Integrable spin chains and cellular automata with medium-range interaction

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We study integrable spin chains and quantum and classical cellular automata with interaction range $\ell \geqslant 3$. This is a family of integrable models for which there was no general theory so far. We develop an algebraic framework for such models, generalizing known methods from nearest-neighbor interacting chains. This leads to a new integrability condition for medium-range Hamiltonians, which can be used to classify such models. A partial classification is performed in specific cases, including $U(1)$-symmetric three-site interacting models, and Hamiltonians that are relevant for interaction-round-a-face models. We find a number of models which appear to be new. As an application we consider quantum brickwork circuits of various types, including those that can accommodate the classical elementary cellular automata on light cone lattices. In this family we find that the so-called Rule150 and Rule105 models are Yang-Baxter integrable with three-site interactions. We present integrable quantum deformations of these models, and derive a set of local conserved charges for them. For the famous Rule54 model we find that it does not belong to the family of integrable three-site models, but we cannot exclude Yang-Baxter integrability with longer interaction ranges.

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I. INTRODUCTION

One-dimensional quantum integrable models are special many-body systems, which allow for exact solutions of their dynamics. Their study goes back to the solutions of the Heisenberg spin chain by Bethe in 1931 [1] and the exact treatment of the two-dimensional (2D) classical Ising model by Onsager in 1944 [2]. It was understood in the 1960s and '70s that a key element appearing in various types of quantum integrable models is the Yang-Baxter equation, independently discovered by Yang [3] and Baxter [4]. A common algebraic framework was afterwards developed by the Faddeev and Leningrad group (see, for example, the historical review in Ref. [5]). These elements of integrability connect seemingly different types of models, such as the 2D integrable statistical physical models (for example, the six-vertex and eight-vertex models), the famous integrable spin chains such as the Heisenberg model or the Hubbard model, nonrelativistic quantum gas models [6], and integrable quantum field theories (iQFT) [7].

A recurring question over the decades has been the classification of (quantum) integrable models, together with an attempt to give a precise definition of what integrability actually is. It appears that there is no single definition encompassing all possible integrable models, but there are two very common elements appearing in integrable models: the existence of a large set of extra conservation laws and a completely elastic and factorized scattering of the physical excitations [8]. Then the attempts for the classification can proceed along the lines of either of the charges [8] or by finding all possible factorized S-matrices as in iQFT [7].

Focusing on quantum spin chains two big families of models have been studied extensively: those with nearest-neighbor (n.n.) interactions, and some long-range models. In the latter case spins at an arbitrary distance can interact, although with strongly decreasing coupling constants. The n.n. chains can be treated with the algebraic methods developed by the Leningrad group [9], which are routinely used today. However, the treatment of the long-range chains is typically more involved. Examples are the Haldane-Shastry chain [10,11] or the Inozemtsev chain [12] or long-range version of the Hubbard model [13]. In such cases the construction of the exact eigenstates and also the charges is typically more complicated than in the n.n. chains; see, for example, Refs. [14–16].

Returning to the nearest-neighbor chains, partial classifications have been achieved in certain specific cases. Integrable nearest-neighbor Hamiltonians are intimately connected with so-called regular solutions of the Yang-Baxter (YB) equation. Thus, a classification can proceed by finding all solutions of the YB equation; this is possible within restricted parameter spaces. For example, it was understood very early that solutions can be found by assuming underlying group or quantum group symmetries [17–21]. However, the (quantum) group symmetric cases do not exhaust all possibilities, and it is also desirable to find the remaining models. It is not possible to list here all known integrable n.n. chains, therefore we just mention a few works that performed classifications with certain restrictions [22–27]. More recently a systematic method was worked out in Refs. [28–32], based on well-established ideas

[33] but leading to more detailed classifications than in prior works.

Despite all of this progress there is a class of models which has so far received relatively little attention: Translationally invariant spin chains where the Hamiltonian has a finite interaction range $\ell \geqslant 3$. We call these models "medium-range spin chains" to distinguish them both from the nearest-neighbor and the long-range cases. It is important that we are interested in models where the finite range Hamiltonian is the smallest dynamics generating charge, so we dismiss those cases when the Hamiltonian is chosen as a linear combination of some of the short range charges of a n.n. interacting chain. These cases can be interesting on their own right (see, for example, Ref. [34]), but we are looking for models with genuinely new interactions. We also exclude those models, where the Hilbert space is a constrained subspace of the usual tensor product space of the spin chains; an important example is the constrained XXZ model and its generalizations treated, for example, in Refs. [35–41] or the supersymmetric spin chains studied in Refs. [42,43]. Such constraints are nonlocal, and we are looking for strictly local models with the usual tensor product Hilbert space.

There are various reasons why the medium-range models can be interesting. First of all there is the obvious academic interest: If one was to uncover all possible integrable spin chains, then clearly one should consider these models as well. We can expect that as we increase the interaction range, more and more possibilities open up, and a full classification becomes less and less feasible in practice. Nevertheless, it is desirable to develop a general theory for such models, and at least some key ideas for the classification, which can be applied in restricted parameter spaces. As a second motivation we can mention various recent research directions where medium-range models were encountered.

A. Medium-range spin chains in the literature

An early example of an interacting medium-range spin chain is the Bariev-model, which has a three-site Hamiltonian [44]. Generally, the three-site models can be pictured as zigzag spin ladders, and this was also used in the presentation of the Bariev model. In this work we stick to the translationally invariant representations. The algebraic explanation of the integrability of the Bariev model was given in Refs. [45,46].

Recently there was interest in medium-range chains which can be solved by free fermions of parafermions. A specific three-site model was found in Ref. [47] with generalizations studied later in Refs. [48–50]. In these models the fermions are "in disguise," which means they are not obtained by the usual Jordan-Wigner transformation. A more general theory for such models was initiated in Ref. [51].

A specific medium-range model called the "folded XXZ model" was investigated in the recent works [52–55]. There are two formulations of the model, and the dynamical Hamiltonian is a four-site or three-site operator, depending on the formulation used. In the three-site formulation the model is seen as a special point of the Bariev model. It was shown in Ref. [54] that the model exhibits Hilbert space fragmentation, and it can be considered as a hard rod deformation of the XX model. Furthermore, its real-time dynamics can be solved exactly in certain special quench problems, thus the model can be considered as one of the simplest interacting spin chains. It is remarkable that a spin chain with four-site interactions has a simpler solution than the famous XXZ chains. This shows that it is worthwhile to explore the medium-range chains.

In the recent work [56] a family of unitary transformations was studied which can generate a medium-range chain starting from a nearest-neighbor model. The techniques applied here originate in quantum information theory, and the transformations are members of the discrete Clifford group.

B. Integrable quantum circuits

We should also mention the recent interest in integrable quantum circuits and classical cellular automata. This is a topic closely connected to integrable Hamiltonians, and some of the models in the literature have medium-range interactions.

The interest in quantum gate models is motivated in part by experimental advances, but also by surprising theoretical results. For example, simple (nonintegrable) models with random unitary gates lead to a number of new results, see, for example, Refs. [57–63], and models with so-called "dual unitary" gates are exactly solvable [64–66]. In the integrable setting there is interest for quantum circuits with unitary gates that span two, three of four sites (in the following we will often use the short term "unitary" instead of "unitary gate").

First of all, a quantum circuit model with two-site unitaries was developed in Ref. [67]: the model serves as an integrable Trotterization (discrete time analog) of the XXZ spin chain. This idea goes back to the light cone regularization of integrable QFTs [68–70]. More recently the same idea was also applied to dissipative systems [71]. The key observation in these works is that the so-called R-matrix itself can be used as a two-site quantum gate, and in certain cases this leads to discrete unitary time evolution with well defined integrability properties. The original integrable spin chains can be recovered in the continuous time limit of the quantum gate models.

An important family of quantum circuits falls outside the realm of nearest-neighbor models. These are the elementary cellular automata on light cone lattices classified in Ref. [72], which can be considered quantum circuits with special three-site unitaries. The most important example is the Rule54 model, which is often called the simplest interacting integrable model [73]. It is a very special model with soliton-like behavior, which allows for exact solutions [74–76] and integrable quantum deformations [77] (see also Ref. [78]). However, the connection with the standard Yang-Baxter integrability remained unknown.

Very recently a new algebraic framework was proposed for these cellular automata [79], by making connection to the so-called interaction round-a-face (IRF) models of statistical physics (see, for example, Refs. [80–83]). In Ref. [79] new transfer matrices were developed for the classical cellular automata and certain quantum deformations of them, and it was conjectured that the new construction gives new quasilocal conserved charges in these models, thus proving their integrability. These IRF models are such that the three-site quantum gates have two control bits on the two sides and one action bit in the middle. If these IRF models are indeed integrable,

then they could serve as integrable Trotterization of some spin chains with three-site Hamiltonians, likely having a very similar structure. However, such connections have not yet been found.

In the recent work of Ref. [84] a cellular automaton was found with a four-site update rule, such that it can be considered as an integrable Trotterization of the folded XXZ model mentioned above. However, the construction in Ref. [84] had some drawbacks: it did not have space reflection symmetry, and the integrability was only proven for a certain diagonal-to-diagonal transfer matrix, which is not adequate to treat the Cauchy problem. Nevertheless, the results of Ref. [84] indicate that the cellular automata and medium-range spin chains are indeed closely related, and can be treated with the usual algebraic methods of integrability.

We should also note that there exists a family of classical cellular automata, where the integrability properties are well understood: these are the so-called box-ball systems [85,86]. Here the update rules cannot be formulated using a simultaneous action of local update rules; instead, they belong to the class of the so-called filter automata [87–90]. The box-ball models are noteworthy, because they display solitonic behavior, and they are connected to a number of question in representation theory of quantum groups, combinatorics, and classical integrability [86]. Recently the hydrodynamic behavior of these models was also studied in Ref. [91]. In our paper we do not treat these models, because we are interested in strictly local systems.

C. The goals of this paper

Motivated by the findings discussed above, in this paper we strive toward a general theory for medium-range integrable models. It is our goal to develop the common algebraic structures, which will be generalizations of the known methods applied for nearest-neighbor models. We stress that up to now there has been no general framework for the medium-range models, and even in those cases where the algebraic background was developed (see, for example, the Bariev model [45,46]), it was based on ad hoc ideas lacking a general understanding. In contrast, in this work we establish the key relations for the medium-range models, focusing in particular on the three-site and four-site interacting cases. A special emphasis will be put on the IRF models treated in Ref. [79]: we show that they can be embedded into our framework, and we disprove some of the conjectures made in Ref. [79]. In particular, we argue that the Rule54 model is not in the family of the three-site interacting Yang-Baxter integrable models, but we do not exclude integrability with longer interaction ranges.

In Sec. II we set the stage for our computations: we introduce the main concepts and also explain and summarize some of our key results. The algebraic structures of integrability are then introduced in Sec. III, which also includes our main results about the medium-range spin chains. Integrable quantum circuits of various types are constructed in Sec. IV. The special class of models related to the elementary cellular automata are considered in Sec. V. Here we also treat the results of Ref. [79]. In Sec. VI we study the four-site interacting models. Open questions are discussed in Sec. VII, and we present some of the technical computations in the Appendices.

II. PRELIMINARIES

In this section we introduce the key concepts regarding integrable spin chains, and we summarize our new results for the medium-range cases. We also introduce the quantum circuits, which can be considered as the discrete time versions of the spin chain models. In this section we avoid the algebraic treatment of the integrability properties, instead we focus on the overall physical properties of these models, most importantly on the set of conserved charges.

First we introduce some notations that we use throughout the work, and afterwards we discuss the spin chains and the quantum circuit models. The algebraic structures behind the integrability are presented later in Secs. III and IV.

A. Notations

We consider homogeneous spin chains with translationally invariant Hamiltonians. The local Hilbert spaces are $V_j = \mathbb{C}^d$ with some fixed $d \geqslant 2$. The full Hilbert space of the model in finite volume L is $\mathcal{H} = \otimes_{j=1}^{L} V_j$. The majority of our abstract results will not depend on the actual value of the local dimension d, but in the concrete examples we consider $d = 2$.

We say that an operator $\mathcal{O}(j)$ is local if its support is restricted to a limited number of sites starting from j, such that the support does not grow with L as we consider longer and longer chains. We use notation $|\mathcal{O}(j)|$ for the range of the local operator (which we also call length). This means that the support of $\mathcal{O}(j)$ with $|\mathcal{O}(j)| = \ell$ is the segment $[j, \ldots, j + \ell - 1]$.

If a local operator has a fixed small range ℓ, then we will also use an alternative notation where we spell out the sites on which it acts. For example, for two-site operators we also write $\mathcal{O}_{j,j+1}$, for three-site operators $\mathcal{O}_{j,j+1,j+2}$, and so on. We will switch between the two notations depending on which is more convenient for the actual computation.

In our concrete examples we will treat spin-1/2 chains. In these cases we use the standard basis of the up and down spins, but we will use the notations $|\circ\rangle = |0\rangle$ (empty site) and $|\bullet\rangle = |1\rangle$ (occupied site) for these basis states, respectively. We use the standard Pauli matrices $\sigma^{x,y,z}$ and also the standard ladder operators $\sigma^{\pm}$, together with the following projectors onto the basis states:

$$P^{\circ} = P^{0} = \frac{1+\sigma^{z}}{2}, \quad P^{\bullet} = P^{1} = \frac{1-\sigma^{z}}{2}. \tag{2.1}$$

An important operator that we will use often is the cyclic shift operator $\mathcal{U}$ that translates the finite chain of length L to the right by one site.

B. Integrable spin chains with nearest-neighbor interactions

In the literature there is no single definition for quantum integrability. However, it is generally accepted that one of the key properties of integrable models is the existence of a large set of additional conserved charges, which commute with each other. Then the integrable models can be classified according to the patterns of how these charges appear in the model [8].

In this paper we focus on local spin chains, where the Hamiltonian is given by a strictly local Hamiltonian density:

$$H = \sum_j h(j). \tag{2.2}$$

Here $h(j)$ is a local operator with some range ℓ. Periodic boundary conditions are understood throughout this work.

The additional conserved charges are a set of operators Q_α, where α is a label which we discuss below. We require that each charge should be extensive with a local density:

$$Q_\alpha = \sum_j q_\alpha(j). \tag{2.3}$$

In this work we restrict ourselves to these strictly local charges, even though it is known that in certain cases so-called quasilocal charges also play an important role [92,93]. Furthermore, there are integrable models where the charges typically grow super-extensively with the volume; see, for example, the discussion of the Haldane-Shastry chain in Ref. [8]. Nevertheless, in this work we focus only on the extensive cases.

It is generally required that the conserved charges commute,

$$[Q_\alpha, Q_\beta] = 0, \tag{2.4}$$

and the Hamiltonian should be a member of the set. The commutativity has to hold in every volume L large enough so that both charges fit into the system.

If these requirements are met, then generally the label α can be chosen simply as the length of the charge density, therefore we will use the convention throughout this work,

$$|q_\alpha(j)| = \alpha. \tag{2.5}$$

Within this class of models the most studied ones are nearest-neighbor interacting ones, thus we can identify $H = Q_2$. In such cases the allowed values for α are the integers starting from 2. If there is also a global $U(1)$-symmetry, then $\alpha = 1$ is also allowed.

Within this class the most important cases are the spin-1/2 chains, for which a full classification (including non-Hermitian cases) was performed in Refs. [28,29]. We do not treat the classification here, instead we just mention the most important examples.

Let us start with a generic (nonintegrable) spin-1/2 chain and let us require space reflection invariance. Then it can be shown that the most general nearest-neighbor Hamiltonian (apart from global $SU(2)$ rotations) is the XYZ model with magnetic fields:

$$H = \sum_j \left(J_x\sigma_j^x\sigma_{j+1}^x + J_y\sigma_j^y\sigma_{j+1}^y + J_z\sigma_j^z\sigma_{j+1}^z + h_x\sigma_j^x + h_y\sigma_j^y + h_z\sigma_j^z\right). \tag{2.6}$$

This model is not integrable except for special cases [94].

One integrable family is when $h_x = h_y = h_z = 0$, and the couplings $J_{x,y,z}$ are arbitrary, this is known as the XYZ model. A special point with $U(1)$ symmetry is the XXZ chain with $J_x = J_y$, which allows for a nonzero h_z. A further special point is the $SU(2)$ invariant Heisenberg spin chain with equal couplings, which allows for arbitrary magnetic fields.

An other special integrable family within Eq. (2.6) are the so-called XYh models, where $J_z = 0$ and $h_x = h_y = 0$. A special model of this family is the quantum Ising chain where also $J_y = 0$. The XYh family can be solved by free fermion techniques [95,96].

C. The Reshetikhin condition

A common property of the nearest-neighbor models is that they satisfy the so-called Reshetikhin condition of integrability. There are multiple formulations of this condition, and now we review the most general one. The algebraic background is treated later in Sec. III.

First of all we quote a conjecture that was presented in Ref. [33]. We put this in a slightly modified form:

Conjecture 1. A nearest-neighbor spin chain with a dynamical Hamiltonian H is integrable iff there exists an extensive three-site charge Q_3 which is functionally independent from H and the possible one-site charges of the model, and which commutes with H for every volume $L \geqslant 3$.

As far as we know no counterexamples have been found so far, but the Conjecture has not yet been proven either. It is important that we added the condition that the Hamiltonian should be dynamical: If this condition is not satisfied, then simple counterexamples can be found, see the discussion in Appendix A.

Now we also present the Reshetikhin condition in a rather general form:

Conjecture 2. If there exists a conserved charge Q_3 commuting with the dynamical two-site Hamiltonian $H = \sum_j h(j)$, then it can be written as $Q_3 = \sum_j q_3(j)$, with

$$q_3(j) = [h(j), h(j+1)] + \tilde{h}(j), \tag{2.7}$$

where $\tilde{h}(j)$ is also a two-site operator.

It might appear that the Conjecture allows for a lot of freedom due to the presence of $\tilde{h}(j)$, but the fact that this operator has to be a two-site operator is rather restrictive.

The conjecture can be proven backwards: If the spin chain is Yang-Baxter integrable, then the precise form of the density $q_3(j)$ follows from the underlying algebraic objects, and it has precisely the form of Eq. (2.7). However, it is not known how to prove the Conjecture without assuming Yang-Baxter integrability. We put forward that $\tilde{h}(j) = 0$ in models where the so-called R-matrix is of *difference form*; this corresponds to the original Reshetikhin condition treated in Ref. [33]. However, $\tilde{h}(j) \neq 0$ in other models such as the Hubbard model [97].

Conjecture 2 was used in the recent works [28–32] for the classification of integrable nearest-neighbor chains in various circumstances. We will not review this classification here, instead we will focus on the generalization of the Reshetikhin condition to medium-range spin chains.

D. Medium-range spin chains

In this work we treat integrable spin chains and closely related quantum gate models where the interaction range is $\ell \geqslant 3$. We call these models "medium-range chains." We propose the following definition:

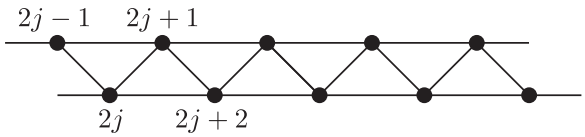

FIG. 1. Graphical illustration of a zigzag spin ladder. It is natural to expect three-site interactions for each plaquet.

Definition 1. A medium-range integrable spin chain is a model which has an infinite set of commuting local charges $\{Q_\alpha\}$ where $\alpha \in \mathcal{S}$ with $\mathcal{S} \subset \mathbb{Z}^+$, such that the lowest dynamical charge (which is regarded as the Hamiltonian) has a range $\ell \geqslant 3$.

Once again it is important to add the requirement of having a dynamics generating charge as the Hamiltonian. A good example for the usefulness of this requirement is the so-called "folded XXZ model" treated in Refs. [52–54], where the first four charges are

$$\begin{aligned} Q_1 &= \sum_{j=1}^{L} \sigma_j^z, \quad Q_2 = \sum_{j=1}^{L} \sigma_j^z \sigma_{j+1}^z, \\ Q_3 &= \sum_j i\big(\sigma_j^z + \sigma_{j+3}^z\big)\big(\sigma_{j+1}^+ \sigma_{j+2}^- - \sigma_{j+1}^- \sigma_{j+2}^+\big), \\ Q_4 &= \sum_{j=1}^{L} \big(1 + \sigma_j^z \sigma_{j+3}^z\big)\big(\sigma_{j+1}^+ \sigma_{j+2}^- + \sigma_{j+1}^- \sigma_{j+2}^+\big). \end{aligned} \tag{2.8}$$

Based on the existence of the charge Q_2 one could regard this model as nearest-neighbor interacting, but Q_2 does not generate nontrivial dynamics: it is also a sum of mutually commuting local operators. Instead, in this model Q_4 is regarded as the Hamiltonian, because Q_4 is the first parity symmetric charge of the model, which generates nontrivial dynamics.

E. Three-site models—General remarks

Let us focus on the case with $\ell = 3$. In this case we identify $H = Q_3$ and we also write

$$H = \sum_j h_{j,j+1,j+2}, \tag{2.9}$$

where $h_{j,j+1,j+2}$ is the three-site Hamiltonian density.

Such models can be interpreted very naturally as a zigzag spin ladder. See Fig. 1. However, we will focus on the translationally invariant representation Eq. (2.9).

Our main results are finding the general algebraic structures behind the three-site models, which lead to a generalization of the Reshetikhin condition. We formulate the following conjecture:

Conjecture 3. A three-site Hamiltonian is integrable, iff the charge $Q_5 = \sum_j q_5(j)$ defined by

$$\begin{aligned} q_5(j) = &[h_{j,j+1,j+2}, h_{j+1,j+2,j+3} + h_{j+2,j+3,j+4}] \\ &+ \tilde{h}_{j,j+1,j+2} \end{aligned} \tag{2.10}$$

commutes with the Hamiltonian in every volume $L \geqslant 5$. Here $\tilde{h}_{j,j+1,j+2}$ is an other three-site operator.

Clearly, this is a generalization of Conjecture 2. The construction of Q_5 through Eq. (2.10) is one of our key results. Its derivation from an underlying algebraic theory is presented in Sec. III C. We stress again that this result is very restrictive: it uses two three-site operators $h_{j,j+1,j+2}$ and $\tilde{h}_{j,j+1,j+2}$ to generate a five site charge.

Based on this result it is possible to perform a classification of integrable spin chains with three-site interactions. This is rather analogous to the ideas used in Refs. [20,21] and later in Refs. [28–32]. The idea is to make an Ansatz for $h_{j,j+1,j+2}$ and $\tilde{h}_{j,j+1,j+2}$, possibly including a number of free parameters, to construct Q_5 using Eq. (2.10) and to check the commutation relation $[H, Q_5] = 0$ on spin chains with medium length. We implemented this strategy using the program `Mathematica` and performed partial classifications on spin 1/2 chains. The generic density $h_{j,j+1,j+2}$ has a total number of $8^2 = 64$ parameters, which is a too large parameter space for practical computations. Therefore, we performed partial classifications along restricted subspaces which can bear physical relevance. The results are presented in Secs. III D and V C.

F. Quantum gates and cellular automata

We also consider brickwork type quantum circuits, where the fundamental local unitaries have a support of ℓ sites. The interest in such models is manifold: On the one hand, they can be understood as integrable models in discrete time, or alternatively as integrable Trotterizations of the continuous time spin chain models. On the other hand, they are interesting because they can lead to classical cellular automata, thus presenting one more link between the worlds of quantum and classical integrability. Finally, they are also relevant to quantum computing and real world experiments.

Let us sketch the general schemes behind our quantum circuit models. First we present the abstract formulation of the update rules, and we give more concrete examples later. It is necessary to start with the most general form, because later in this work we consider multiple types of constructions.

We build systems with Floquet-type discrete time evolution, such that the equal time update rules are given by local unitaries. Let us fix an interaction range ℓ, and consider a local unitary $U^{(\ell)}(j)$ which acts on the segment $[j, \ldots, j + \ell - 1]$ of the spin chain. Typically these unitaries will also depend on a continuous parameter u (the spectral parameter) and on a small number of extra parameters characterizing a family of models. Then we construct a brickwork type update rule for the whole spin chain using the single unitaries. We build a Floquet-type cycle with time period τ:

$$\mathcal{V} = \mathcal{V}_\tau \ldots \mathcal{V}_1, \tag{2.11}$$

such that each update step $\mathcal{V}_j$ with $j = 1 \ldots \tau$ is a product of commuting local unitaries acting at the same time. We formalize it as

$$\mathcal{V}_l = \prod_k U^{(\ell)}(x_k + \Delta_l). \tag{2.12}$$

Here x_k are coordinates that specify the placement of the local unitaries within a single time update, and Δ_l is a displacement which depends on the discrete time index l, signaling the position within the Floquet-type cycle.

The local unitaries within a given time step should commute with each other, such that the order of the product Eq. (2.12) does not matter. This requirement can be important for practical purposes (implementation of the quantum circuits in experiments), but also for theoretical reasons. In the most general case the commutativity holds if the supports are nonoverlapping, i.e., $x_{k+1} \geqslant x_k + \ell$. Nevertheless, the supports can have a nonzero overlap, if the commutativity is guaranteed by other means, for example, if the local unitaries act diagonally on the overlapping sites.

The simplest example for the brickwork construction discussed above is the alternating circuit discussed, for example, in Ref. [67]. In this case $\tau = 2$, we can choose $x_k = 2k$, and $\Delta_l = l$ with $l = 1, 2$. For a graphical representation see Fig. 8 later in Sec. IV. We can build similar structures with interaction range $\ell = 3$, the most obvious choice is $\tau = 3$, $x_k = 3k$, and $\Delta_l = l$ with $l = 1, 2, 3$ (see Fig. 12). Such a brickwork circuit was introduced in Ref. [84]. Later we will also present other types of constructions.

As mentioned earlier, the local unitaries typically have a spectral parameter u which can be tuned freely. This means that we can build families of quantum circuits. These families can have special points with very specific physical behavior.

For example, in the most typical case the unitaries become equal to the identity at the special point $u = 0$. Furthermore, the first order expansion in u gives a local Hamiltonian h with interaction range ℓ. Assuming $u \in \mathbb{R}$ this is formalized as

$$U^{(\ell)}(u|j) = 1 + iuh_{j,\ldots,j+\ell-1} + \mathcal{O}(u^2). \tag{2.13}$$

In such a case the Floquet circle $\mathcal{V}$ can act as a Trotterization of the global Hamiltonian H:

$$\mathcal{V} = 1 + iucH + \mathcal{O}(u^2), \tag{2.14}$$

where c is a real number that depends on the details of the construction, such as the Floquet period τ, the coordinate differences $x_{k+1} - x_k$ and the displacements Δ_l in Eq. (2.12).

We intend to construct quantum circuits with precisely such a behavior, so that H is one of our medium-range integrable Hamiltonians. Furthermore, we require that the quantum circuit itself should have certain integrability properties. These depend on the particular construction, and will be discussed in detail in IV; the local unitaries will be derived from the so-called Lax operators of the medium-range model.

In some models the local unitaries become deterministic for a special value u of the rapidity parameter. This means that $U^{(\ell)}(j)$ simply just permutes the states in the computational basis (possibly with some phases added), without creating any linear combinations. The states of the computational basis can be considered *classical*, because every spin has a fixed value; if the local unitaries are deterministic then classical states are mapped to classical states during time evolution. This means that the quantum circuit can be considered a *classical cellular automaton* at this special point u. An integrable example for such model was presented recently in Ref. [84]. An other important class for such models are the interaction-round-a-face models treated in Ref. [79], which lead to the elementary cellular automata on light-cone lattices. In the next subsection we discuss these models in detail.

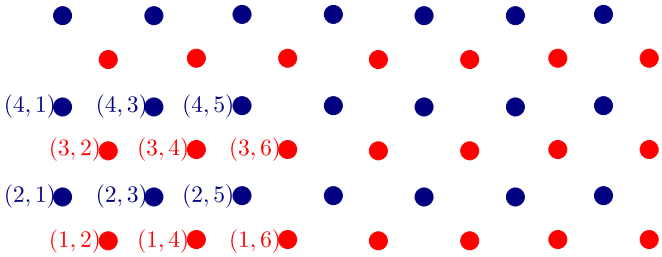

FIG. 2. The light cone lattice for the elementary cellular automata. We assign coordinates (t, x) to the sites, where t is interpreted as a time variable. The x coordinates are increased by steps of 2, and they take even (odd) values if the t coordinate is odd (even), respectively. The update of the cellular automata proceeds in the time direction upwards, and each spin is given a new value using the state of 3 of its neighbors (to the directions Southwest, South, and Southeast). For example, the spin at position (3,2) is given a value using the spins at (2,1), (1,2), and (2,3).

G. Elementary cellular automata on light cone lattices

These are classical two-state models where the variables are defined on a light cone lattice; see Fig. 2. The vertical dimension is interpreted as the direction of time. Each cell is updated depending on the state of its three neighbors (to the Southwest, South, and Southeast), and the update rules are homogeneous both in space and time. Accordingly, there are $2^{2^3} = 256$ such models, and they have been studied and classified in the seminal works [72,98]. The nomenclature for these models follows the original proposal of Wolfram [99] (see also Ref. [72]). Recently these cellular automata attracted considerable attention due to the integrability properties of some of its members: the Rule54, Rule150, and Rule201 models (see the review in Ref. [73] and also Refs. [100,101]).

As the update rules depend on three bits, it is tempting to look for a connection with our three-site interacting Hamiltonians and quantum gate models. Therefore, we provide here a formulation of the models which fits into the framework given above. Afterward, we provide a simple classification of the physically interesting models. Finally, we summarize our main results, with the technical computation presented later in Sec. IV.

First we transform the light cone lattice into a regular rectangular lattice. The idea is to add new sites to the light cone lattice to the centers of the faces; see Fig. 3. Then on this rectangular lattice we formulate a Floquet-type update rule with period $\tau = 2$, such that at each step the odd or even sites are updated, respectively. In this formulation the local update is performed by a three-site $U^{(3)}$ which is actually deterministic in the computational basis. Furthermore, it has a structure which was discussed already for the IRF-type Hamiltonians above: The quantum gate acts diagonally on the first and last bits, whereas it has an action bit in the middle. In this particular case we have

$$U^{(3)}(j) = \sum_{a,b=0,1} P_j^a f_{j+1}^{ab} P_{j+2}^b, \tag{2.15}$$

where P_j^a is a projector to basis state a acting on site j, and f_{j+1}^{ab} is a collection of four matrices acting on site $j + 1$. Then

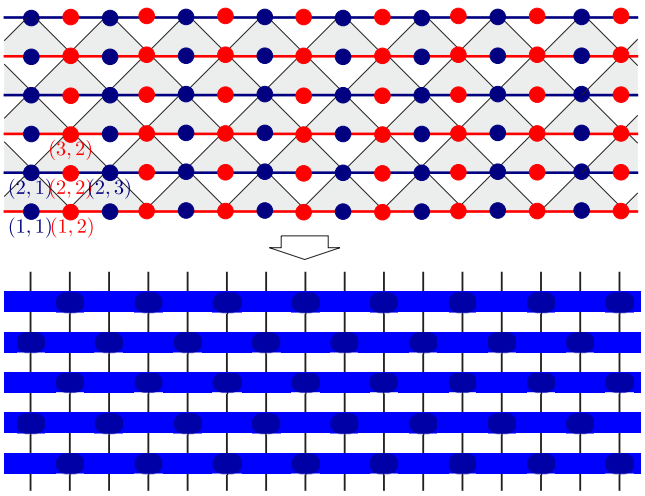

FIG. 3. Two different representations for the cellular automata on the light cone lattices. On the top we complement the original arrangement into a rectangular lattice, by adding new sites to the centers of the faces of the original lattice. The spins at the newly added sites are taken to be identical with those immediately below them, for example, the state of the new site at (2,2) is copied from the spin at (1,2). In this way we can formulate an update rule using three-site unitaries on a rectangular lattice. For example, the spin at (3,2) is given a value using the three spins (2,1), (2,2), and (2,3) from the previous row. The gray triangles show the direction of the update steps. – On the bottom we show a representation using quantum gates. Now the spin variables live on the vertices and three-site unitaries update them. The unitary gates are placed so that the neighboring pairs overlap at a control bit, which are shown by the darker shaded circles.

the full update rule is specified by

$$\mathcal{V} = \mathcal{V}_2\mathcal{V}_1, \tag{2.16}$$

with

$$\mathcal{V}_l = \prod_{k=1}^{L/2} U^{(3)}(2k+l), \quad l = 1, 2. \tag{2.17}$$

The neighboring three-site unitaries overlap at one site, but they commute because they act diagonally on the boundary sites. Thus, Eq. (2.17) is well defined without specifying the order of the action the quantum gates.

Let us now discuss the classification of these models. We wish to have deterministic time evolution (without phases), and we also require time reversibility, which follows from the requirement of unitary. Therefore, the only possibilities are

$$f^{ab} = 1 \quad \text{or} \quad f^{ab} = \sigma^x. \tag{2.18}$$

The choices Eq. (2.18) leave us with $2^4 = 16$ models. If we also require space reflection invariance, then we end up with $2^3 = 8$ models. Those two models where all f^{ab} matrices are identical are completely trivial, which leaves us with 6 models. Of these six models we can choose the following four, which are not related to each other by overall spin reflection [79]:

$$\text{Rule54: } f^{00} = 1, \quad f^{01} = f^{10} = f^{11} = \sigma^x, \tag{2.19}$$

$$\text{Rule105: } f^{00} = f^{11} = \sigma^x, \quad f^{01} = f^{10} = 1, \tag{2.20}$$

$$\text{Rule150: } f^{00} = f^{11} = 1, \quad f^{01} = f^{10} = \sigma^x, \tag{2.21}$$

$$\text{Rule201: } f^{00} = \sigma^x, \quad f^{01} = f^{10} = f^{11} = 1. \tag{2.22}$$

An additional two new models can be obtained by a complete spin reflection of the Rule54 and Rule201 models.

The Rule105 and Rule150 models are not completely independent either, because their f-matrices are obtained from each other by a multiplication with σ^x. This means that

$$\mathcal{V}_k^{(150)} = X_k\mathcal{V}_k^{(105)} = \mathcal{V}_k^{(105)}X_k, \quad k = 1, 2, \tag{2.23}$$

where we defined

$$X_k = \prod_{j=1}^{L/2} \sigma_{2j+k}^x, \quad k = 1, 2. \tag{2.24}$$

We can also observe the commutation relations

$$\left[\mathcal{V}_1^{(105)}, X_2\right] = \left[\mathcal{V}_2^{(105)}, X_1\right] = 0, \tag{2.25}$$

and similarly for the operators of the Rule150 model. Altogether this implies that the combined Floquet steps are related as

$$\mathcal{V}^{(150)} = X\mathcal{V}^{(105)}, \tag{2.26}$$

where X is the global spin reflection operator given by

$$X = X_2X_1 = \prod_{j=1}^{L} \sigma_j^x. \tag{2.27}$$

From these relations we can also derive

$$(\mathcal{V}^{(150)})^2 = (\mathcal{V}^{(105)})^2. \tag{2.28}$$

Thus, the physical behavior of the two models could be considered the same, up to a staggered global spin reflection.

An important property of these models is that the two different possibilities for the Floquet time step are actually inverses of each other:

$$\mathcal{V}_1\mathcal{V}_2 = (\mathcal{V}_2\mathcal{V}_1)^{-1}, \tag{2.29}$$

which follows simply from

$$(\mathcal{V}_1)^2 = (\mathcal{V}_2)^2 = 1. \tag{2.30}$$

As a result the two Floquet operators actually commute with each other:

$$[\mathcal{V}_1\mathcal{V}_2, \mathcal{V}_2\mathcal{V}_1] = [\mathcal{V}_1\mathcal{V}_2, \mathcal{U}^{-1}\mathcal{V}_1\mathcal{V}_2\mathcal{U}] = 0. \tag{2.31}$$

The four models listed above have been studied in a number of works recently (see the review in Ref. [73] for the Rule54 model and also Refs. [100,101] for the Rule150 and Rule201 models); nevertheless, the algebraic background for their observed integrability properties was not understood for a long time. Recently a new framework was introduced in Ref. [79] which claimed to solve this problem. We also treat these cellular automata; our main results are as follows.

We find that the Rule105 and Rule150 models can be embedded into our framework of three-site interacting models. We find a rapidity dependent family of commuting transfer matrices which includes the time evolution operator of the model as a particular case. This family of transfer matrices is regular, and we derive a set of local conserved charges that commute with the discrete time evolution operator of the cellular automata. Even though we use a different formalism, we show explicitly that our construction is identical to that one of Ref. [79] for these special class of models.

However, for the Rule54 and Rule201 we find that they are not in the family of three-site interacting integrable models. In the case of the Rule54 model we also show that the transfer matrices of Ref. [79] are algebraically dependent on three known conserved charges of the model, therefore those transfer matrices do not yield new information; this is presented in Sec. V E.

III. INTEGRABILITY STRUCTURES

In this section we present the integrability structures behind the spin chains under consideration. We start with a brief treatment of the nearest-neighbor chains, and afterwards we turn to our new results.

A. Nearest-neighbor interacting spin chains

We construct a transfer matrix which serves as a generating function for the conserved charges of the model under consideration. For an introduction into the methods we refer the reader to Refs. [9,102].

First we construct the monodromy matrix as follows. We take an auxiliary space $\mathbb{C}^{d'}$. The Lax operator $\mathcal{L}_{a,j}(u)$ acts on the tensor product of the auxiliary space (denoted by the index a) and a physical space with site index j. The variable u is called spectral parameter. In those cases when the transfer matrix generates the Hamiltonian and the other charges we have $d' = d$.

The monodromy matrix for a finite volume L is defined as

$$M_a(u) = \mathcal{L}_{a,L}(u) \dots \mathcal{L}_{a,2}(u)\mathcal{L}_{a,1}(u), \tag{3.1}$$

and the transfer matrix is

$$t(u) = \mathrm{Tr}_a\, M_a(u). \tag{3.2}$$

The transfer matrices form a commuting set of operators if the Lax operators satisfy the following exchange relations, where a and b denote two auxiliary spaces:

$$R_{b,a}(v, \mu)\mathcal{L}_{b,j}(v)\mathcal{L}_{a,j}(\mu) = \mathcal{L}_{a,j}(\mu)\mathcal{L}_{b,j}(v)R_{b,a}(v, \mu). \tag{3.3}$$

Here $R(u, v)$ is the so-called R-matrix which satisfies the Yang-Baxter relations

$$\begin{aligned} &R_{12}(\lambda_1, \lambda_2)R_{13}(\lambda_1, \lambda_3)R_{23}(\lambda_2, \lambda_3) \\ &\quad = R_{23}(\lambda_2, \lambda_3)R_{13}(\lambda_1, \lambda_3)R_{12}(\lambda_1, \lambda_2). \end{aligned} \tag{3.4}$$

Figure 4 shows the graphical presentation of the R-matrix. In the models of physical relevance the R-matrix also satisfies the so-called regularity property

$$R_{ab}(u, u) \sim \mathcal{P}_{ab}, \tag{3.5}$$

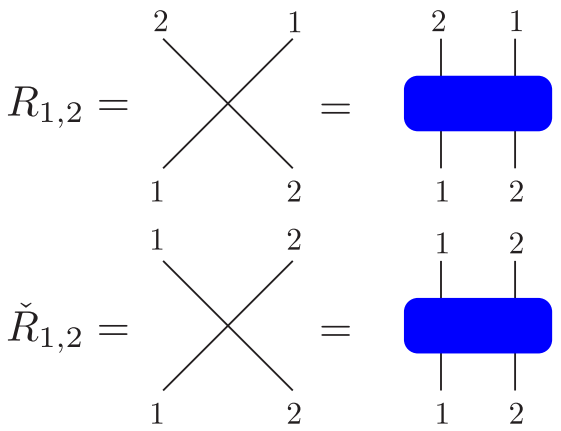

FIG. 4. Graphical illustration of the operators $\check{R}_{1,2}$ and $R_{1,2}$; we suppressed the dependence on the rapidity parameters. On the left we show the usual notation which comes from the vertex models. On the right we depict the same operators as quantum gates. The two matrices differ in a permutation, and in this notation $\check{R}_{1,2}$ acts such that the two vector spaces are kept in place.

where $\mathcal{P}_{ab}$ is the permutation operator acting on the tensor product space.

If the regularity condition holds, then the following inversion can be established:

$$R_{12}(\lambda, \mu)R_{21}(\mu, \lambda) \sim 1, \tag{3.6}$$

where

$$R_{21}(\mu, \lambda) = \mathcal{P}R_{12}(\mu, \lambda)\mathcal{P}. \tag{3.7}$$

For the sake of completeness we present the derivation of Eq. (3.6) using the Yang-Baxter equations and Eq. (3.5) in Appendix C.

One can use the R-matrix itself as a Lax operator:

$$\mathcal{L}_{a,j}(\mu) = R_{a,j}(\mu, \xi_0), \tag{3.8}$$

where ξ_0 is a fixed parameter of the model. In such a case the YB relation is equivalent to the RLL relation and the transfer matrix reads as

$$t(u) = \mathrm{Tr}_a R_{a,L}(u, \xi_0) \dots R_{a,2}(u, \xi_0)R_{a,1}(u, \xi_0). \tag{3.9}$$

There is an alternative way to define a transfer matrix, where the ordering of the sites is the opposite, and the role of the auxiliary and physical spaces is exchanged:

$$\bar{t}(u) = \mathrm{Tr}_a R_{1,a}(\xi_0, u)R_{2,a}(\xi_0, u) \dots R_{L,a}(\xi_0, u). \tag{3.10}$$

It can be proven using the Yang-Baxter relation that

$$[t(u), \bar{t}(v)] = 0. \tag{3.11}$$

In some of our constructions below it will be more convenient to use Eq. (3.10) instead of Eq. (3.9). In Figs. 5 and 6 we can see the graphical presentations of these two transfer matrices.

The regularity condition ensures that at the special point ξ_0 we have the initial conditions

$$t(\xi_0) = \mathcal{U}, \quad \bar{t}(\xi_0) = \mathcal{U}^{-1}, \tag{3.12}$$

where $\mathcal{U}$ is the cyclic shift operator on the chain.

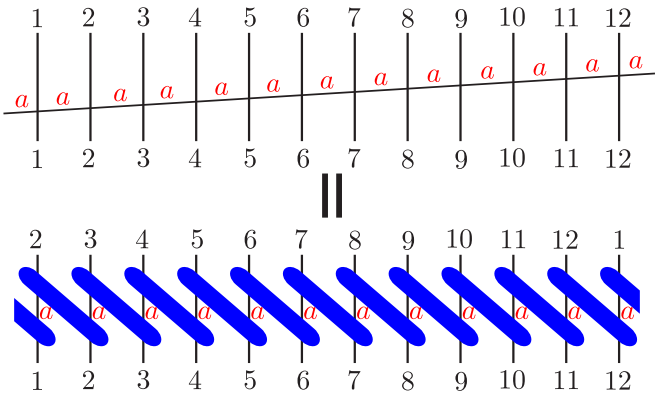

FIG. 5. Graphical illustration of transfer matrix Eq. (3.9). Here a denotes the auxiliary space. The first representation is the usual from the literature, which shows the transfer matrix as a concatenation of Lax operators. The second picture shows the same object using a succession of quantum gates. The two representations are not very different, but generalizations of the second one will be more convenient in the more complicated cases that will follow.

A commuting set of local charges is then constructed as

$$Q_\alpha \quad \sim \quad (\partial_u)^{\alpha-1} \log(t(u))\big|_{u=\xi_0}. \tag{3.13}$$

In many models the R-matrix is of difference form, which means

$$R(u, v) = R(u - v). \tag{3.14}$$

In such a case the parameter ξ_0 is irrelevant, and it is conventional to set it to $\xi_0 = 0$. However, we will consider the generic case where the R-matrix is not necessarily of difference form.

Let us investigate the first few charges in detail. Performing the first derivative of Eq. (3.13) we get the nearest-neighbor Hamiltonian

$$H = Q_2 = \sum h_{j,j+1}, \tag{3.15}$$

with

$$h_{j,j+1} = \partial_u \check{\mathcal{L}}_{j,j+1}(u)\big|_{u=\xi_0}, \tag{3.16}$$

where

$$\check{\mathcal{L}}_{j,j+1}(u) = \mathcal{P}_{j,j+1} R_{j,j+1}(u, \xi_0). \tag{3.17}$$

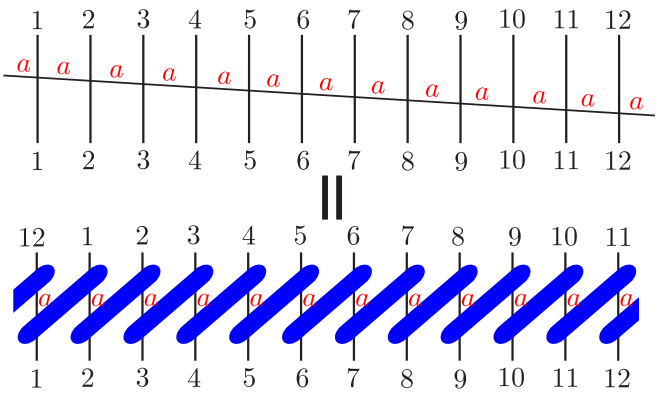

FIG. 6. Graphical illustration of transfer matrix Eq. (3.10).

For this operation it is crucial that the regularity condition is satisfied.

For the third charge we get the general expression

$$Q_3 = \sum_j [h_{j,j+1}, h_{j+1,j+2}] + \check{\mathcal{L}}''_{j,j+1}(\xi_0) - h^2_{j,j+1}. \tag{3.18}$$

We can see that in addition to the commutator we have two-site operators, and altogether this expression takes the form of Eq. (2.7) announced earlier.

Assuming that the R-matrix has difference form and setting $\xi_0 = 0$ then the following inversion relation holds:

$$\check{\mathcal{L}}(u)\check{\mathcal{L}}(-u) = 1. \tag{3.19}$$

This implies that the last two terms in Eq. (3.18) cancel, which can be seen after taking the second derivatives of Eq. (3.19) with respect to u and substituting $u = 0$. In this case we end up with

$$Q_3 = \sum_j [h_{j,j+1}, h_{j+1,j+2}]. \tag{3.20}$$

We can see that Eq. (3.20) follows from Eq. (3.6) if the R-matrix is of difference form. However, in other cases it does not hold generally. Perhaps the most famous example where it does not hold is the Hubbard model and its inhomogeneous versions [103].

The form of Eq. (3.18) yields the original version of the Reshetikhin condition used, for example, in Ref. [33].

B. Three-site interactions

Let us now consider a three-site interacting model, defined by the Hamiltonian

$$H = \sum_j h_{j,j+1,j+2}. \tag{3.21}$$

Below we conjecture a generic form of the Lax operator for such models. We motivate our conjecture by some simple ideas. We do not assume the existence of a proper translationally invariant Lax operator from the start, instead we develop arguments that motivate its existence and its properties.

The key idea is to build a nearest-neighbor chain out of our model by grouping together (or gluing) every two spins into blocks. Therefore, we consider our spin chain in an even volume $L = 2k$. We pair the spins, and label the pairs using the original coordinates, for example, $(j, j + 1)$. Then we obtain a new model with k sites and local dimension d^2. The Hamiltonian for the new model can be written as

$$\tilde{H} = \sum_{j=1}^{L/2} \tilde{h}_{j,j+1}, \tag{3.22}$$

where we can choose, for example,

$$\tilde{h}_{j,j+1} = h_{2j,2j+1,2j+2} + h_{2j+1,2j+2,2j+3}. \tag{3.23}$$

Similarly we can construct commuting higher charges for the glued model by using the charges of the original one, and thus we obtain a nearest-neighbor integrable chain with local dimension d^2. In our arguments below we will switch back and forth between viewing the spin chains and the charges in

the original and the glued representations. This will gives us crucial clues about the integrability structures.

First we look at the glued chain. It has a set of commuting local charges, thus we can assume that it is Yang-Baxter integrable in the usual way. Thus, there should exist an auxiliary space A and an R-matrix which generates the charges for this glued chain. The auxiliary space should have the same dimension as the physical spaces, which are now the tensor product spaces $(j, j+1)$. Therefore, we construct the auxiliary space V_A as $V_a \otimes V_b$ where the two spaces labeled a and b are isomorphic to the physical spaces of the original chain. In this way we obtain a commuting set of transfer matrices

$$t(u) = \mathrm{Tr}_A R_{A,(L-1,L)}(u,0)\dots R_{A,(3,4)}(u,0)R_{A,(1,2)}(u,0), \tag{3.24}$$

which generate the Hamiltonian and the charges of the glued chain. Here we used the same letter for the R-matrix as before; the distinction between the different R-matrices is made by denoting explicitly the indices of the spaces on which they act.

Above we set the inhomogeneity parameter of the R-matrix to $\xi_0 = 0$, which is just a choice for the zero point of the rapidity parameters. Generally, we can consider families of models by varying ξ_0, see, for example, Ref. [103], for deformations of the Hubbard model. However, picking a particular model we are always free to set $\xi_0 = 0$ by a reparametrization.

Since the glued chain is a nearest-neighbor interacting model we can assume that the R-matrix is regular, i.e.,

$$R_{(a,b),(j,j+1)}(0,0) = \mathcal{P}_{(a,b),(j,j+1)} = \mathcal{P}_{a,j}\mathcal{P}_{b,j+1}. \tag{3.25}$$

From this it follows that the charges derived from Eq. (3.24) are all local on the glued chain, and thus also on the original chain.

Let us then return to the original spin chain. The transfer matrix constructed above can be understood as a nonlocal operator acting on the original Hilbert space. The Taylor expansion of $t(u)$ on the glued chain gives the glued charges, and if we view $t(u)$ as an operator acting on the original chain, then we see that it generates the charges of the original model. This is a crucial observation.

In the original spin chain all charges are translationally invariant, but the gluing procedure explicitly breaks this invariance. The transfer matrix Eq. (3.24) enjoys two-site invariance by construction:

$$t(u) = \mathcal{U}^{-2} t(u) \mathcal{U}^2, \tag{3.26}$$

where $\mathcal{U}$ is the translation operator of the original chain, thus $\mathcal{U}^2$ describes a single-site translation in the glued chain. However, the charges of the original chain are one-site invariant, and they are the Taylor coefficients of $t(u)$ if viewed as an operator acting on the original chain. This leads to the conclusion that the transfer matrix should also be translationally invariant:

$$t(u) = \mathcal{U}^{-1} t(u) \mathcal{U}. \tag{3.27}$$

This is a very strong condition. It implies that the two different gluing procedures (where we group sites $(2j, 2j+1)$ or $(2j+1, 2j+2)$, respectively) should lead to the same global transfer matrix:

$$\begin{aligned}&\mathrm{Tr}_{a,b} R_{(a,b),(L-1,L)}(u,0)\dots R_{(a,b),(1,2)}(u,0)\\ &\quad = \mathrm{Tr}_{a,b} R_{(a,b),(L,1)}(u,0)\dots R_{(a,b),(2,3)}(u,0).\end{aligned} \tag{3.28}$$

This relation motivates the existence of a proper Lax operator for the original chain, so that we could bypass the gluing procedure. We expect that the only way that Eq. (3.28) can be satisfied is if the corresponding R-matrix factorizes into a product of Lax operators. We formulate the following:

Conjecture 4. If the condition Eq. (3.28) holds in every even volume L, then the R-matrix of the glued chain factorizes as

$$R_{(a,b),(j,j+1)}(u,0) = \mathcal{L}_{a,b,j+1}(u)\mathcal{L}_{a,b,j}(u), \tag{3.29}$$

where $\mathcal{L}_{a,b,j}(u)$ is a proper Lax operator for the original chain which satisfies the following RLL relation:

$$R_{AB}(u,v)\mathcal{L}_{A,j}(u)\mathcal{L}_{B,j}(v) = \mathcal{L}_{B,j}(v)\mathcal{L}_{A,j}(u)R_{AB}(u,v), \tag{3.30}$$

where A and B stand for pairs of auxiliary spaces, and j labels a physical space.

We did not find a proof for this Conjecture, but it is easy to see that the assumption Eq. (3.29) naturally satisfies Eq. (3.28).

It is a simple consequence of Conjecture 4. that if the glued R-matrix is regular then the Lax operator satisfies the three-site regularity condition

$$\mathcal{L}_{ab,j}(0) = \mathcal{P}_{a,j}\mathcal{P}_{b,j}. \tag{3.31}$$

This follows simply from the observation

$$\begin{aligned}R_{(1,2),(3,4)}(0,0) &= \mathcal{P}_{2,4}\mathcal{P}_{1,3} = \mathcal{P}_{2,4}\mathcal{P}_{1,2}\mathcal{P}_{1,2}\mathcal{P}_{1,3}\\ &= (\mathcal{P}_{1,4}\mathcal{P}_{2,4})(\mathcal{P}_{1,3}\mathcal{P}_{2,3}) = \mathcal{L}_{1,2,4}(0)\mathcal{L}_{1,2,3}(0).\end{aligned} \tag{3.32}$$

Strictly speaking, Eq. (3.32) does not imply Eq. (3.31), but we conjecture that all other choices for $\mathcal{L}_{ab,j}(0)$ can be transformed to $\mathcal{P}_{a,j}\mathcal{P}_{b,j}$ after an appropriate gauge transformation in the auxiliary spaces.

In general, the RLL equations do not have unique solutions (up to normalization) if the R-matrix has gauge invariance

$$[R_{A,B}(u,v), G_A(u)G_B(v)] = 0, \tag{3.33}$$

where $G_A(u)$ is a spectral parameter dependent $d \times d$ matrix. Indeed, assuming the gauge invariance the transformed Lax operator

$$G_A(u)\mathcal{L}_{A,j}(u) \tag{3.34}$$

is also a solution of the RLL Eq. (3.30). For the practical examples such symmetry of R-matrix is excluded and only global symmetry (spectral parameter independent symmetry) is allowed. In the following we concentrate on R-matrices with no gauge invariance.

Although we cannot prove Conjecture 4, we can prove the reverse statement:

Theorem 1. Taking a regular R-matrix $R_{A,B}(u)$ with no gauge invariance and a Lax operator $\mathcal{L}_{A,j}(u)$ which satisfy the RLL relation Eq. (3.30) and the regularity condition Eq. (3.31) then the R-matrix is factorized as Eq. (3.29).

The proof is presented in Appendix D.

Let us now consider the transfer matrix of the original three-site interacting case. We can now write it as

$$t(u) = \mathrm{Tr}_{a,b}\mathcal{L}_{a,b,L}(u)\ldots\mathcal{L}_{a,b,1}(u). \tag{3.35}$$

This representation of the transfer matrix is manifestly translationally invariant; the formula already appeared in Ref. [84].

The relation Sec. (3.31) leads to the initial condition

$$t(0) = \mathcal{U}^2. \tag{3.36}$$

Let us now define the operator $\check{\mathcal{L}}_{a,b,j}(u)$ through

$$\mathcal{L}_{a,b,j}(u) = \mathcal{P}_{a,j}\mathcal{P}_{b,j}\check{\mathcal{L}}_{a,b,j}(u). \tag{3.37}$$

The condition Eq. (3.31) leads to

$$\check{\mathcal{L}}_{a,b,j}(0) = 1. \tag{3.38}$$

Computing the first logarithmic derivative of the transfer matrix as

$$H = t^{-1}(0)\,\partial_u t(u)|_{u=0}, \tag{3.39}$$

we obtain Eq. (3.21) with

$$h_{j,j+1,j+2} = \partial_u \check{\mathcal{L}}_{j,j+1,j+2}(u)\big|_{u=0}. \tag{3.40}$$

Here we used

$$t^{-1}(0) = \mathcal{U}^{-2}. \tag{3.41}$$

Summarizing these findings we formulate the following:

Conjecture 5. Every integrable three-site Hamiltonian Eq. (3.21) has a three-site Lax operator in the form

$$\mathcal{L}_{1,2,3}(u) = \mathcal{P}_{13}\mathcal{P}_{23}[1 + uh_{123} + \mathcal{O}(u^2)], \tag{3.42}$$

and there exists an R-matrix for which the RLL-relation is satisfied

$$R_{AB}(u, v)\mathcal{L}_{A,j}(u)\mathcal{L}_{B,j}(v) = \mathcal{L}_{B,j}(v)\mathcal{L}_{A,j}(u)R_{AB}(u, v), \tag{3.43}$$

such that the R-matrix factorizes as Eq. (3.29). In the RLL relation above A and B stand for pairs of auxiliary spaces.

The assumptions leading to this Conjecture were the integrability of the glued chain, the translational invariance of all charges and the corresponding transfer matrix when viewed as operators acting on the original chain, and finally the assumption that the regularity condition Eq. (3.32) implies Eq. (3.31) up to an irrelevant gauge transformation.

Let us now also discuss two trivial solutions to the above relations, which bring us back to the nearest-neighbor chains.

We can choose

$$\mathcal{L}_{a,b,j}(u) = \mathcal{L}_{a,j}(u)\mathcal{L}_{b,j}(u), \tag{3.44}$$

where $\mathcal{L}_{a,j}(u)$ is a Lax operator of a n.n. model. This choice satisfies all the requirements listed above. If we denote by $t^{(3)}(u)$ the transfer matrix constructed out of Eq. (3.44) using Eq. (3.35) and by $t^{(2)}(u)$ the simple transfer matrix constructed from $\mathcal{L}_{a,j}(u)$ according to Eq. (3.2), then we obtain the relation

$$t^{(3)}(u) = [t^{(2)}(u)]^2. \tag{3.45}$$

This implies that from $t^{(3)}(u)$ we would obtain the same nearest-neighbor Hamiltonian as from $t^{(2)}(u)$, but multiplied with factor of 2.

An alternative trivial choice is

$$\mathcal{L}_{a,b,c}(u) = \mathcal{P}_{a,b}\mathcal{L}_{a,c}(u). \tag{3.46}$$

It can be seen that this leads to two decoupled spin chains that are placed on the odd and even sublattices of the original spin chain, such that we have nearest-neighbor interactions within each sublattice.

These trivial examples bring us to an important conclusion: *the real source of the three-site interaction is a coupling of the auxiliary spaces which cannot be factorized as in Eq. (3.44) or as in Eq. (3.46).*

C. Conserved charges in the three-site interacting case

Let us now consider the higher conserved charges in the three-site interacting models, which are computed from the higher logarithmic derivatives of the transfer matrix. The next charge is computed from

$$(\partial_u)^2 \log[t(u)] = t^{-1}(u)t''(u) - [t^{-1}(u)t'(u)]^2 \tag{3.47}$$

after taking the derivatives and eventually substituting $u = 0$. Taking into account the definition Eq. (3.35), the initial conditions Eq. (3.31), and also the inverse Eq. (3.41) we obtain a five-site operator, which can be written as

$$Q_5 = \sum_j [h_{j,j+1,j+2}, h_{j+1,j+2,j+3} + h_{j+2,j+3,j+4}] - (h_{j,j+1,j+2})^2 + \check{\mathcal{L}}''_{j,j+1,j+2}(0). \tag{3.48}$$

This is a generalization of Eq. (3.18) to the three-site interacting case. We see that the density of Q_5 depends on a term which is completely determined by the Hamiltonian density, but it also includes an additional three-site operator, which was included in Eq. (2.10) that we announced earlier.

The simplest cases are those when the following inversion relation holds:

$$\check{\mathcal{L}}_{a,b,j}(u)\check{\mathcal{L}}_{a,b,j}(-u) = 1. \tag{3.49}$$

Taking second derivative in u and substituting $u = 0$ we obtain that the last two terms in Eq. (3.48) cancel.

At present it is not clear whether all three-site interacting models satisfy Eq. (3.49). In our classification we found that we can always choose conventions such that Eq. (3.49) holds. In the case of the $U(1)$-invariant models we actually allowed for an additional three-site operator in the density of Q_5, performed the classification using the condition $[H, Q_5] = 0$ and did not find additional models. However, this might be a peculiarity of the $U(1)$-invariant models.

We also note a gauge freedom which does actually change the representation of the charge Q_5. Considering a Hamiltonian density $h_{1,2,3}$ we can construct a new one by

$$h'_{1,2,3} = h_{1,2,3} + g_{1,2} - g_{2,3}, \tag{3.50}$$

where $g_{1,2}$ is an arbitrary two-site operator. Clearly, the density $h'_{1,2,3}$ leads to the same global Hamiltonian, because the additional terms add up telescopically to zero. However, the commutator in Eq. (3.48) will be a different operator.

The dependence on $g_{1,2}$ does not drop out, whereas the global Q_5 charge cannot change. This paradox is resolved by noting that the three-site operator in the second line of Eq. (3.48) also changes, because the Lax operator needs to be modified so that its first derivative can reproduce Eq. (3.50). Altogether this modification cancels the additional terms that appear from the commutator in Eq. (3.48), so that Q_5 does not change as expected. In our concrete examples we always found a gauge where Eq. (3.49) holds.

Let us now also consider the higher charges. Taking further derivatives we see that the range of the charges increases by two sites after every new derivative. This means that the allowed indices α for the charges Q_α are $3, 5, 7, \ldots$ with $H = Q_3$. This is clearly different from the n.n. chains where typically all integers are allowed.

In specific cases it can happen that there is a one-site or a two-site charge commuting with the transfer matrix above; examples will be shown below. In all such cases we found that the smaller charges are not dynamics generating. If they are nontrivial, then the model has to be nearest-neighbor interacting.

D. Partial classification for three-site interacting spin-1/2 chains

Our method is to make an Ansatz for $h_{j,j+1,j+2}$ and $\tilde{h}_{j,j+1,j+2}$, to compute Q_5 through Eq. (2.10), and finally to enforce the commutativity $[H, Q_5] = 0$. We find that this relation indeed gives us a number of interesting new models. We repeat this procedure for different cases with different Ansatz, see below. Afterward, we also look for the corresponding Lax operators and R-matrices. The idea for finding the Lax operator is rather simple: We are looking for a one-parameter family of three-site operators, within the same Ansatz as specified for the Hamiltonian density, and we enforce that the transfer matrix Eq. (3.35) commutes with the Hamiltonian. Afterward, we also check the initial condition Eq. (3.31) and the first derivative according to Eq. (3.40). Finally, the R-matrices can be found simply from Eq. (3.3) which becomes a linear equation for them. The Yang-Baxter relation for the R-matrices can be checked afterwards.

It is important for the classification to exclude "trivial" solutions which would not lead to new physical behaviour. Such trivial cases include simply taking a nearest-neighbor Hamiltonian density $h^{(nn)}_{j,j+1}$ and choosing either $h_{j,j+1,j+2} = h^{(nn)}_{j,j+1}$ or $h_{j,j+1,j+2} = h^{(nn)}_{j,j+2}$. The first choice simply just gives back the original two-site model, whereas the second choice gives two decoupled nearest-neighbor chains living on the odd and even sublattices of the new model. We encountered both cases among the results of the classification, but we will not include them in the lists to be presented below.

Curiously we found that in some restricted parameter spaces $\tilde{h}_{j,j+1,j+2} = 0$, for example, this holds for all $U(1)$-invariant models. However, at present we cannot exclude models in other classes with a nonzero $\tilde{h}_{j,j+1,j+2}$.

We performed the classification in three specific cases.

1. $SU(2)$ invariant models

It is relatively easy to impose $SU(2)$ invariance on the three-site Hamiltonian density $h_{j,j+1,j+2}$: we require that it has to be built as a sum of permutation operators that act on the three sites $j, j+1, j+2$. We do not impose space reflection invariance. With these conditions we found **no nontrivial three-site models**. Trivial solutions include $h_{j,j+1,j+2} = \mathcal{P}_{j,j+1}$ which describes the Heisenberg spin chain, $h_{j,j+1,j+2} = \mathcal{P}_{j,j+2}$ which describes two independent Heisenberg chains on two sublattices, and $h_{j,j+1,j+2} = q_3(j)$ with $q_3(j)$ being the density of the third charge in the Heisenberg chain.

2. $U(1)$ invariant models with space reflection invariance

We investigated models where the Hamiltonian commutes with the charge $Q_1 = S_z$, which generates a global $U(1)$ group. We also required space reflection invariance, but allowing for a gauge freedom of the type Eq. (3.50).

We found two families of models.

The Bariev model. It is given by the Hamiltonian

$$H = \sum_j [\sigma_j^- \sigma_{j+2}^+ + \sigma_j^+ \sigma_{j+2}^-] \frac{1 - U\sigma_{j+1}^z}{2}, \tag{3.51}$$

where U is a coupling constant. The model was first proposed in Ref. [44] as a zigzag spin ladder. Special points of the model are $U = \pm 1$ where it becomes identical to the folded XXZ model in the bond picture [52–54]. We investigated the fundamental Lax and R-matrices of the model given in Ref. [45] and found that they satisfy the equations derived above, including the initial condition Eq. (3.31) and the factorization Eq. (3.29) (for the Lax operators see also Refs. [46,104]). To obtain the desired formulas we just applied certain permutations on the basis vectors so that Eqs. (3.31) and (3.29) would hold in the form given above.

The hard rod deformed XXZ model. It is given by

$$H = \sum_j [\sigma_j^- P^\bullet_{j+1} \sigma_{j+2}^+ + \sigma_j^+ P^\bullet_{j+1} \sigma_{j+2}^- - \Delta(P^\circ_j P^\bullet_{j+1} P^\bullet_{j+2} + P^\bullet_j P^\bullet_{j+1} P^\circ_{j+2})]. \tag{3.52}$$

Here Δ is a coupling constant. Up to our best knowledge this is a new model, but it is closely related to the so-called constrained XXZ model treated earlier in Refs. [35,38–41]. The complete solution of the new model and the discussion of its special physical properties will be discussed in an upcoming publication. We note that at the special point $\Delta = 0$ this model also becomes equal to the folded XXZ model in the bond picture. Thus, these two families of models intersect at the points $\Delta = 0$ and $U = 1$.

3. Hamiltonians of the IRF type

A further special class of models are those when the three-site operator $h_{j,j+1,j+2}$ acts diagonally on the first and the last sites. This means that the spins at site j and $j+2$ can be considered as control bits that influence the action on the site $j+1$. The most general form for such an operator is

$$h_{j,j+1,j+2} = \sum_{a,b=0,1} P_j^a h_{j+1}^{ab} P_{j+2}^b, \tag{3.53}$$

where now h^{ab} stands for a collection of four Hermitian matrices corresponding to the indices $a, b = 0, 1$.

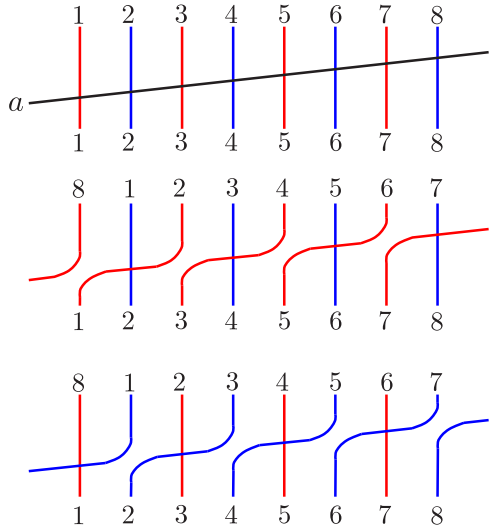

FIG. 7. Graphical illustration of transfer matrices $t(u)$, $t(\mu)$, and $t(\nu)$. The corresponding spectral parameters of black, red and blue lines are u, μ and ν, respectively. The line avoidings are a result of the regularity condition Eq. (3.5).

The search for such Hamiltonians is motivated by recent studies on quantum gates and cellular automata, which we discussed in Sec. II G. In particular, such Hamiltonians can be considered as continuous time version of the IRF models treated in Ref. [79].

We treat these models separately in Sec. V C.

IV. INTEGRABLE QUANTUM CIRCUITS

In this section we present our results for the brickwork type quantum circuits. We introduce a number of closely related constructions, with different types of integrability properties.

Let us recall the general formulas for the brickwork circuits as explained in Sec. II F. We are building Floquet-type cycles with time period τ:

$$\mathcal{V} = \mathcal{V}_\tau \dots \mathcal{V}_1, \tag{4.1}$$

with the update steps being

$$\mathcal{V}_l = \prod_k U^{(\ell)}(x_k + \Delta_l). \tag{4.2}$$

Here x_k are coordinates for the unitaries and Δ_l are the displacements that distinguish the different single step updates within the Floquet cycle.

A. Integrable Trotterization for nearest-neighbor interacting chains

Here we review the construction of Ref. [67], which can be applied for integrable nearest-neighbor chains. The key ideas go back to the light cone regularization of the quantum field theories; see, for example, Refs. [68–70].

We build a brickwork quantum circuit using two-site unitaries ($\ell = 2$) with Floquet period $\tau = 2$. Correspondingly, the coordinates for the unitaries are $x_k = 2k$ and the shift is $\Delta_l = l$, see Fig. 8.

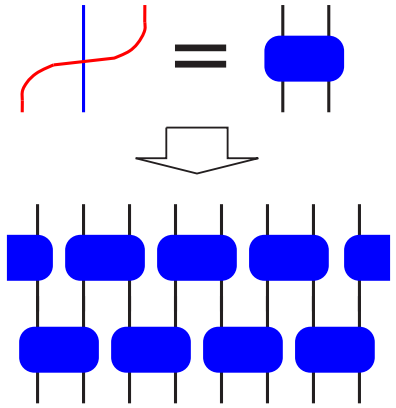

FIG. 8. Graphical illustration of the period-2 Floquet cycle $[t(\nu)]^{-1}t(\mu)$.

The starting point is the R-matrix $R(u, v)$ which is supposed to be a regular solution of the YB Eqs. (3.4). We do not assume that the R-matrix is of difference form.

On a chain of length $L = 2k$ we build an *inhomogeneous* transfer matrix with alternating inhomogeneities μ, ν as

$$t(u) = \mathrm{Tr}_a[R_{a,L}(u, \nu)R_{a,L-1}(u, \mu)\dots R_{a,2}(u, \nu)R_{a,1}(u, \mu)]. \tag{4.3}$$

Using the regularity condition Eq. (3.5) we obtain two special points for the transfer matrix, where it becomes a product of distinct quantum gates multiplied by an overall translation (see Fig. 7):

$$t(\mu) = \mathcal{U}\check{R}_{L-1,L}(\mu, \nu)\dots\check{R}_{1,2}(\mu, \nu), \tag{4.4}$$

$$t(\nu) = \mathcal{U}\check{R}_{L,1}(\nu, \mu)\dots\check{R}_{2,3}(\nu, \mu). \tag{4.5}$$

Let us assume that the inversion relation Eq. (3.6) holds without scalar factors

$$\check{R}_{1,2}(u, v)\check{R}_{1,2}(v, u) = 1. \tag{4.6}$$

Then we obtain

$$[t(\nu)]^{-1} = \check{R}_{L,1}(\mu, \nu)\dots\check{R}_{2,3}(\mu, \nu)\mathcal{U}^{-1}. \tag{4.7}$$

Finally, we see that the operator product

$$[t(\nu)]^{-1}t(\mu) \tag{4.8}$$

can be interpreted as a period-2 Floquet cycle of the form Eq. (2.11) with a two-site gate

$$U^{(2)}(j) = \check{R}_{j,j+1}(\mu, \nu); \tag{4.9}$$

see Fig. 8.

The requirement of unitarity puts constraints on the R-matrix and the spectral parameters μ, ν. However, in the typical cases there are simple choices which fulfill unitarity, which depend on the real analyticity of the R-matrix. It follows from Eq. (4.6) that the R-matrix is unitary for a pair μ, ν if

$$(\check{R}_{1,2}(\mu, \nu))^\dagger = \check{R}_{1,2}(\nu, \mu). \tag{4.10}$$

In the simple case of the XXZ spin chain with $\Delta = \cosh(\eta)$ we can choose the following representation of the R-matrix:

$$\check{R}(\mu,\nu) = \begin{pmatrix} 1 & & & \\ & c(\mu-\nu) & b(\mu-\nu) & \\ & b(\mu-\nu) & c(\mu-\nu) & \\ & & & 1 \end{pmatrix}, \tag{4.11}$$

with

$$c(u) = \frac{\sinh(\eta)}{\sinh(u+\eta)}, \quad b(u) = \frac{\sinh(u)}{\sinh(u+\eta)}. \tag{4.12}$$

It can be seen that $\check{R}(\mu,\nu)$ is unitary if either η is real ($\Delta > 1$) and $\mu - \nu$ is purely imaginary, or if η is purely imaginary ($\Delta < 1$) and $\mu - \nu$ is real.

B. Integrable quantum circuits for three-site models—Construction 1

Now we construct quantum circuits for the three-site interacting models. Such circuits can be built for every model which fits into our framework laid out in Sec. III. The specific case of the IRF type models is treated later in Sec. V A, where we present a different type of quantum circuit adapted to the special form of those Lax operators.

We present two different Floquet circles for the three-site models. In the first case we generalize the results from the previous subsection to the present case: this is a rather straightforward construction from a technical point of view, but it leads to brickwork circuits with "untouched" sites. An alternative construction is presented in the next subsection. That one leads to a tightly packed brickwork circuit, but its integrability structure is more involved.

In the first case we use the glued chain, where we group together pairs of sites of the original chain, see the derivations in Sec. III B. Then the idea is to generalize the definition Eq. (4.3) to the present case with the grouped sites. In this way we obtain a quantum circuit with four-site unitaries, because the R-matrix of the glued chain acts on pairs of sites. However, at special points we can make use of the factorization Eq. (3.29) in order to obtain the three-site unitaries.

We take a chain of length $L = 4k$ and construct an inhomogeneous transfer matrix for the grouped sites with alternating inhomogeneities μ, ν:

$$t(u) = \mathrm{Tr}_{ab}[R_{(a,b)(4k-1,4k)}(u,\nu)\ldots \times R_{(a,b)(3,4)}(u,\nu)R_{(a,b)(1,2)}(u,\mu)]. \tag{4.13}$$

Here a, b stand for the two auxiliary spaces of the model. This family of transfer matrices is commuting. Special points are $u = \mu, \nu$ with

$$t(\mu) = \mathcal{U}^2\check{R}_{(4k-3,4k-2)(4k-1,4k)}(\mu,\nu)\ldots\check{R}_{(1,2)(3,4)}(\mu,\nu),$$
$$t(\nu) = \mathcal{U}^2\check{R}_{(4k-1,4k)(1,2)}(\nu,\mu)\ldots\check{R}_{(3,4)(5,6)}(\nu,\mu). \tag{4.14}$$

Note the appearance of $\mathcal{U}^2$, the translation operator by two sites.

Similar to the nearest-neighbor case, we take now the inverse of $t(\mu)$, which becomes

$$t^{-1}(\nu) = \check{R}_{(4k-1,4k)(1,2)}(\mu,\nu)\ldots\check{R}_{(3,4)(5,6)}(\mu,\nu)\mathcal{U}^{-2}. \tag{4.15}$$

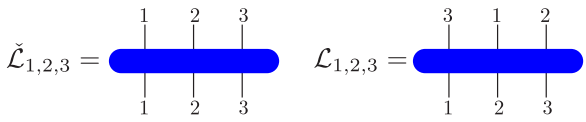

FIG. 9. Graphical illustration of operators $\check{\mathcal{L}}_{123}$ and $\mathcal{L}_{123}$.

Finally, we define the Floquet cycle as

$$\mathcal{V} = t^{-1}(\nu)t(\mu) = \check{R}_{(4k-1,4k)(1,2)}(\mu,\nu)\ldots\check{R}_{(3,4)(5,6)}(\mu,\nu) \times \check{R}_{(4k-3,4k-2)(4k,4k-1)}(\mu,\nu)\ldots\check{R}_{(1,2)(3,4)}(\mu,\nu). \tag{4.16}$$

This can be understood as a cycle with period $\tau = 2$ and with the four-site gates

$$U^{(4)}(j) = \check{R}_{(j,j+1)(j+2,j+3)}(\mu,\nu). \tag{4.17}$$

The coordinates of the gates are $x_k = 4k$ and the displacements are $\Delta_l = 2l$ with $l = 1, 2$. Similar to the nearest-neighbor cases we need to impose restrictions on μ, ν to obtain a gate which is unitary. This restriction depends on the model.

A quantum circuit with three-site gates is obtained by substituting $\nu = 0$. Then we use the factorization

$$\check{R}_{(j,j+1),(j+2,j+3)}(\mu,0) = \check{\mathcal{L}}_{j+1,j+2,j+3}(\mu)\check{\mathcal{L}}_{j,j+1,j+2}(\mu), \tag{4.18}$$

which follows from Eq. (3.29). For a graphical interpretation of this relation see Figs. 9 and 10. Substituting this factorization into Eq. (4.16) we obtain a Floquet cycle with period $\tau = 4$, three-site gates

$$U^{(3)}(j) = \check{\mathcal{L}}_{j,j+1,j+2}(\mu), \tag{4.19}$$

coordinates $x_k = 4k$, and displacements $\Delta_l = l$ with $l = 1, 2, 3, 4$. For a graphical interpretation of this quantum circuit see Fig. 11.

Disadvantages of this construction are that the quantum circuit does not have left-right symmetry, and that the three-site unitaries are not tightly packed: every fourth spin is left untouched at every time step.

C. Integrable quantum circuits for three-site models—Construction 2

Now we also present a quantum circuit which is tightly packed. We take three-site gates defined by Eq. (4.19) and construct a circuit with period $\tau = 3$, coordinates $x_k = 3k$, and displacements $\Delta_l = l$ with $l = 1, 2, 3$. For a graphical interpretation see Fig. 12.

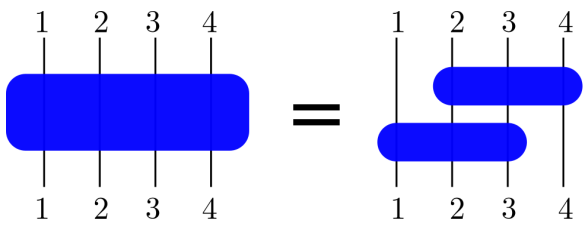

FIG. 10. Graphical illustration of Eq. (4.18).

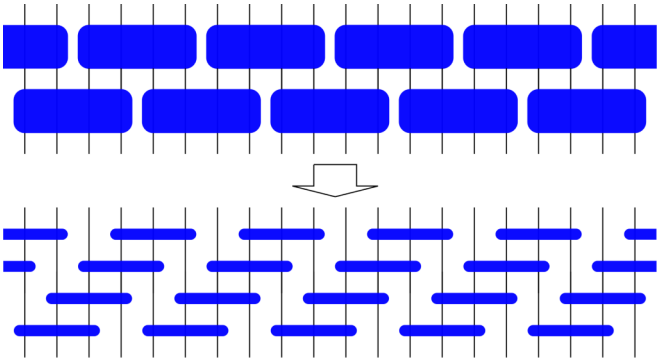

FIG. 11. In the top of the figure we can see the period 2 Floquet cycle for the glued chain. We changed the R-matrices from Fig. 8 to $\check{R}_{(12),(34)}(\mu,\nu)$. In the bottom we substitute $\nu=0$ and use the factorization property Eq. (4.18). Thus, we get a period 4 Floquet cycle with three-site gates so that every fourth spin is untouched at every step.

Such a circuit was already introduced in Ref. [84], however, the integrability was only shown for the diagonal-to-diagonal transfer matrices, which are identical to the ones defined by Eq. (3.35) (for a pictorial interpretation see Fig. 13). Now we also develop the commuting row-to-row transfer matrices for this quantum circuit.

We start with the three-site Lax operator $\check{\mathcal{L}}(u)$ and the associated R-matrix $\check{R}_{ab,(j,j+1)}(u,v)$. We construct an operator acting on five spaces:

$$\begin{aligned}\check{\mathcal{R}}_{1,2,3,4,5}(\theta,u) &= \check{\mathcal{L}}^{-1}_{1,2,3}(u)\check{R}_{2,3,4,5}(\theta,u)\check{\mathcal{L}}_{1,2,3}(\theta)\\ &= \check{\mathcal{L}}_{3,4,5}(\theta)\check{R}_{1,2,3,4}(\theta,u)\check{\mathcal{L}}^{-1}_{3,4,5}(u). \qquad (4.20)\end{aligned}$$

For the transfer matrices we will also need an operator which acts on one more space with a permutation, therefore we define

$$\mathcal{R}_{(1,2,3),(4,5,6)}(\theta,u) = \mathcal{P}_{1,4}\mathcal{P}_{2,5}\mathcal{P}_{3,6}\check{\mathcal{R}}_{1,2,3,4,5}(\theta,u). \qquad (4.21)$$

This matrix satisfies the YB equation

$$\begin{aligned}&\mathcal{R}_{(1,2,3),A}(\theta,u)\mathcal{R}_{(1,2,3),B}(\theta,v)\mathcal{R}_{A,B}(u,v)w\\ &\quad= \mathcal{R}_{A,B}(u,v)\mathcal{R}_{(1,2,3),B}(\theta,v)\mathcal{R}_{(1,2,3),A}(\theta,u), \qquad (4.22)\end{aligned}$$

where $A=(4,5,6)$ and $B=(7,8,9)$ stand for additional two triplets of auxiliary spaces. Relation Eq. (4.22) can be checked by direct substitution of the definitions above, and making use of the RLL relations Eq. (3.3) and YB relations Eq. (3.4) applied to the R-matrix in question.

Then we a construct a transfer matrix for our chain after grouping together triplets of physical spaces. The precise

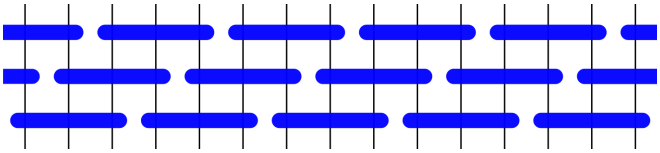

FIG. 12. A tightly packed quantum circuit with three-site gates. This network has periodicity 3 in both the space and time directions. Accordingly, we can prove the existence of commuting transfer matrices built from three rows.

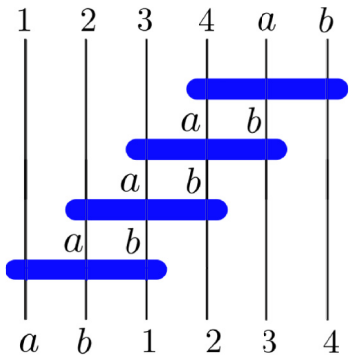

FIG. 13. Graphical interpretation of diagonal to diagonal transfer matrices, which are identical to those defined in Eq. (3.35), but drawn simply in a different arrangement, compare also with Fig. 5. This transfer matrix can also be used to build the circuit shown in 12, this was first worked out in Ref. [84].

formula with auxiliary space $A=(a,b,c)$ reads

$$\begin{aligned}t(u) = \mathrm{tr}_A[&\mathcal{R}_{(1,2,3),A}(\theta,u)\mathcal{R}_{(4,5,6),A}(\theta,u)\ldots\\ &\times\mathcal{R}_{(L-5,L-4,L-3),A}(\theta,u)\mathcal{R}_{(L-2,L-1,L),A}(\theta,u)]. \qquad (4.23)\end{aligned}$$

Note that the relative ordering of the physical triplets is such that we proceed backwards on the chain, as in Eq. (3.10). This is due to certain technical details, so that in the end we can obtain the desired quantum circuit.

These transfer matrices commute, if we regard θ as a fixed parameter. The special point $u=\theta$ gives the translation operator by three sites:

$$t(\theta) = \mathcal{U}^{-3}. \qquad (4.24)$$

The other special point is obtained by setting $u=0$. In this case we get

$$t(\theta)^{-1}t(0) = \mathcal{V}_3\mathcal{V}_2\mathcal{V}_1, \qquad (4.25)$$

where the equal time update steps $\mathcal{V}_j$ are defined by

$$\mathcal{V}_j = \prod_k U^{(3)}(3k+j), \quad U^{(3)}(j) = \check{\mathcal{L}}_{j,j+1,j+2}(\theta). \qquad (4.26)$$

For the proof of the initial condition Eq. (4.25) we need to use the factorization condition Eq. (3.29) which eventually leads to

$$\check{\mathcal{R}}_{1,2,3,4,5}(\theta,0) = \check{\mathcal{L}}_{3,4,5}(\theta)\check{\mathcal{L}}_{2,3,4}(\theta)\check{\mathcal{L}}_{1,2,3}(\theta), \qquad (4.27)$$

where we also used the initial condition $\check{\mathcal{L}}_{1,2,3}(0)=1$. A graphical interpretation of this equation (applied for the six-site object $\mathcal{R}_{1,2,3,4,5,6}$) is given in Fig 14. Multiplying the operators thus obtained, together with the permutations introduced in Eq. (4.21) will eventually lead to Eq. (4.25). A graphical proof is shown on Fig. 15.

V. INTERACTION-ROUND-A-FACE TYPE MODELS

In this section we study the IRF type models. Our motivations come from recent results in the literature about elementary cellular automata, see the discussion in Sec. II G. It is our goal to embed these models into the algebraic framework of medium-range models. We will see that the special

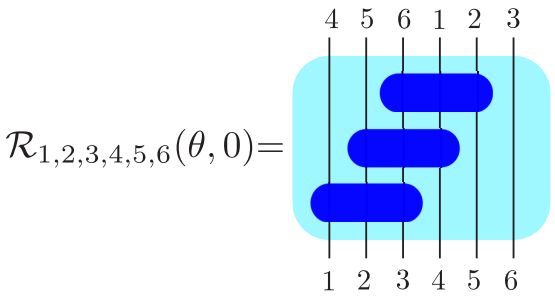

FIG. 14. Graphical representation for the factorization of $\mathcal{R}_{1,2,3,4,5,6}(\theta,0)$ into the three-site gates given by $\mathcal{L}(\theta)$. Note that the last vector space is also involved in the permutations, which is necessary in order to build the desired transfer matrix.

structure of these models leads to unique constructions for the quantum circuits, and also to the discovery of new algebraic structures that are connected to the "face weight formulation" of the Yang-Baxter relation.

We are looking for three-site integrable models where the Lax operator has the special form

$$\check{\mathcal{L}}_{j,j+1,j+2}(u)=\sum_{a,b=0,1}P_j^a f_{j+1}^{ab}(u)P_{j+2}^b, \tag{5.1}$$

where $f^{ab}(u)$ is a collection of four u-dependent matrices. Such Lax operators will be used to build quantum circuits: they will play the role of the three-site unitaries $U^{(3)}(j)$. The assumption Eq. (5.1) leads to unique algebraic constructions and quantum circuits, which would be meaningless without the special structure of the Lax operator.

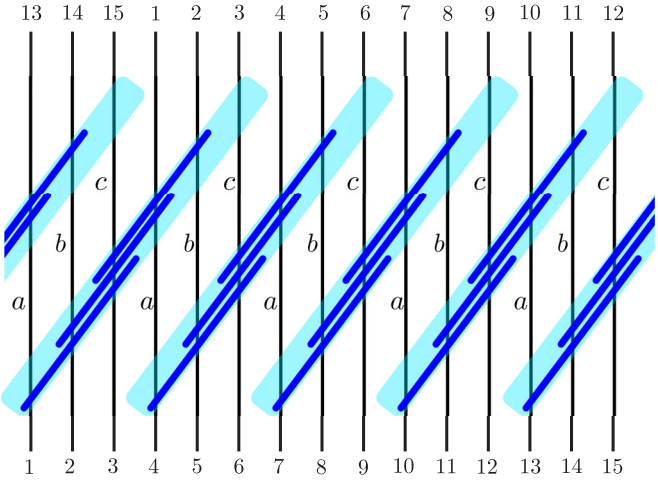

FIG. 15. Graphical proof of Eq. (4.25). The labels (a, b, c) stand for the triplet of auxiliary spaces which are present in the definition Eq. (4.23). The big lightly shaded rectangles stand for the action of the $\mathcal{R}$ operators. Within each big rectangle we denoted the factorization into the product of $\mathcal{L}$ operators, as shown in Fig. 14. Then the quantum circuit of Fig. 12 is obtained by "straightening out" the angles of the three-site gates, noticing that they perfectly fit together to build the tightly packed circuit. Notice that this circuit also inlcudes a translation by three sites, which is canceled by $t^{-1}(\theta)=\mathcal{U}^3$ in Eq. (4.25).

Later in Sec. V C we perform a classification of such models, and in Sec. V D we also discuss the concrete cases that eventually lead to the elementary cellular automata.

A. Integrability structures

In general we have R- and Lax-matrices which satisfy the RLL relation which we now write in the form

$$\check{R}_{23,45}(u,v)\check{\mathcal{L}}_{123}(u)\check{\mathcal{L}}_{345}(v)=\check{\mathcal{L}}_{123}(v)\check{\mathcal{L}}_{345}(u)\check{R}_{12,34}(u,v). \tag{5.2}$$

It follows from Eq. (5.1) that now the Lax-operators satisfy an extra condition

$$[\check{\mathcal{L}}_{123}(u),\check{\mathcal{L}}_{345}(v)]=0. \tag{5.3}$$

Using this requirement the RLL relation reads as

$$\check{\mathcal{L}}_{345}(u)^{-1}\check{R}_{23,45}(u,v)\check{\mathcal{L}}_{345}(v)=\check{\mathcal{L}}_{123}(v)\check{R}_{12,34}(u,v)\check{\mathcal{L}}_{123}(u)^{-1}. \tag{5.4}$$

We can see that the (left-hand side) l.h.s. and the (right-hand side) r.h.s. act trivially on the spaces 1 and 5, respectively, therefore they have to be equal to a three-site operator which we denote as $\check{\mathcal{G}}_{234}$. Thus, we find

$$\check{\mathcal{G}}_{234}(u,v)=\check{\mathcal{L}}_{345}(u)^{-1}\check{R}_{23,45}(u,v)\check{\mathcal{L}}_{345}(v), \tag{5.5}$$

$$\check{\mathcal{G}}_{234}(u,v)=\check{\mathcal{L}}_{123}(v)\check{R}_{12,34}(u,v)\check{\mathcal{L}}_{123}(u)^{-1}. \tag{5.6}$$

We can express the R-matrices with $\mathcal{G}$ and $\mathcal{L}$ in two ways:

$$\check{R}_{12,34}(u,v)=\check{\mathcal{L}}_{123}(v)^{-1}\check{\mathcal{G}}_{234}(u,v)\check{\mathcal{L}}_{123}(u), \tag{5.7}$$

$$\check{R}_{23,45}(u,v)=\check{\mathcal{L}}_{345}(u)\check{\mathcal{G}}_{234}(u,v)\check{\mathcal{L}}_{345}(v)^{-1}, \tag{5.8}$$

or equivalently

$$\check{R}_{12,34}(u,v)=\check{\mathcal{L}}_{234}(u)\check{\mathcal{G}}_{123}(u,v)\check{\mathcal{L}}_{234}(v)^{-1}. \tag{5.9}$$

The consistency of the two expressions for the R-matrix leads to the equation

$$\check{\mathcal{G}}_{234}(u,v)\check{\mathcal{L}}_{123}(u)\check{\mathcal{L}}_{234}(v)=\check{\mathcal{L}}_{123}(v)\check{\mathcal{L}}_{234}(u)\check{\mathcal{G}}_{123}(u,v). \tag{5.10}$$

This relation is similar to Eq. (5.2), but there are important differences: Here the supports for the Lax operators overlap at two spaces at both the l.h.s. and the r.h.s., whereas in Eq. (5.2) they overlap only at a single space. We call this equation the GLL relation. Below we show that it is equivalent to the "face weight" formulation of the RLL relation.

We can easily calculate this G-operator at special values of spectral parameters. Using the regularity of the R-matrix and Eq. (5.5) we get

$$\check{\mathcal{G}}_{123}(v,v)=1. \tag{5.11}$$

Using the factorization of the R-matrix and Eqs. (5.9) and (5.7) we obtain that

$$\check{\mathcal{G}}_{123}(u,0)=\check{\mathcal{L}}_{123}(u), \tag{5.12}$$

$$\check{\mathcal{G}}_{123}(0,v)=\check{\mathcal{L}}_{123}(v)^{-1}. \tag{5.13}$$

From Eq. (5.5) we can also derive the inversion property of the G-operator

$$\check{\mathcal{G}}_{123}(u,v)\check{\mathcal{G}}_{123}(v,u)=1. \tag{5.14}$$

Equations (5.9), (5.7), (5.5), and (5.6) imply that the R- and G-operators act diagonally on the first and last sites.

We also know that the R-matrix satisfies the YB equation

$$\begin{aligned}&\check{R}_{34,56}(u_1,u_2)\check{R}_{12,34}(u_1,u_3)\check{R}_{34,56}(u_2,u_3)\\&\quad=\check{R}_{12,34}(u_2,u_3)\check{R}_{34,56}(u_1,u_3)\check{R}_{12,34}(u_1,u_2).\end{aligned} \tag{5.15}$$

Substituting Eqs. (5.9) and (5.7) we can easily show that the G-operator also satisfies a YB type equation

$$\begin{aligned}&\check{\mathcal{G}}_{234}(u_1,u_2)\check{\mathcal{G}}_{123}(u_1,u_3)\check{\mathcal{G}}_{234}(u_2,u_3)\\&\quad=\check{\mathcal{G}}_{123}(u_2,u_3)\check{\mathcal{G}}_{234}(u_1,u_3)\check{\mathcal{G}}_{123}(u_1,u_2).\end{aligned} \tag{5.16}$$

Below we show that this is equivalent to the "face weight" formulation of the Yang-Baxter relation.

To see this we introduce a new notation for the Lax operator, by making use of its special form:

$$\check{\mathcal{L}}(u)=\sum_{i,j,k,l}M^{il}_{kj}(u)P_i\otimes E^l_k\otimes P_j. \tag{5.17}$$

Assuming that the G-operator has a similar form we write it as

$$\check{\mathcal{G}}(u,v)=\sum_{a,b,c,d}(g_{bc})^a_d(u,v)P_a\otimes E^c_b\otimes P_d. \tag{5.18}$$

Then the GLL relation is expressed as

$$\begin{aligned}&\sum_s(g_{bs})^i_r(u,v)M^{il}_{sj}(u)M^{sj}_{rq}(v)\\&\quad=\sum_s M^{il}_{bs}(v)M^{bs}_{rq}(u)(g_{sj})^l_q(u,v),\end{aligned} \tag{5.19}$$

which is a relation used in Ref. [79]. This connection will be discussed further in Sec. V E.

B. Quantum circuits

Let us now focus on the quantum circuits. We intend to build brickwork circuits which can accommodate the elementary cellular automata. It is clear that the constructions discussed in Sec. IV are not appropriate for this purpose, because there the local unitaries are too far away from each other. Instead, we need to build "tightly packed" quantum circuits where every pair of neighboring quantum gates is overlapping at the common control bit. This will enable us to treat some of the elementary cellular automata discussed in Sec. II G.

Motivated by the discussion in Sec. II G we build a Floquet-type time evolution operator as

$$\mathcal{V}=\mathcal{V}_2\mathcal{V}_1, \tag{5.20}$$

where the operators $\mathcal{V}_{1,2}$ are built from three-site unitaries that we choose as

$$U^{(3)}(j)=\check{\mathcal{L}}_{j,j+1,j+2}(\theta). \tag{5.21}$$

The number θ will be a fixed parameter of the quantum circuit.

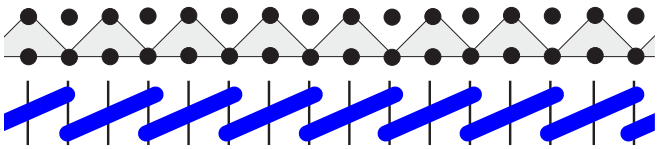

FIG. 16. Lax representation of the time evaluation operator $\mathcal{V}_2$.

The update steps are then given by

$$\begin{aligned}\mathcal{V}_1&=\check{\mathcal{L}}_{1,2,3}(\theta)\check{\mathcal{L}}_{3,4,5}(\theta)\ldots\check{\mathcal{L}}_{L-3,L-2,L-1}(\theta)\check{\mathcal{L}}_{L-1,L,1}(\theta),\\\mathcal{V}_2&=\check{\mathcal{L}}_{2,3,4}(\theta)\check{\mathcal{L}}_{4,5,6}(\theta)\ldots\check{\mathcal{L}}_{L-2,L-1,L}(\theta)\check{\mathcal{L}}_{L,1,2}(\theta).\end{aligned} \tag{5.22}$$

Notice that every pair of neighboring Lax operators overlaps at a common site. For a graphical interpretation see see Fig. 16.

The complete Floquet time step can be expressed alternatively as

$$\begin{aligned}\mathcal{V}=&\mathcal{U}^2\mathrm{tr}_{ab}[\mathcal{L}_{1,2,b}\mathcal{L}_{1,2,a}\mathcal{L}_{3,4,b}\mathcal{L}_{3,4,a}\ldots\\&\times\mathcal{L}_{L-3,L-2,b}\mathcal{L}_{L-3,L-2,a}\mathcal{L}_{L-1,L,b}\mathcal{L}_{L-1,L,a}].\end{aligned} \tag{5.23}$$

For simplicity we suppressed the dependence on θ. For a graphical proof of the rewriting see Fig. 17.

We can now use the factorization of the R-matrix, which we write in the form

$$R_{(12),(34)}(\theta,0)=\mathcal{L}_{1,2,4}(\theta)\mathcal{L}_{1,2,3}(\theta). \tag{5.24}$$

Using this relation we can express the Floquet update step as

$$\begin{aligned}\mathcal{V}=&\mathcal{U}^2\mathrm{tr}_A[R_{(1,2),A}(\theta,0)R_{(3,4),A}(\theta,0)\ldots\\&\times R_{(L-3,L-2),A}(\theta,0)R_{(L-1,L),A}(\theta,0)],\end{aligned} \tag{5.25}$$

where $A=(a,b)$ stands for a pair of auxiliary spaces. Defining the transfer matrix

$$\begin{aligned}t(u)=&\mathrm{tr}_A[R_{(1,2),A}(\theta,u)R_{(3,4),A}(\theta,u)\ldots\\&\times R_{(L-3,L-2),A}(\theta,u)R_{(L-1,L),A}(\theta,u)]\end{aligned} \tag{5.26}$$

we obtain that

$$\mathcal{V}=t(\theta)^{-1}t(0), \tag{5.27}$$

where we used that

$$t(\theta)=\mathcal{U}^{-2}. \tag{5.28}$$

The transfer matrices Eq. (5.26) form a commuting family:

$$[t(u),t(v)]=0. \tag{5.29}$$

The variable θ plays the role of an inhomogeneity parameter for this commuting family. Note that Eq. (5.26) is a generalization of Eq. (3.10) and not of Eq. (3.9).

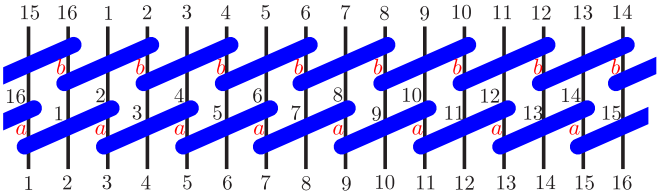

FIG. 17. Lax representation of the time evaluation operator $\mathcal{V}_2\mathcal{V}_1$.

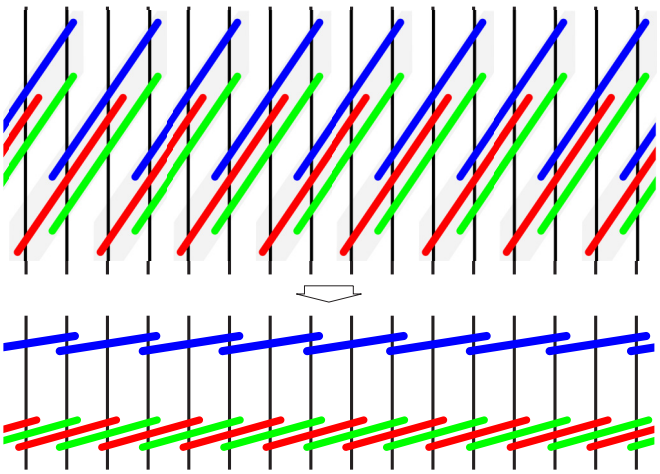

FIG. 18. Graphical illustration of the transfer matrix Eq. (5.26). The blue, red and green boxes are the operators $\check{\mathcal{L}}(\theta)$, $\check{\mathcal{G}}(\theta,u)$ and $\check{\mathcal{L}}(u)^{-1}$, respectively. We use the commutativity Eq. (5.3) to separate the action of the upper (blue) layer of gates. However, the lower layer cannot be simplified further, because there the consecutive operators overlap at two sites each.

We can also define the rapidity-dependent update rule

$$\mathcal{V}(u) = t(\theta)^{-1}t(u). \tag{5.30}$$

Clearly, these operators commute with each other, and thus they commute also with the "physical" update step which is obtained at $u = 0$.

The operators $\mathcal{V}(u)$ are nonlocal for generic u. However, similar to the case of a standard transfer matrix they lead to extensive and local charges. The initial condition $\mathcal{V}(\theta) = 1$ and the definition of the transfer matrix $t(u)$ lead to the extensive four-site operator

$$Q_4' = \partial_u \mathcal{V}(u)|_{u=\theta}. \tag{5.31}$$

The transfer matrix is only two-site invariant, which is inherited by Q_4', similar to the update rule $\mathcal{V}$ which is not translationally invariant either.

Higher charges could be obtained from the derivative of the logarithm of the transfer matrix, or with the boost operator method [97] applied to transfer matrix Eq. (5.26).

Simplified formulas for the transfer matrix can be obtained using the $\check{\mathcal{G}}$ operators introduced above. We substitute the expression

$$\check{R}_{12,34}(\theta,u) = \check{\mathcal{L}}_{234}(\theta)\check{\mathcal{G}}_{123}(\theta,u)\check{\mathcal{L}}_{234}(u)^{-1} \tag{5.32}$$

into the definition Eq. (5.26). This substitution is depicted pictorially in the top of Fig. 18. We can see here that the transfer matrix can be written as

$$t(u) = \mathcal{V}_2\tilde{t}(u), \tag{5.33}$$

where

$$\tilde{t}(u) = \mathrm{tr}_{a,b}[\mathcal{G}_{1,a,b}(\theta,u)\mathcal{L}_{2,a,b}(u)^{-1}\mathcal{G}_{3,a,b}(\theta,u)\mathcal{L}_{4,a,b}(u)^{-1}\dots \times \mathcal{G}_{L-1,a,b}(\theta,u)\mathcal{L}_{L,a,b}(u)^{-1}]. \tag{5.34}$$

For this rewriting we used again the fact that the $\check{\mathcal{L}}$ operators commute if they share a control bit.

The operator $\tilde{t}(u)$ is completely identical to the transfer matrices defined in Ref. [79], which can be seen after proper identifications are made. To this aim we need to use the representations Eqs. (5.17) and (5.18) for the $\check{\mathcal{L}}$ and $\check{\mathcal{G}}$ matrices. After substitution we obtain a formula identical to the one presented in Ref. [79]; see Eq. (5.66).

Our derivation in this subsection assumed the regularity condition for the R-matrix, which leads to the factorization Eq. (5.24). However, an alternative derivation is also possible, without this assumption. We could start with the definition Eq. (5.26) for a proper R-matrix, and we then could still derive the alternative form Eq. (5.33). In concrete cases it could be shown that this transfer matrix is related to cellular automata. Such a derivation would completely bypass the requirement of the regularity. However, in this work we are interested in cases which yield local conserved charges. Furthermore, we found that if the regularity condition does not hold then the concrete models do not have more conserved charges at all, see the example of the Rule54 model in Sec. V E. Therefore, we do not discuss solutions without the regularity condition.

C. Partial classification

Here we perform a partial classification of three-site models, where the Lax operators have the special structure Eq. (5.1). The methods for the classification are essentially the same as in Sec. III. We are looking for Lax operators satisfying the RLL relations, and we perform a classification based on the Hamiltonian densities that are derived from the Lax operators: we apply the generalized Reshetikhin condition to find the integrable cases.

It is important the Hamiltonians that we find this way don't commute with the transfer matrices defined in the previous subsection, because the transfer matrices involve the inhomogeneities as well. The Hamiltonians only commute with homogeneous transfer matrices as defined in Eq. (3.24). However, we can also regard the Hamiltonians we find below as new integrable models on their own right.

It follows from the Ansatz Eq. (5.1) and the derivation rule Eq. (3.40) that the Hamiltonians in question have the structure given by Eq. (3.53) with the action matrices being

$$h^{ab} = \partial_u f^{ab}(u)\big|_{u=0}. \tag{5.35}$$

Therefore, we need to classify three-site Hamiltonians with the particular structure given by Eq. (3.53), where the outer two spins act as control bits, and the middle spin is an action bit. For this special class of models we assume that the inversion relation Eq. (3.19) holds, therefore we exclude the possibility of having a nonzero $\tilde{h}_{j,j+1,j+2}$ in the construction of Q_5, see Eq. (2.10).

The Ansatz Eq. (3.53) has a total number of 16 real parameters, because there are four g-matrices which are Hermitian. Subtracting the identity component and performing a $U(1)$ rotation the number of parameters could be narrowed down to 14. However, we found this parameter space to be too big for a first classification attempt. Instead, we selected an even more restricted Ansatz given explicitly by

$$h_{123} = A\sigma_2^x + B\sigma_2^z + C\sigma_1^z\sigma_2^x + D\sigma_2^x\sigma_3^z + E\sigma_1^z\sigma_2^z\sigma_3^z + F\sigma_1^z\sigma_2^x\sigma_3^z + G\sigma_1^z\sigma_3^z. \tag{5.36}$$

Apart from an overall multiplicative normalization this Ansatz has six free parameters, which makes the classification of integrable cases relatively easy. A Hermitian operator is obtained if all parameters are real, and in this case all matrix elements are real in the computational basis.

Within this parameter space we found three nontrivial integrable models. Now we list these models together with a brief discussion of their main properties. Their application as quantum gate models and classical cellular automata is discussed later in Sec. V D; here we focus on their properties as integrable Hamiltonians.

We argue that two of the models can be related to nearest-neighbor chains by a bond-site transformation. This transformation was used recently in Refs. [54,84] and it is explained in detail in Appendix B.

1. The bond-site transformed XYZ model

In this case the Hamiltonian density is written in the compact form

$$h_{123} = J_x\sigma_2^x - J_y\sigma_1^z\sigma_2^x\sigma_3^z + J_z\sigma_1^z\sigma_3^z. \tag{5.37}$$

This model can be seen as the bond-site transformed version of the XYZ model (we suggest to call it the $bXYZ$ model). The Hamiltonian satisfies the requirements of the bond-site transformation discussed in Appendix B: it is spin reflection invariant and the first and last bits are control bits. Using Eqs. (B2) for the transformation of the operators we see immediately that in the bond picture the model becomes identical to the XYZ model with the couplings as given above. Thus, it describes interacting dynamics of domain walls (DW), where the creation and annihilation of pairs of DW's is also allowed.

A special point of the model is when $J_x = J_y$, which becomes the bond-site transformation of the XXZ model. In this case the Hamiltonian commutes with the $U(1)$-charge

$$Q_2 = \sum_j \sigma_j^z\sigma_{j+1}^z, \tag{5.38}$$

which is interpreted as the domain wall number, which is conserved. This model was already presented in Refs. [56,105].

An other special case is when $J_y = 0$. In this case the model describes two decoupled quantum Ising chains on the even and odd sublattices, such that the parameter J_x can be interpreted as a magnetic field. Switching on $J_y \neq 0$ we obtain a Bariev-type coupling between the two sublattices, therefore we could also call this system the Bariev-Ising model.

The Lax operator is found using the known solution for the XYZ model and the bond-site transformation:

$$\begin{aligned}\check{\mathcal{L}}_{1,2,3}(u) = {}& \frac{1}{2}\frac{\mathrm{sn}(\eta) + \mathrm{sn}(u)\sigma_2^x}{\mathrm{sn}(\eta) + \mathrm{sn}(u)}\left(1 - \sigma_1^z\sigma_3^z\right) \\ & + \frac{1}{2}\frac{\mathrm{sn}(u+\eta) + k\,\mathrm{sn}(\eta)\mathrm{sn}(u)\mathrm{sn}(u+\eta)\sigma_2^x}{\mathrm{sn}(\eta) + \mathrm{sn}(u)} \\ & \times \left(1 + \sigma_1^z\sigma_3^z\right),\end{aligned} \tag{5.39}$$

where $\mathrm{sn}(u) = \mathrm{sn}(u;k)$ and

$$\frac{J_y}{J_x} = \frac{1 - k\mathrm{sn}^2(\eta)}{1 + k\mathrm{sn}^2(\eta)} \quad \frac{J_z}{J_x} = \frac{\mathrm{cn}(\eta)\mathrm{dn}(\eta)}{1 + k\mathrm{sn}^2(\eta)}. \tag{5.40}$$

This Lax operator satisfies the inversion relation Eq. (3.49),

$$\check{\mathcal{L}}_{1,2,3}(u)\check{\mathcal{L}}_{1,2,3}(-u) = 1. \tag{5.41}$$

In this model the G-operator can be obtained from the Lax operator in a very natural way,

$$\check{\mathcal{G}}_{123}(u, v) = \check{\mathcal{L}}_{123}(u - v). \tag{5.42}$$

Taking $k \to 0$ we obtain the XXZ limit of the model

$$\begin{aligned}\check{\mathcal{L}}_{1,2,3}(u) = {}& (P_1^\circ P_3^\circ + P_1^\bullet P_3^\bullet)\frac{\sin(u+\eta)}{\sin(u) + \sin(\eta)} \\ & + (P_1^\circ P_3^\bullet + P_1^\bullet P_3^\circ)\frac{\sin(u)\sigma_2^x + \sin(\eta)}{\sin(u) + \sin(\eta)}.\end{aligned} \tag{5.43}$$

We can also take the XXX limit as $\eta \to 0$ and $u = \eta v$. We obtain the following Lax matrix

$$\begin{aligned}\check{\mathcal{L}}_{1,2,3}(v) = {}& (P_1^\circ P_3^\circ + P_1^\bullet P_3^\bullet) \\ & + (P_1^\circ P_3^\bullet + P_1^\bullet P_3^\circ)\frac{v\sigma_2^x + 1}{v + 1}.\end{aligned} \tag{5.44}$$

2. Twisted XX model with n.n.n. coupling

In this model the Hamiltonian density is

$$h_{123} = \sigma_1^z\sigma_2^x + \kappa\sigma_2^x\sigma_3^z + G\sigma_1^z\sigma_3^z. \tag{5.45}$$

These are actually two different models depending on the sign $\kappa = \pm 1$; the real parameter G is a coupling constant. The form of the Hamiltonian density respects the Ansatz Eq. (5.36), but perhaps a more familiar way of writing the global Hamiltonian is

$$H = \sum_j \sigma_j^x\sigma_{j+1}^y \pm \sigma_j^y\sigma_{j+1}^x + G\sigma_j^x\sigma_{j+2}^x. \tag{5.46}$$

Here we performed a rotation such that the Pauli matrices are cyclically exchanged as $\sigma^x \to \sigma^y \to \sigma^z$. In the case of a minus sign we can further express this as

$$H = \sum_j 2i(\sigma_j^+\sigma_{j+1}^- - \sigma_j^-\sigma_{j+1}^+) + G\sigma_j^x\sigma_{j+2}^x, \tag{5.47}$$

which can be interpreted as a twisted XX model with a next-to-nearest-neighbor interaction term.

In the case of a plus sign in Eq. (5.45) we do not get such an interpretation.

An alternative interpretation of the model is found by performing a bond-site transformation. First we perform a transformation $\sigma^x \leftrightarrow \sigma^y$ so that the Hamiltonian density becomes

$$h_{123} = \sigma_1^z\sigma_2^y + \kappa\sigma_2^y\sigma_3^z + G\sigma_1^z\sigma_3^z. \tag{5.48}$$

This operator is spin-flip invariant, therefore we can apply the bond-site transformation discussed in Sec. B. Then we obtain a two site interacting model with Hamiltonian density

$$h_{12} = \sigma_1^y\sigma_2^x + \kappa\sigma_1^x\sigma_2^y + G\sigma_1^z\sigma_2^z. \tag{5.49}$$

If $\kappa = -1$, then the original Hamiltonian commutes with the $U(1)$-charge given by Eq. (5.38), and the model defined by Eq. (5.49) commutes with the global S^z operator. In fact, this case can be interpreted as the XXZ model with a homogeneous twist, where the kinetic term is the Dzyaloshinskii-Moriya interaction term. Thus, the model describes the interacting dynamics of the domain walls, with a twisted kinetic term.

For the model with $\kappa = 1$ we did not find a translationally invariant $U(1)$-charge, and the kinetic term describes the creation and annihilation of pairs of domain walls.

We found the Lax operator for both models. It is given by

$$\check{\mathcal{L}}_{123}(u) = G\frac{e^{2u}-1}{(e^u-1)^2-4G^2} \times \left(\frac{2G\kappa}{e^u-1} + \left(\sigma_1^z\sigma_2^x + \kappa\sigma_2^x\sigma_3^z\right) + \frac{e^u-1+2G^2}{G(e^u+1)}\sigma_1^z\sigma_3^z\right). \tag{5.50}$$

Relation Eq. (3.49) holds with this parametrization. This operator is unitary if u is purely imaginary.

The G-operator (which immediately gives the R-matrix as well) reads as

$$\check{\mathcal{G}}_{123}(u,v) = \kappa\frac{(4G^2-1)e^v - e^u + e^ue^v + 1}{2G(e^u-e^v)} + \left(\sigma_1^z\sigma_2^x + \kappa\sigma_2^x\sigma_3^z\right) + G\frac{(4G^2-3)e^v + e^u + e^ue^v + 1}{(2G^2-1)(e^u+e^v)+e^ue^v+1}\sigma_1^z\sigma_3^z. \tag{5.51}$$

Substituting the special point $G = 1$ we get

$$\check{\mathcal{L}}_{123}(u) = \frac{e^u-1}{e^u-3} \times \left(\frac{2\kappa}{e^u-1} + \left(\sigma_1^z\sigma_2^x + \kappa\sigma_2^x\sigma_3^z\right) + \sigma_1^z\sigma_3^z\right). \tag{5.52}$$

A special point is $u = i\pi$, at which the unitary operator becomes deterministic; this will lead to an elementary cellular automata, see Sec. V D below.

3. *Integrable deformation of the PXP model*

This model has no free parameters, just a sign $\kappa = \pm 1$:

$$h_{123} = \sigma_2^x + \kappa\left(\sigma_1^z\sigma_2^x + \sigma_2^x\sigma_3^z\right) + \sqrt{2}\sigma_1^z\sigma_2^z\sigma_3^z - \sigma_1^z\sigma_2^x\sigma_3^z. \tag{5.53}$$

In the case of $\kappa = 1$ the Hamiltonian density can be expressed as

$$h_{123} = -4P_1^\bullet\sigma_2^xP_3^\bullet + 2\sigma_2^x + \sqrt{2}\sigma_1^z\sigma_2^z\sigma_3^z, \tag{5.54}$$

while for $\kappa = -1$ we would obtain a similar model with $P^\bullet$ replaced by P°. These models can be seen as an integrable deformation of the PXP model [106]. However, if we remain in the parameter space of our Ansatz, then there is no free parameter, so we cannot tune the "operator distance" from the PXP Hamiltonian.

It is likely that the models Eq. (5.53) are just particular cases of a continuous family of models which stretches outside our Ansatz. We leave the exploration of the bigger parameter space to future works.

For this model we find the Lax operator

$$\check{\mathcal{L}}_{123}(u) = \frac{1+uh_{123}}{1+\sqrt{6}u}. \tag{5.55}$$

Simple computation shows that

$$(h_{123})^2 = 6. \tag{5.56}$$

This implies that Eq. (3.49) is satisfied. In this case a unitary gate is obtained for u being purely imaginary.

For this specific model we did not find a bond-site transformation, which would make it locally equivalent to a n.n. chain.

D. Elementary cellular automata

The construction of Sec. V A can be applied for every IRF type three-site model treated in Sec. V C: in this way we obtain families of quantum cellular automata with varying numbers of free parameters. All of these models are Yang-Baxter integrable. Now we are looking for specific cases that can accommodate the elementary cellular automata discussed in Sec. II G.

First we consider the $bXYZ$ model Eq. (5.37) at the special point $J_x = J_y = J_z$, in which case the Lax operator is given by Eq. (5.44). Taking the $v \to \infty$ limit we obtain the three-site unitary

$$U^{(3)}(1) = (P_1^\bullet P_3^\circ + P_1^\circ P_3^\bullet)\sigma_2^x + P_1^\bullet P_3^\bullet + P_1^\circ P_3^\circ. \tag{5.57}$$

We recognize that this is the update rule for the classical Rule150 model given by Eq. (2.21). Thus, we obtained a Yang-Baxter integrable three parameter family of quantum cellular automata (with the parameters being J_y/J_x, J_z/J_x and v, or alternatively k, η, and v), which includes the Rule150 model at special points. At this special point the first nontrivial local conserved charge is

$$Q_4' = \sum_j \sigma_{2j}^x\sigma_{2j+1}^x + \sigma_{2j-1}^z\sigma_{2j}^y\sigma_{2j+1}^y\sigma_{2j+2}^z + \sigma_{2j-1}^z\sigma_{2j}^z\sigma_{2j+1}^z\sigma_{2j+2}^z. \tag{5.58}$$

Let us now perform the bond-site transformation of Appendix B directly on the quantum cellular automata. In the bond picture we obtain two-site gates that are given directly by the R-matrices of the XXX, XXZ and XYZ models. In the XXZ case the two-site gate is given by Eq. (4.11), unitary time evolution is obtained if $\eta \in \mathbb{R}$ and $v \in i\mathbb{R}$ or vice versa. The classical Rule150 model is obtained after taking the special limits $\eta \to 0$ and $v \to \infty$, in which case the R-matrix Eq. (4.11) becomes a permutation operator (swap gate). This implies that the Rule150 model describes free movement of domain walls. The XXZ version can be seen as an interacting deformation where the total number of DW's is conserved. Finally, the XYZ case is the most general model in this family, where domain walls can be created or annihilated in pairs.

Let us also consider the Model of Sec. V C 2 with the sign $\kappa = 1$ and the coupling constant $G = 1$, for which the Lax operator and thus the three-site unitary is given by Eq. (5.52). Further substituting $u = i\pi$ we obtain

$$U^{(3)}(1) = \tfrac{1}{2}\left(-1 + \sigma_1^z\sigma_2^x + \sigma_2^x\sigma_3^z + \sigma_1^z\sigma_3^z\right), \tag{5.59}$$

This is also a deterministic quantum gate, which gives the f matrices

$$f^{00} = -f^{11} = \sigma^x, \quad f^{01} = f^{10} = -1. \tag{5.60}$$

We can see that apart from simple signs these f-matrices are equal to those of the Rule105 model given by Eq. (2.20). As already argued in Ref. [84], if the quantum gates are deterministic, then the phases are irrelevant for the simulation of a classical cellular automata. Thus, the two-parameter family of quantum gates Eq. (5.52) can be considered as a deformation

of the actual Rule105 model, which is included at the special point $G = 1$ and $u = i\pi$.

For this model and the specific values $G = 1$ and $u = i\pi$ the definition Eq. (5.31) gives the local conserved charge

$$Q'_4 = \sum_j \sigma^y_{2j}\sigma^y_{2j+1} + \sigma^z_{2j-1}\sigma^x_{2j}\sigma^x_{2j+1}\sigma^z_{2j+2} + \sigma^z_{2j-1}\sigma^z_{2j}\sigma^z_{2j+1}\sigma^z_{2j+2}. \tag{5.61}$$

Performing the transformation $\sigma^x \leftrightarrow \sigma^y$ mentioned above we obtain the same charge as in Eq. (5.58).

The charges Eqs. (5.58) and (5.61) commute with the time evolution of the update rules given by Eqs. (2.21) and (5.60), respectively. The update rules are deterministic, therefore if we choose a "classical" initial state (an element of the computational basis) then it will stay classical. This also means that for the classical time evolution we can disregard the the σ^x and σ^y operators, because their mean values in the classical states are zero. This leads to the following classical charge for the Rule105 and Rule150 models:

$$Q_4^{(cl)} = \sum_j \sigma^z_{2j-1}\sigma^z_{2j}\sigma^z_{2j+1}\sigma^z_{2j+2}. \tag{5.62}$$

This charge is conserved by both classical cellular automata. Taking further derivatives of the logarithm of the transfer matrix we could obtain further quantum and classical charges for these models. If we consider the quantum models, then the relative signs in Eq. (5.60) have to be taken into account. So far we have not yet found a quantum model which would describe the Rule105 model without these signs, but this could be just a limitation of our Ansatz Eq. (5.36).

Regarding the Rule54 and Rule201 models we did not find any three-site Hamiltonian, which would lead to Lax operators and transfer matrices that would actually accommodate these classical cellular automata. This is in accordance with the findings of Ref. [79]. Regarding the Rule54 model it was claimed in Ref. [79] that there are no translationally invariant local charges up to interaction range $\ell = 5$. This clearly shows that for the Rule54 model we cannot have a Lax operator acting on three sites, because it would give a translationally invariant charge Q'_4 with range $\ell = 4$. The alerted reader might object that our Q'_4 derived in Eq. (5.31) is invariant with respect to a two site shift only. However, in the case of these cellular automata we also have the inversion relations Eq. (2.29) which implies that the two-site invariant charge Q'_4 commuting with $\mathcal{V}_2\mathcal{V}_1$ has to commute with $\mathcal{V}_1\mathcal{V}_2$ as well, leading eventually to a translationally invariant version of Q'_4 commuting with both $\mathcal{V}_2\mathcal{V}_1$ and $\mathcal{V}_1\mathcal{V}_2$. Altogether we reach the Conclusion that the Rule54 model is not Yang-Baxter integrable with three-site interactions.

In Sec. V E below we also analyze the recent construction of Ref. [79] for these models, and we reach the same conclusion: the transfer matrices built in Ref. [79] only have a diagonal dressing using a known charge and thus do not lead to extra conserved charges.

However, it is known that there is a local conserved charge for the Rule54 model with interaction range $\ell = 6$: it is the Hamiltonian derived in Ref. [77]. This suggests that perhaps the true algebraic background for the model lies within the family of 6-site interacting models. We return to this question in the Discussions (Sec. VII).

E. Discussion of the results of Ref. [79] for the IRF models

Recently an algebraic framework for the integrability of the Rule54 and related models was proposed in Ref. [79]. Here we review this construction, we point out connections with our results, and we also disprove some of the conjectures made in Ref. [79].

Let us start with a brief discussion of integrable 2D statistical physical models. There are three different sorts of commonly used models: spin models, vertex models, and interaction round a face (IRF) models. Accordingly, there are three different types of Yang-Baxter equations, one for each family. The different formulations can always be transformed into each other, although this might not be convenient and it can lead to an increase in the local dimensions. For a summary of the different formulations see the introductory sections of Refs. [107,108].

Nowadays the most commonly used formulation is the one based on vertex models; this is also what was used throughout the present work. It was a new idea of Ref. [79] to construct transfer matrices for the classical cellular automata (and for certain deformations thereof) using the IRF language.

Now we review the construction of Ref. [79], by focusing on the Rule54 model without deformation. We will show that the transfer matrices of Ref. [79] have an identical structure as in our quantum circuits discussed above.

The time evolution operator of Ref. [79] is built exactly in the same way as in Eqs. (2.16) and (2.17) with the three-site gates having the structure given by Eq. (2.15). Afterward, a commuting family of transfer matrices is built using two matrices $L^{j_1,j_2}_{i_1,i_2}(\lambda)$ and $M^{j_1,j_2}_{i_1,i_2}(\lambda)$ which describe *face weights* in the IRF language. Both matrices have four indices ranging from 1 to 2, and they can be represented most easily as 4×4 matrices using the conventions for the tensor product:

$$L = \begin{pmatrix} L^{0,0}_{0,0} & L^{0,1}_{0,0} & L^{1,0}_{0,0} & L^{1,1}_{0,0} \\ L^{0,0}_{0,1} & L^{0,1}_{0,1} & L^{1,0}_{0,1} & L^{1,1}_{0,1} \\ L^{0,0}_{1,0} & L^{0,1}_{1,0} & L^{1,0}_{1,0} & L^{1,1}_{1,0} \\ L^{0,0}_{1,1} & L^{0,1}_{1,1} & L^{1,0}_{1,1} & L^{1,1}_{1,1} \end{pmatrix}. \tag{5.63}$$

The number λ is interpreted again as a spectral parameter. The explicit form of the L and M matrices is given by

$$L(\lambda) = \begin{pmatrix} 1 & & & 1 \\ 1 & & & 1 \\ & \lambda^2 & & \lambda \\ & \lambda & & 1 \end{pmatrix}, \tag{5.64}$$

$$M(\lambda) = \begin{pmatrix} 1 & & & 1 \\ & 1/\lambda & & 1/\lambda \\ & 1 & 1/\lambda & \\ 1 & & 1/\lambda & \end{pmatrix}. \tag{5.65}$$

The transfer matrices $\mathcal{I}(\lambda)$ are defined component-wise as

$$\mathcal{I}^{j_1,j_2,\ldots,L}_{i_1,i_2,\ldots,i_L}(\lambda) = \prod_{x=1}^{L/2} M^{j_{2x-1},j_{2x}}_{i_{2x-1},i_{2x}}(\lambda) L^{j_{2x},j_{2x+1}}_{i_{2x},i_{2x+1}}(\lambda). \tag{5.66}$$

There is no summation over repeated indices.

It is then proven in Ref. [79] that the transfer matrices commute with each other and also with the time evolution

operator:

$$[\mathcal{I}(\lambda), \mathcal{V}] = 0. \tag{5.67}$$

This is shown using the "face weight" formulation of the Yang-Baxter relation discussed above.

This construction of Ref. [79] is completely identical with our quantum circuits of Sec. V A after proper identifications are made. It was already shown in Sec. V A that our GLL and GGG relations are identical to the "face weight" formulation of the Yang-Baxter relation given by Eq. (5.19). Furthermore, we recognize the structural similarity between the transfer matrices Eqs. (5.34) and (5.66). This leads to the following correspondences:

$$\check{\mathcal{L}}_{123}(\theta) \equiv f, \tag{5.68}$$

$$\check{\mathcal{L}}_{123}(u) \equiv M, \tag{5.69}$$

$$\check{\mathcal{G}}_{234}(\theta, u) \equiv L, \tag{5.70}$$

$$\check{\mathcal{G}}_{123}(u_1, u_2) \equiv g, \tag{5.71}$$

where on the l.h.s. we listed our operators, and the r.h.s. contains the objects defined in Ref. [79]. For the identification of the indices see Eqs. (5.17) and (5.18).

Let us now show that in the particular case of the Rule54 model the transfer matrix Eq. (5.66) does not yield new conserved charges.

First of all we consider two known conserved operators in this model: the translation operator $\mathcal{U}$ and the particle current defined as

$$\mathcal{J} = \sum_{x=1}^{L/2} \left(\sigma^z_{2x-1}\sigma^z_{2x} - \sigma^z_{2x}\sigma^z_{2x+1}\right). \tag{5.72}$$

This operator anticommutes with both the shift and the single step update operators:

$$\{\mathcal{J}, \mathcal{U}\} = \{\mathcal{J}, \mathcal{V}_1\} = \{\mathcal{J}, \mathcal{V}_2\} = 0. \tag{5.73}$$

It follows that it commutes with the Floquet-cycle operator $\mathcal{V} = \mathcal{V}_2\mathcal{V}_1$:

$$[\mathcal{J}, \mathcal{V}] = 0. \tag{5.74}$$

The translation operator intertwines the two update steps:

$$\mathcal{V}_1\mathcal{U} = \mathcal{U}\mathcal{V}_2. \tag{5.75}$$

Strictly speaking $\mathcal{U}$ is not conserved by the Floquet cycle $\mathcal{V}$, because it interchanges the odd and even sites. However, $\mathcal{U}^2$ is conserved.

It was conjectured in Ref. [79] that new quasilocal charges can be obtained from the transfer matrix Eq. (5.66). On the contrary, we show here that $\mathcal{I}(\lambda)$ is functionally dependent on the time evolution operator and the two conserved operators $\mathcal{U}$ and $\mathcal{J}$.

First we note that the matrix $L^{j_1,j_2}_{i_1,i_2}(\lambda)$ is diagonal in the indices $j_2 \leftrightarrow i_1$, and it can be factorized as

$$L^{j_1,j_2}_{i_1,i_2}(\lambda) = \delta_{i_1,j_2}\lambda^{A^{j_1}_{i_1}+B^{j_2}_{i_2}}, \tag{5.76}$$

where

$$A^{j_1}_{i_1} = \delta_{j_1,0}\delta_{i_1,1}, \quad B^{j_2}_{i_2} = \delta_{j_2,1}\delta_{i_2,0}. \tag{5.77}$$

The factorization above means that the λ-dependence can be separated into index pairs to the left and to the right. It follows that the transfer matrix Eq. (5.66) can be written as

$$\mathcal{I}^{j_1,j_2,\ldots,j_L}_{i_1,i_2,\ldots,i_L}(\lambda) = \prod_{x=1}^{L/2} \tilde{M}^{j_{2x-1},j_{2x}}_{i_{2x-1},i_{2x}}(\lambda)\delta_{i_{2x},j_{2x+1}}, \tag{5.78}$$

where

$$\tilde{M}^{j_1,j_2}_{i_1,i_2}(\lambda) = \lambda^{B^{j_1}_{i_1}} M^{j_1,j_2}_{i_1,i_2}(\lambda)\lambda^{A^{j_2}_{i_2}}. \tag{5.79}$$

Once again there is no summation over repeated indices.

Furthermore, the same operator can be written as $\mathcal{I}(\lambda) = \mathcal{U}\tilde{\mathcal{I}}(\lambda)$, where now the components of $\tilde{\mathcal{I}}(\lambda)$ are

$$\tilde{\mathcal{I}}^{j_1,j_2,\ldots,L}_{i_1,i_2,\ldots,i_L}(\lambda) = \prod_{x=1}^{L/2} \tilde{M}^{j_{2x-2},j_{2x-1}}_{i_{2x-1},i_{2x}}(\lambda)\delta_{i_{2x},j_{2x}}. \tag{5.80}$$

We can see that this operator acts as the identity on the even sites, which become control bits for the action on the odd sites. To be more precise, the same operator can be written as a product of commuting three-site unitaries

$$\tilde{\mathcal{I}}(\lambda) = \prod_{x=1}^{L/2} U^{(3)}(2x|\lambda), \tag{5.81}$$

where $U^{(3)}(2x|\lambda)$ has the form of Eq. (2.15) with the λ-dependent f-matrices given through the matrix elements

$$[f^{ab}(\lambda)]^j_i = \tilde{M}^{aj}_{ib}(\lambda). \tag{5.82}$$

Considering the concrete components of $\tilde{M}$ we can write the individual f-matrices as

$$f^{11} = \sigma^x, \quad f^{00} = 1 \tag{5.83}$$

and

$$f^{10} = \begin{pmatrix} \lambda & \\ & 1/\lambda \end{pmatrix}\sigma^x, \quad f^{01} = \begin{pmatrix} 1/\lambda & \\ & \lambda \end{pmatrix}\sigma^x. \tag{5.84}$$

Comparing to Eq. (2.19) we see that these are λ-deformed versions of the original f-matrices of the model. Thus, we can write

$$\tilde{\mathcal{I}}(1) = \mathcal{V}_2, \tag{5.85}$$

where $\mathcal{V}_{1,2}$ are the two operators that define the update rules, see Eqs. (2.16) and (2.17).

Collecting the factors of λ as we multiply the equal time quantum gates we obtain

$$\tilde{\mathcal{I}}(\lambda) = \lambda^{\mathcal{J}/2}\,\mathcal{V}_2, \tag{5.86}$$

where $\mathcal{J}$ is the particle current operator defined in Eq. (5.72). Going back to the actual transfer matrix we get

$$\mathcal{I}(\lambda) = \mathcal{U}\,\lambda^{\mathcal{J}/2}\,\mathcal{V}_2. \tag{5.87}$$

This formula means that the transfer matrix $\mathcal{I}(\lambda)$ is functionally dependent on three known operators: the cyclic shift, the conserved particle current, and the single step update rule. From this formula it follows that $\mathcal{I}(\lambda)$ is unitary if $|\lambda| = 1$; this was an unexplained observation of Ref. [79]. Finally, for the product of two transfer matrices we obtain

$$\mathcal{I}(\lambda_2)\mathcal{I}(\lambda_1) = \mathcal{U}^2(\lambda_1\lambda_2)^{-\mathcal{J}}\mathcal{V}. \tag{5.88}$$

Here we used the anticommutation relations Eq. (5.73) and the definition of the Floquet cycle $\mathcal{V}$. This proves the commutativity of the transfer matrices. Furthermore, choosing

$\lambda_1 = \lambda_2$ we find that the squared transfer matrix is simply just a combination of the two-site translation, the conserved particle current, and the Floquet update rule.

We interpret this result as follows: Even though the Rule54 model seems integrable, the construction of Ref. [79] cannot be considered as a proof of it, because Ref. [79] fails to introduce new charges on top of the existing ones. The same conclusion can be reached for the deformed Rule54 model, where the M-matrices are modified but the L-matrices are kept the same [79], so that the key steps of our computation here can be applied in the same way.

VI. FOUR-SITE INTERACTIONS

It is relatively straightforward to generalize the results of the previous sections to models with four-site interactions. In Sec. III B the key ideas were obtained after we constructed a nearest-neighbor chain by gluing pair of sites together. In the case of four-site interactions we need to group together triplets of spins, thus obtaining a nearest-neighbor chain for the glued sites. This n.n. chain is integrable, therefore we expect that it has a regular R-matrix. We have glued together three sites, therefore the auxiliary space for this R-matrix has to be a tensor product of three auxiliary spaces a, b, c. We can then construct transfer matrices in an analogous way as in Eq. (3.24) but now with $R_{(a,b,c),(j,j+1,j+2)}(u, 0)$ which acts on the triplets of physical sites and auxiliary spaces.

Going further, we need to satisfy the condition that the charges of the original chain are translationally invariant, and as an effect we expect that the transfer matrix will also be translationally invariant. This condition leads to the factorization of the R-matrix as

$$R_{(a,b,c),(j,j+1,j+2)}(u, 0) = \mathcal{L}_{a,b,c,j+2}(u)\mathcal{L}_{a,b,c,j+1}(u)\mathcal{L}_{a,b,c,j}(u). \tag{6.1}$$

Here $\mathcal{L}_{a,b,c,j}(u)$ is the Lax operator acting on three auxiliary spaces and a single physical space.

The transfer matrix is then constructed as

$$t(u) = \mathrm{Tr}_{a,b,c}\mathcal{L}_{a,b,c,L}(u)\ldots\mathcal{L}_{a,b,c,1}(u). \tag{6.2}$$

The regularity condition for the R-matrix implies the initial condition

$$\mathcal{L}_{a,b,c,j}(0) = \mathcal{P}_{a,j}\mathcal{P}_{b,j}\mathcal{P}_{c,j}, \tag{6.3}$$

which leads to

$$t(0) = \mathcal{U}^3. \tag{6.4}$$

Writing the Lax operator as

$$\mathcal{L}_{a,b,c,j}(u) = \mathcal{P}_{a,j}\mathcal{P}_{b,j}\mathcal{P}_{c,j}\check{\mathcal{L}}_{a,b,c,j}(u), \tag{6.5}$$

we compute the four-site Hamiltonian density as

$$h_{1,2,3,4} = \partial_u \check{\mathcal{L}}_{1,2,3,4}(u)\big|_{u=0}. \tag{6.6}$$

For the Lax operator we expect the inversion relation

$$\check{\mathcal{L}}_{a,b,c,j}(u)\check{\mathcal{L}}_{a,b,c,j}(-u) = 1. \tag{6.7}$$

From this we can compute the next conserved charge from the transfer matrix. It will be a seven-site operator

$$Q_7 = \sum_j q_7(j), \tag{6.8}$$

with

$$q_7(1) = \left[h_{1,2,3,4}, \sum_{k=1}^{3} h_{1+k,2+k,3+k,4+k}\right]. \tag{6.9}$$

The commutativity of H and Q_7 can be used as an integrability criterion, which can serve as a starting point for classifying four-site interacting models.

As an initial step in this direction we classified all $SU(2)$ invariant models with space reflection symmetry. Sorting out the trivial cases we found only one new model, with the Hamiltonian density being

$$h_{1,2,3,4} = 2(\mathcal{P}_{1,4} - 1)(\mathcal{P}_{2,3} - 1) - \mathcal{P}_{1,3} - \mathcal{P}_{2,4}. \tag{6.10}$$

Given the huge literature of integrable models we cannot be entirely certain that the model has not yet appeared in the literature, possibly in some other form. In any case it appears to be new.

Going further in the classification, an obvious next step is to consider the $U(1)$-invariant models. This opens up a bigger parameter space, and we leave its exploration to future works. We note that the folded XXZ model treated in Refs. [52–54] belongs to this class, and its Hamiltonian is the four-site charge Q_4 of Eq. (2.8). In the next subsection we derive an integrable quantum circuit for this particular model.

Finally, we stress that (in parallel with the three-site interacting case) we were not able to prove the factorization Eq. (6.1), therefore we regard it as a conjecture. Furthermore, it is not clear whether all integrable solutions can be put in a form which satisfies the inversion relation Eq. (6.7). We leave these problems to future research.

A. Integrable quantum circuit for the folded XXZ model

A brickwork type quantum circuit for the folded XXZ model was introduced in Ref. [84]. The idea is to build a Floquet cycle of length $\tau = 3$, with four-site unitaries $U^{(4)}$ placed at coordinates $x_k = 3k$ and with the displacements $\Delta_l = l$ (see Sec. II F for the explanation notations). The four-site unitaries are given by the Lax operator, which reads [84]

$$U^{(4)}(j|u) = \check{\mathcal{L}}_{1,2,3,4}(u) = P_j^{\bullet}P_{j+3}^{\circ} + P_j^{\circ}P_{j+3}^{\bullet} + (P_j^{\bullet}P_{j+3}^{\bullet} + P_j^{\circ}P_{j+3}^{\circ})U^{(2)}_{j+1,j+2}(u), \tag{6.11}$$

where $U^{(2)}_{j+1,j+2}(u)$ is a two-site unitary given by the explicit matrix representation

$$U^{(2)}(u) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \mathrm{sech}(u) & i\tanh(u) & 0 \\ 0 & i\tanh(u) & \mathrm{sech}(u) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{6.12}$$

This matrix is obtained simply from the known R-matrix of the XX model. Note that Eq. (6.11) has the same structure as the corresponding charge Q_4: it has two control bits and two action bits. As an effect, the unitaries commute even if they overlap at the control bits. This enables us to build a Floquet cycle which has periodicity 3 both in the temporal and the spatial directions. With this we have completely specified the quantum circuit. For a graphical interpretation see the upper graph in Fig. 19.

In Ref. [84] the integrability of this circuit was established in the bond picture (after performing the bond-site transforma-

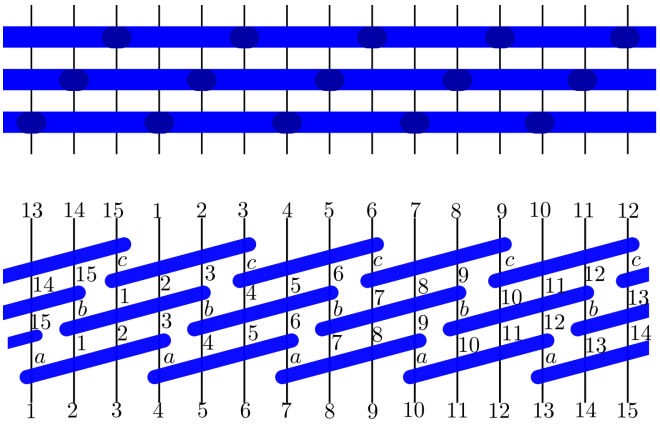

FIG. 19. Time step operator and its transfer matrix representation. This construction applies to models with four-site interactions where the outer two spins are control bits. These control bits are depicted as shaded circles in the figure above. An example is the folded XXZ model.

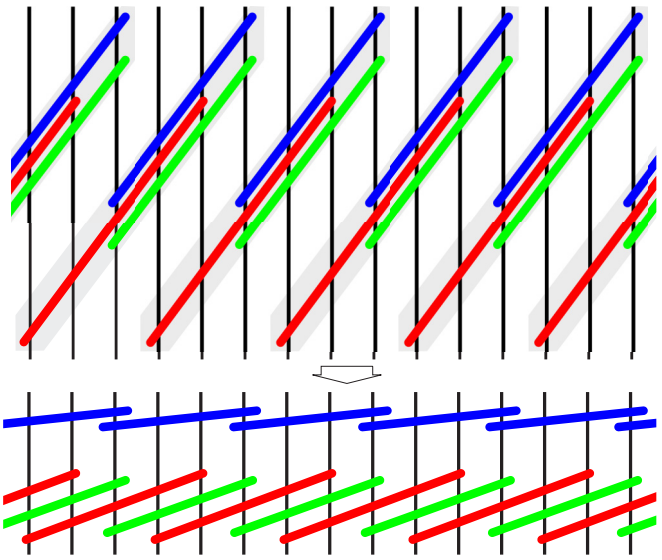

FIG. 20. Transfer matrix with the operator $\check{\mathcal{G}}$.

tion discussed in Appendix B), where the building blocks are three-site unitaries. In Ref. [84] diagonal-to-diagonal transfer matrices were constructed, in the same way as in Sec. IV B.

Now we show that there exists a commuting family of row-to-row transfer matrices in the original picture of this model. This complements the results of Ref. [84].

First we start with the discussion of the integrability properties of the special class of four-site models, where the Lax operators satisfies an additional condition

$$[\check{\mathcal{L}}_{1234}(u), \check{\mathcal{L}}_{4567}(v)] = 0, \tag{6.13}$$

i.e., the first and the last sites are control bits. The consequence of this property is that there exists an five-site operator $\check{\mathcal{G}}$ for which the R-matrix factorizes as

$$\begin{aligned}\check{R}_{123456}(u,v) =& \check{\mathcal{L}}_{1234}(v)^{-1}\check{\mathcal{G}}_{23456}(u,v)\check{\mathcal{L}}_{1234}(u)\\ =& \check{\mathcal{L}}_{3456}(u)\check{\mathcal{G}}_{12345}(u,v)\check{\mathcal{L}}_{3456}(v)^{-1}.\end{aligned} \tag{6.14}$$

The consistency of these factorizations requires the GLL relation

$$\begin{aligned}&\check{\mathcal{G}}_{23456}(u,v)\check{\mathcal{L}}_{1234}(u)\check{\mathcal{L}}_{3456}(v)\\ &\quad= \check{\mathcal{L}}_{1234}(v)\check{\mathcal{L}}_{3456}(u)\check{\mathcal{G}}_{12345}(u,v).\end{aligned} \tag{6.15}$$

Let us now construct the single step update rule as

$$\mathcal{V}_1 = \check{\mathcal{L}}_{1,2,3,4}(\theta)\check{\mathcal{L}}_{4,5,6,7}(\theta)\ldots\check{\mathcal{L}}_{L-2,L-1,L,1}(\theta), \tag{6.16}$$

where θ will be a fixed parameter of the quantum circuit. For the Floquet cycle we obtain

$$\begin{aligned}\mathcal{V} = \mathcal{V}_3\mathcal{V}_2\mathcal{V}_1 =& \mathcal{U}^3\\ &\times \times \mathrm{tr}_{abc}[\mathcal{L}_{1,2,3,c}(\theta)\mathcal{L}_{1,2,3,b}(\theta)\mathcal{L}_{1,2,3,a}(\theta)\\ &\times \mathcal{L}_{4,5,6,c}(\theta)\mathcal{L}_{4,5,6,b}(\theta)\mathcal{L}_{4,5,6,a}(\theta)\ldots\\ &\times \mathcal{L}_{L-2,L-1,L,c}(\theta)\mathcal{L}_{L-2,L-1,L,b}(\theta)\mathcal{L}_{L-2,L-1,L,a}(\theta)].\end{aligned} \tag{6.17}$$

Applying the factorization formula

$$\check{R}_{123456}(\theta,0) = \check{\mathcal{L}}_{3456}(\theta)\check{\mathcal{L}}_{2345}(\theta)\check{\mathcal{L}}_{1234}(\theta), \tag{6.18}$$

we can define a transfer matrix [with auxiliary space $A = (a,b,c)$]

$$\begin{aligned}t(u) =& \mathrm{tr}_A[R_{(1,2,3),A}(\theta,u)R_{(4,5,6),A}(\theta,u)\ldots\\ &\times R_{(L-5,L-4,L-3),A}(\theta,u)R_{(L-2,L-1,L),A}(\theta,u)],\end{aligned} \tag{6.19}$$

which generates the time step as

$$\mathcal{V} = t^{-1}(\theta)t(0). \tag{6.20}$$

These transfer matrices commute:

$$[t(u), t(v)] = 0. \tag{6.21}$$

With this we have established a commuting family of transfer matrices that includes the update rule of the quantum circuit at the special point $u = 0$.

The transfer matrix can be rewritten using the factorization Eq. (6.14). We find

$$t(u) = \mathcal{V}_3\tilde{t}(u), \tag{6.22}$$

where

$$\begin{aligned}\tilde{t}(u) =& \mathrm{tr}_{a,b,c}[\mathcal{G}_{1,2,a,b,c}(\theta,u)\mathcal{L}_{3,a,b,c}(-u)\mathcal{G}_{4,5,a,b,c}(\theta,u)\\ &\times \mathcal{L}_{6,a,b}(-u)\ldots\\ &\times \mathcal{G}_{L-2,L-1,a,b,c}(\theta,u)\mathcal{L}_{L,a,b,c}(-u)],\end{aligned} \tag{6.23}$$

where

$$\mathcal{G}_{1,2,3,4,5}(\theta,u) = \mathcal{P}_{1,5}\mathcal{P}_{2,5}\mathcal{P}_{3,5}\mathcal{P}_{1,4}\mathcal{P}_{2,4}\mathcal{P}_{3,4}\check{\mathcal{G}}_{1,2,3,4,5}(\theta,u). \tag{6.24}$$

For a graphical interpretation of the transfer matrix and its factorization see Fig. 20.

VII. DISCUSSION

In this paper we treated integrable spin chains with medium-range interaction, focusing on cases with three-site and four-site interactions. We presented a new algebraic framework which can lead to a classification of such models, and to the construction of new quantum and classical cellular automata. As it was explained in the Introduction, two of the most general problems in the field of integrability is the *classification of all integrable models* and clarifying the

essential features of integrability. Our results can be seen as a contribution to this multi decade endeavor. In the paper we treated the three- and four-site interacting models in detail, but the generalization to longer interaction ranges is rather straightforward.

We presented partial classifications for the three- and four-site spin-1/2 models, and we found a number of new models. Given the enormous literature of integrable models it is always difficult to know whether a model is indeed new; we did our best in the search of the literature and our models appear to be new. We recall that our models are translationally invariant, and in the three-site interacting case they can be pictured as zigzag spin ladders. To our best knowledge the only translationally invariant integrable three-site chain the literature is the Bariev model [44]; other constructions naturally involve a staggering of some of the parameters (see, for example, Refs. [109–112]) and thus they are not in the category of models that we are investigating.

In the family of $SU(2)$-invariant spin chains with reflection symmetry we did not find a nontrivial three-site model, and we found only one new four-site model given by Eq. (6.10). In the family of $U(1)$-invariant three-site chains (again with space reflection symmetry) we found two families: the Bariev model and the hard rod deformed XXZ model given by Eq. (3.52). The latter will be analyzed in detail in an upcoming publication.

A further interesting family of models is that of the IRF type Hamiltonians and quantum gates. These theories are very similar to known restricted solid on solid (RSOS) models [80,81], their Hamiltonians have the same structure; see, for example, Ref. [83]. However, in the case of the RSOS theories the Hilbert space is restricted (it consists of certain paths), while in our case it is simply the tensor product space of the spin chains.

For these models we also used the same formulation of our algebraic methods, as opposed to the "face weight" formulation of the Yang-Baxter relations typically used in the RSOS (or IRF) framework. However, in Sec. V A we showed that the two formulations are indeed identical in these special cases. This also implies that our models are solutions to the "face weight" formulation of the Yang-Baxter relation. We believe that the connection between the RSOS models and our new Hamiltonians deserves further study.

The family of the IRF type Hamiltonians accommodates some of the elementary cellular automata that have been studied recently [73,79]. We found that out of the classical cellular automata treated in Ref. [79] the Rule150 and Rule105 models are Yang-Baxter integrable, and they can be deformed into quantum cellular automata. We also gave a recipe for computing extensive local charges for these quantum and classical cellular automata, and we derived the concrete formulas for the first charge of the Rule150 and Rule105 models. Putting everything together, our construction can be seen as a remarkable link between classical and quantum integrable models.

In contrast, we did not find such three-site structures for the famous Rule54 model. We pointed out that the construction of Ref. [79] does not yield new conserved charges on top of the known ones, and the transfer matrices derived there are functionally dependent on the known charges. Thus, the problem of the integrability of the Rule54 model is still open. A very important piece of the puzzle was presented in Ref. [77], where a six site interacting Hamiltonian was constructed, which commutes with the Floquet update rule of the Rule54 model. This suggest that the model could lie in the family of six site interacting models. Preliminary computations show that this is indeed the case: we found a new local extensive charge with interaction range $\ell = 10$ using the proper generalization of our methods. We will present this result in a future work.

It would be interesting to continue the partial classification of medium-range models, extending our results to more complicated or four-site interacting cases or to higher-dimensional local spaces. In both cases a much larger parameter space opens up, and a clear physical motivation is needed to formulate the restrictions for the Hamiltonians. Symmetries can be chosen as guiding principles, together with special assumptions on the structure of the Hamiltonian. A known four-site interacting model is the folded XXZ model treated in Refs. [52–54]. This Hamiltonian has a particular structure: it has two control bits and two action bits, and its algebraic treatment leads to a Yang-Baxter integrable classical cellular automaton (see Ref. [84] and Sec. VI A). It would be interesting to classify models with a similar structure, potentially leading to new cellular automata with four-site update rules.

An other interesting question is whether our constructions exhaust all possibilities for integrable quantum circuits. The IRF type circuits show very clearly that if the Lax operators have a special structure, then this allows the construction of special brickwork circuits, which would be meaningless for other types of Lax operators. Therefore, it cannot be excluded, that some other sorts of special circuits can be built if we impose some other special structure on the building blocks.

In this regard let us return to the so-called box-ball systems mentioned in the Introduction [85,86]. These are classical cellular automata with a less local update procedure, which is performed by acting with a certain transfer matrix which does not factorize into commuting local unitary operators. Theses systems are special cases of so-called filter automata [87–90]. The crucial ingredient of such a construction is a Lax operator which becomes deterministic at some special points, but the regularity condition (that would lead to strictly local update rules) is not required. Our solutions for the integrable Lax operators could also be used to construct such filter automata.

In this paper we discussed the physical properties of our models only in passing. We explained that the bond-site transformed XYZ model of Sec. V C describes interacting dynamics of domain walls, with or without domain wall number conservation. And we will publish a paper dealing specifically with the hard rod deformed XXZ model found in Sec. III D. We believe that the other new spin chain and quantum gate models also deserve further attention.

Finally, let us mention that our methods could be relevant for also the AdS/CFT conjecture. It is known that in the planar limit the dilatation operator of the gauge theory is essentially an integrable Hamiltonian with long-range interaction [113,114]. The spectrum of this Hamiltonian is now understood using the so-called quantum spectral curve method [115–117], but there is no clear understanding of the actual Hamiltonian on the operator level. It is known that it is a long-range deformation of an integrable nearest-neighbor chain, but

it is not clear how to perform the long-range deformation in a finite volume [118]. Our methods could give a recipe for this problem: perhaps there is a truncation scheme where we could gradually increase the interaction range of the chains while still using our present methods at each step. This appears to be a promising direction for future work.

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APPENDIX A: COUNTEREXAMPLE TO THE ORIGINAL CONJECTURE OF REF. [33]

Here we discuss a counterexample to the original conjecture of Ref. [33] regarding the integrability of nearest-neighbor spin chains. In Ref. [33] it was claimed that a sufficient condition of integrability is the existence of a three-site charge which commutes with the Hamiltonian. However, it was not stressed in Ref. [33] that the Hamiltonian has to be dynamical.

For example, consider the family of models defined by the two charges

$$Q_2 = \sum_j \sigma_j^z \sigma_{j+1}^z,$$
$$Q_3 = \sum_j \left(1 - \sigma_j^z \sigma_{j+2}^z\right)\left(\sigma_{j+1}^x + \kappa \sigma_{j+1}^z\right). \tag{A1}$$

Here $\kappa \in \mathbb{R}$ is a coupling constant. Direct computation shows that $[Q_3, Q_2] = 0$ for every κ. The model is integrable for $\kappa = 0$, it is a special point of the bond-site transformed XYZ model considered in Sec. V C. However, a nonzero κ introduces a term which our classification found to be nonintegrable. To confirm that the model is indeed nonintegrable, we investigated the level spacing distribution for $\kappa = 1$ and confirmed the Wigner-Dyson statistics characteristic for chaotic models. This computation was performed by Dávid Szász-Schagrin and we are thankful to him.

This example shows that if the nearest-neighbor charge Q_2 is not dynamical, then the existence of a commuting charge Q_3 is not enough to ensure integrability of the model.

APPENDIX B: BOND-SITE TRANSFORMATION

A number of models that we encountered in this work together with the folded XXZ model treated in Refs. [52–54] allow for an alternative description after performing a bond-site transformation. This is a nonlocal transformation, and in the models of interest it leads to Hamiltonians with shorter interaction range. The bond-site transformation is a special case of the more general Clifford transformations treated recently in Ref. [56]; here we just treat this simple case.

The first observation is that in some models the dynamics generating Hamiltonian (be it a three-site or four-site operator) commutes with the nondynamical charge

$$Q_2 = \sum_j \frac{1 - \sigma_j^z \sigma_{j+1}^z}{2}. \tag{B1}$$

Here we chose the conventions such that Q_2 has zero eigenvalue on ferromagnetic states in the computational basis. Then the nonzero contributions to Q_2 originate from nearest neighbors where the two spins are different. Such a situation can be interpreted as a domain wall (DW), and then Q_2 is seen as the total DW number which is conserved. It is then natural to expect that the Hamiltonian can be interpreted as an operator that generates dynamics for the DW's.

This is seen explicitly by performing a bond-site transformation, either in finite volume with open boundary conditions or directly in infinite volume. The idea is to put spin-1/2 variables on the bonds between lattice sites, and to perform a change of basis starting from the original computational basis. For each bond we write down a ∘ (up spin) if the two neighboring spins are identical, and a • (down spin) if they are different. This is a highly nonlocal transformation, which can be inverted (up to simple complications at the boundaries). Then we also obtain a new Hamiltonian in the new basis.

Such a transformation can be performed for any spin chain with interaction range ℓ. The new Hamiltonian will be local if the original one respects spin reflection invariance. Nevertheless, the new interaction will generally have range $\ell + 1$ in the bond picture. It is important that the bond-site transformation can be performed even if Q_2 is not conserved: in this case domain walls can be created or annihilated. The only requirement for the locality of the transformation is the spin-flip invariance in a given basis.

The utility of the transformation shows itself if the new model has a smaller interaction range. A range of $\ell - 1$ can be obtained if a further special condition holds: The original Hamiltonian density should be such that it does not change the spins at the first and the last sites of its support. Then only the bonds within the support of length ℓ are modified, which means that in the bond basis the interaction range will be $\ell - 1$.

A concrete example for the site-bond transformation was presented in Ref. [54] in the case of the folded XXZ model. There the first few charges are given by Eq. (2.8). The charge Q_4 indeed preserves the first and last spins, and the domain wall number given by Q_2 is also conserved. After the bond-site transformation the charge Q_4 becomes identical to the three-site Hamiltonian Eq. (3.52) with $\Delta = 0$, which is interpreted as the hard rod deformation of the XX model.

Further examples for the bond-site transformation are presented in Sec. (V C). In those cases the original Hamiltonian is a three-site operator, which preserves the first and the last spins, acting nontrivially on the middle spin. In certain cases these models can be transformed into a nearest-neighbor chain. In these three-site interacting cases the transformation rules for a subset of the allowed operators are found to be

$$1 \otimes \sigma^x \otimes 1 \leftrightarrow \sigma^x \otimes \sigma^x, \tag{B2}$$
$$-\sigma^z \otimes \sigma^x \otimes \sigma^z \leftrightarrow \sigma^y \otimes \sigma^y, \tag{B3}$$
$$\sigma^z \otimes 1 \otimes \sigma^z \leftrightarrow \sigma^z \otimes \sigma^z, \tag{B4}$$
$$\sigma^z \otimes \sigma^y \otimes 1 \leftrightarrow \sigma^y \otimes \sigma^x, \tag{B5}$$
$$1 \otimes \sigma^y \otimes \sigma^z \leftrightarrow \sigma^x \otimes \sigma^y. \tag{B6}$$

On the l.h.s. above we listed the three-site interacting operators allowed by the requirements, which are transformed into the two site operators on the r.h.s.

APPENDIX C: INVERSION RELATION FOR THE *R*-MATRICES

Here we show that the regularity property Eq. (3.5) of the R-matrix and its inversion relation Eq. (3.6) are not independent properties.

Substituting $\lambda_1 = \lambda_3$ to the YB Eq. (3.4) we get

$$R_{12}(\lambda_1,\lambda_2)R_{13}(\lambda_1,\lambda_1)R_{23}(\lambda_2,\lambda_1) = R_{23}(\lambda_2,\lambda_1)R_{13}(\lambda_1,\lambda_1)R_{12}(\lambda_1,\lambda_2). \tag{C1}$$

Using the regularity property Eq. (3.5) we obtain that

$$R_{12}(\lambda_1,\lambda_2)R_{21}(\lambda_2,\lambda_1) = R_{23}(\lambda_2,\lambda_1)R_{32}(\lambda_1,\lambda_2). \tag{C2}$$

We can see that the left- and the right-hand sides act trivially on 3 and 1 spaces, respectively. Therefore, they have to be equal to an operator X_2 acting only on the second space. Writing out the rapidity dependence we get

$$R_{12}(\lambda_1,\lambda_2)R_{21}(\lambda_2,\lambda_1) = X_2(\lambda_1,\lambda_2), \tag{C3}$$

$$R_{23}(\lambda_2,\lambda_1)R_{32}(\lambda_1,\lambda_2) = X_2(\lambda_1,\lambda_2). \tag{C4}$$

The second equation can be rewritten as

$$R_{12}(\lambda_2,\lambda_1)R_{21}(\lambda_1,\lambda_2) = X_1(\lambda_1,\lambda_2). \tag{C5}$$

Substituting back to Eq. (C3) we obtain that

$$X_1(\lambda_2,\lambda_1) = X_2(\lambda_1,\lambda_2). \tag{C6}$$

Since the l.h.s. and the r.h.s. act on different spaces the operator X should be proportional to the identity, i.e.,

$$R_{12}(\lambda,\mu)R_{21}(\mu,\lambda) \sim 1. \tag{C7}$$

APPENDIX D: FACTORIZATION PROPERTY OF THE *R*-MATRIX

Here we prove Theorem 1.

Substitute $v = 0$ to the RLL relation we get

$$R_{A,(12)}(u,0)\mathcal{L}_{A,3}(u)\mathcal{L}_{(12),3}(0) = \mathcal{L}_{(12),3}(0)\mathcal{L}_{A,3}(u)R_{A,(12)}(u,0). \tag{D1}$$

Now let us use the regularity of the Lax operator to obtain

$$R_{A,(12)}(u,0)\mathcal{L}_{A,3}(u) = \mathcal{L}_{A,2}(u)\tilde{R}_{A,(31)}(u,0). \tag{D2}$$

After a simple rearrangement we get

$$\mathcal{L}_{A,2}(u)^{-1}R_{A,(12)}(u,0) = R_{A,(31)}(u,0)\mathcal{L}_{A,3}(u)^{-1}. \tag{D3}$$

We can see that the l.h.s. and the r.h.s. act trivially on the spaces 3 and 2, respectively, therefore they have to be equal to an operator that acts only on space 1:

$$\mathcal{L}_{A,2}(u)^{-1}R_{A,(12)}(u,0) = X_{A,1}(u), \tag{D4}$$

$$R_{A,(31)}(u,0)\mathcal{L}_{A,3}(u)^{-1} = X_{A,1}(u). \tag{D5}$$

The second equation can be written as

$$R_{A,(12)}(u,0) = X_{A,2}\mathcal{L}_{A,1}(u). \tag{D6}$$

Substituting back to Eq. (D4) we obtain that

$$X_{A,2}(u)\mathcal{L}_{A,1}(u) = \mathcal{L}_{A,2}(u)X_{A,1}(u), \tag{D7}$$

therefore

$$\mathcal{L}_{A,2}(u)^{-1}X_{A,2}(u) = X_{A,1}(u)\mathcal{L}_{A,1}(u)^{-1}. \tag{D8}$$

Since the l.h.s. and the r.h.s. act trivially on spaces 1 and 2 they have to be equal to an operator acting only on the auxiliary space A:

$$\mathcal{L}_{A,2}(u)^{-1}X_{A,2}(u) = Y_A(u), \tag{D9}$$

$$X_{A,1}(u)\mathcal{L}_{A,1}(u)^{-1} = Y_A(u). \tag{D10}$$

From the first equation we obtain

$$X_{A,1}(u) = \mathcal{L}_{A,1}(u)Y_A(u). \tag{D11}$$

Substituting back to Eq. (D10) we obtain that

$$[\mathcal{L}_{A,1}(u), Y_A(u)] = 0. \tag{D12}$$

Substituting back to Eq. (D6) the R-matrix reads as

$$R_{A,(12)}(u,0) = \mathcal{L}_{A,2}(u)\mathcal{L}_{A,1}(u)Y_A(u). \tag{D13}$$

We are almost ready. The only remaining thing is to prove that the operator $Y_A(u)$ has to proportional to the identity.

We also know that the R-matrix is regular, i.e.,

$$R_{A,(12)}(0,0) = P_{A,(12)}, \tag{D14}$$

therefore

$$Y_A(0) \sim 1. \tag{D15}$$

Let us substitute $\lambda_1 = u$, $\lambda_2 = v$, and $\lambda_3 = 0$ to the YB equation.

$$R_{A,B}(u,v)R_{A,(12)}(u,0)R_{B,(12)}(v,0) = R_{B,(12)}(v,0)R_{A,(12)}(u,0)R_{A,B}(u,v). \tag{D16}$$

Using Eq. (D13) we obtain that

$$R_{A,B}(u,v)\mathcal{L}_{A,2}(u)\mathcal{L}_{B,2}(v)\mathcal{L}_{A,1}(u)\mathcal{L}_{B,1}(v)Y_A(u)Y_B(v) = \mathcal{L}_{B,2}(v)\mathcal{L}_{A,2}(u)\mathcal{L}_{B,1}(v)\mathcal{L}_{A,1}(u)Y_A(u)Y_B(v)R_{A,B}(u,v). \tag{D17}$$

Using the RLL relation on the l.h.s. we obtain that

$$R_{A,B}(u,v)\mathcal{L}_{A,2}(u)\mathcal{L}_{B,2}(v)\mathcal{L}_{A,1}(u)\mathcal{L}_{B,1}(v)Y_A(u)Y_B(v) = \mathcal{L}_{B,2}(v)\mathcal{L}_{A,2}(u)\mathcal{L}_{B,1}(v)\mathcal{L}_{A,1}(u)R_{A,B}(u,v)Y_A(u)Y_B(v). \tag{D18}$$

Substituting back to Eq. (D17) we obtain that

$$[R_{A,B}(u,v), Y_A(u)Y_B(v)] = 0. \tag{D19}$$

The operator $Y_A(u)$ can only be nontrivial if the R-matrix has gauge symmetry (spectral parameter dependent symmetry).We assumed that such symmetry is excluded, therefore

$$Y_A(u) = Y_A. \tag{D20}$$

Using Eq. (D15) we can see that the operator Y_A has to proportional to the identity.

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