $\mathbb{C}$. □

We have similar results at ∞. Indeed,

$$\mathfrak{Y}_\infty(z) = A(q^{-1}z)A(q^{-2}z)A(q^{-3}z)\cdots$$

defines an element of $\mathrm{GL}_n(\mathcal{O}_{\mathbb{P}^1(\mathbb{C}),\infty})$ such that

$$\mathfrak{Y}_\infty(qz) = A(z)\mathfrak{Y}_\infty(z) \quad \text{and} \quad \mathfrak{Y}_\infty(\infty) = I_n .$$

This functional equation shows that $\mathfrak{Y}_\infty(z)$ can be extended into a meromorphic function over $\mathbb{P}^1(\mathbb{C}) \setminus \{0\}$:

$$\mathfrak{Y}_0(z) \in \mathrm{GL}_n\big(\mathcal{M}(\mathbb{P}^1(\mathbb{C}) \setminus \{0\})\big) .$$

We let

$$R_\infty = \mathbb{C}(z)\Big[\mathfrak{Y}_\infty(z), \Big(\det\big(\mathfrak{Y}_\infty(z)\big)\Big)^{-1}\Big]$$

be the $\mathbb{C}(z)$-algebra generated by the entries of $\mathfrak{Y}_\infty(z)$ and the inverse of its determinant. This ring has a natural structure of difference ring extension of $(\mathbb{C}(z), \sigma_q)$. It is an integral domain, therefore its total Picard–Vessiot ring K_∞ is nothing but the field of fractions of R_∞:

$$K_\infty = \mathbb{C}(z)\big(\mathfrak{Y}_\infty(z)\big) .$$

Proposition 9.9 ([15, Sect. 3]) *The difference ring R_∞ is a Picard–Vessiot ring for the q-difference system (6) over $\mathbb{C}(z)$. Hence, the difference field K_∞ is a total Picard–Vessiot ring for this system over $\mathbb{C}(z)$.*

So, we have two Picard–Vessiot rings R_0 and R_∞. Theorem 5.5 ensures that they are isomorphic as difference rings extensions of $(\mathbb{C}(z), \sigma_q)$. In order to describe such an isomorphism, we introduce Birkhoff's connection matrix.

Definition 9.10 The Birkhoff connection matrix is defined by

$$\mathcal{P}(z) = \mathfrak{Y}_0(z)^{-1}\mathfrak{Y}_\infty(z) \in \mathrm{GL}_n\big(\mathcal{M}(\mathbb{C}^\times)\big).$$

It is easily seen that

$$\mathcal{P}(qz) = \mathcal{P}(z).$$

So, one can consider $\mathcal{P}(z)$ as meromorphic function over the complex torus $\mathbb{C}^\times/q^{\mathbb{Z}}$ (i.e., as an elliptic function).

We let S be the set of poles of $\mathcal{P}(z)$ or $\mathcal{P}(z)^{-1}$ in $\mathbb{C}^\times$.

Theorem 9.11 ([15, Theorem 3.1]) *For any $v \in \mathbb{C}^\times \setminus S$, there exists a unique isomorphism of difference ring extensions of $(\mathbb{C}(z), \sigma_q)$*

$$\tau_v : R_\infty \to R_0$$

such that

$$\tau_v\big(\mathfrak{Y}_\infty(z)\big) = \mathfrak{Y}_0(z)\mathcal{P}(v) .$$

It induces an isomorphism of difference field extensions of $(\mathbb{C}(z), \sigma_q)$

$$\tau_v : K_\infty \to K_0 .$$

Proof Let $X = (X_{i,j})_{1\le i,j\le n}$ be indeterminates over $\mathbb{C}(z)$. Consider the unique $\mathbb{C}(z)$-algebra morphism

$$\varphi_0 : \mathbb{C}(z)[X] \to \mathbb{C}(z)[\mathfrak{Y}_0(z)]$$

such that $\varphi_0(X) = \mathfrak{Y}_0(z)$ and let $I_0 = \ker(\varphi_0)$ (i.e., I_0 is the ideal of the algebraic relations with coefficients in $\mathbb{C}(z)$ among the entries of $\mathfrak{Y}_0(z)$). We denote by

$$\overline{\varphi_0}\colon \mathbb{C}(z)[X]/I_0 \to \mathbb{C}(z)[\mathfrak{Y}_0(z)]$$

the $\mathbb{C}(z)$-algebra isomorphism induced by φ_0.

We define φ_∞, I_∞ and $\overline{\varphi_\infty}$ similarly.

Consider $P(X) \in I_\infty$, so that $P\big(\mathfrak{Y}_\infty(z)\big) = P\big(\mathfrak{Y}_0(z)\mathcal{P}(z)\big) = 0$. Therefore, the function $P\big(\mathfrak{Y}_0(z)\mathcal{P}(v)\big)$, meromorphic over $\mathbb{C}$, vanishes at $q^k v$ for all integer k large enough. It follows that $P\big(\mathfrak{Y}_0(z)\mathcal{P}(v)\big) = 0$, i.e., $P\big(X\mathcal{P}(v)\big) \in I_0$. Hence, we have a well-defined ring morphism

$$\begin{aligned} \mathbb{C}(z)[X]/I_\infty &\to \mathbb{C}(z)[X]/I_0 \\ P(X) &\mapsto P\big(X\mathcal{P}(v)\big). \end{aligned}$$

This is actually a ring isomorphism; its inverse is given by

$$\begin{aligned} \mathbb{C}(z)[X]/I_0 &\to \mathbb{C}(z)[X]/I_\infty \\ P(X) &\mapsto P(X\mathcal{P}(v)^{-1}) \ . \end{aligned}$$

Therefore,

$$\overline{\varphi_0} \circ \iota \circ \overline{\varphi_\infty}^{-1} : \mathbb{C}(z)[\mathfrak{Y}_\infty(z)] \to \mathbb{C}(z)[\mathfrak{Y}_0(z)]$$

is a ring isomorphism. It induces (by localization) ring isomorphisms $R_\infty \to R_0$ and $K_\infty \to K_0$ with the expected properties. □

Therefore, for all $v, w \in \mathbb{C}^\times \setminus S$,

$$\tau_v^{-1}\tau_w \in \mathrm{Gal}^\phi\big(R_\infty/\mathbb{C}(z)\big)$$

and, hence,

$$\mathcal{P}(v)^{-1}\mathcal{P}(w) \in G_{\mathrm{gal}}$$

where G_{gal} denotes the image of the linear representation

$$\rho_{\mathrm{gal}}\colon \mathrm{Gal}^\phi\big(R_\infty/\mathbb{C}(z)\big) \to \mathrm{GL}_n(\mathbb{C})$$

attached to the fundamental matrix of solutions $\mathfrak{Y}_\infty(z)$.

Definition 9.12 We denote by G_{Bir} the subgroup of $\mathrm{GL}_n(\mathbb{C})$ generated by $\mathcal{P}(v)^{-1}\mathcal{P}(w)$ for all $v, w \in \mathbb{C}^\times \setminus S$.

Theorem 9.13 ([15, Theorem 3.3]) *We have*

$$G_{\mathrm{gal}} = G_{\mathrm{Bir}} .$$

Proof We admit that G_{Bir} is Zariski-closed and refer to [15, Proposition 3.2] for the proof. According to Galois correspondence, it is sufficient to prove that $K_\infty^{G_{\mathrm{Bir}}} \subset \mathbb{C}$. Consider $f(z) \in K_\infty^{G_{\mathrm{Bir}}}$. So, $f(z) = P\big(\mathfrak{Y}_\infty(z)\big)$ for some $P(X) = A(X)/B(X)$ with $A(X), B(X) \in \mathbb{C}(z)[X]$ such that $B\big(\mathfrak{Y}_\infty(z)\big) \neq 0$. Since $f(z) \in K_\infty^{G_{\mathrm{Bir}}}$, we have $f(z) = P\big(\mathfrak{Y}_\infty(z)\big) = P\big(\mathfrak{Y}_\infty(z)\mathcal{P}(v)^{-1}\mathcal{P}(w)\big)$ for all $v, w \in \mathbb{C}^\times \setminus S$. For $v = z$ and for w fixed, we get $f(z) = P(\mathfrak{Y}_0(z)\mathcal{P}(w)^{-1})$. Therefore, $f(z)$, which is a priori meromorphic over $\mathbb{P}^1(\mathbb{C}) \setminus \{0\}$, is also meromorphic at 0; thus, it is meromorphic over the whole $\mathbb{P}^1(\mathbb{C})$ and, hence, belongs to $\mathbb{C}(z)$. The Galois correspondence ensures that $G_{\mathrm{Bir}} = G_{\mathrm{gal}}$. □

Remark 9.14 What does $\mathcal{P}(z)$ says about $\sigma_q Y = AY$? Consider two q-difference systems $\sigma_q Y = A_1 Y$ and $\sigma_q Y = A_2 Y$ with $A_1, A_2 \in \mathrm{GL}_n\big(\mathbb{C}(z)\big)$. We denote by $\mathcal{P}_1(z) = \mathfrak{Y}_{1,0}(z)^{-1}\mathfrak{Y}_{1,\infty}(z)$ and $\mathcal{P}_2(z) = \mathfrak{Y}_{2,0}(z)^{-1}\mathfrak{Y}_{2,\infty}(z)$ the corresponding connection matrices (with obvious notations). Assume that

$$\mathcal{P}_1(z) = \mathcal{P}_2(z) .$$

Then, we have

$$\mathfrak{Y}_{2,0}(z)\mathfrak{Y}_{1,0}(z)^{-1} = \mathfrak{Y}_{2,\infty}(z)\mathfrak{Y}_{1,\infty}(z)^{-1} =: R(z) .$$

Note that $R(z)$ is meromorphic over $\mathbb{P}_1(\mathbb{C}) \setminus \{\infty\}$ (this follows from the first expression for $R(z)$) and $\mathbb{P}_1(\mathbb{C}) \setminus \{0\}$ (this follows from the second expression for $R(z)$) so it is meromorphic over $\mathbb{P}_1(\mathbb{C})$ and, hence,

$$R(z) \in \mathrm{GL}_n\big(\mathbb{C}(z)\big) .$$

Moreover, we have $R(qz) = A_2(z)R(z)A_1(z)^{-1}$. So, the q-difference system $\sigma_q Y = A_2 Y$ is obtained form $\sigma_q Y = A_1 Y$ by using the linear change of unknown function

$$Y \rightsquigarrow RY .$$

We say that the two q-difference systems above are isomorphic over $\mathbb{C}(z)$.

9.3 From Connection Matrices to Monodromy

One can consider differential equations as degenerations of q-difference equations as q tends to 1. We have attached (Galoisian) analytic invariants to both differential and q-difference systems, namely the monodromy representation and the connection

matrices. The aim of this section is to understand what happens to the connection matrices as q tends to 1. We follow Sauloy in [30].

We fix $\tau \in \mathbb{C}$ such that $\Im(\tau) > 0$. For all $\epsilon > 0$, we set $q_\epsilon = \mathrm{e}^{2\pi \mathrm{i} \tau \epsilon}$. So, $|q_\epsilon| < 1$ and q_ϵ tends to 1 as $\epsilon > 0$ tends to 0.

Consider a differential system

$$Y'(z) = \widetilde{B}(z) Y(z) \quad \text{with } \widetilde{B}(z) \in \mathrm{M}_n\big(\mathbb{C}(z)\big) \,. \tag{7}$$

We deform this differential system into a family of q_ϵ-difference equations

$$Y(q_\epsilon z) = A_\epsilon(z) Y(z) \quad \text{with } A_\epsilon(z) \in \mathrm{GL}_n\big(\mathbb{C}(z)\big) \tag{8}$$

parameterized by $\epsilon > 0$. By deformation, we mean the following. The previous q_ϵ-difference systems can be rewritten as follows:

$$D_{q_\epsilon} Y(z) = B_\epsilon(z) Y(z) \tag{9}$$

where

$$B_\epsilon(z) = \frac{A_\epsilon(z) - I_n}{(q_\epsilon - 1)z} \quad \text{and} \quad D_{q_\epsilon} Y(z) = \frac{Y(q_\epsilon z) - Y(z)}{(q_\epsilon - 1)z} \,.$$

Roughly speaking, we say that the family of systems (8) deforms the differential system (7) if $B_\epsilon(z)$ tends to $\widetilde{B}(z)$ as $\epsilon > 0$ tends to 0, so that the systems (9) tend to the differential system (7) as $\epsilon > 0$ tends to 0.

We shall now state more precisely our hypotheses:

• We assume that the differential system (7) is regular at 0 and ∞, i.e., that there exists $\mathfrak{Y}_0(z) \in \mathrm{GL}_n(\mathcal{O}_{\mathbb{P}^1(\mathbb{C}),0})$ such that

$$\mathfrak{Y}_0'(z) = \widetilde{B}(z) \mathfrak{Y}_0(z) \quad \text{and} \quad \mathfrak{Y}_0(0) = I_n$$

and that there exists $\mathfrak{Y}_\infty(z) \in \mathrm{GL}_n(\mathcal{O}_{\mathbb{P}^1(\mathbb{C}),\infty})$ such that

$$\mathfrak{Y}_\infty'(z) = \widetilde{B}(z) \mathfrak{Y}_\infty(z) \quad \text{and} \quad \mathfrak{Y}_\infty(\infty) = I_n \,.$$

• We assume that the q_ϵ-difference systems (8) are regular at 0 and ∞, and we denote by $\mathcal{P}_\epsilon(z)$ the corresponding connection matrices.

• We denote the singularities of $\widetilde{B}(z)$ (in $\mathbb{C}^\times$) by $\tilde{z}_1, \dots, \tilde{z}_R$. We set $\tilde{z}_0 = 1$. We assume that the spirals $\tilde{z}_j \mathrm{e}^{2\pi \mathrm{i} \tau \mathbb{R}}$ are pairwise distinct. We index $\tilde{z}_0, \dots, \tilde{z}_R$ in such a way that a positive circle around 0 meats the spirals $\tilde{z}_0 \mathrm{e}^{2\pi \mathrm{i} \tau \mathbb{R}}, \dots, \tilde{z}_R \mathrm{e}^{2\pi \mathrm{i} \tau \mathbb{R}}$ in this order.

• We assume that $B_\epsilon(z)$ converges uniformly to $\widetilde{B}(z)$ on every compact subset of $\mathbb{C}^\times \setminus \{\tilde{z}_0, \dots, \tilde{z}_R\}$ as $\epsilon > 0$ tends to 0.

We denote by $\widetilde{U}_0, \dots, \widetilde{U}_R$ the connected components of $\mathbb{C}^\times \setminus \bigcup_{j=1}^r \tilde{z}_j \mathrm{e}^{2\pi \mathrm{i} \tau \mathbb{R}}$ where $\widetilde{U}_j$ has $\tilde{z}_j$ and $\tilde{z}_{j+1}$ on its boundary.

Theorem 9.15 ([30, Sect. 4]) *Under the previous assumptions, we have*:

- *For all* $j \in \{0, \dots, r\}$, *there exists* $\widetilde{\mathcal{P}}_j \in \mathrm{GL}_n(\mathbb{C})$ *such that* $\mathcal{P}_\epsilon(z)$ *tends to* $\widetilde{\mathcal{P}}_j$ *on* $\widetilde{U}_j$ *as* $\epsilon > 0$ *tends to* 0.
- *The monodromy matrix around* $\tilde{z}_j$ *in the basis* $\mathfrak{Y}_0(z)$ *is given by* $\widetilde{\mathcal{P}}_j \widetilde{\mathcal{P}}_{j-1}^{-1}$.

Remark 9.16 For a very general study of the behavior of the q-difference Galois groups as q tends to 1, we refer to André's [3].

Remark 9.17 The results established by Etingof have been extended to the regular singular q-difference systems by van der Put and Singer in [23] and by Sauloy in [31], following distinct approaches.

10 Computing Difference Galois Groups

Hendricks developed algorithms in [19, 20] in order to compute the difference Galois groups of linear difference or q-difference equations of order 2 with coefficients in $\overline{\mathbb{Q}}(z)$ and $\bigcup_{j\geq 1} \overline{\mathbb{Q}}(z^{1/j})$ respectively. It relies on the classification of the algebraic subgroups of $\mathrm{GL}_2(\overline{\mathbb{Q}})$. For the difference Galois groups of Mahler equations of order 2 with coefficients in $\bigcup_{j\geq 1} \overline{\mathbb{Q}}(z^{1/j})$, we refer to [29]. For calculations of difference Galois groups of finite difference equations of order 2 on an elliptic curve, we refer to [11].

What about equations of higher order?

Feng has recently given in [16] an algorithm to compute the Galois groups of linear difference equations over $\overline{\mathbb{Q}}(z)$.

For the Galoisian properties of "classical equations," especially of the generalized q-hypergeometric equations, we refer to [26–28]. The methods combine algebra and analysis.

We also emphasize that André's main result in [3] gives a powerful tool to compute the difference Galois groups of difference equations deforming a given differential equations whose differential Galois group is known.

11 Parameterized Difference Galois Theory

In the recent years, several authors have developed "parameterized" differential or difference Galois theories. The starting point was the seminal work of Cassidy and Singer in [9]. This section is a brief introduction to the parameterized difference Galois theory developed by Hardouin and Singer in [17]. This theory is typically adapted to the study of the algebraic relations among the successive derivatives of the entries of a fundamental matrix of solutions of a given difference system. For instance, it has been used in loc. cit. to give a short proof of Hölder's theorem, concerning Euler's Gamma function, which satisfies

$$\Gamma(z+1) = z\Gamma(z)\ .$$

Theorem 11.1 (Hölder) *Euler's Gamma function is hypertranscendental, i.e., the successive derivatives* $\Gamma(z), \Gamma'(z), \Gamma''(z), \ldots$ *are algebraically independent over* $\mathbb{C}(z)$.

Another application is given by the following result, which was first proved by Hardouin and Singer in special cases (see http://www4.ncsu.edu/~singer/papers/worksheet.pdf). The full result follows from the main results of [12] or of [4].

Theorem 11.2 *Let* $y_1(z), y_2(z)$ *be linearly independent solutions of the q-hypergeometric equation*

$$y(q^2z) - \frac{2az-2}{a^2z-1}y(qz) + \frac{z-1}{a^2z-q^2}y(z) = 0$$

where $a \in \mathbb{C}^\times \setminus q^{\mathbb{Z}}$ *and* $a^2 \in q^{\mathbb{Z}}$ *and* $|q| \neq 1$. *Then* $y_1(z), y_2(z), y_1(qz)$ *and their successive derivatives are algebraically independent over the field of q-invariant meromorphic functions over* $\mathbb{C}^\times$.

Also, the parameterized difference Galois theory has been used by Dreyfus et al. [13] in order to study the generating series of automatic sequences. Let us recall that the generating series $f(z) = \sum_{k\geq 0} s_k z^k$ of any p-automatic sequence $(s_k)_{k\geq 0} \in \overline{\mathbb{Q}}^{\mathbb{N}}$ (and, actually, of any p-regular sequence) satisfies a Mahlerian difference system, i.e., a difference system of the form

$$F(z^p) = A(z)F(z)$$

where

$$F(z) = \big(f(z), f(z^p), \ldots, f(z^{p^{n-1}})\big)^t \quad \text{and} \quad A(z) \in \mathrm{GL}_n\big(\mathbb{C}(z)\big)$$

for some positive integer n; see Mendès France's [21], Randé's [25], Dumas' [14], Becker's [5], Adamczewski and Bell's [1], and the references therein. The famous examples are the generating series of the Thue–Morse, the paper-folding, the Baum–Sweet and the Rudin–Shapiro sequences (see Allouche and Shallit's book [2]). The study of the algebraic relations between such series and their successive derivatives is a classical problem, and we have shown in [13] that the parameterized difference Galois theory is a very convenient tool in this context. For instance, we were able to prove the following result, where $f_{\mathrm{BS}}(z)$ and $f_{\mathrm{RS}}(z)$ are the generating series of the Baum–Sweet and Rudin–Shapiro series.

Theorem 11.3 ([13, Introduction]) *The series* $f_{\mathrm{BS}}(z), f_{\mathrm{BS}}(z^2), f_{\mathrm{RS}}(z), f_{\mathrm{RS}}(-z)$ *and all their successive derivatives are algebraically independent over* $\mathbb{C}(z)$.

11.1 A Short Introduction to Parameterized Difference Galois Theory

The general setting of the parameterized difference Galois theory developed in [17] is the following. Instead of a difference field (k, ϕ), we consider a differential difference field (k, ϕ, δ), i.e., k is a field, ϕ is a field automorphism of k and $\delta: k \to k$ is a derivation (this means that δ is an additive map satisfying Leibniz rule) such that

$$\phi \circ \delta = \delta \circ \phi \, .$$

Example 11.4 1. In the example of Hölder's theorem, one can take $k = \mathbb{C}(z)$, $\phi: f(z) \mapsto f(z+1)$, $\delta = \mathrm{d}/\mathrm{d}z$.
2. $k = \mathbb{C}(z)$, $\phi: f(z) \mapsto f(qz)$, $\delta = z\mathrm{d}/\mathrm{d}z$.

We want to study (the solutions of) a linear difference system

$$\phi(Y) = AY \quad \text{with } A \in \mathrm{GL}_n(k) \, . \tag{10}$$

The difference rings used in difference Galois theory are replaced by the differential difference rings, i.e., by 3-uples (R, ϕ, δ) where R is a ring, $\phi: R \to R$ is a ring automorphism and $\delta: R \to R$ is a derivation such that $\phi \circ \delta = \delta \circ \phi$. We denote by C the field of constants of the difference field (k, ϕ).

There are natural notions of differential difference ring extensions, ideals, isomorphisms, etc., similar to the notions of difference ring extensions, ideals, isomorphisms, etc., introduced in Sect. 4. For instance, a differential difference ring $(\widetilde{R}, \tilde{\phi}, \tilde{\delta})$ is a differential difference ring extension of the differential difference ring (R, ϕ, δ) if $\widetilde{R}$ is a ring extension of R, $\tilde{\phi}_{|R} = \phi$ and $\tilde{\delta}_{|R} = \delta$; in this case, we will often denote $\tilde{\phi}$ by ϕ and $\tilde{\delta}$ by δ. We refer the reader to [17] for the details.

Definition 11.5 ([17, Definition 2.3]) A parameterized Picard–Vessiot ring for (10) over (k, ϕ, δ) is a differential difference ring extension R of (k, ϕ, δ) such that

1. there exists $\mathfrak{Y} \in \mathrm{GL}_n(R)$ such that $\phi(\mathfrak{Y}) = A\mathfrak{Y}$ (such a $\mathfrak{Y}$ is called a fundamental matrix of solutions of (4));
2. R is generated, as a (k, δ)-algebra, by the entries of $\mathfrak{Y}$ and $\det(\mathfrak{Y})^{-1}$, i.e., R is generated as a k-algebra by the entries of $\mathfrak{Y}$ and $\det(\mathfrak{Y})^{-1}$ and they successive transforms by δ.
3. R is a simple differential difference ring, i.e., the only ideals of R stable by ϕ and δ are $\{0\}$ and R.

As in difference Galois theory, we need to impose restrictions on the field of constants C in order to have a nice parameterized Picard–Vessiot theory. Unfortunately, the requirement that C is algebraically closed is not sufficient. The usual requirement is that C is differentially closed. This is not only a property of the field C but a property of C endowed with the derivation $\delta: C \to C$ (δ

induces a map $C \to C$ because ϕ and δ commute). Roughly speaking, the fact that (C, δ) is differentially closed means that, for any polynomials $P_1(y_1, \dots, y_s), \dots, P_R(y_1, \dots, y_s), Q(y_1, \dots, y_s)$ in the $\delta^i(y_j)$ (here, $\delta^i(y_j)$ is a suggestive notation for indeterminates over C) and with coefficients in C, if

$$P_1(y_1, \dots, y_s) = 0, \dots, P_R(y_1, \dots, y_s) = 0, \quad Q(y_1, \dots, y_s) \neq 0 \tag{11}$$

has a solution $\tilde{y}_1, \dots, \tilde{y}_s$ is some differential field extension (F, D) of (C, δ) (i.e., F is a field extension of C, $D: F \to F$ is a derivation such that $D_{|C} = \delta$, and the Eq. (11) are satisfied if we replace y_i by $\widetilde{y_i}$ and δ by D), then it has a solution in (C, δ).

Proposition 11.6 ([17, Proposition 2.4]) *Assume that k is of characteristic* 0 *and that C is differentially closed. Then, up to isomorphism of differential difference fields over* (k, ϕ, δ), *there exists a unique parameterized Picard–Vessiot ring for the difference system* (10) *over* (k, ϕ).

Moreover, we have $R^\phi = C$.

We let R be a parameterized Picard–Vessiot rings for the difference system (10) over (k, ϕ, δ). The parameterized difference Galois group is then defined as follows.

Definition 11.7 ([17, Definition 2.5]) The parameterized difference Galois group $\mathrm{Gal}^{(\phi,\delta)}(R/k)$ over (k, ϕ, δ) of (10) is the group of the k-linear ring automorphisms of R commuting with ϕ and δ:

$$\mathrm{Gal}^{(\phi,\delta)}(R/k) := \{\sigma \in \mathrm{Aut}(R/k) \mid \phi \circ \sigma = \sigma \circ \phi \text{ and } \delta \circ \sigma = \sigma \circ \delta\}.$$

As in difference Galois theory, one can see $\mathrm{Gal}^{(\phi,\delta)}(R/k)$ as a subgroup of $\mathrm{GL}_n(C)$ via the faithful representation

$$\begin{aligned} \rho_{\mathrm{gal}}: \mathrm{Gal}^{(\phi,\delta)}(R/k) &\to \mathrm{GL}_n(C) \\ \sigma &\mapsto C(\sigma) \end{aligned}$$

where $C(\sigma)$ is determined by the equality $\sigma(\mathfrak{Y}) = \mathfrak{Y}C(\sigma)$.

A crucial result is then:

Theorem 11.8 ([17, Theorem 2.6]) *The image of* ρ_{gal}, *which will be denoted by* $G_{\mathrm{gal}}^{(\phi,\delta)}$, *is a* differential algebraic *subgroup of* $\mathrm{GL}_n(C)$.

This means that the image of ρ_{gal} is

- a subgroup of $\mathrm{GL}_n(C)$ and
- the zero-locus in $\mathrm{GL}_n(C)$ of a set of differential polynomials in $C\left[\left(\delta^k(X_{i,j})\right)_{1 \le i,j \le n}, \det X^{-1}\right]$.

One can prove that the parameterized difference Galois groups reflect the algebraic relations among the entries of a fundamental matrix of solutions and their successive derivatives, in a similar way that the difference Galois groups reflect the algebraic relations among the entries of a fundamental matrix of solutions.

11.2 From Parameterized to Nonparameterized Difference Galois Theory: Applications

We maintain the hypotheses and notations of the previous section. We let S be the k-algebra generated by the entries of $\mathfrak{Y}$ and $\det(\mathfrak{Y})^{-1}$. Then, it can be shown that (S, ϕ) is a Picard–Vessiot ring for the difference system (10) over (k, ϕ). We denote by G^{ϕ}_{gal} the group $\mathrm{Gal}^{\phi}(S/k)$ seen as a subgroup of $\mathrm{GL}_n(C)$ via the faithful representation attached to $\mathfrak{Y}$.

Theorem 11.9 ([17, Proposition 2.8]) *The differential algebraic group $G^{(\phi,\delta)}_{\mathrm{gal}}$ is a Zariski-dense subgroup of the algebraic group G^{ϕ}_{gal}.*

In some cases, e.g., if G^{ϕ}_{gal} has few differential algebraic subgroups, this is strong information. For instance, it has been proved by Cassidy in [8] that the Zariki-dense proper algebraic subgroups of $\mathrm{SL}_n(C)$ are conjugate to $\mathrm{SL}_n(C^{\delta})$, where

$$C^{\delta} = \{f \in C \mid \delta(f) = 0\}.$$

Whence the following result.

Theorem 11.10 *Assume that $G^{\phi}_{\mathrm{gal}} = \mathrm{SL}_n(C)$. Then, we have*:

- *either $G^{(\phi,\delta)}_{\mathrm{gal}} = G^{\phi}_{\mathrm{gal}} = \mathrm{SL}_n(C)$;*
- *or $G^{(\phi,\delta)}_{\mathrm{gal}}$ is conjugate to $\mathrm{SL}_n(C^{\delta})$.*

Moreover, the difference between the former and the later case can be reformulated as an integrability condition:

Proposition 11.11 ([17, Proposition 2.9]) *The differential algebraic group $G^{(\phi,\delta)}_{\mathrm{gal}}$ is conjugate to a subgroup of $\mathrm{GL}_n(C^{\delta})$ if and only if there exists $B \in k^{n\times n}$ such that*

$$\phi(B) = ABA^{-1} + \delta(A)A^{-1}\ .$$

In this case, there exists $Y \in \mathrm{GL}_n(R)$ such that

$$\phi(Y) = AY \quad \text{and} \quad \delta(Y) = BY\ .$$

For instance, these are the main ingredients behind the proofs of Theorem 11.2.

12 Answers to Selected Exercises

Answer to Exercise 4.4 Indeed, we have $\phi(I) \subset I$, thus $I \subset \phi^{-1}(I)$. But $\phi^{-1}(I)$ is a difference ideal of R. So, we have either $\phi^{-1}(I) = I$ or $\phi^{-1}(I) = R$. The latter case is excluded.

Answer to Exercise 4.5 Assume that $(R/I, \overline{\phi})$ is a difference ring. Prove that there is a 1–1 correspondence between the difference ideals of R containing I and the difference ideals of R/I given by $J \mapsto \pi^{-1}(J)$ where $\pi : R \to R/I$ is the canonical morphism.

Answer to Exercise 4.6 1 Indeed, we have $\phi(I) \subset I$ and, hence, $I \subset \phi^{-1}(I)$. Therefore, we have the ascending chain of ideals $I \subset \phi^{-1}(I) \subset \phi^{-2}(I) \subset \cdots$. Since R is Noetherian, there exists a positive integer j such that $\phi^{-j}(I) = \phi^{-(j+1)}(I)$, whence $\phi(I) = I$.

2 Let $(X_n)_{n\in\mathbb{Z}}$ be a family of indeterminates over a field k and consider the difference ring (R, ϕ) where $R = k[(X_n)_{n\in\mathbb{Z}}]$ and where ϕ is the unique k-algebra endomorphism of R such that $\phi(X_n) = X_{n+1}$. Then, $I = (X_0, X_1, \dots)$ is a difference ideal of (R, ϕ) and we have $\phi(I) \subsetneq I$.

Answer to Exercise 4.14 1 Let $f \in k'^{\phi}$. Let $P(X) \in k[X]$ be the minimal polynomial of f over k (in particular, $P(X)$ is monic). Then, $P^{\phi}(X) - P(X) \in k[X]$ has degree $< \deg P(X)$ and vanishes at f. Therefore, $P^{\phi}(X) - P(X) = 0$, i.e., the coefficients of $P(X)$ belong to k^{ϕ} and, hence, f is algebraic over k^{ϕ}.

2 Consider for instance $\mathbb{C}$ endowed with the complex conjugation.

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References

1. B. Adamczewski, J.P. Bell, A problem about Mahler functions (2013), arXiv:1303.2019
2. J.P. Allouche, J. Shallit, *Automatic Sequences*: *Theory*, *Applications*, *Generalizations* (Cambridge University Press, Cambridge, 2003)
3. Y. André, Différentielles non commutatives et théorie de Galois différentielle ou aux différences. Ann. Sci. École Norm. Sup. (4) **34**(5), 685–739 (2001)
4. C.E. Arreche, M.F. Singer, Galois groups for integrable and projectively integrable linear differential equations (2016), arXiv:1608.00015
5. P.G. Becker, *k*-regular power series and Mahler-type functional equations. J. Number Theory **49**(3), 269–286 (1994)
6. D. Bertrand, Groupes algébriques et équations différentielles linéaires, in *Séminaire Bourbaki*. Astérisque, vol. 1991/1992, no. 206 (Société Mathématique de France, Paris, 1992), pp. 183–204
7. F. Beukers, Differential Galois theory, in *From Number Theory to Physics*, ed. by M. Waldschmidt, P. Moussa, J.M. Luck, C. Itzykson (Springer, Berlin/Heidelberg, 1992), pp. 413–439
8. P.J. Cassidy, The classification of the semisimple differential algebraic groups and the linear semisimple differential algebraic Lie algebras. J. Algebra **121**(1), 169–238 (1989)

9. P.J. Cassidy, M.F. Singer, Galois theory of parameterized differential equations and linear differential algebraic groups, in *Differential Equations and Quantum Groups*, ed. by D. Bertrand, B. Enriquez, C. Mitschi, C. Sabbah, R. Schäfke. IRMA Lectures in Mathematics and Theoretical Physics, vol. 9 (European Mathematical Society, Zürich, 2007), pp. 113–155
10. L. Di Vizio, Approche galoisienne de la transcendance différentielle (2012), arXiv:1404.3611
11. T. Dreyfus, J. Roques, Galois groups of difference equations of order two on elliptic curves. SIGMA, Symmetry Integr. Geom. Methods Appl. **11**, 003 (2015)
12. T. Dreyfus, C. Hardouin, J. Roques, Functional relations for solutions of q-difference equations (2016), arXiv:1603.06771
13. T. Dreyfus, C. Hardouin, J. Roques, Hypertranscendence of solutions of Mahler equations. J. Eur. Math. Soc. (to appear)
14. P. Dumas, Récurrences mahlériennes, suites automatiques, études asymptotiques. Ph.D. thesis, Université Bordeaux 1 (1993)
15. P.I. Etingof, Galois groups and connection matrices of q-difference equations. Electron. Res. Announc. Am. Math. Soc. **1**(1), 1–9 (1995)
16. R. Feng, On the computation of the Galois group of linear difference equations (2015), arXiv:1503.02239
17. C. Hardouin, M.F. Singer, Differential Galois theory of linear difference equations. Math. Ann. **342**(2), 333–377 (2008)
18. C. Hardouin, J. Sauloy, M.F. Singer, *Galois Theories of Linear Difference Equations*: *An Introduction*. Mathematical Surveys and Monographs, vol. 211 (American Mathematical Society, Providence, 2016)
19. P.A. Hendriks, An algorithm for computing a standard form for second-order linear q-difference equations. J. Pure Appl. Algebra **117/118**, 331–352 (1997)
20. P.A. Hendriks, An algorithm determining the difference Galois group of second order linear difference equations. J. Symb. Comput. **26**(4), 445–461 (1998)
21. M. Mendès France, Nombres algébriques et théorie des automates. Enseign. Math. (2) **26**(3-4), 193–199 (1980)
22. M. van der Put, Recent work on differential Galois theory, in *Séminaire Bourbaki*. Astérisque, vol. 1997/1998, no. 252 (Société Mathématique de France, Paris, 1998), pp. 341–367
23. M. van der Put, M.F. Singer, *Galois Theory of Difference Equations*. Lecture Notes in Mathematics, vol. 1666 (Springer, Berlin/Heidelberg, 1997)
24. M. van der Put, M.F. Singer, *Galois Theory of Linear Differential Equations*. Grundlehren der Mathematischen Wissenschaften, vol. 328 (Springer, Berlin/Heidelberg, 2003)
25. B. Randé, Équations fonctionnelles de Mahler et applications aux suites p-régulières. Ph.D. thesis, Université Bordeaux 1 (1992)
26. J. Roques, Galois groups of the basic hypergeometric equations. Pac. J. Math. **235**(2), 303–322 (2008)
27. J. Roques, Generalized basic hypergeometric equations. Invent. Math. **184**(3), 499–528 (2011)
28. J. Roques, On classical irregular q-difference equations. Compos. Math. **148**(5), 1624–1644 (2012)
29. J. Roques, On the algebraic relations between Mahler functions. Trans. Am. Math. Soc. (to appear)
30. J. Sauloy, Systèmes aux q-différences singuliers réguliers: classification, matrice de connexion et monodromie. Ann. Inst. Fourier (Grenoble) **50**(4), 1021–1071 (2000)
31. J. Sauloy, Galois theory of Fuchsian q-difference equations. Ann. Sci. École Norm. Sup. (4) **36**(6), 925–968 (2003)
32. J. Sauloy, *Introduction to Differential Galois Theory* (2012). https://www.math.univ-toulouse.fr/~sauloy/
33. M.F. Singer, Galois theory of linear differential equations, in *Algebraic Theory of Differential Equations*, ed. by M.A.H. MacCallum, A.V. Mikhailov. London Mathematical Society Lecture Note Series, vol. 357 (Cambridge University Press, Cambridge, 2009), pp. 1–82

Lectures on Quantum Integrability: Lattices, Symmetries and Physics

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Abstract These lectures notes are intended as a friendly introduction to the many-body physics and methods of integrability. They were presented during the ASIDE12, a school preceding the SIDE12 conference. The aimed audience of them are mathematicians with interests in integrability and physics.

1 Introduction

In this introductory section we give a meaning to all the three keywords: physical applications, lattices and symmetries, referred to in the title. We illustrate main concepts with a simple model of many-body physics.

1.1 Physics

We start with a quick overview of problems and questions that we face in quantum physics (of many-body systems), and that we want integrable models to help us with.

The central role in quantum physics is played by the Hamiltonian. That is a Hermitian operator $H = H^\dagger$, acting in some Hilbert space $\mathcal{H}$, governing the time evolution of the system

$$\mathrm{i}\partial_t|a\rangle = H|a\rangle \ . \tag{1}$$

Main task is to find eigenstates and eigenenergies

$$H|a\rangle = E_a|a\rangle \ . \tag{2}$$

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The time evolution of the eigenstates is straightforward

$$|a(t)\rangle = \mathrm{e}^{-\mathrm{i}E_a t}|a\rangle \ . \tag{3}$$

Once we know the spectrum (the eigenstates) every state of the system can be written as a superposition (a linear combination) of them. The time evolution of a generic state follows then from time evolution of the eigenstates. Traditionally, models that exhibit an exact solution to the eigenvalue problem (2) are called exactly solvable models.

Among all the states an important role for physical applications is played by the ground states. In thermal equilibrium the probability that the system is in a certain eigenstate $|a\rangle$ is proportional to $\exp(-E_a/T)$. At low temperatures T the physics is reigned by the properties of states with the lowest energy—the ground states. We shall denote a ground state by $|\mathrm{gs}\rangle$.

The mere knowledge of the ground state is not enough to infer its physical properties. These are best explored through expectation values of physical operators or, in other words, correlation functions. They answer physical questions like: what is the average density of particles in a gas? What are the fluctuations around this average densities. Is there a correlation between fluctuations at different places (and/or at different times). To each observable in quantum physics there is an associated Hermitian operator. For example if we denote by $n(x)$ an operator counting particles at position x an example of a correlation function would be

$$S_0(x_1, x_2) = \langle \mathrm{gs}|n(x_1)n(x_2)|\mathrm{gs}\rangle \ . \tag{4}$$

This object measures correlations between particles at positions x_1 and x_2. For the computation of correlation functions the least that we need is an action of the operators (like $n(x)$) on the eigenstates. Correlation functions are objects that are accessible experimentally.

At nonzero temperatures the system is in a thermal state. Inferring its properties is achieved by studying the partition function

$$Z = \mathrm{tr}\big(\exp(-\beta H)\big) = \sum_a \exp(-\beta E_a) \ , \quad \beta = 1/T \ , \tag{5}$$

where the summation extends over all eigenstates. Similarly to the zero temperature case, we can learn more about a thermal state by computing correlation functions. At finite temperatures, the density-density correlation function is

$$S_T(x_1, x_2) = \frac{1}{Z}\sum_a \exp(-\beta E_a)\langle a|n(x_1)n(x_2)|a\rangle, \tag{6}$$

where again we sum over all eigenstates.

So far we discussed isolated systems that we assumed to be in thermal equilibrium. There is a lot of interesting and much less understood physics in out-

of-equilibrium situations. We divide the out-of-equilibrium situations in 2 rough categories: driven and quenched systems. The first category refers to systems which are under a constant exertion of an external force. This could be an oscillating magnetic field or leads at the edges pumping particles through the system. Generally such systems approach some steady state characterized by a constant flow of particles or energy. Characterization of such steady state is the first step in understanding physics of driven systems.

The second category, quenched systems, refers to an abrupt change of the Hamiltonian. The ingredients that we have introduced are sufficient to formulate this problem explicitly. Let us say at times $t < 0$ the system is in an eigenstate $|a_0\rangle$ of a Hamiltonian H_0. Now, at time $t = 0$ we abruptly change the Hamiltonian from H_0 to H. The change can be anything. We could change mass of particles, turn on an external magnetic field or even change interactions between particles. Bizarre as these may sound, all these processes are experimentally feasible. Afterwards the system is let alone. The time evolution following the quench is

$$|a(t)\rangle = \mathrm{e}^{-\mathrm{i}Ht}|a_0\rangle = \sum_b \mathrm{e}^{-\mathrm{i}E_b t} \underbrace{\langle b|a_0\rangle}_{\text{overlap}} |b\rangle \ , \tag{7}$$

where we used a resolution of the identity

$$\sum_b |b\rangle\langle b| = 1 \ , \tag{8}$$

in terms of the eigenstates of the post-quench Hamiltonian H. A new ingredient appearing is an overlap (a scalar product) $c_{ba} = \langle b|a_0\rangle$ of the initial state $|a_0\rangle$ with eigenstates of the post-quench Hamiltonian H.

Instead of looking at the post-quench state $|a(t)\rangle$ itself, it is again instructive to look at correlation functions. The density-density correlation function is now

$$S_{\text{quench}}(x_1, x_2; t) = \sum_{b,c} \mathrm{e}^{-\mathrm{i}(E_b - E_c)t} c_{ba} c^*_{ca} \langle c|n(x_1)n(x_2)|b\rangle \ . \tag{9}$$

The main question that we try to answer with studying quenches is whether the system equilibrates, and if so whether the equilibrium is thermal

$$\lim_{t\to\infty} S_{\text{quench}}(x_1, x_2; t) \stackrel{?}{=} S_T(x_1, x_2) \ . \tag{10}$$

The quench process provides a clear-cut and neat formulation of an otherwise vast subject of nonequilibrium dynamics. In its simplicity and viable experimental realization lies its power.

Concluding, in the perfect world we would be able to: (1) diagonalize a Hamiltonian and understand the structure of its eigenstates; (2) compute correlations functions in various, physically relevant, situations. The second point requires

(2a) identification of physical operators and knowledge of their action on the eigenstates and (2b) knowledge of the overlaps between eigenstates of different Hamiltonians.

These lectures are dedicated to the Algebraic Bethe Ansatz which is a method of studying quantum integrable models. Within its framework it provides solution to (1) and (2a) of the above list. The applicability of the Algebraic Bethe Ansatz in the computation of the overlaps remains unknown.

1.2 Lattices

The second keyword in the theme list are lattices. We consider only models defined on a one-dimensional lattice, say of L sites (Fig. 1). Hilbert space factorizes

$$\mathcal{H} = \otimes_{j=1}^{L} \mathsf{h}_j = \mathsf{h}^{\otimes L} . \tag{11}$$

All the sites are identical and the Hilbert spaces in the tensor product are all isomorphic. The dimension of the full Hilbert space is $\dim \mathcal{H} = (\dim \mathsf{h})^L$. The operators acting on such Hilbert space admit a natural hierarchy. There are on-site operators, such that act nontrivially only on a single site, two-site operators that act nontrivially only on two neighboring sites, etc. We supply an operator o with an index k to indicate that it acts nontrivially only on the kth site

$$o_k = \underbrace{1 \otimes 1 \ldots 1}_{(k-1) \text{ times}} \otimes o \otimes \underbrace{1 \otimes \cdots \otimes 1}_{(L-k-1) \text{ times}} , \quad o \colon \mathsf{h}_k \to \mathsf{h}_k . \tag{12}$$

We construct multiple site operators from one-site operators, for example $o_k o_{k+1} o_{k+2}$. These are local operators. A nonlocal operator would be a product of large number of local operators such as $o_k o_{k+1} \cdots o_{k+j}$ with j comparable with the lattice length L.

We introduce also a notion of local charges. These are local operators summed over the whole lattice. For example

$$Q_j = \sum_{k=1}^{L} o_k o_{k+1} \cdots o_{k+j} . \tag{13}$$

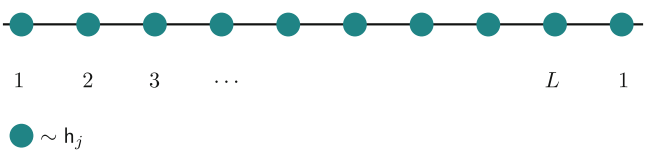

Fig. 1 A lattice model of L latices sites and with the periodic boundary condition: after the Lth lattice site there is again the first lattice site and so on. At each lattice site there is a Hilbert space related to local degrees of freedom

This operator is well defined in a system with the periodic boundary conditions where $o_{N+j} = o_j$. A nonlocal charge is a nonlocal operator summed over the whole lattice or in other words it is Q_j with j of the order of L.

1.3 Symmetries

The last keyword is the symmetries. A symmetry of a system implies invariance of observables under some operations. This operation can be, for example, a rotation, a translation (also in the time direction) or inversion of spins. Such symmetries reflect ambiguity in choosing what time is $t = 0$, which lattice site is the first one (remember the periodic boundary conditions) or which direction is up. To every corresponding operation we associate an unitary operator U which realizes this operation. The state $|a\rangle$ transforms into $U|a\rangle$ which we write as

$$|a\rangle \to U|a\rangle \ . \tag{14}$$

The unitarity of U implies that the normalization is respected

$$\langle a|U^\dagger U|a\rangle = \langle a|a\rangle \ , \tag{15}$$

where we used that the dual state transforms as

$$\langle a| \to \langle a|U^\dagger \ . \tag{16}$$

Together with states also operators are influenced by the symmetry transformation, transforming like

$$\mathcal{O} \to U\mathcal{O}U^\dagger \ , \tag{17}$$

which implies that expectation values are invariant under the transformation

$$\langle a|\mathcal{O}|b\rangle \to \langle a|U^\dagger U\mathcal{O}U^\dagger U|b\rangle = \langle a|\mathcal{O}|b\rangle \ . \tag{18}$$

An important class of transformations are those that can be generated by a Hermitian operator Q, namely

$$U(\epsilon) = \mathrm{e}^{\mathrm{i}\epsilon Q} \ . \tag{19}$$

Invariance of the Hamiltonian under such transformations: $H \to U(\epsilon)HU^\dagger(\epsilon) = H$ implies that Hamiltonian commutes with the generator Q

$$[H, Q] = 0 \ . \tag{20}$$

Commutation with the Hamiltonian implies that an expectation value of Q is time independent. We call such operators conserved charges.

Among all the models there is a special group of quantum integrable models. The precise definition of quantum integrability is still missing, but a working definition is the following. Quantum lattice integrable models are models in which there are local conserved charges Q_j (thus commuting with the Hamiltonian). The number of (functionally) independent charges is of the order of the number of lattice sites. These charges can be found within the Algebraic Bethe Ansatz method.

A crucial ingredient of the above definition of quantum integrability is that the charges in question are local. Indeed for every model there are conserved operators which are simply projectors on eigenstates $P_\alpha = |\alpha\rangle\langle\alpha|$. There is $(\dim \mathsf{h})^L$ of them. These are however nonlocal operators and therefore they do not tell us much about the local physics encoded for example in correlation functions. All that they mean is that the eigenstates have a simple time evolution, according to (3). Local conserved charges restrict the dynamics and provide more valuable information about the eigenstates.

We conclude this section by giving examples of two important transformations. The simplest example of a transformation which is built-in quantum physics is the time translation. Formally integrating the Schrödinger equation (1) we find

$$|a(t)\rangle = \mathrm{e}^{-\mathrm{i}Ht}|a(0)\rangle \ , \tag{21}$$

which identifies

$$U(t) = \mathrm{e}^{-\mathrm{i}Ht} \ , \tag{22}$$

as a unitary operator (H is Hermitian) translating in time. The Hamiltonian is a generator of this operation. Equivalently we can think of time evolving the operators while keeping the states intact such that

$$\langle a(t)|\mathcal{O}|a(t)\rangle = \langle a(0)|\mathrm{e}^{\mathrm{i}Ht}\mathcal{O}\mathrm{e}^{-\mathrm{i}Ht}|a(0)\rangle \ , \tag{23}$$

which gives that

$$\mathcal{O}(t) = \mathrm{e}^{\mathrm{i}Ht}\mathcal{O}\mathrm{e}^{-\mathrm{i}Ht} \ . \tag{24}$$

Other types of transformations are spatial translations. On the lattice they can be generated from a permutation operator of two lattice sites denoted by $\mathcal{P}_{ij}$ fulfilling

$$\mathcal{P}_{ij} = \mathcal{P}_{ij}^\dagger \ , \quad \mathcal{P}_{ij} = \mathcal{P}_{ji} \ . \tag{25}$$

The most important translation is the shift operator

$$U = \mathcal{P}_{12}\mathcal{P}_{23}\cdots\mathcal{P}_{L-1,L} \ , \tag{26}$$

which shifts a local operator by one lattice site to the right

$$o_{j+1} = U o_j U^\dagger \,. \tag{27}$$

Just as the Hamiltonian is a generator of the time translation, so is the momentum operator a generator of a spatial translation

$$U = \mathrm{e}^{-\mathrm{i}P} \,. \tag{28}$$

We say that Hamiltonian is translationally invariant if it commutes with the momentum operator. A generic local operator acting at site $j+1$ at time t can then be expressed as

$$o_{j+1}(t) = \mathrm{e}^{\mathrm{i}(Ht-Pj)} o_1 \mathrm{e}^{-\mathrm{i}(Ht-Pj)} \,. \tag{29}$$

After this lightning introduction to quantum physics let us consider a concrete example of a lattice model, the free lattice fermions in 1D.

1.4 Free Lattice Fermions in 1D

In this section we consider a lattice model of free (spinless) fermions. This model will serve as an illustration to the basic concepts without obscuring them with technicalities. We will diagonalize the Hamiltonian, describe the spectrum and find local conserved charges. We choose the spinless fermion example (instead of a spin model) to simplify the presentation. This model is connected to a spin model through a Jordan-Wigner transformation (see Sect. 2.2).

The Hamiltonian of free and spinless lattice fermions contains only a kinetic energy (see Fig. 2) and reads

$$H = -t \sum_{j=1}^{L} \left(c_j^+ c_{j+1}^- - c_j^- c_{j+1}^+ \right) \,, \tag{30}$$

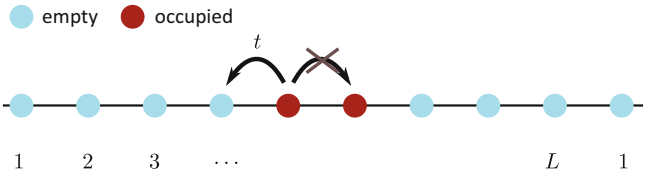

Fig. 2 A lattice model of spinless fermions. Each lattice site can be occupied by at most one fermion. Particles can move to the left or to the right with $t = 1$ amplitude. We impose the periodic boundary conditions

where operators $c_j^{\pm}$ obey the fermionic algebra

$$\{c_j^+, c_k^-\} = \delta_{jk} , \quad \{c_j^{\pm}, c_k^{\pm}\} = 0 . \tag{31}$$

We assume the periodic boundary conditions: $c_{N+1}^{\pm} = c_1^{\pm}$ and set $t = 1$.

The Hamiltonian (30) is invariant under translations. To expose this symmetry let us write the permutation operator in terms of the fermionic operators

$$\mathcal{P}_{ij} = 1 - (c_i^+ - c_j^+)(c_i^- - c_j^-) . \tag{32}$$

Exercise 1.1 Verify that $\mathcal{P}_{ij} c_j^+ = c_i^+ \mathcal{P}_{ij}$ and that $\mathcal{P}_{ij}\mathcal{P}_{ij} = 1$. Recall that the shift operator is

$$U = \mathcal{P}_{12}\mathcal{P}_{23} \cdots \mathcal{P}_{L-1,L} .$$

and show that $U c_j^{\pm} = c_{j+1}^{\pm} U$. Finally show that $UHU^{\dagger} = H$ which proves the translational invariance of the Hamiltonian.

We will transform the Hamiltonian to the Fourier (momentum) space to take advantage of the translational invariance. Because the system is noninteracting this will be enough to actually diagonalize the Hamiltonian.

As a prototype of the Fourier transform we could define

$$c_{\lambda}^{\pm} = \sum_{j=1}^{L} e^{\pm ij\lambda} c_j^{\pm}, \tag{33}$$

where λ is so far just a real number. The constraints on λ come from the periodic boundary condition and the discrete space (lattice).

Exercise 1.2 Show that the periodic boundary condition restricts value of λ to $\lambda = 2\pi/L \times I$ where I (a quantum number) is an integer. Show that the lattice causes the λ and $\lambda + 2\pi$ to be equivalent thus imposing a further constraint on the quantum numbers to belong to a finite set $\mathrm{BZ} = \{0, \ldots, L-1\}$ (Brillouin zone).

The inverse Fourier transform is then given by

$$c_j^{\pm} = \frac{1}{L} \sum_{\lambda \in \mathrm{BZ}} e^{\mp ij\lambda} c_{\lambda}^{\pm} , \tag{34}$$

with the summation extending over the Brillouin zone. The anticommutation relations of the new operators are

$$\{c_{\lambda}^+, c_{\mu}^-\} = L\delta_{\lambda,\mu}, \quad \{c_{\lambda}^{\pm}, c_{\mu}^{\pm}\} = 0 . \tag{35}$$

Exercise 1.3 Diagonalize the Hamiltonian (30) by writing it in the momentum space.

In the momentum space we find

$$H = -\frac{2}{L}\sum_{\lambda} n_\lambda \cos\lambda\,, \qquad n_\lambda = c_\lambda^+ c_\lambda^- \,. \tag{36}$$

The Hamiltonian commutes with the particle number operator

$$n = \sum_{j=1}^{L} c_j^+ c_j^- = \frac{1}{L}\sum_{\lambda} n_\lambda \,. \tag{37}$$

and thus the Hilbert space is a tensor product of Hilbert spaces with a fixed number of particles n: $\mathcal{H} = \otimes_{n=0}^{L}\mathcal{H}_n$. The maximal number of particles is L because at most one fermion can occupy a single lattice site.

Exercise 1.4 Derive commutation relations between n_λ, n and $c_\mu^\pm$. There is a useful identity

$$[AB, C] = A\{B, C\} - \{A, C\}B = A[B, C] + [A, C]B \,. \tag{38}$$

The operators $c_\lambda^\pm$ provide maps between Hilbert spaces with different number of particles

$$c_\lambda^+ \colon \mathcal{H}_n \to \mathcal{H}_{n+1}, \quad n = 0, \ldots, L-1; \qquad c_\lambda^- \colon \mathcal{H}_n \to \mathcal{H}_{n-1}, \quad n = 1, \ldots, L.$$

The subspace $\mathcal{H}_0$ is spanned by a single state, the vacuum $|0\rangle \in \mathcal{H}_0$, characterized by

$$c_\lambda^- |0\rangle = 0 \,. \tag{39}$$

We take the vacuum to be normalized: $\langle 0|0\rangle = 1$. A generic eigenstate with n particles can be written as

$$|\lambda_1, \ldots, \lambda_n\rangle = c_{\lambda_1} \ldots c_{\lambda_n}|0\rangle = \prod_{j=1}^{n} c_{\lambda_j}^+ |0\rangle \,, \tag{40}$$

where we agree that the product is developed from the left to the right. A choice of a convention is necessary because of the anticommutation relation of the fermionic operators. Due to the Fermi statistics $\left(c_\lambda^+\right)^2 = 0$ and therefore all λ_js (and consequently quantum numbers I_j) must be distinct. This is the Pauli principle. The action of the Hamiltonian gives the eigenenergies

$$H|\lambda_1, \ldots, \lambda_n\rangle = -\frac{2}{L}\sum_{j=1}^{n} \cos(\lambda_j)\ |\lambda_1, \ldots, \lambda_n\rangle. \tag{41}$$

Exercise 1.5 Find quantum numbers of the ground state of the Hamiltonian with, for example, $n = 5$ particles.

An important characteristic of an eigenstate is its momentum. To this end let us first consider relations between action of the shift operator and the creation/annihilation operators.

Exercise 1.6 Show that: $Uc_\lambda^\pm = \mathrm{e}^{\mp \mathrm{i}\lambda} c_\lambda^\pm U$. Observe that vacuum is invariant under U, that is $U|0\rangle = |0\rangle$ and compute action of U on eigenstates $|\lambda_1, \ldots, \lambda_N\rangle$.

Defining the momentum operator P through $U = \mathrm{e}^{-\mathrm{i}P}$ we find that

$$P|\lambda_1, \ldots, \lambda_N\rangle = \left(\sum_{j=1}^{N} \lambda_j + \mathrm{mod}\ 2\pi \right) |\lambda_1, \ldots, \lambda_N\rangle \ . \tag{42}$$

As a final step we will find local conserved charges. Note that because n_λ commutes with the Hamiltonian any operator of the form

$$Q = \sum_{\lambda \in \mathrm{BZ}} n_\lambda f(\lambda) \ . \tag{43}$$

is a conserved charge. Among all operators of this form we want to find these that are local in the real space. Motivated by the form of the Hamiltonian we define

$$Q_n^+ = -\frac{2}{L} \sum_{\lambda \in \mathrm{BZ}} n_\lambda \cos(n\lambda), \qquad Q_n^- = -\frac{2}{L} \sum_{\lambda \in \mathrm{BZ}} n_\lambda \sin(n\lambda) \ . \tag{44}$$

Exercise 1.7 Compute the expressions for the conserved charges in the real space.

In the real space we find that indeed these are local charges.

$$Q_n^+ = -\sum_{j=1}^{L} \left(c_j^+ c_{j+n}^- - c_j^- c_{j-n}^+ \right) , \quad Q_n^- = -\mathrm{i} \sum_{j=1}^{L} \left(c_j^+ c_{j+n}^- + c_j^- c_{j-n}^+ \right) . \tag{45}$$

Note that the charges are complete, knowledge of their expectation values uniquely identifies an eigenstate. We can characterize each eigenstate by either specifying the Fourier modes occupation numbers n_λ or by expectation values of these conserved charges.

To conclude let us list what we have done. We diagonalized the free fermions Hamiltonian, we found its spectrum and described local conserved charges. Thus this model is a prototype of a quantum integrable model. The key element in its diagonalization was a relation between the physical operators $c_j^\pm$ and operators $c_\lambda^\pm$ in terms of which the Hamiltonian is diagonal. For a noninteracting model like the one at hand this relation is simply the Fourier transform and $c_\lambda^\pm$ follows the same commutation relations as the physical operators. For interacting integrable models

things are more complicated. As we shall see, the algebra of operators diagonalizing the Hamiltonian is more complicated. Furthermore, the transformation between them and physical operators is not any longer a Fourier transform but a more complicated "Quantum Inverse Scattering" transform.

1.5 Literature

A standard introduction to quantum mechanics is Dirac's evergreen *The Principles of Quantum Mechanics* [6]. For a notion of classical integrability (not discussed here) check *Mathematical Methods of Classical Mechanics* by Arnold [1]. For a concise discussion of quantum integrability and difficulties with its definition see the article by Caux and Mossel [3]. A standard book on the many body physics and condensed matter in one dimension is *Quantum Physics in One Dimension* by Giamarchi [12].

Zooming into the world of integrable models a list of books includes

- Gaudin, *The Bethe Wavefunction* [11]. A classical book summarizing the early times of the integrable quantum models in a single uniform treatment. Available in English only since 2014.
- Baxter, *Exactly Solved Models in Statistical Mechanics* [2]. A classic of integrability in the classical statistical models.
- Sutherland, *Beautiful Models* [20]. A very inviting and pleasing journey through the world of integrability. Highly recommended.
- Korepin et al., *Quantum Inverse Scattering Method and Correlation Functions* [14]. As the title suggests, the book is focused on cracking the problem of computing correlation functions of integrable models. It contains a very detailed introduction to some quantum integrable models and to quantum integrability in general.
- Takahashi, *Thermodynamic of One-Dimensional Soluble Models* [22]. A throughout discussion on thermodynamics of the spin chains. Early version of the book is available online [21].
- Essler et al., *The One-Dimensional Hubbard Model* [8]. A complete treatment of the 1D Hubbard model (a model of spinfull interacting fermions) from the Bethe Ansatz point of view.

There are a lot of lecture notes on quantum integrability that are available online. Here we name few of our favorites

- Nepomechie, *A Spin Chain Primer* [18]. A very short and focused introduction to the Algebraic Bethe Ansatz of the XXX model.
- Fadeev, *How Algebraic Bethe Ansatz works for integrable model* [9]. The title is self explanatory.
- Franchini, *An introduction to integrable techniques for one-dimensional quantum systems* [10]. The complete lectures notes on the Bethe Ansatz applied to spin chains and Lieb-Liniger model (a gas of bosonic particles).

- Doikou et al., *Introduction to Quantum Integrability* [7]. The most mathematical (in this list) introduction to the quantum integrability with a lot of focus on highlighting the algebraic structures behind the quantum spin chains (like XXX and XXZ).
- Deguchi, *Introduction to solvable lattice models in statistical and mathematical physics* [4]. A throughout discussion of the integrability in the context of classical statistical physics (the 6-vertex model and alike). Connections with quantum spin chains (XXZ) and quantum groups are elucidated.

2 The XXX Model

In this section we introduce the XXX model. This model is also known as the Heisenberg model. It is a model of magnetism: it describes spins (magnetic moments) placed regularly along a 1d chain and interacting with nearest neighbors. The interaction depends on the relative orientation of the neighboring spins. We place the chain in an external magnetic field which we choose to be in the z direction. We consider the spin $1/2$ case. The Hamiltonian is

$$\begin{aligned} H_{\mathrm{XXX}} &= \sum_{j=1}^{L} \left(J \mathbf{s}_j \cdot \mathbf{s}_{j+1} + h s_j^z \right) \\ &= J \sum_{j=1}^{L} \left(s_j^x s_{j+1}^x + s_j^y s_{j+1}^y + s_j^z s_{j+1}^z \right) + h \sum_{j=1}^{L} s_j^z \,. \end{aligned} \tag{46}$$

We assume periodic boundary conditions: $s_{N+1}^{\alpha} = s_1^{\alpha}$ with $\alpha = x, y, z$. The spin operators on a single site obey the su(2) algebra

$$[s_j^x, s_j^y] = i s_j^z \,, \quad [s_j^y, s_j^z] = i s_j^x \,, \quad [s_j^z, s_j^x] = i s_j^y \,, \tag{47}$$

and commute with spin operators of other sites

$$[s_j^{\alpha}, s_k^{\beta}] = 0 \,, \quad j \neq k \text{ and } \alpha, \beta = x, y, z \,. \tag{48}$$

The local Hilbert space is a two-dimensional complex vector space. An element of it we write as

$$|a\rangle = \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}_{[j]} \,. \tag{49}$$

The spin operators are represented by 2×2 unitary matrices

$$s_j^x = \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \,, \quad s_j^y = \frac{1}{2} \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} \,, \quad s_j^z = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} . \tag{50}$$

There is a fourth linearly independent from s_j^α matrix, the identity matrix. Any operator on a single site can be written as a certain linear combination of these 4 matrices. Any operator acting on a whole chain can be written as a tensor product of local operators.

As a basis of a local Hilbert space we choose the eigenvectors of the s^z operators and denote them

$$|\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} , \quad |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} . \tag{51}$$

The last part of the Hamiltonian, describing interaction with the external magnetic field is very simple because the operator

$$S^z = \sum_{j=1}^{L} s_j^z , \tag{52}$$

commutes with the Hamiltonian. Therefore adding the magnetic field simply shifts the energies of the eigenstates leaving the eigenstates intact. While discussing the diagonalization of the XXX model we set $h = 0$.

Exercise 2.1 Consider an anisotropic generalization of the XXX model, the so called XYZ model

$$H_{\mathrm{XYZ}} = \sum_{j=1}^{L} \left(J_x s_j^x s_{j+1}^x + J_y s_j^y s_{j+1}^y + J_z s_j^z s_{j+1}^z \right) . \tag{53}$$

Find the condition (on J_x, J_y, J_z) under which the total z-spin operator S_z commutes with this Hamiltonian.

2.1 Spin Lowering and Raising Operators

For a better understanding of the XXX model it is convenient to introduce the spin lowering s_j^- and raising s_j^+ operators. Observe the following relations

$$\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} |\uparrow\rangle = 0 , \quad \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} |\downarrow\rangle = |\uparrow\rangle . \tag{54}$$

These matrices define the spin raising operator s_j^+. Similarly we can define a spin lowering operator s_j^-.

Exercise 2.2 Find the matrix representation of the s_j^- operators. Find the expression for $s_j^\pm$ in terms of the original s_j^α operators. Write the XXX Hamiltonian using these new operators.

The spin lowering operators are given by

$$s_j^\pm = s_j^x \pm i s_j^y \,. \tag{55}$$

Expressing the Hamiltonian in terms of the new operators we find

$$H_{\mathrm{XXX}} = J \sum_{j=1}^{L} \Big(\tfrac{1}{2} \underbrace{(s_j^+ s_{j+1}^- + s_j^- s_{j+1}^+)}_{\text{kinetic}} + \underbrace{s_j^z s_{j+1}^z}_{\text{interaction}} \Big) + hS^z \,. \tag{56}$$

The first two terms describe now a process of exchanging spin at neighboring sites. If we think about a spin up as a particle and a spin down as a hole (absence of a particle), then the first term describes hopping of this particle. The second term describes interaction of the neighboring spins (or particles and holes).

The Hamiltonian commutes with the total z-spin operator S_z so the Hilbert space factorizes in product of Hilbert spaces, each with fixed value of the magnetization S_z. For a spin $1/2$ chain of length L the possible values of S_z are

$$S_z = -L/2, -(L-1)/2, \ldots, (L-1)/2, L/2 \,. \tag{57}$$

The two fully polarized states

$$|\Uparrow\rangle = \underbrace{|\uparrow\rangle \otimes \cdots \otimes |\uparrow\rangle}_{L \text{ times}} \,, \quad |\Downarrow\rangle = \underbrace{|\downarrow\rangle \otimes \cdots \otimes lvert\, \downarrow\rangle}_{L \text{ times}} \,, \tag{58}$$

with $S_z = \pm L/2$, are eigenstates of H_{XXX} with eigenvalues $L(J/4 \pm h/2)$.

2.2 Lattice Fermions and Spin Chains

A distinctive feature of the 1d physics is transmutability of bosonic and fermionic particles and spins. This short section introduces the Jordan–Wigner transformation that relates fermionic degrees of freedom to spins.

Recall that spinless fermions obey the following anticommutation relations

$$\{c_j^+, c_k^-\} = \delta_{jk}, \quad \{c_j^\pm, c_k^\pm\} = 0 \,, \tag{59}$$

whereas the spin 1/2 operators $s_j^\pm$, s_j^z commute on different sites and on a single site obey

$$[s_j^+, s_j^-] = 2s_j^z, \quad [s_j^z, s_j^\pm] = \pm s_j^\pm \,, \tag{60}$$

and additionally

$$\{s_j^+, s_j^-\} = 1 \ . \tag{61}$$

Therefore the spins on a single lattice behave like fermions, but they commute, instead of anticommuting on different lattice sites. This can be fixed by introducing a Jordan-Wigner string

$$s_j^+ = c_j^+ \underbrace{\exp\left(\mathrm{i}\pi \sum_{k<j} n_k\right)}_{\text{Jordan–Wigner string}}, \quad s_j^- = \exp\left(-\mathrm{i}\pi \sum_{k<j} n_k\right) c_j^- \ , \quad s_j^z = n_j - \frac{1}{2} \ , \tag{62}$$

where $n_j = c_j^+ c_j^-$.

Exercise 2.3 Show that operators $s_j^\pm$ and s_j^z defined through the Jordan–Wigner transformation obey the spin $1/2$ commutation relations.

What model of fermions corresponds to the XXX spin chain?

Exercise 2.4 Using the Jordan-Wigner transformation write a model of spinless fermions corresponding to the XXX spin chain. What spin model describes the free fermions of Sect. 1.4?

3 The Algebraic Bethe Ansatz

In this section we formulate the Algebraic Bethe Ansatz (ABA) for the XXX spin chain. The central object of the ABA is a transfer matrix. The transfer matrix is an operator acting in the Hilbert space of the XXX spin chain and containing the XXX Hamiltonian. The ABA provides means of diagonalizing the transfer matrix. The transfer matrix is also a generating function for a family of local operators commuting with the XXX Hamiltonian thus showing the integrability of the XXX model.

The transfer matrix is built of Lax operators which we now introduce. The Hamiltonian is a sum over two-sites operators

$$H_{\mathrm{XXX}} = J \sum_{j=1}^{L} H_{j,j+1} \ , \quad H_{j,j+1} = s_j^x s_{j+1}^x + s_j^y s_{j+1}^y + s_j^z s_{j+1}^z \ . \tag{63}$$

Using the matrix representation of the operators we observe that the two-site Hamiltonian is closely related to the permutation operator. Recall that in our notation

$$o_1 o_2 = (o \otimes o)_{[12]} \tag{64}$$

which gives

$$s_1^x s_2^x = \frac{1}{4}\begin{pmatrix} & & & 1 \\ & & 1 & \\ & 1 & & \\ 1 & & & \end{pmatrix}_{[12]} , \quad s_1^y s_2^y = \frac{1}{4}\begin{pmatrix} & & & -1 \\ & & 1 & \\ & 1 & & \\ -1 & & & \end{pmatrix}_{[12]} ,$$
$$s_1^z s_2^z = \frac{1}{4}\begin{pmatrix} 1 & & & \\ & -1 & & \\ & & -1 & \\ & & & 1 \end{pmatrix}_{[12]} \tag{65}$$

and

$$H_{12} = \tfrac{1}{2}\mathcal{P}_{12} - \tfrac{1}{4}1_{12} \tag{66}$$

where 1 is the 4×4 identity matrix and the permutation operator is

$$\mathcal{P}_{12} = \begin{pmatrix} 1 & & & \\ & & 1 & \\ & 1 & & \\ & & & 1 \end{pmatrix}_{[12]} , \quad \mathcal{P}_{12}(|a\rangle \otimes |b\rangle) = |b\rangle \otimes |a\rangle . \tag{67}$$

Diagonalization of the two-site Hamiltonian is equivalent to finding the eigenstates of the permutation operator. We find $2^2 = 4$ eigenstates

$$|\uparrow\rangle \otimes |\uparrow\rangle , \quad |\downarrow\rangle \otimes |\downarrow\rangle , \quad |\downarrow\rangle \otimes |\uparrow\rangle + |\uparrow\rangle \otimes |\downarrow\rangle ; \quad |\downarrow\rangle \otimes |\uparrow\rangle - |\uparrow\rangle \otimes |\downarrow\rangle . \tag{68}$$

Note that besides the two fully polarized states there are two states that are superpositions of states in which some spins are up and some down.

The Lax operator, that we introduce in the next section, is a certain deformation of the two-site Hamiltonian.

3.1 Transfer Matrix

Define the Lax operator $L_{0j} : \mathsf{h}_0 \otimes \mathsf{h}_j \to \mathsf{h}_0 \otimes \mathsf{h}_j$ such that

$$L_{0j}(\lambda) = \left(\lambda - \frac{\mathrm{i}}{2}\right) 1_{0j} + \mathrm{i}\, \mathcal{P}_{0j} . \tag{69}$$

Note that $L_{0j}(0) = 2iH_{0j}$. The Lax operator acts in a tensor product of an auxiliary space (h_0) and the physical Hilbert space at the jth lattice site. The auxiliary space is isomorphic with the single lattice site space and can be thought of as also

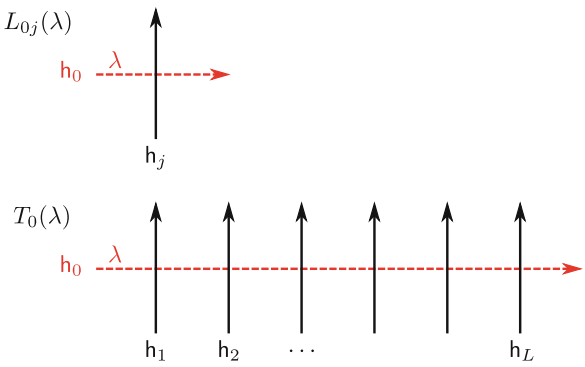

Fig. 3 The Lax operator and the monodromy matrix

representing a single spin $1/2$ degree of freedom. We should think about the Lax operator as a propagator of this auxiliary spin through a single lattice site. This propagation depends on three factors: the spin of the lattice site, the value of the virtual spin and the rapidity λ of the virtual spin (see Fig. 3). To enforce this interpretation we can write the Lax operator as a matrix in the auxiliary space

$$L_{0j}(\lambda) = \begin{pmatrix} \lambda + is_j^z & 2is_j^- \\ 2is_j^+ & \lambda - is_j^z \end{pmatrix}_{[0]} . \tag{70}$$

Taking product of the Lax operators we obtain a propagator (monodromy matrix) of the virtual spin through the whole chain

$$T_0(\lambda) = L_{0L}(\lambda) \times \cdots \times L_{02}(\lambda) L_{01}(\lambda) . \tag{71}$$

The monodromy matrix depends on the spin and the rapidity of the virtual particle and on the configuration of all spins of the chain. In the auxiliary space, the monodromy matrix can be written as a matrix of operators

$$T_0(\lambda) = \begin{pmatrix} A(\lambda) & B(\lambda) \\ C(\lambda) & D(\lambda) \end{pmatrix}_{[0]} . \tag{72}$$

The matrix elements $A, B, \ldots,$ are operators acting in the physical Hilbert space $\mathcal{H}$ and parametrized by λ. Their explicit form can be found by a repetitive multiplication of Lax operators.

Trace of the monodromy matrix, called the transfer matrix,

$$\tau(\lambda) = \mathrm{tr}_0\, T_0(\lambda) = A(\lambda) + D(\lambda) , \tag{73}$$

describes a propagation of the virtual spin through the whole chain with the same in and out spins. An eigenstate of the transfer matrix is a special configuration of lattice spins through which the virtual spin propagates invisibly. We will now show that the transfer matrix contains the momentum operator and the XXX Hamiltonian.

Of importance is behavior of the transfer matrix around $\lambda = \mathrm{i}/2$. Observe that

$$L_{0j}(\mathrm{i}/2) = \mathrm{i}P_{0j} \tag{74}$$

and thus

$$\begin{aligned}\tau(\mathrm{i}/2) = \mathrm{tr}_0\, T_0(\mathrm{i}/2) &= \mathrm{tr}_0\big(L_{0L}(\mathrm{i}/2)L_{0L-1}(\mathrm{i}/2)\cdots L_{01}(\mathrm{i}/2)\big)\\ &= \mathrm{i}^L\,\mathrm{tr}_0(\mathcal{P}_{0L}\mathcal{P}_{0L-1}\cdots\mathcal{P}_{01})\ .\end{aligned} \tag{75}$$

A product of the permutation operators can be reorganized, using the formula

$$\mathcal{P}_{0L}\mathcal{P}_{0L-1} = \mathcal{P}_{L,L-1}\mathcal{P}_{0L}, \tag{76}$$

we find

$$\begin{aligned}\tau(\mathrm{i}/2) &= \mathrm{i}^L\,\mathrm{tr}_0(\mathcal{P}_{L,L-1}\mathcal{P}_{L,L-2}\cdots\mathcal{P}_{L1}\mathcal{P}_{0L})\\ &= \mathrm{i}^L\mathcal{P}_{L,L-1}\mathcal{P}_{L,L-2}\cdots\mathcal{P}_{L1} = i^L\mathcal{P}_{1,2}\mathcal{P}_{2,3}\ldots\mathcal{P}_{L-1,L} = i^L U\ .\end{aligned} \tag{77}$$

Therefore the transfer matrix at $\mathrm{i}/2$ is just the shift operator. From the relation $U = \mathrm{e}^{-\mathrm{i}P}$ between the momentum operator P and the shift operator U we find

$$P = \mathrm{i}\log\mathrm{i}^{-L}\tau(\mathrm{i}/2)\ . \tag{78}$$

Exercise 3.1 Show first that

$$\tau'(\mathrm{i}/2) = \mathrm{i}^{L-1}\sum_{j=1}^{L}\mathcal{P}_{1,2}\cdots\mathcal{P}_{j-1,j+1}\ldots\mathcal{P}_{L-1,L}\ .$$

Consider now the log derivative of $\tau(\lambda)$ at $\lambda = \mathrm{i}/2$

$$\frac{\partial}{\partial\lambda}\log\tau(\lambda) = \tau^{-1}(\lambda)\frac{\partial}{\partial\lambda}\tau(\lambda)\ .$$

Show that it contains the XXX Hamiltonian.

The relation between the transfer matrix and the XXX Hamiltonian is the following

$$H = \frac{J}{2}\left(\mathrm{i}\frac{\partial}{\partial\lambda}\log\tau(\lambda)|_{\lambda=\mathrm{i}/2} - \frac{L}{2}\right), \tag{79}$$

since

$$\frac{\partial}{\partial\lambda}\log\tau(\lambda)|_{\lambda=i/2} = -i\sum_{j=1}^{L}\mathcal{P}_{j,j+1}\ . \tag{80}$$

Taking higher log derivatives of the transfer matrix we get a family of local charges enumerated by an integer n

$$Q_n \sim \frac{\partial^n}{\partial \lambda^n} \log \tau(\lambda)|_{\lambda=\mathrm{i}/2} \,. \tag{81}$$

Exercise 3.2 Compute Q_2 and observe that this is a local operator. The computations are a bit long and we provide a partial result

$$\tau^{-1}(\mathrm{i}/2)\tau''(\mathrm{i}/2) = -2\sum_{j>k+1}^{L} \mathcal{P}_{k-1,k}\mathcal{P}_{j-1,j} - 2\sum_{k=1}^{L} \mathcal{P}_{k,k+1}\mathcal{P}_{k-1,k} \,. \tag{82}$$

The ABA construction has just shown that the XXX Hamiltonian can be generated from the transfer matrix. The next step is to find the eigenstates. The XXX Hamiltonian commutes with the transfer matrix (we will see this in the next section) and therefore we can look for the eigenstates of the transfer matrix itself.

3.2 Diagonalizing the Transfer Matrix

Recall that the monodromy matrix contains 4 operators, 2 of them (A and D) make the transfer matrix. The remaining two could be used as a creation and annihilation operators. To materialize this idea we need to know a single eigenstate of the transfer matrix and we need commutation relations between the operators forming the monodromy matrix. We know actually two eigenstates of the transfer matrix, these are the fully polarized states $|\Uparrow\rangle$ and $|\Downarrow\rangle$ that we introduced earlier.

Exercise 3.3 Show that the states $|\Uparrow\rangle$ and $|\Downarrow\rangle$ are indeed eigenstates of the transfer matrix using its explicit construction as a trace of a monodromy matrix which in turn is a product of local Lax operators. Find the eigenvalues.

For the "up" state we find

$$\tau(\lambda)|\Uparrow\rangle = \left[\left(\lambda + \frac{\mathrm{i}}{2}\right)^L + \left(\lambda - \frac{\mathrm{i}}{2}\right)^L\right]|\Uparrow\rangle \,. \tag{83}$$

We could now try to obtain other eigenstates using the $B(\lambda)$ operator. We make an ansatz

$$|\mu_1, \ldots, \mu_M\rangle = \prod_{j=1}^{M} B(\mu_j)|\Uparrow\rangle \,. \tag{84}$$

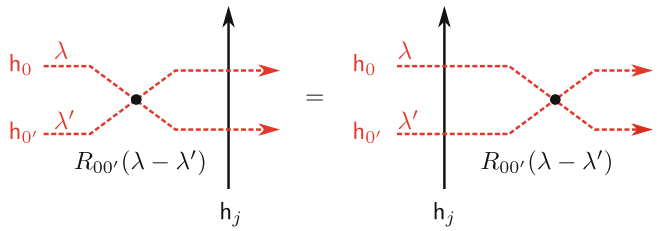

Fig. 4 The intertwining relation for the Lax operator

To check if $|\mu_1, \ldots, \mu_M\rangle$ is an eigenstate of $\tau(\lambda)$ we need commutation relations between A, D and B. Because the monodromy matrix is made of the Lax operators we consider first the commutation relation between matrix elements of the Lax operator.

The Lax operator obeys the commutation relation (see Fig. 4)

$$R_{00'}(\lambda-\lambda')L_{0j}(\lambda)L_{0'j}(\lambda') = L_{0'j}(\lambda')L_{0j}(\lambda)R_{00'}(\lambda-\lambda') \,, \tag{85}$$

where R is a matrix

$$R(\lambda) = \begin{pmatrix} \lambda+\mathrm{i} & & & \\ & \lambda & \mathrm{i} & \\ & \mathrm{i} & \lambda & \\ & & & \lambda+\mathrm{i} \end{pmatrix} = \begin{pmatrix} a(\lambda) & & & \\ & b(\lambda) & c(\lambda) & \\ & c(\lambda) & b(\lambda) & \\ & & & a(\lambda) \end{pmatrix} . \tag{86}$$

The R-matrix and the Lax operator are related

$$L_{ab}(\lambda) = R_{ab}(\lambda - \mathrm{i}/2) \,, \tag{87}$$

which implies that the R-matrix obeys the Yang–Baxter equation

$$R_{ab}(\lambda-\lambda')R_{ac}(\lambda)R_{bc}(\lambda') = R_{bc}(\lambda')R_{ac}(\lambda)R_{12}(\lambda-\lambda') \,. \tag{88}$$

Exercise 3.4 Verify that the R-matrix (86) indeed solves the Yang–Baxter equation. Symbolic computation software is of great help in performing such task.

The commutation relation (85) implies an analogous relation for the monodromy matrices (see Fig. 5)

$$R_{00'}(\lambda-\lambda')T_0(\lambda)T_{0'}(\lambda') = T_{0'}(\lambda')T_0(\lambda)R_{00'}(\lambda-\lambda') \,. \tag{89}$$

Exercise 3.5 Show that the commutation relation for the Lax operators implies the corresponding relation for the monodromy matrices. Start with the $L = 2$ case.

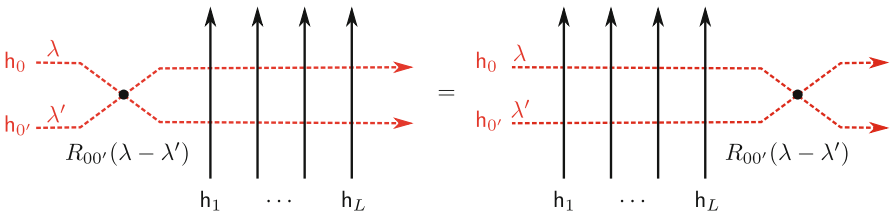

Fig. 5 The commutation relation for the monodromy matrix

Taking traces over the auxiliary spaces in (89) we find that the transfer matrices with different rapidities commute

$$[\tau(\lambda), \tau(\lambda')] = 0 \,. \tag{90}$$

Recall that the transfer matrix contains the Hamiltonian, thus we found that there is a one-parameter family of operators commuting with the XXX Hamiltonian.

$$[\tau(\lambda), H] = 0 \,. \tag{91}$$

Expanding the transfer matrix $\tau(\lambda)$ as in (81), we find that Q_j's are local conserved charges. Thus showing the integrability of the XXX model.

The R-matrix provides commutation relations between operators A, B, etc. Deriving the relations is a straightforward computation using the intertwining relation (89) and the R-matrix (86). As a result we find, among others, the following relations

$$[B(\lambda), B(\lambda')] = 0 \,, \tag{92}$$

$$A(\lambda)B(\lambda') = \frac{a(\lambda'-\lambda)}{b(\lambda'-\lambda)}B(\lambda')A(\lambda) - \frac{c(\lambda'-\lambda)}{b(\lambda'-\lambda)}B(\lambda)A(\lambda') \,, \tag{93}$$

$$D(\lambda)B(\lambda') = \frac{a(\lambda-\lambda')}{b(\lambda-\lambda')}B(\lambda')D(\lambda) - \frac{c(\lambda-\lambda')}{b(\lambda-\lambda')}B(\lambda)D(\lambda') \,, \tag{94}$$

$$[B(\lambda), C(\lambda')] = \frac{c(\lambda-\lambda')}{b(\lambda-\lambda')}\big(D(\lambda')A(\lambda) - D(\lambda)A(\lambda')\big) \,. \tag{95}$$

Exercise 3.6 Verify these commutation relations. Again, with a software capable of performing symbolic computations it is a straightforward task to do.

We can now get back to the ansatz for the eigenstate of the transfer matrix. We proposed

$$|\mu_1, \ldots, \mu_M\rangle = \prod_{j=1}^{M} B(\mu_j)|\Uparrow\rangle, \tag{96}$$

as an eigenstate. Acting with $A(\lambda)$ and $D(\lambda)$ we get results of the following structure

$$A(\lambda)|\mu_1,\dots,\mu_M\rangle = \Lambda(\lambda,\{\mu\})|\mu_1,\dots,\mu_M\rangle + \sum_{a=1}^{M}\Lambda_a B(\mu)\prod_{b=1,j\neq a}^{M} B(\mu_j)|\Uparrow\rangle\,, \tag{97}$$

$$D(\lambda)|\mu_1,\dots,\mu_M\rangle = \tilde{\Lambda}(\lambda,\{\mu\})|\mu_1,\dots,\mu_M\rangle + \sum_{a=1}^{M}\tilde{\Lambda}_a B(\mu)\prod_{b=1,j\neq a}^{M} B(\mu_j)|\Uparrow\rangle\,. \tag{98}$$

Exercise 3.7 Derive explicit expressions for Λs. The general pattern can be easily guessed as from considering $M = 2$ and $M = 3$ cases.

For $|\mu_1,\dots,\mu_M\rangle$ to be an eigenstate of $\tau(\lambda)$ we need $\Lambda_a + \tilde{\Lambda}_a = 0$ which yields the following equations

$$\left(\frac{\mu_a+\frac{\mathrm{i}}{2}}{\mu_a-\frac{\mathrm{i}}{2}}\right)^L = \prod_{b=1,b\neq a}^{M}\frac{\mu_a-\mu_b+\mathrm{i}}{\mu_a-\mu_b-\mathrm{i}}\,,\quad a=1,\dots,M\,. \tag{99}$$

These are the celebrated Bethe equations (for the XXX spin chain). The eigenvalue of the transfer matrix $(\Lambda+\tilde{\Lambda})$ is

$$\begin{aligned}\tau(\lambda,\{\mu\}) &= \Lambda(\lambda,\{\mu\}) + \tilde{\Lambda}(\lambda,\{\mu\})\\ &= \left(\lambda+\frac{\mathrm{i}}{2}\right)^L\prod_{a=1}^{M}\frac{a(\mu_a-\lambda)}{b(\mu_a-\lambda)} + \left(\lambda-\frac{\mathrm{i}}{2}\right)^L\prod_{a=1}^{M}\frac{a(\lambda-\mu_a)}{b(\lambda-\mu_a)}\\ &= \left(\lambda+\frac{\mathrm{i}}{2}\right)^L\prod_{a=1}^{M}\frac{\lambda-\mu_a-\mathrm{i}}{\lambda-\mu_a} + \left(\lambda-\frac{\mathrm{i}}{2}\right)^L\prod_{a=1}^{M}\frac{\lambda-\mu_a+\mathrm{i}}{\lambda-\mu_a}\,.\end{aligned} \tag{100}$$

From the eigenvalue of the transfer matrix we can find the momenta and energies of the states. Recall that

$$P = \mathrm{i}\log \mathrm{i}^{-L}\tau(\mathrm{i}/2)\,,\quad H = \frac{J}{2}\left(\mathrm{i}\frac{\partial}{\partial\lambda}\log\tau(\lambda)|_{\lambda=\mathrm{i}/2} - \frac{L}{2}\right). \tag{101}$$

We find

$$P_\mu = \sum_{a=1}^{M} p(\mu_a)\,,\qquad p(\mu) = i\log\frac{\mu+\mathrm{i}/2}{\mu-\mathrm{i}/2}\,, \tag{102}$$

$$E_\mu = \sum_{a=1}^{M}\epsilon(\mu_a) + \frac{JL}{4}\,,\qquad \epsilon(\mu) = -\frac{J}{2}\frac{1}{\mu^2+\frac{1}{4}}\,. \tag{103}$$

Exercise 3.8 Show these equations.

We can eliminate the rapidity μ to find a dispersion relation

$$\epsilon(p) = J(\cos p - 1) \ . \tag{104}$$

The magnetization in the z direction S^z is

$$S^z|\mu_1, \dots \mu_M\rangle = \left(\frac{L}{2} - M\right)|\mu_1, \dots, \mu_M\rangle \ . \tag{105}$$

Finally let us just state that the dual states are created with the C operators

$$\langle\mu_1, \dots, \mu_M| = \langle\Uparrow| \prod_{j=1}^{M} C(\mu_j) \ , \tag{106}$$

and they are the Bethe states (eigenstates of the XXX Hamiltonian) if μ_js obey the same Bethe equations (99).

3.3 Bethe Equations and Their Solutions: Physics

The Bethe equations (99) can be rewritten in a logarithmic form using an identity

$$\frac{x + \mathrm{i}}{x - \mathrm{i}} = \exp[2\mathrm{i}\,\mathrm{atan}(1/x)] = \exp[\mathrm{i}\pi - 2\mathrm{i}\,\mathrm{atan}(x)] \ . \tag{107}$$

This yields

$$\exp\bigl(-2iL\,\mathrm{atan}(2\mu_a)\bigr) = (-1)^{M-L-1} \exp\left(-2\mathrm{i}\sum_{\substack{b=1 \\ b\neq a}}^{M} \mathrm{atan}(\mu_a - \mu_b)\right) , \qquad a = 1, \dots, M \tag{108}$$

and upon taking the logarithm we find

$$\mathrm{atan}(2\mu_a) = \frac{\pi}{L} I_a + \frac{1}{L} \sum_{b=1}^{M} \mathrm{atan}(\mu_a - \mu_b) \ , \quad a = 1, \dots, M \ , \tag{109}$$

where quantum numbers I_a defined through $(-1)^{M-L-1} = \exp(2\pi I_j)$ are half-odd integers (if $L - M$ is even) or integers (if $L - M$ is odd). Quantum numbers are bounded and this can be seen from sending one rapidity to infinity. Then

$$\lim_{\mu_a\to\infty}\left(\operatorname{atan}(2\mu_a)-\frac{1}{L}\sum_{b=1}^{M}\operatorname{atan}(\mu_a-\mu_b)\right)=\frac{\pi}{2}-\frac{\pi(M-1)}{2L}\,. \tag{110}$$

For the rapidities to be finite the quantum numbers should be bounded

$$|I_a|<I_\infty=\frac{L-M+1}{2}\,. \tag{111}$$

We are interested in the structure of the ground state and excitations above it. The situations are different for the ferromagnetic ($J<0$) and antiferromagnetic ($J>0$) cases. We start with the former.

3.3.1 Ferromagnetic Chain: Magnons

In the ferromagnetic sector the spins tend to align parallel to each other and in the absence of the magnetic field the ground state is given by one of the fully polarized states. The excitations are given by states with nonzero M. For large chains ($L\to\infty$) we can neglect the interacting part of the Bethe equations and get

$$\operatorname{atan}(2\mu_a)=\frac{\pi}{L}I_a+\mathcal{O}(1/L)\,. \tag{112}$$

Therefore the excitations are (approximately) free particles with a spin 1 and dispersion relation $\epsilon_0(p)=|J|(1-\cos p)$. We call them magnons.

Magnons can form bound states. Consider Bethe equations for $M=2$ in the product form

$$\left(\frac{\mu_1+\frac{\mathrm{i}}{2}}{\mu_1-\frac{\mathrm{i}}{2}}\right)^L=\frac{\mu_1-\mu_2+\mathrm{i}}{\mu_1-\mu_2-\mathrm{i}}\,, \tag{113}$$

$$\left(\frac{\mu_2+\frac{\mathrm{i}}{2}}{\mu_2-\frac{\mathrm{i}}{2}}\right)^L=\frac{\mu_2-\mu_1+\mathrm{i}}{\mu_2-\mu_1-\mathrm{i}}\,. \tag{114}$$

We can allow the rapidities μ_a to be complex under a condition that the momentum $p(\mu_a)+p(\mu_b)$ is real. This turns into a constraint

$$\left(\frac{\mu_1+\frac{\mathrm{i}}{2}}{\mu_1-\frac{\mathrm{i}}{2}}\right)^L\left(\frac{\mu_2+\frac{\mathrm{i}}{2}}{\mu_2-\frac{\mathrm{i}}{2}}\right)^L=1\,. \tag{115}$$

If the imaginary part of μ_1 is nonzero then the LHS of the Bethe equations behaves exponentially in L. For the Bethe equations to hold in the limit $L\to\infty$ we need that

$$\mu_1-\mu_2=\pm\mathrm{i}\,. \tag{116}$$

Because the Bethe equations are symmetric we can postulate that

$$\mu_1 = \mu_{1/2} + \frac{\mathrm{i}}{2}\,, \quad \mu_2 = \mu_{1/2} - \frac{\mathrm{i}}{2}\,, \tag{117}$$

with a real $\mu_{1/2}$. The momentum and energy of this state are

$$P = p(\mu_{1/2} + \mathrm{i}/2) + p(\mu_{1/2} - \mathrm{i}/2) = -\mathrm{i}\log\frac{\mu_{1/2} + \mathrm{i}}{\mu_{1/2} - \mathrm{i}}, \tag{118}$$

$$E = \epsilon(\mu_{1/2} + \mathrm{i}/2) + \epsilon(\mu_{1/2} - \mathrm{i}/2) = |J|\frac{1}{\mu_{1/2}^2 + 1}. \tag{119}$$

Eliminating the rapidity $\mu_{1/2}$ we find the dispersion relation

$$\epsilon_{1/2}(p) = \frac{|J|}{2}(1 - \cos p)\,. \tag{120}$$

This state is interpreted as a stable bound state because it has a lower energy than the sum of two free magnons

$$\epsilon_{1/2}(p) < \epsilon_0(p - p_1) + \epsilon(p_1)\,. \tag{121}$$

There exist also bound states of more than two magnons, forming a regular (for $L \to \infty$) pattern in the complex plane

$$\lambda_{m,a} = \lambda_{m,0} + \mathrm{i}a/2\,, \quad a = -m, \ldots, m\,. \tag{122}$$

with m half integers. In general, these are called string solutions to the Bethe equations. The whole Hilbert space is thus spanned (for large L) by magnons and their bound states.

3.3.2 Antiferromagnet: Spinons

We consider now the antiferromagnetic regime. As we switch the sign of J a fundamental thing happens. The reference state is not anymore a ground state. If the magnetic field is zero then the ground state of an antiferromagnet should have $S^z = L/2 - M = 0$ which sets $2M = L$. Therefore the number of rapidities is of the same order as the number of lattice sites. The ground states is now the state with $M = L/2$ and with the minimal energy. The Bethe equations (109) are

$$\mathrm{atan}(2\mu_a) = \frac{\pi}{L}I_a + \frac{1}{L}\sum_{b=1}^{M}\mathrm{atan}(\mu_a - \mu_b)\,, \quad a = 1, \ldots, M\,, \tag{123}$$

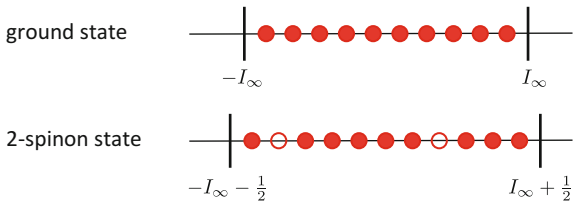

Fig. 6 We consider a chain of $N = 20$ lattice sites at the zero external magnetic field. Quantum numbers for the ground state and a 2-spinon excited state are depicted

We now assume that the ground state is formed by finite and real rapidities (recall that in the ferromagnetic sector bound states had lower energy, thus now they have higher). It can also be shown that the quantum numbers should be all distinct. According to (110) the quantum numbers are limited by

$$|I_a| < I_\infty^{h=0} = \frac{M+1}{2} , \tag{124}$$

and the ground state quantum numbers occupy the whole allowed interval (see Fig. 6). Explicitly we can write them as

$$I_a^{\mathrm{GS}} = a - \frac{M+1}{2} , \quad a = 1, \dots, M . \tag{125}$$

In a nonzero magnetic field there is a bit of space between I_M and I_∞ and excited states can be created by choosing a different set of quantum numbers. In the zero magnetic case the way to create an excited state is to either send some rapidities to infinity, delete some rapidities or to consider complex solutions. We will consider deleting some rapidities. Thus let us delete one B operator and consider a state with $M-1$. The quantum numbers are now bounded by (we have $M = L/2 - 1$)

$$I_\infty = \frac{L-M+1}{2} = \frac{M}{2} + 1 = I_\infty^{h=0} + \frac{1}{2} . \tag{126}$$

So the bounds on the quantum numbers extend giving one extra space. We have also one less quantum number to occupy thus in total there are two holes that characterize an excited state. The positions of holes can be chosen freely (in the allowed range). Because we erased one B operator the spin of this state is 1. However we should interpret it as an excited state having two excitations, spinons, of spin $\frac{1}{2}$. We associate a spinon with a choice of a position of a hole. The dispersion relation of a spinon is given by (for a derivation we refer for example to [10])

$$\epsilon_{\mathrm{sp}}(p) = \frac{\pi}{2} |\sin p| , \quad -\pi < p \leq 0 . \tag{127}$$

If we were to consider all possible states we would find that their total number is 2^L as required by the dimension of the Hilbert space. This requires careful analysis of possible configuration of quantum numbers in states with strings, infinite

rapidities and holes. In the end we would find that the elementary excitation is a spinon which appears always in pairs (for even number of lattice sites).

We will not discuss the structure of the Bethe states any further, let us note however that understanding it is crucial for computing the correlation functions.

4 Other Spin Chains

The aim of this section is to provide a quick reference of the quantum integrable models. We focus exclusively on the lattice models.

- The XX model

$$H_{\mathrm{XX}} = J_x \sum_{j=1}^{N} \left(s_j^x s_{j+1}^x + s_j^y s_{j+1}^y\right) + h \sum_{j=1}^{N} s_j^z \,,$$

  The XX model is equivalent to the free fermions model. See Sect. 2.2.
- The Ising model (in the transverse field)

$$H_{\mathrm{Ising}} = J_x \sum_{j=1}^{N} s_j^z s_{j+1}^z + \left(h \sum_{j=1}^{N} s_j^x\right) \,,$$

  The Ising model is also equivalent to a free fermionic theory, but of Majorana fermions. Can be solved exactly and correlation functions can be also computed.
- The XXX model

$$H_{\mathrm{XXX}} = J_x \sum_{j=1}^{N} \left(s_j^x s_{j+1}^x + s_j^y s_{j+1}^y + s_j^z s_{j+1}^z\right) + h \sum_{j=1}^{N} s_j^z \,,$$

  this is a fully interacting spin chain. It can not be mapped to a free theory.

  All these three models are a special case of the XXZ model

$$H_{\mathrm{XXZ}} = J_x \sum_{j=1}^{N} \left(s_j^x s_{j+1}^x + s_j^y s_{j+1}^y + \Delta s_j^z s_{j+1}^z\right) + h \sum_{j=1}^{N} s_j^z \,.$$

The XXZ model corresponds to a deformation of the XXX (for which $\Delta = 1$). This deformation breaks the sl(2) symmetry of the XXX chain. However this breaking is under control and the symmetry of the XXZ chain is a symmetry of the quantum group $\left(U_q(\mathrm{sl}(2)\right)$. In the next section we will discuss the XXZ model in a greater detail.

The models that we described so far had spin $\frac{1}{2}$. There are also integrable models of higher spins. However, if we naively take the XXX model and choose the $s = 1$ representation such a model will not be integrable. The correct generalization is

$$H_{\mathrm{XXX}}^{(s=1)} = \frac{J}{4}\sum_{j=1}^{N}\Big(\mathbf{s}_j\mathbf{s}_{j+1} - \big(\mathbf{s}_j\mathbf{s}_{j+1}\big)^2\Big)\ . \tag{128}$$

We will shed a light on why this model is integrable in the next section.

Another viable modification of the XXX model is to couple spins more than one lattice site apart. Such couplings render the model, generally speaking, nonintegrable.

5 Constructing an Integrable Model

Let us take one more look at the construction of the XXX model and try to generalize it. The central object is the R-matrix solving the Yang–Baxter equation

$$\begin{aligned} R_{ab}(\lambda_a-\lambda_b)R_{ac}(\lambda_a-\lambda_c)R_{bc}(\lambda_b-\lambda_c) \\ = R_{bc}(\lambda_b-\lambda_c)R_{ac}(\lambda_a-\lambda_c)R_{ab}(\lambda_a-\lambda_b)\ . \end{aligned} \tag{129}$$

Assume that we have such a matrix at our disposal. Then we can define a Lax operator

$$L_{0j}(\lambda) = R_{0j}(\lambda - \mathrm{i}/2)\ . \tag{130}$$

The shift of the argument of the R-matrix is here only for convenience, it leads to a more symmetric Bethe equations. We also relabeled the vector spaces to emphasize that the Lax operator acts in a tensor product of the auxiliary matrix and the local Hilbert space. This also means that the local Hilbert space must be isomorphic to the auxiliary space. Redefining the rapidities we find the intertwining relation for the Lax operator

$$R_{00'}(\lambda-\lambda')L_{0j}(\lambda)L_{0'j}(\lambda') = L_{0'j}(\lambda')L_{0j}(\lambda)R_{00'}(\lambda-\lambda')\ . \tag{131}$$

As earlier, we can define the monodromy matrix. In fact we can define a slightly more general monodromy matrix by introducing anisotropies ξ_j at each lattice sites such that

$$T_0(\lambda) = L_{0L}(\lambda-\xi_L)\ldots L_{02}(\lambda-\xi_2)L_{01}(\lambda-\xi_1)\ . \tag{132}$$

Such modification does not influence the main property of the monodromy matrix, it is still intertwined with the same R-matrix

$$R_{00'}(\lambda-\lambda')T_0(\lambda)T_{0'}(\lambda') = T_{0'}(\lambda')T_0(\lambda)R_{00'}(\lambda-\lambda')\ . \tag{133}$$

However introduction of anisotropies breaks the translational symmetry and to obtain a local Hamiltonian (like the XXX model) the anisotropies should be set to zero. When discussing latter the quantum inverse scattering method the anisotropies turn out to be useful as an intermediate technical tool.

We can again read-off the commutation relations between matrix elements of the monodromy matrix. Moreover, the transfer matrix $\tau(\lambda) = \mathrm{tr}_0\, T_0(\lambda)$ commutes for different values of the rapidity

$$[\tau(\lambda), \tau(\mu)] = 0\ . \tag{134}$$

If the R-matrix has the property that

$$R_{00'}(0) = \mathcal{P}_{00'}\ , \tag{135}$$

we can look at the transfer matrix $\tau(\lambda)$ around $\lambda = \mathrm{i}/2$ (remember the shift in the definition of the Lax operator). This will lead to local operators. In fact we immediately obtain that $\tau(\mathrm{i}/2)$ gives the shift operator. What we get as a Hamiltonian, recall that

$$H \sim \frac{\partial}{\partial\lambda} \log \tau(\lambda)|_{\lambda=\mathrm{i}/2}\ , \tag{136}$$

depends on the derivative of the R-matrix around $\lambda = 0$.

This brings us to the problem of finding R-matrices obeying the Yang-Baxter equation. This is generally achieved using the framework of Quantum Groups which leads to universal R-matrices and their representation theory. We will not go into the details, instead consider an example of the trigonometric R-matrix which corresponds to the fundamental representation of the $U_q\big(\mathrm{sl}(2)\big)$.

$$R(\lambda) = \begin{pmatrix} a(\lambda) & & & \\ & b(\lambda) & c(\lambda) & \\ & c(\lambda) & b(\lambda) & \\ & & & a(\lambda) \end{pmatrix}\ . \tag{137}$$

This matrix has the same structure as the R-matrix (86) of the XXX model, only the entries are trigonometric functions instead of polynomials

$$a(\lambda) = \sinh(\lambda + \eta), \qquad b(\lambda) = \sinh(\lambda), \qquad c(\lambda) = \sinh(\eta)\ . \tag{138}$$

Exercise 5.1 Show that the Hamiltonian resulting from the trigonometric R-matrix is the XXZ Hamiltonian. Namely, you should find that after an appropriate rescaling of the Hamiltonian the coupling constants are $J_x = J_y = 1$ and $J_z = \cosh\eta$.

Diagonalizing the transfer matrix is also straightforward and follows the same procedure as in the XXX case.

Exercise 5.2 Write down the Bethe equations for the XXZ model and eigenvalues of the transfer matrix.

Finally let us comment that finding higher spin integrable spin chains that generalize XXX or XXZ requires finding the R-matrix of $U_q\big(\mathrm{sl}(2)\big)$ in a higher representation. This problem is addressed by the representation theory of quantum groups. Following this procedure gives the spin-1 model reported in (128).

6 Thermodynamics

As noted earlier, despite diagonalizing the XXX model, inferring physical properties is still challenging because they are obscured by the Bethe equations. For example, even computing the energy of the ground state (for the antiferromagnetic case) is not straightforward. A simplification occurs if we consider a thermodynamic limit, that is a limit of a very long chain, $L \to \infty$. We will now derive an exact (in the $L \to \infty$ limit) expression for the ground state energy.

We consider the XXX spin chain in zero magnetic field. The ground state quantum numbers are $I_a^{\mathrm{GS}} = a - (L/4 + 1/2)$ with $a = 1, \ldots, L/2$, and occupy the whole allowed interval bounded by $I_\infty = L/4 + 1/2$.

Let us define a density of quantum numbers and a density of rapidities

$$\rho(x) = \frac{1}{L}\sum_{j=1}^{M} \delta(x - I_j/L) \,, \tag{139}$$

$$\rho(\lambda) = \frac{1}{L}\sum_{j=1}^{M} \delta(\lambda - \mu_a) \,. \tag{140}$$

This two functions are not independent but are related through the Bethe equations. To this end we define a function

$$\pi x(\lambda) = \operatorname{atan}(2\lambda) - \frac{1}{L}\sum_{b=1}^{M} \operatorname{atan}(\lambda - \mu_b) = \operatorname{atan}(2\lambda) - \int \mathrm{d}\mu\, \rho(\mu) \operatorname{atan}(\lambda - \mu) \,. \tag{141}$$

From the definition, $x(\mu_a) = I_a/L$. From the properties of the Dirac δ-function we have

$$\rho(\lambda) = \rho(x)\frac{\mathrm{d}x}{\mathrm{d}\lambda} \,. \tag{142}$$

For the ground state the all the possible quantum numbers are occupied so $\rho(x) = 1$. This gives an integral equation for $\rho(\lambda)$

$$\pi\rho(\lambda) = \frac{2}{1+4\lambda^2} - \int_{-\infty}^{\infty} \mathrm{d}\mu \, \frac{\rho(\mu)}{1+(\mu-\lambda)^2} \, . \tag{143}$$

This integral equation can be solved through Fourier transform

Exercise 6.1 Find $\rho(\lambda)$ solving (143).

The ground state rapidity distribution for the XXX spin chain at zero magnetic field is

$$\rho(\lambda) = \frac{1}{2\cosh(\pi\lambda)} \, . \tag{144}$$

We can now compute two physical quantities. First, we can verify that magnetization is zero by computing

$$s_z/L = \frac{1}{2} - \int_{-\infty}^{\infty} \mathrm{d}\lambda \, \rho(\lambda) = 0 \, . \tag{145}$$

Second, we can compute the energy of the ground state

$$E_{\mathrm{GS}}/L = -\frac{J}{2} \int_{-\infty}^{\infty} \mathrm{d}\lambda \, \frac{\rho(\lambda)}{\lambda^2 + \frac{1}{4}} + \frac{J}{4} = -J \ln 2 + \frac{J}{4} \, . \tag{146}$$

If the magnetic field is not zero, the quantum numbers of the ground state do not occupy the whole accessible interval. Therefore, there is a maximal rapidity, call it λ_F and the density of rapidities is zero outside the interval $[-\lambda_F, \lambda_F]$. As the magnetic field goes to zero, λ_F approaches infinity and we go back to the previous, zero magnetic field, situation. In general, the magnetization is now

$$s_z/L = \frac{1}{2} - \int_{-\lambda_F}^{\lambda_F} \mathrm{d}\lambda \, \rho(\lambda) \tag{147}$$

while the energy is

$$E_{\mathrm{GS}}/L = -\frac{J}{2} \int_{-\lambda_F}^{\lambda_F} \mathrm{d}\lambda \, \frac{\rho(\lambda)}{\lambda^2 + \frac{1}{4}} + \frac{J}{4} \, . \tag{148}$$

In general, to compute other thermodynamic quantities like partition function we need to be able to study the thermodynamic limit of all the states in the Hilbert space, not only of the ground state. The complexity of the problem increases tremendously if we recall that the structure of the Hilbert space is complicated: states with infinite

rapidities, string solutions, exceptional states. Nevertheless there is a solution and we refer (for example) to Takahashii's notes [21] and book [22] for details.

7 Correlation Functions

We have the eigenstates and we recognized the ground states. It is time now for the correlation functions. Studying the correlation functions is a notoriously difficult problem and we will only scratch its surface. Let us first identify required blocks.

For example, let us look at the correlation between the z-components of spins at two lattice sites. Invariance under translations implies that the correlation function depends only on the relative distance between the lattice sites. We have

$$S^z(l) = \langle gs|s_j^z s_{j+l}^z|\mathrm{gs}\rangle \ . \tag{149}$$

Because we identified the eigenstates of the model we can write (and use) a resolution of the identity

$$\sum_a |a\rangle\langle a| = 1 \ . \tag{150}$$

Summation means going over all possible quantum numbers enumerating the eigenstates. Inserting the resolution of the identity between the operators in the correlation function we get

$$S^z(l) = \sum_a \langle \mathrm{gs}|s_j^z|a\rangle\langle a|s_{j+l}^z|\mathrm{gs}\rangle \ , \tag{151}$$

which shows the role of form factors (matrix elements) $\langle a|s_j^z|b\rangle$ as the building blocks of the correlation functions. In this section we will study the form factors. Note that

$$\langle a|s_j^\alpha|b\rangle = \mathrm{e}^{\mathrm{i}j(P_b - P_a)}\langle a|s_1^\alpha|b\rangle \ . \tag{152}$$

To compute the form factors we need three elements.

1. We need to take care that states are normalized

$$\langle a|a\rangle = \langle \Uparrow| \prod_{j=1}^{M} C(\lambda_j) \prod_{j=1}^{M} B(\lambda_j)|\Uparrow\rangle = 1 \ . \tag{153}$$

2. We need to know the action of spin operators like s_j^z on the Bethe states

$$s_j^z \prod_{j=1}^{M} B(\lambda_j)|\Uparrow\rangle = ? \tag{154}$$

Generally speaking on the right hand side we will have some expression involving the B or C operators. This leads us to the third ingredient.

3. We need to know the scalar product between the Bethe state and an arbitrary state (not an eigenstate)

$$S_M(\{\mu\},\{\lambda\}) = \underbrace{\langle \Uparrow | \prod_{j=1}^{M} C(\mu_j)}_{\text{Bethe state}} \underbrace{\prod_{j=1}^{M} B(\lambda_j) | \Uparrow \rangle}_{\lambda_j \text{arbitrary}} . \tag{155}$$

After identifying the ingredients let us look at them in some detail.

7.1 Scalar Products

We start with the scalar products. Technically if we know the scalar product S_M we can always derive from it an expression for the norm. Therefore, the first ingredient is contained in the third. The formula for the scalar product is in principle easy to compute. We only need to commute all the C operators through all the B operators and use that the reference state is annihilated by C.

Exercise 7.1 Derive the scalar product formula for $M = 1$ case using directly the commutation relations between the B and C operators from (92). Note that if both states are Bethe states than the scalar product vanishes unless the rapidities are identical. If rapidities are the same we get a norm of the Bethe state.

Unfortunately for large M the complexity increases tremendously. This can be handled efficiently in two ways. One is to derive a recursion relation connecting a scalar product S_M with a scalar product of S_{M-1}. This approach was developed in [19]. Another option is to use the so-called F-basis which helps with solving the permutative problem. The F-basis was introduced in [16] and further applied in the our present context in [13]. We will introduce the F-basis in the next section while describing the inverse scattering method. Regarding the scalar product let us just cite the result.

$$S_M(\{\mu\},\{\lambda\}) = \prod_{j=1}^{M} \left(\mu_j - \frac{\mathrm{i}}{2}\right)^L \left(\lambda_j - \frac{\mathrm{i}}{2}\right)^L \times \frac{\det_M(\{\mu\},\{\lambda\})}{\prod_{j>k}^{M}(\mu_k - \mu_j)(\lambda_j - \lambda_k)} , \tag{156}$$

where the $M \times M$ matrix H is

$$H_{ab} = \frac{i}{\mu_a - \lambda_b} \left(\left(\frac{\lambda_b + \mathrm{i}/2}{\lambda_b - \mathrm{i}/2} \right)^L \prod_{k \neq a}^{M} (\mu_k - \lambda_b + i) - \prod_{k \neq a}^{M} (\mu_k - \lambda_b - i) \right) . \tag{157}$$

For the proof of this formula we refer to the original papers that we mentioned above.

Exercise 7.2 Derive an expression for the norm of the Bethe state by taking a limit $\lambda_j \to \mu_j$. An extra care is needed in computing the limit for the H_{aa} elements of the matrix.

7.2 The Inverse Scattering Problem

The inverse scattering transform is a transformation between the physical operators, like local spin operators at lattice site j and the A, B, C, D operators of the monodromy matrix that we use to describe the eigenstates. Such a transformation is a generalization of the Fourier transform. Recall that in the case of the free fermions the physical operators $c_j^{\pm}$ are related to the $c_\lambda^{\pm}$ operators that describe the eigenstates through

$$c_j^{\pm} = \frac{1}{L}\sum_{\lambda} \mathrm{e}^{\mp ij\lambda} c_\lambda^{\pm} \,. \tag{158}$$

For the spin operators in the XXX model the relations are the following

$$s_j^{-} = \prod_{k=1}^{j-1}\big(A(\xi_k)+D(\xi_k)\big)B(\xi_j)\prod_{k=j+1}^{L}\big(A(\xi_k)+D(\xi_k)\big)\,, \tag{159}$$

$$s_j^{+} = \prod_{k=1}^{j-1}\big(A(\xi_k)+D(\xi_k)\big)C(\xi_j)\prod_{k=j+1}^{L}\big(A(\xi_k)+D(\xi_k)\big)\,, \tag{160}$$

$$s_j^{z} = \prod_{k=1}^{j-1}\big(A(\xi_k)+D(\xi_k)\big)\big(A(\xi_j)-D(\xi_j)\big)\prod_{k=j+1}^{L}\big(A(\xi_k)+D(\xi_k)\big)\,. \tag{161}$$

First we can note that the operator $A(\xi_k)+D(\xi_k)$ acts as translation operator through the kth site. Because of the anisotropies the translation is not anymore a symmetry unless we translate through the whole chain. Thus, we can expect that

$$\prod_{k=1}^{L}\big(A(\xi_k)+D(\xi_k)\big) = 1\,. \tag{162}$$

This is supported by an observation that the fourth operator, linearly independent from $s_j^{\pm}$ and s_j^{z}, is the identity operator. We see that a linearly independent combination of the A, B C, D operators from these appearing on the right-hand side is $A + D$ which then gives (162).

We will sketch a derivation of the inverse scattering transform. Let us start with the spin operators on the first lattice. This is the simplest case and the general expression can be obtained from this particular one with the help of the F-basis.

To derive expressions between s_1^α and transfer matrix operators we consider the following object

$$\mathrm{tr}_0\big(s_0^\alpha T_{0;1,\dots L}(\lambda)\big)\ . \tag{163}$$

Simply writing the transfer matrix and the spin operator as a 2×2 matrices we find

$$\mathrm{tr}_0\big(s_0^\alpha T_{0,1\dots L}(\lambda)\big) = \begin{cases} B(\lambda), & \alpha = -, \\ C(\lambda), & \alpha = +, \\ A(\lambda) - D(\lambda), & \alpha = z. \end{cases} \tag{164}$$

These expressions hold for arbitrary λ. Recall now that if we evaluate the transfer matrix at $\lambda = \xi_k$, then the kth Lax operator becomes the permutation operator. Thus if we set $\lambda = \xi_1$ we get

$$\begin{aligned} \mathrm{tr}_0\big(s_0^\alpha T_{0;1\dots L}(\xi_1)\big) &= \mathrm{tr}_0\big(s_0^\alpha \mathcal{P}_{0,1} L_{0,2}(\xi_1-\xi_2)\cdots L_{0,L}(\xi_1-\xi_L)\big) \\ &= \mathrm{tr}_0\big(s_0^\alpha L_{1,2}(\xi_1-\xi_2)\cdots L_{1,L}(\xi_1-\xi_L)\mathcal{P}_{0,j}\big) \\ &= s_1^\alpha L_{1,2}(\xi_1-\xi_2)\cdots L_{1,L}(\xi_1-\xi_L)\ . \end{aligned} \tag{165}$$

The product of Lax operators is simple to compute

Exercise 7.3 Show that

$$L_{1,2}(\xi_1-\xi_2)\cdots L_{1,L}(\xi_1-\xi_L) = A(\xi_1) + D(\xi_1)\ .$$

Do not be intimidated by this equality, start with writing the right-hand side as a trace of the transfer matrix.

We find

$$\mathrm{tr}_0\big(s_0^\alpha T_{0;1\dots L}(\xi_1)\big) = s_1^\alpha\big(A(\xi_1) + D(\xi_1)\big)\ , \tag{166}$$

and for example for the s_1^- operator we find

$$s_1^- = B(\xi_1)\big(A(\xi_1)+D(\xi_1)\big)^{-1} = B(\xi_1)\prod_{k=2}^{L}\big(A(\xi_k)+D(\xi_k)\big)\ , \tag{167}$$

in agreement with (159). The computation for an arbitrary position of the spin operators are similar because we can effectively pretend that each lattice site is the first one. There exists a basis, the F-basis, in which we are free to rearrange the

lattice sites as we wish without changing the transfer matrix. Thus our strategy is the following. We start with the expression of the form

$$\mathrm{tr}_0\big(s_0^\alpha T_{0,1\dots L}(\xi_j)\big)\ . \tag{168}$$

We change to the F-basis, we permute the lattice sites such that the jth lattice site is the first one and then we go back to the original basis. The transformation to the F-basis, the F-matrix, depends on the ordering of the lattice sites. We define the transformation as

$$\widetilde{T}_{0;1\dots L}(\lambda) = F_{1\dots L} T_{0;1\dots L}(\lambda) F^{-1}_{1\dots L}\ , \tag{169}$$

and the premise is that $\widetilde{T}$ does not depend on the reordering of the lattice sites, that is

$$\widetilde{T}_{0;\pi(1)\dots\pi(L)}(\lambda,\xi_{\pi(1)},\dots,\xi_{\pi(L)}) = \widetilde{T}_{0;1\dots L}(\lambda;\xi_1,\dots,\xi_L)\ ,\quad \pi\in S_L\ , \tag{170}$$

where S_L is a group of permutations of L elements. Then we obtain

$$\mathrm{tr}_0\big(s_0^\alpha T_{0;1\dots L}(\xi_j)\big) = F^{-1}_{1\dots L} F_{j\dots j-1}\,\mathrm{tr}_0\big(s_0^\alpha T_{0;jj+1\dots j-1}(\xi_j)\big) F^{-1}_{j\dots j-1} F_{1\dots L}\ . \tag{171}$$

The term in the middle is nothing else but (166) for the lattice labelled $j, j+1$, and so on until $j-1$. Therefore

$$\mathrm{tr}_0\big(s_0^\alpha T_{0;jj+1\dots j-1}(\xi_j)\big) = s_j^\alpha\ . \tag{172}$$

To complete the derivation we need to compute the products of F-matrices and prove that indeed in the F-basis the transfer matrix is independent of a permutation of the lattice sites.

To this end we have to finally introduce properly the F-basis. The main observation is that the R-matrix (equivalently the Lax operator) factorizes

$$R_{ab}(\lambda) = a(\lambda) F^{-1}_{ba}(-\lambda) F_{ab}(\lambda)\ , \tag{173}$$

where

$$F_{ab}(\lambda) = \begin{pmatrix} 1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & c(\lambda)/a(\lambda) & b(\lambda)/a(\lambda) & 0\\ 0 & 0 & 0 & 1\end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & \mathrm{i}/(\lambda+\mathrm{i}) & \lambda/(\lambda+\mathrm{i}) & 0\\ 0 & 0 & 0 & 1\end{pmatrix}\ , \tag{174}$$

and $F_{ba} = P_{ab} F_{ab} P_{ab}$.

Exercise 7.4 Show that the factorization indeed holds.

Note that the F-matrix can be written as (we renormalize the R-matrix by dividing by $a(\lambda)$)

$$F_{ab}(\lambda) = e_a^{(11)} + e_a^{22} R_{ab}(\lambda) = e_b^{(11)} R_{ab}(\lambda) + e_b^{(22)} \tag{175}$$

where $e_a^{(ij)}$ is a matrix which in space a has only one nonzero element at position (i,j)

$$\begin{aligned} e_a^{(11)} &= \begin{pmatrix} 1 & & \\ & 1 & \\ & & \end{pmatrix}, \qquad e_a^{(22)} = \begin{pmatrix} & & \\ & 1 & \\ & & 1 \end{pmatrix}, \\ e_b^{(11)} &= \begin{pmatrix} 1 & & \\ & & \\ & & 1 \end{pmatrix}, \qquad e_b^{(22)} = \begin{pmatrix} & & \\ 1 & & \\ & & 1 \end{pmatrix}. \end{aligned} \tag{176}$$

The R-matrix (after the normalization) is unitary

$$R_{ab}(\lambda)^\dagger = R_{ba}(-\lambda) = \big(R_{ab}(\lambda)\big)^{-1} \tag{177}$$

Let us now extend the factorization property on products of R-matrices. Define partial R-matrices

$$R_{1,2\ldots L}(\lambda;\{\xi\}) = R_{1,L}(\lambda-\xi_L) R_{1,L-1}(\lambda-\xi_{L-1}) \ldots R_{1,2}(\lambda-\xi_2)\,, \tag{178}$$

$$R_{1\ldots L-1,L}(\lambda;\{\xi\}) = R_{1,L}(\xi_1-\lambda) R_{2,L}(\xi_2-\lambda) \ldots R_{L-1,L}(\xi_{L-1}-\lambda)\,. \tag{179}$$

Note that the first expression with $\lambda = \xi_1$ is nothing else but a monodromy matrix $\tau(\xi_1) = A(\xi_1) + D(\xi_1)$. We define now partial F-matrices through a generalization of (175)

$$F_{1,2\ldots L}(\lambda;\{\xi\}) = e_1^{(11)} + e_1^{(22)} R_{1,2\ldots L}(\lambda;\{\xi\})\,, \tag{180}$$

$$F_{1\ldots L-1,L}(\lambda;\{\xi\}) = e_L^{(11)} R_{1\ldots L-1,L}(\lambda;\{\xi\}) + e_L^{(22)}\,. \tag{181}$$

Just from the definition it follows that the partial F-matrices almost factorize also the product of R-matrices

$$F_{2\ldots L,1}(\lambda;\{\xi\}) R_{1,2\ldots L}(\lambda;\{\xi\}) = F_{1,2\ldots L}(\lambda;\{\xi\})\,. \tag{182}$$

Exercise 7.5 Show this relation.

We say almost because the partial F-matrices appearing in this formula are not easily relatable to each other, as the ones in the original formula (173) for the single R-matrix. To this end we define F-matrices (without the adjective partial) through the following recursion relation

$$\begin{aligned} F_{1\dots L}(\{\xi\}) &= F_{2\dots L}(\{\xi\})F_{1,2\dots L}(\xi_1;\{\xi\}) \\ &= F_{1\dots L-1}(\{\xi\})F_{1\dots L-1,L}(\xi_L;\{\xi\}) \ . \end{aligned} \tag{183}$$

To simplify the notation we will now skip the arguments of the F-matrices

$$F_{1\dots L} = F_{1\dots L}(\{\xi\}) = F_{1\dots L}(\xi_1,\dots\xi_L) \ . \tag{184}$$

From the definition of the F-matrices and property (182) of the partial F-matrices we get

$$F_{2\dots L1}R_{1,2\dots L}(\xi_1) = F_{1\dots L} \ , \tag{185}$$

or in other words

$$R_{1,2\dots L}(\xi_1) = F^{-1}_{2\dots L1}F_{1\dots L} \ . \tag{186}$$

This relation can be easily propagated to obtain

$$F^{-1}_{j\dots j-1}F_{1\dots L} = R_{j-1,j\dots j-2}(\xi_{j-1})\cdots R_{1,2\dots L}(\xi_1) \ . \tag{187}$$

On the other hand, recall that the product of the R-matrices evaluates at $\lambda = \xi_j$ to

$$R_{j,j\dots j-1}(\xi_j) = A(\xi_j) + D(\xi_j) \ . \tag{188}$$

Combining these results we get the sought after expression for the product of F-matrices

$$F^{-1}_{j\dots j-1}F_{1\dots L} = \prod_{k=1}^{j-1}\big(A(\xi_k) + D(\xi_k)\big) \ . \tag{189}$$

Using this expression in (171) we find the formulas for the inverse scattering transform.

The complete the proof we still need to show that the transfer matrix in the F-basis is independent of the permutation of the lattice sites. To simplify the presentation we will just prove that the transfer matrix in the F-basis is invariant under a shift by one lattice site. Iterating the procedure we obtain invariance under an arbitrary shift and this is enough for our purposes. Invariance under the action of the full symmetry group S_L can also be proven and we refer to the original literature for the details [16].

What we need to show is the following equality

$$F_{1\ldots L}T_{0,1\ldots L}F^{-1}_{1\ldots L} = F_{2\ldots 1}T_{0,2\ldots 1}F^{-1}_{2\ldots 1}\ . \tag{190}$$

Using the factorization (186) of the partial R-matrices we find

$$R_{1,2\ldots L}T_{0,1\ldots L} = T_{0,2\ldots 1}R_{1,2\ldots L}. \tag{191}$$

That the both sides are equal follows from the definition (178) of the partial R-matrices, the definition of the transfer matrix, and the RLL relation between the R-matrices and Lax operators. This completes the derivation of the inverse scattering transform. A general approach to the inverse scattering transform for XXZ spin chains can be found in [17] and [5].

Exercise 7.6 Show equality (191).

We are now in the position to write the form factors of local spin operators. For example for the s_j^- operator we have

$$\begin{aligned}\langle \mu_1,\ldots,\mu_{M-1}|s_j^-|\lambda_1,\ldots,\lambda_M\rangle \\ = \langle \mu_1,\ldots,\mu_{M-1}|\prod_{k=1}^{j-1}\big(A(\xi_k)+D(\xi_k)\big)B(\xi_j) \\ \times\prod_{k=j+1}^{L}\big(A(\xi_k)+D(\xi_k)\big)|\lambda_1,\ldots,\lambda_M\rangle\ .\end{aligned} \tag{192}$$

If the left and right states are Bethe states then they are eigenstates of the transfer matrix $(A+D)$ and we know their eigenvalues. The remaining part can be computed using the scalar product formula where the left side is the Bethe state but the right state not because of the extra B operator.

To compute a correlation function knowing the form factors requires summation over the eigenstates, as in (151) that we repeat here

$$S^z(k) = \sum_{|a\rangle\in\mathcal{H}}\langle \mathrm{gs}|s_j^z|a\rangle\langle a|s_{j+k}^z|\mathrm{gs}\rangle \tag{193}$$

It is very difficult to handle such sum analytically however it is possible to evaluate it numerically. A materialization of this idea is the ABACUS algorithm which computes the correlation functions of various integrable models, in and out of the equilibrium. It allows to match the theoretical predictions coming from the Algebraic Bethe Ansatz with the real world experimental measurements (for an example see [15]). This fulfills our initial aim of employing integrable models in a study of many-body physics.

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References

1. V.I. Arnold, *Mathematical Methods of Classical Mechanics*. Graduate Texts in Mathematics, vol. 60 (Springer, Berlin, 1978)
2. R.J. Baxter, *Exactly Solved Models in Statistical Mechanics* (Academic, London, 1982)
3. J.-S. Caux, J. Mossel, Remarks on the notion of quantum integrability. J. Stat. Mech. Theory Exp. **2011**, P02023 (2011)
4. T. Deguchi, Introduction to solvable lattice models in statistical and mathematical physics, in *Classical and Quantum Nonlinear Integrable Systems*, ed. by A. Kundu. Mathematical and Computational Physics, chap. 5, pp. 107–146 (Institute of Physics, Bristol, 2003)
5. T. Deguchi, C. Matsui, Form factors of integrable higher-spin XXZ chains and the affine quantum-group symmetry. Nucl. Phys. B **814**(3), 405–438 (2009)
6. P.A.M. Dirac, *The Principles of Quantum Mechanics*, 4th edn. (Clarendon Press, Oxford, 1959)
7. A. Doikou, S. Evangelisti, G. Feverati, N. Karaiskos, Introduction to quantum integrability. Int. J. Modern Phys. A **25**(17), 3307–3351 (2010)
8. F.H.L. Essler, H. Frahm, F. Göhmann, A. Klümper, V.E. Korepin, *The One-Dimensional Hubbard Model* (Cambridge University Press, Cambridge, 2005)
9. L.D. Faddeev, How the algebraic Bethe ansatz works for integrable models, in *Symétries Quantiques*, ed. by A. Connes, K. Gawedzki, J. Zinn-Justin (North-Holland, Amsterdam, 1998), pp. 149–219
10. F. Franchini, *An Introduction to Integrable Techniques for One-Dimensional Quantum Systems*. Springer Briefs in Mathematical Physics, vol. 16 (Springer, Cham, 2017)
11. M. Gaudin, *La fonction d'onde de Bethe* (Masson, Paris, 1983)
12. T. Giamarchi, *Quantum Physics in One Dimension* (Oxford University Press, Oxford, 2004)
13. N. Kitanine, J.-M. Maillet, V. Terras, Form factors of the XXZ Heisenberg spin-$\frac{1}{2}$ finite chain. Nuclear Phys. B **554**(3), 647–678 (1999)
14. V.E. Korepin, N.M. Bogoliubov, A.G. Izergin, *Quantum Inverse Scattering Method and Correlation Functions*. Cambridge Monographs on Mathematical Physics (Cambridge University Press, Cambridge, 1993)
15. B. Lake, D.A. Tennant, J.-S. Caux, T. Barthel, U. Schollwöck, S.E. Nagler, C.D. Frost, Multispinon continua at zero and finite temperature in a near-ideal Heisenberg chain. Phys. Rev. Lett. **111**(13), 137205 (2013)
16. J.-M. Maillet, J. Sánchez de Santos, Drinfeld twists and algebraic Bethe ansatz, in *L. D. Faddeev's Seminar on Mathematical Physics*, ed. by M. Semenov-Tian-Shansky. American Mathematical Society Translation Series 2, vol. 201 (American Mathematical Society, Providence, 2000), pp. 137–178
17. J.-M. Maillet, V. Terras, On the quantum inverse scattering problem. Nucl. Phys. B **575**(3), 627–644 (2000)
18. R.I. Nepomechie, A spin chain primer. Int. J. Modern Phys. B **13**(24-25), 2973–2985 (1999)
19. N.A. Slavnov, Calculation of scalar products of wave functions and form-factors in the framework of the algebraic Bethe ansatz. Theor. Math. Phys. **79**(2), 502–508 (1989)
20. B. Sutherland, *Beautiful Models* (World Scientific, Singapore, 2004)
21. M. Takahashi, Thermodynamical Bethe ansatz and condensed matter, in *Conformal Field Theories and Integrable Models*, ed. by Z. Horváth, L. Palla. Lecture Notes in Physics, vol. 498 (Springer, Berlin, 1997), pp. 204–250
22. M. Takahashi, *Thermodynamics of One-Dimensional Solvable Models* (Cambridge University Press, Cambridge, 1999)

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