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Cellular automata and spin chains: a medium range connection

Supervisor:

Prof. Francesco Ravanini

Submitted by:

Lorenzo Salvi

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Abstract

A cellular automaton is an extremely simple physical system: it has both a discrete time and space dimension. While they were initially developed as a new paradigm for quantum computation, it was soon realized that cellular automata were able to display very interesting behaviours like integrability and large-scale diffusive transport. Indeed rule 54, an elementary cellular automaton, is widely considered the simplest physical system to display integrability, making it the perfect toy model to study various properties of classical and quantum integrability and how they connect.

Since a cellular automaton is a fully discrete system it is natural to ask what is the corresponding model in the continuum, if it exists. Recently a new algebraic framework was developed that made it possible to generate classes of integrable quantum spin chains with medium range interactions while also building their corresponding discretization, in the form of quantum cellular automata. In this work we will study what it means for an system to be integrable, both in the classical and quantum realm; then we will describe the structure behind cellular automata and we will show the connection between integrable spin chains and quantum cellular automata. Finally we will try to extend this framework to a more complex system, the class of Restricted Solid-on-Solid models.

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Chapter 1

Introduction

Let's imagine one of the simplest non-trivial physical system possible: we take a string of zeros and ones of finite length and we define a rule that evolves the string by one discrete time-step; this rule is also very simple, depending only on a small neighbourhood. This class of systems is called cellular automaton and, despite their apparent triviality, they can accommodate highly non-trivial dynamical properties.

While cellular automata were first developed in the 1950s by von Neumann as a model for self-replicating machines in [1], they soon realized that cellular automata were a versatile tool to model phenomena with local interactions. A first attempt at classification and formalization of cellular automata was given by Wolfram in [2]; the long-time behaviour shown by the automata is extremely varied, from randomness to uniformity and periodically repeating sub-structures.

Already in 1993 it was noted by Bobenko et al. in [3] that a particular automaton, rule 54, showed the presence of soliton-like scattering, a characteristic of integrable systems. Integrability is a nebulous property, with a clear definition only for classical systems. In general we expect that an integrable system has enough conserved quantities to make it completely solvable, at least in principle.

Historically, quantum integrable models were discovered in two different areas of physics:

from quantum mechanics Bethe in [4] was able to solve completely the XXX spin chain by a method called coordinate Bethe ansatz, later augmented by Yang and Yang to solve XXZ chain; from statistical mechanics the six-vertex model was solved by Lieb and Sutherland in the 1970s using the transfer-matrix method and the coordinate Bethe ansatz, revealing a connection between two very different classes of models.

The underlying structure was recognized and codified by Fadeev et al. in a framework called quantum inverse scattering method; this method is based on a specific notion of integrability called Yang-Baxter integrability that is based on the existence of an operator, called R-matrix that is the solution of the Yang-Baxter equation. The R-matrix can be used to find the tower of conserved quantities and, ultimately, the eigenvectors and eigenvalues of the model through a process called algebraic Bethe ansatz, a sort of second quantization of the coordinate Bethe ansatz.

A cellular automaton that is Yang-Baxter integrable could be the perfect toy model to study both exact large scale behaviour and how integrability behaves under quantization. Despite the initial observation about the possible integrability of rule 54, a rigorous integration in the Yang-Baxter formalism turned out to be a highly non-trivial task. Indeed methods taken from the field of quantum information were used to describe the equilibrium and out-of-equilibrium dynamics of rule 54, finding even the exact thermalization dynamics of the model in [5].

Recently, a connection between spin chains with medium range interactions and quantum cellular automata was found; in particular the quantum cellular automata was found to be the Trotterization, or time discretization, of the folded XXZ chain, a spin chain with a three site interaction length. Then the established methods for spin chains were applied to prove both the integrability of the quantum automaton and of its classical limit.

To employ this connection a framework was developed to generate classes of integrable medium range spin chains and compute their quantum automata limit; in this way it was proven that automatons, like rule 150 and rule 105, are integrable, while rule 54 was

not found as the classical limit of any of the model studied.

In chapter 1 of this work we will study the meaning of classical integrability, both in the Liouville sense and in the Yang-Baxter sense. Then we will extend the construction to the quantum case.

In chapter 2 we will instead focus on cellular automata, by first giving a thorough description of classical automata and a subset of this models called elementary automata. Then we will extend the models to the quantum case and to a more general description that admits time-dependent and periodic evolution operators that we will need in the next section.

In chapter 3 we will explain what a medium range spin chain is and how we can build classes of this chains that are already integrable. We will also describe the discretization procedure that leads to the integrable quantum cellular automata and their classical limit, when it exists.

In chapter 4 we will apply this framework to a different class of higher spin chains, the RSOS quantum chains.

Chapter 2

Integrability

Finding an exact solution for a dynamical system is, in general, a complex and often unsolvable task. In fact we can expect a generic dynamical system to have a small number of conserved charges, if at all, relative to the number of the degrees of freedom; this leads to chaotic behaviour making it impossible to write down explicit solutions.
There is however a subset of dynamical systems called integrable system that can, theoretically, be completely solved. Even thought the requirement of integrability is extremely strong there are many physical systems that, at least as a good approximation, seems to be integrable. One of the most famous examples is that of solitons: solitary non-linear waves that preserve their shape as they evolve. They were first observed by Russel in 1834 and later they were understood as a pretty general solution of a class of integrable PDEs like the Korteweg-de Vries equation or the Sine-Gordon equation [6].
The definition of integrability is clear in a classical, finite-dimensional setting. We discuss this case in the next section, commenting on the quantum case later.

2.1 Classical Integrability

The space of states of a classical system with n degrees of freedom is a $2n$-dimensional space, called the phase space, parametrized by $q_i \in \mathbb{R}$ coordinates and $p_i \in \mathbb{R}$ conjugated

momenta, where $i = 1, ..., n$. The equation of motion is given as the solution of a first order differential system:

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial q_i} \tag{2.1}$$

It depends on a special function $H(q_i, p_i)$ called the Hamiltonian.

On phase space is defined a bilinear, antisymmetric product between functions $F, G \in \mathcal{F}$, where $\mathcal{F}$ is the space of real smooth functions, called the Poisson bracket:

$$\{F, G\} = \sum_i \frac{\partial F}{\partial p_i}\frac{\partial G}{\partial q_i} - \frac{\partial G}{\partial p_i}\frac{\partial F}{\partial q_i} \tag{2.2}$$

This product induces a symplectic structure on phase space that characterizes Hamiltonian dynamics.

The time evolution of any function $F(q_i, p_i) \in \mathcal{F}$ is given by

$$\dot{F} = \{H, F\} \tag{2.3}$$

From this we can see that any function F that satisfies $\{F, H\} = 0$ is conserved by the time evolution.

We say that a system with a $2n$-dimensional phase space is Liouville integrable if it has n independent conserved quantities in involution [7]:

$$\{F_i, F_j\} = 0, \quad i, j = 1, ..., n \quad \text{with} \quad F_1 = H \tag{2.4}$$

This system is solvable, due to Liouville theorem:

Theorem 2.1.1 (Liouville Theorem:) *The equations of motion of a Liouville integrable system can be solved by quadratures.*

Given this theorem, there exists a canonical transformation that gives as new momenta the conserved quantities F_i

$$(p_i, q_i) \longrightarrow (F_i, \varphi_i) \tag{2.5}$$

The equations of motion in the new coordinates are very simple

$$\dot{F}_i = 0$$
$$\dot{\varphi}_i = \frac{\partial H}{\partial F_i} = \Omega_i$$

and the solution can be found by integration:

$$F_i(t) = \alpha$$
$$\varphi_i(t) = \Omega_i t + \phi_i(0)$$

Although Liouville's theorem guarantees the existence of a set of variables where the solution becomes linear in time, it does not provide an explicit way to construct the new set.

1D Harmonic Oscillator Let's consider the harmonic oscillator as the simplest example [8]. The Hamiltonian is given by [1]

$$H = \frac{p^2}{2} + \frac{\omega^2 q^2}{2} = E \tag{2.6}$$

We can make a change of variable to

$$p = F \cos\varphi \tag{2.7}$$
$$q = \frac{F}{\omega} \sin\varphi \tag{2.8}$$

[1] The mass has been chosen as $m = 1$ here to simplify the notation.

The Hamiltonian becomes

$$H = \frac{F^2}{2}\cos^2\varphi + \frac{\omega^2 F^2}{2\omega^2}\sin^2\varphi = \frac{F^2}{2} = E \tag{2.9}$$

so we find that $F = \sqrt{2E}$. The equation of motion then take the linear form

$$\varphi(t) = \omega t + \varphi(0) \tag{2.10}$$

For some models we can introduce a way to find the integrals of motion using a couple of n-dimensional square matrices called the Lax pair L, M, where $L_{i,j}, M_{i,j} \in \mathcal{F}$ [8]. The dynamics of the matrix L is given by

$$\dot{L} = [L, M] \tag{2.11}$$

This implies that the traces of powers of L

$$Q_j = \operatorname{Tr} L^j, \quad j = 1, ..., n \tag{2.12}$$

are conserved by the time evolution since

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\operatorname{Tr}(L^m) =& m \operatorname{Tr}\left(L^{m-1}\dot{L}\right) \\
=& m \operatorname{Tr}\left(L^{m-1}[M, L]\right) \\
=& m \operatorname{Tr}\left(L^{m-1}ML - L^{m-1}LM\right) \\
=& m \operatorname{Tr}(ML^m) - m \operatorname{Tr}(ML^m) \\
=& 0
\end{aligned} \tag{2.13}$$

1D Harmonic Oscillator The Lax pair of a standard harmonic oscillator [9] can be found to be

$$L = \frac{1}{2}\begin{pmatrix} p & \omega q \\ \omega q & -p \end{pmatrix}, \quad M = \frac{1}{2}\begin{pmatrix} 0 & -\omega \\ \omega & 0 \end{pmatrix} \tag{2.14}$$

The equation of motion 2.11 is satisfied and we can find the Hamiltonian as the trace of L^2

$$\mathrm{Tr}(L^2) = \frac{1}{4}\,\mathrm{Tr}\begin{pmatrix} p^2+\omega^2 q^2 & 0 \\ 0 & p^2+\omega^2 q^2 \end{pmatrix} = \frac{p^2}{2} + \frac{\omega^2 q^2}{2} \tag{2.15}$$

Assuming that L can be diagonalized by a matrix U

$$L = U\Lambda U^{-1} \tag{2.16}$$

Then we can recast the evolution equation 2.11 as

$$\dot{\Lambda} = [B, \Lambda] = 0 \tag{2.17}$$

so we get an equivalent set of conserved charges given by the n eigenvalues of L.

Now we have to determine if the conserved charges are in involution. Since we want to compute the Poisson brackets between function-valued matrices we need to introduce some notation first.

Given $A, B \in \mathcal{M}$, the space of $\mathcal{F}$-valued $n \times n$ matrices, we can define a Poisson bracket as a map $\mathcal{M} \otimes \mathcal{M} \to \mathcal{M} \otimes \mathcal{M}$ given by

$$\{A, B\} = \sum_{\alpha\beta} \{A_\alpha, B_\beta\}\, E_\alpha E_\beta \tag{2.18}$$

where E_α is a basis for $\mathcal{M}$ [7].

Theorem 2.1.2 *The eigenvalues of L are in involution if and only if there exists $r \in$*

$\mathcal{M} \otimes \mathcal{M}$ *such that*

$$\{L_1, L_2\} = [r_{12}, L_1] - [r_{21}, L_2] \tag{2.19}$$

where the indices refer to which space in the tensor product the matrix operates on, e.g. $A_3 = I \otimes I \otimes A \otimes I ... I$, and r_{21} is the permutation of r_{12}.

If the matrix r is constant the Jacobi identity gives as a constraint the following equation

$$[r_{12}, r_{13}] + [r_{12}, r_{23}] + [r_{32}, r_{13}] = 0 \tag{2.20}$$

If $r_{12} = -r_{21}$ this condition is called the classical Yang-Baxter equation and r is called the classical r-matrix.

When dealing with systems with an infinite number of degrees of freedom this construction is no longer adequate but we can augment it by introducing a non-physical spectral parameter $z \in \mathrm{C}$ such that $L = L(z), M = M(z)$; this is done to avoid the use of infinite dimensional matrices.

The equation of motion remains the same but the Yang-Baxter equation becomes:

$$[r_{12}(z_1 - z_2), r_{13}(z_1)] + [r_{12}(z_1 - z_2), r_{23}(z_2)] + [r_{13}(z_1), r_{23}(z_2)] = 0 \tag{2.21}$$

where we assumed that the r-matrix is antisymmetric and that it depends only on the difference of the spectral parameters.

To find the conserved charges we need to define a new quantity, the transfer matrix

$$t(z) = \mathrm{Tr}\, L(z) \tag{2.22}$$

Since the transfer matrix is defined in terms of $L(z)$ it's conserved in time and in involution with itself

$$\{t(z_1), t(z_2)\} = 0 \tag{2.23}$$

So if we expand the transfer matrix in terms of its spectral parameter

$$t(z) = \sum_{i=1} Q_i z^i, \quad i \in \mathrm{Z}^+ \tag{2.24}$$

we find an infinite number of conserved charges Q_i in involution and independent of the spectral parameter.

2.2 Quantum Integrability

A notion of integrability is present also in quantized systems, although a precise definition of what it means for a quantum system to be integrable is still up for debate. Mimicking the classical construction we can require the existence of a set of N independent and local charges in involution, where N is the number of degrees of freedom. Both the requirement of locality and independence are not trivial to define clearly in a quantized system [7]. Since we will study spin chain we can give a widely accepted definition of integrable spin chain: a local quantum spin chain model is integrable if there exists infinitely many local conserved quantities in involution and whose densities are local with respect to each other [8][10].

We can extend the formalism that we developed in the classical case can to give a recipe to build the conserved charges of a system given a quantum R-matrix. The method is called Quantum Inverse Scattering method (QISM) [11].

Let's consider a chain of N sites, where each site is described by the standard Hilbert space of a spin-$\frac{1}{2}$ system, $\mathcal{H}_i = \mathbb{C}^2$. The total Hilbert space therefore is the tensor product $\mathcal{H} = \bigotimes_{i=1}^{N} \mathbb{C}^2$ and the Hamiltonian of the chain $H = H(\sigma_k^\alpha)$ will depend on the spin operators $\sigma_k^\alpha = I \otimes ... \otimes \sigma^\alpha \otimes ... \otimes I$ with $\alpha = x, y, z$, where the lower index refers to the site on the chain on which the operator acts.

As we can easily deduce the σ_k^α can be represented by $2^N \times 2^N$ matrices, hence the Hamiltonian will also be a $2^N \times 2^N$ matrix [12].

The basic approach to solve this system would be to diagonalize the Hamiltonian, numerically or analytically, to find the energy spectrum; but, as the length of the chain grows, it becomes unwieldy and ultimately impossible to diagonalize explicitly so other tools were developed, like QISM.

Let's introduce an operator $\mathcal{L}_{a,i}(z_i)$ called the Lax operator that acts on the tensor product $\mathcal{V}_a \otimes \mathcal{H}_i$ of an auxiliary space $\mathcal{V}_a$, normally identified as $\mathbb{C}^2$, and the Hilbert space of a single lattice site. The introduction of a non-physical space seems arbitrary but it will be fundamental to obtain the conserved charges [13].

The Lax operator is given as the solution of the RLL equation:

$$R_{ab}(z_a, z_b)\mathcal{L}_{a,j}(z_a)\mathcal{L}_{b,j}(z_b) = \mathcal{L}_{b,j}(z_b)\mathcal{L}_{a,j}(z_a)R_{ab}(z_a, z_b) \tag{2.25}$$

The operator $R_{ab}(z_a, z_b)$, called the R-matrix, acts non-trivially on the tensor product $\mathcal{V}_a \otimes \mathcal{V}_b$ and as the identity on $\mathcal{H}$ and it must be a solution of the quantum Yang-Baxter equation:

$$R_{ab}\left(z_a, z_b\right) R_{ac}\left(z_a, z_c\right) R_{bc}\left(z_b, z_c\right) = R_{bc}\left(z_b, z_c\right) R_{ac}\left(z_a, z_c\right) R_{ab}\left(z_a, z_b\right) \tag{2.26}$$

There is no general, algorithmic way to find the R-matrix of a given model so class of solutions of the YB equation were found using tools from the theory of quantum groups. Notice that, given a R-matrix, there are many possible Lax operators that are solution of the RLL equation; one operator that is always the solution is the R-matrix itself.

We can perform a "classical" limit of the quantum R-matrix as follows

$$R_{ab}(z_a, z_b) = k(z_a, z_b)(\mathbb{I}_{ab} + \hbar r_{ab}(z_a, z_b) + \mathcal{O}(\hbar^2)) \tag{2.27}$$

where we find $r_{ab}(z_a, z_b)$, a classical r-matrix, and $k(z_a, z_b)$ is a scalar function.

If the R-matrix depends only on the difference of the spectral parameters

$$R_{ab}(z_a, z_b) = R_{ab}(z_a - z_b) \tag{2.28}$$

it is said to be of difference form.

Taking the ordered product of the Lax operators at every lattice sites we can define a new operator, the monodromy matrix:

$$T_a(z_a) = \mathcal{L}_{a,N}(z_a)\mathcal{L}_{a,N-1}(z_a)...\mathcal{L}_{a,1}(z_a) \tag{2.29}$$

It is also possible to choose the opposite order for the product

$$\bar{T}_a(z_a) = \mathcal{L}_{a,1}(z_a)\mathcal{L}_{a,2}(z_a)...\mathcal{L}_{a,N}(z_a) \tag{2.30}$$

The monodromy matrix is a 2×2 matrix in the space V_a such that $T^{ij}(z)$ are operators acting in the total Hilbert space $\mathcal{H}$ of the chain. In the standard notation [14]

$$T(z) = \begin{pmatrix} A(z) & B(z) \\ C(z) & D(z) \end{pmatrix} \tag{2.31}$$

Due to the RLL equation the monodromy matrix automatically satisfies the following relation, called RTT equation

$$R(z_a, z_b)(T(z_a) \otimes \mathbf{1})(\mathbf{1} \otimes T(z_b)) = (\mathbf{1} \otimes T(z_b))(T(z_a) \otimes \mathbf{1})R(z_a, z_b) \tag{2.32}$$

It holds on the product of three spaces: $V_a \otimes V_b \otimes \mathcal{H}$, where $T(z_a)$ acts on $V_a \otimes \mathcal{H}$.

We can add back the indices to make it clearer which auxiliary space every operator is

acting on

$$R_{ab}(z_a, z_b)T_a(z_a)T_b(z_b) = T_b(z_b)T_a(z_a)R_{ab}(z_a, z_b) \tag{2.33}$$

If we multiply the RTT equation by $R^{-1}_{ab}(z_a, z_b)$ from the right and we take the trace on $V_a \otimes V_b$ we obtain

$$\mathrm{Tr}_{ab}\left[T_a(z_a)T_b(z_b)\right] = \mathrm{Tr}_{ab}\left[T_b(z_b)T_a(z_a)\right] \tag{2.34}$$

but since the trace of the tensor product is equal to the product of the traces we find

$$\mathrm{Tr}_a\, T_a(z_a)\, \mathrm{Tr}_b\, T_b(z_b) = \mathrm{Tr}_b\, T(z_b)\, \mathrm{Tr}_a\, T_a(z_a) \tag{2.35}$$

where

$$\mathcal{T}(z) = \mathrm{Tr}\, T(z) = A(z) + D(z) \tag{2.36}$$

is called transfer matrix [15].

We can expand the operator $\mathcal{T}(z)$ in a power series over z centered in some point z_0

$$\mathcal{T}(z) = \sum_i (z - z_0)^i Q_i \tag{2.37}$$

to find the coefficients Q_i: this are commuting operators acting on $\mathcal{H}$ and correspond to the conserved charges of the chain.

Sometimes instead we can use the logarithm of the transfer matrix [16]

$$log\mathcal{T}(z) = \sum_i (z - z_0)^i Q_i \tag{2.38}$$

so that the charges can be found as the logarithmic derivative of the trasnfer matrix

$$Q_\alpha = \frac{d^{\alpha-1}}{dz^{\alpha-1}} \log \mathcal{T}(z)|_{z=z_0} \tag{2.39}$$

For most physical systems the R-matrix is regular, that is it satisfies the following condition

$$R_{ab}(z,z) = k\mathcal{P}_{ab} \tag{2.40}$$

where $\mathcal{P}_{ab}$ is the permutation operator that acts on $V_a \otimes V_b$. Such condition imply that the momentum is a conserved charge or, equivalently, the tower of conserved charges commutes with the operator of cyclic permutations.

XXZ model To give an example of the QISM construction let's consider the XXZ periodic spin chain [8], with Hamiltonian given by

$$\mathcal{H} = -\frac{J}{2}\sum_{i=1}^{N}(\sigma_i^x\sigma_{i+1}^x + \sigma_i^y\sigma_{i+1}^y + \Delta\sigma_i^z\sigma_{i+1}^z) \tag{2.41}$$

The model is local and has nearest neighbour interaction. The R-matrix is given by

$$R(z) = \begin{pmatrix} \sinh(z+\eta) & 0 & 0 & 0 \\ 0 & \sinh z & \sinh\eta & 0 \\ 0 & \sinh\eta & \sinh z & 0 \\ 0 & 0 & 0 & \sinh(z+\eta) \end{pmatrix} \tag{2.42}$$

where z is the spectral parameter and η is related to Δ.
This matrix is of difference form, it satisfies the YB equation and it's regular since

$$R(0) = \sinh\eta\mathcal{P} \tag{2.43}$$

We assume as the Lax operator the following solution of the RLL equation

$$\mathcal{L}_{\alpha,i}(z) = \begin{pmatrix} \sinh(z+\frac{\eta}{2}(1+\sigma_i^z)) & \sigma_i^- \sinh(\frac{\eta}{2}) \\ \sigma_i^+ \sinh(\frac{\eta}{2}) & \sinh(z+\frac{\eta}{2}(1-\sigma_i^z)) \end{pmatrix} \tag{2.44}$$

Since the Lax operator $\mathcal{L}_{\alpha,i}(0) \propto \mathcal{P}_{\alpha,i}$ and so $\mathrm{Tr}_\alpha \mathcal{L}_{\alpha,i}(0) \propto \mathbb{I}_i$ then the first conserved charge is

$$Q_1 = \log \mathcal{T}(0) = (\sinh \eta)^N \mathcal{P}_{12} \dots \mathcal{P}_{N-1,N} = i\hat{\mathbb{P}} \tag{2.45}$$

which correspond to the momentum. The second charge is

$$Q_2 = \frac{d}{dz} \log \mathcal{T}(z)|_{z=0} = \mathcal{T}^{-1}(0)\mathcal{T}'(0) \tag{2.46}$$

This is longer to compute so let's consider only $N = 3$, then

$$\begin{aligned} Q_2 =& (\sinh^{-3} \eta \mathcal{P}_{23}\mathcal{P}_{23}\mathcal{P}_{12})(\mathrm{Tr}_\alpha(\mathcal{L}'_{\alpha,3}(0)\mathcal{L}_{\alpha,2}(0)\mathcal{L}_{\alpha,1}(0) + \\ &+ \mathrm{Tr}_\alpha(\mathcal{L}_{\alpha,3}(0)\mathcal{L}'_{\alpha,2}(0)\mathcal{L}_{\alpha,1}(0) + \mathrm{Tr}_\alpha(\mathcal{L}_{\alpha,3}(0)\mathcal{L}_{\alpha,2}(0)\mathcal{L}'_{\alpha,1}(0)) \\ &= \frac{1}{\sinh \eta}(\mathcal{P}_{23}\mathcal{L}'_{23}(0) + \mathcal{P}_{12}\mathcal{L}'_{12}(0) + \mathcal{P}_{31}\mathcal{L}'_{31}(0)) \\ &= \sum_{i=1}^{3} \mathcal{P}_{i,i+1}\mathcal{L}'_{i,i+1}(0) = \mathcal{H} \end{aligned} \tag{2.47}$$

In a similar way we can compute the analytic expression for every conserved charge.

Chapter 3

Cellular Automata

First developed in the 1950s by Von Neumann and Ulam, a cellular automaton is one of the simplest, non-trivial, dynamical systems that can be built: it's composed of a discrete set of identical cells defined on a lattice. The cellular automaton evolves in discrete time steps according to a local transition rule that is homogeneous in space and time and depends on the state of neighbouring cells only, ensuring a finite propagation speed.

From a physical point of view we can interpret cellular automata in a twofold way. First we can use them as a discretization of a dynamical system originally defined on the continuum, as we will do in the case of spin chains; second, we can build cellular automata as original models for physical phenomena.

Even by considering just the simplest class of cellular automata, they can display a great variety of behaviours, including integrability [17][18].

3.1 Classical Automata

A cellular automaton is a fully discretized system, both in space and time, which evolves thanks to a local rule that is fixed for every point in space and time.

Let's consider a simple example: we take a one dimensional lattice of length N such that

every lattice site $x = 1, \ldots, N$ can assume the value $c_x = 0$ or $c_x = 11$; then we choose a function such that the value of the site x at time $t + 1$ is given by

$$f_x(c_{x-1}, c_x, c_{x+1}) = c_x + c_{x+1} + c_{x-1}$$

where the function depends on the value of the site $x + 1$ and $x - 1$ and we implicitly assume a $\bmod 2$ in the sum. So, if we have $c_{x-1} = 0, c_x = 1, c_{x+1} = 0$ then $f_x(0, 1, 0) = 1$ is the new value of the site x at the next time step.

If we apply this function to every point in the lattice we obtain the single-step time evolution of the lattice and thus we defined a classical cellular automaton, in particular an elementary cellular automaton, that we will describe later in more details.

The formal definition of a cellular automaton (CA) is a set of 4 elements $(L, \Sigma, \mathcal{N}, f)$ such that:

- L is a d-dimensional space, normally a lattice indexed by integers so $L = \mathbb{Z}^d$
- Σ is a finite set of possible cell states with the cardinality $|\Sigma|$ being called the cell dimension
- $\mathcal{N}_x \subseteq L$ is a finite neighborhood scheme such that $\mathcal{N}_x = \mathcal{N}_y \quad \forall x, y \in L$
- we call classical configuration a function $c : L \to \Sigma$ that assigns an element of Σ to each lattice point, so that the space of all configurations is Σ_L
- $f_x : \Sigma_{\mathcal{N}_x} \to \Sigma_x$ is a local transition rule that evolves the state of the cell x from time t to $t + 1$

So the local transition function f_x takes the states of the neighbours $\mathcal{N}_x$ of x at the current timestep $t \in \mathbb{Z}$ and it determines the state of x at time $t + 1$.

By considering the local transition rule for every $x \in L$ we can derive a global transition rule:

$$f : \Sigma_L \to \Sigma_L \quad f(c)(x) = f_x\left(\{c(y); y \in N_x\}\right)$$

Notice that CAs are homogeneous in space, since the local transition function is the same for every cell, and they are also homogeneous in time, since $f \neq f(t)$.

Le The connection between the local transition function and the global behaviour of the CA is the most important and most complex question to study, and if we want to relate CA to a physical systems there are first a few issues to resolve.

First, we want to understand if CAs admit some notion of reversibility, since it's a fundamental property of the microscopic physical systems that we want to simulate.

We can find two notion of reversability:

- standard reversability: a CA is said to be reversible if the global map f is bijective
- structural reversability: a CA is said to be structurally reversible if it is reversible and the inverse map is still a CA

Clearly the most interesting definition is the second one. While in the quantum setting this two notions of reversability are equivalent, there are examples of classical CA which have a non-local inverse map (for example see [19]).

It has been proven by Amoroso and Pratt in [20] that, for one-dimensional CAs, there exist algorithms based on the automaton local rule to determine if it's bijective, and so reversible. This result does not generalize to higher dimensions but it's not an issue since we will consider only one-dimensional CA in a standard lattice so $L = \mathbb{Z}$. This will also greatly simplify the general structure since neighborhood schemes are only classified by their length in one dimension.

Another important issue regarding classical cellular automata is if we can build it using local operations on the cells. We say that an automaton is locally implementable if its single step evolution $t \to t+1$ can be decomposed in a finite sequence of local operations on non-overlapping groups of cells called blocks.

For example we could build a localized automaton via Margolous block structure: an automaton has Margoulous block structure if the single time step is implemented by

a finite number of layers of local transformations; in each layer cells are grouped into non-overlapping blocks and each block undergoes a local transformation, where in each layer the blocks are identical.

It has been proven [21] that all of the structurally reversible CAs in one (and two) dimensions admit a Margolous block realization with no more than two (four) layers, combined with shift-like transformations.

3.1.1 Elementary Automata

The simplest examples of CA are characterized by a one dimensional space ($L = \mathbb{Z}$), only two possible states for a cell ($\Sigma = 0, 1$) and only nearest neighbours "interactions" ($\mathcal{N}_x = \{x-1, x, x+1\}$). There are exactly 256 possible local transition functions, since there are 8 combinations of states in $\mathcal{N}_x$ and $2^8 = 256$. The name of the elementary CA is given by their rule: since the local transition function can be expressed as an 8 bit code, ranging from 00000000 to 11111111, we can translate from binary to decimals obtaining a number from 0 to 255, which is the name of the CA.

This CA have been classified by Wolfram [22] in four qualitative categories depending on their large scale behaviour:

- the evolution leads to a homogeneous state (e.g. rule 0,4,16)
- the evolution leads to a set of separated, simple, stable or periodic structures (e.g. rule 8, 56, 40)
- the evolution leads to a chaotic pattern (e.g. rule 6,22,46)
- the evolution leads to complex localized structures, sometimes long-lived (e.g. rule 20, 52)

We give some examples in figure 3.1 Given that the state of the cell at position x is $c(x) = c_x$ the local transition rule will be a function of the two nearest neighbours so

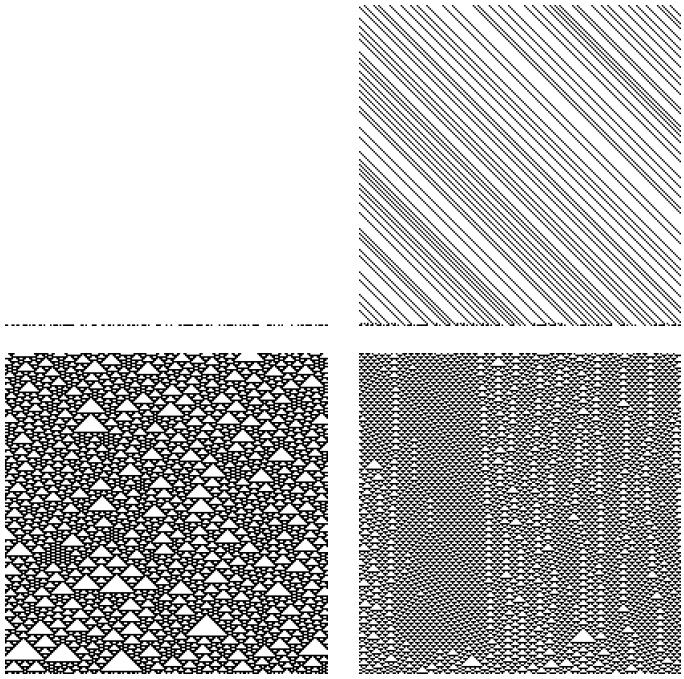

Fig. 3.1. Examples of CA for the four classes with random initial conditions. Up-Left: Rule 0, Class I; Up-Right: Rule 24, Class II; Down-Left: Rule 126, Class III; Down-Right: Rule 54, Class IV.

$c'_x = f_x(c_{x-1}, c_x, c_{x+1})$, where the apex in c'_x indicates that it's the time-evolved state of the cell x . To find the most interesting CA we consider a light-cone lattice and we enforce two symmetry constraints [3]:

- left-right symmetry: $f_x(c_{x+1}, c_x, c_{x-1})$
- up-down symmetry: if $c'_x = f_x(c_{x-1}, c_x, c_{x+1})$ then $c_x = f_{x'}(c_{x-1}, c'_x, c_{x+1})$

These constraints reduce the number of possible CA to 8: rule 204, 51, 150, 105, 108, 147, 54 and 201. We can further reduce these elementary CAs by rewriting the local transition rule using a different parametrization. Consider the maps $c'_x = c_x + \theta_x(c_{x-1}, c_{x+1})$, if we require that $\theta_x(c_{x-1}, c_{x+1}) = \theta_x(c_{x+1}, c_{x-1})$ (i.e. left-right symmetry) then the maps depends only on 8 combinations of states and with the identification $f_x(c_{x-1}, c_x, c_{x+1}) = c_x + \theta_x(c_{x-1}, c_{x+1})$ we recover the exact 8 CAs as before.

We can explicitly write our new eight possible local transition functions:

$$\begin{aligned}
&204\text{: } \theta^0 = 0, && 108\text{: } \theta^4 = c_{x-1}c_{x+1},\\
&51\text{: } \theta^1 = 1, && 147\text{: } \theta^5 = c_{x-1}v_{x+1} + 1,\\
&150\text{: } \theta^2 = c_{x-1} + c_{x+1}, && 54\text{: } \theta^6 = c_{x-1}c_{x+1} + c_{x-1} + c_{x+1},\\
&105\text{: } \theta^3 = c_{x-1} + c_{x+1} + 1, && 201\text{: } \theta^7 = c_{x-1}c_{x+1} + c_{x-1} + c_{x+1} + 1,
\end{aligned}$$

The four rules on the left are affine, since they contain only sums of the states, while on the right we have also products of states. By exchanging the two states $\{0\} \leftrightarrow \{1\}$ we can see that $\theta^4 \simeq \theta^7$, $\theta^5 \simeq \theta^6$, $\theta^0 \simeq \theta^1$ and $\theta^2 \simeq \theta^3$ so we get only four inequivalent CAs: rule 54, 201, 150 and 51. Rule 51 is trivial while Rule 108 does not have an interacting dynamics. Indeed, by interpreting the 0's as the vacuum and the 1's as a particle, we can see that the world-lines of the particles are vertical, i.e. they are at rest.
Instead rule 54 shows something much more interesting: in figure 3.2 we can see particles moving towards the left (left-movers) and particles moving towards the right (right-movers) in a straight line. When a left-mover and a right-mover interacts the two particles pass through each other, but with a time shift (a shift of one lattice point upward), a scattering behaviour typical of solitonic and other integrable systems.

This similarity is more qualitative then quantitative but it spurred the curiosity towards possible relationships between integrable lattice systems and cellular automata. But to explore possible links we need to introduce first quantum cellular automata.

3.2 Quantum Automata

Formally the only difference between a classical and quantum CA lies in the fact that each lattice point $x \in L$ can take as value an element of a basis Σ of an Hilbert space $\mathcal{H}_x$. Naturally the local transition map will become an operator that will act on an appropriate tensor product of $\mathcal{H}_x$ and this operator must be unitary. For this reason the

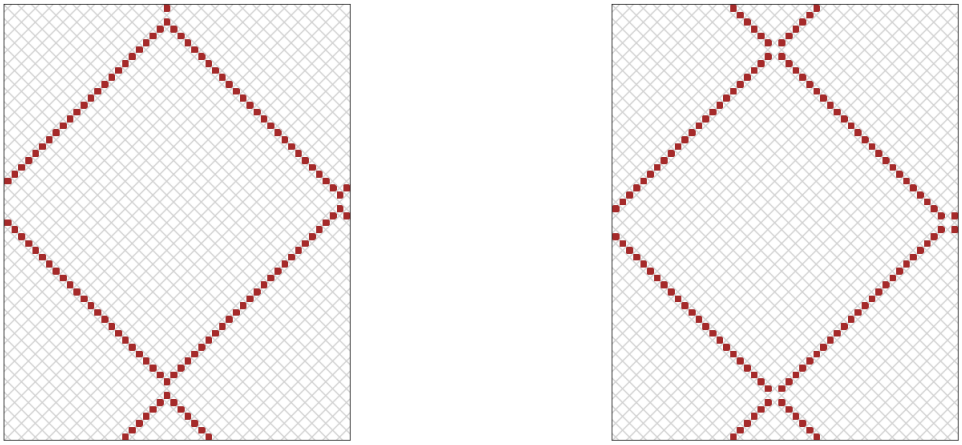

Fig. 3.2. Evolution of Rule 54 (left) and Rule 150 (right) in a light-cone lattice with two initial points. Notice the difference in the interaction between the two propagating particles.

operator itself is also called unitary.

To be precise a quantum cellular automaton is a set of 4 elements $(L, \Sigma, \mathcal{N}, U_x)$ such that:

- L is a d-dimensional space, normally a lattice indexed by integers so $L = \mathbb{Z}^d$
- Σ is a finite set of (orthogonal) basis states
- $\mathcal{N}_x \subseteq L$ is a finite neighborhood scheme such that $\mathcal{N}_x = \mathcal{N}_y \quad \forall x, y \in L$
- $U_x \in U(\bigotimes_{\mathcal{N}_x} \mathcal{H}_x)$ is a unitary operator that acts on the tensor product of the Hilbert spaces of every point $y \in \mathcal{N}_x$ and it evolves the state of the site in $x \in L$

We must further require that the local evolution operator must commute with translations of itself along the lattice:

$$[U_x, U_y] = 0 \quad \forall x, y \in L$$

so that we can apply the local operators in parallel on L without worrying about ordering ambiguities or issues with simultaneity.

The global evolution then can be described as

$$U = \prod_x U_x$$

which is a well defined operator on L.

Technically this description is not general enough to accommodate all possible quantum CAs: for example, considering $L = \mathbb{Z}$, it's not possible to define a unitary operator that implements a simple shift. This is related to the fact that in the classical case, when we are updating the lattice, we are formally conducting two operations at once: we are first reading (and storing) the current state of the cell and then we are updating the value of the cell based on the rule. In a quantum system we must thread more carefully, due to the no-cloning theorem; we can circumvent the issue by adding ancillary spaces to store the necessary informations and by using two different operators, one for reading the current state of the lattice and performing the computation, and one for updating each cell with the new value. In the model that we will see further along the updating operator will simply be given by the identity operator so it will not be explicitly shown.

The issues that we have shown regarding reversibility in a classical CA do not appear in the quantum case due to the unitarity of the time evolution. In fact a quantum CA with neighborhood scheme $\mathcal{N}_x$ and global evolution U is always structurally reversible with the inverse CA having the time evolution given by U^{-1} and scheme $\mathcal{N}_x = x - \mathcal{N}_x$.

The structure of a quantum CA has a lot of similarities to the standard description of quantum circuits. Indeed, it has been build has a possible alternative model of computation. Further, it has been proven that a quantum CA can be simulated by a quantum circuit and vice-versa, thereby giving us an efficient and simple tool to write explicitly the local evolution operators in term of unitary quantum gates, as we will see.

In this work we will focus in particular on 1-dimensional, finite CAs with periodic boundary conditions with neighborhoods of length three and four. We will be interested in understanding the relations between the local evolution and possible global phenomena like integrability and diffusive transport at the mesoscopic level. To do this we will study which physical system, if any, we get in the continuous-time limit.

3.2.1 Brickwork QCA

A small extension of the previous framework is given by brickwork quantum cellular automata [23]. This models are characterized by a discrete and periodic time evolution (Floquet system), namely the unitary gates are time dependent and the global evolution operator is periodic.

Let's consider a time dependent unitary operator

$$U^{(l)}_{x_k+\Delta_t} \tag{3.1}$$

Here in the apex we indicate the length of the neighbourhood. This operator acts on the site $x_k + \Delta_t$ where Δ_t is a time-dependent displacement.

Then we build the global evolution operator at time t as

$$\mathcal{V}_t = \prod_k U^{(l)}_{x_k+\Delta_t} \tag{3.2}$$

and the global evolution operator with time period τ as

$$\mathcal{V} = \mathcal{V}_\tau \dots \mathcal{V}_1 \tag{3.3}$$

In the cases of interest to us the unitaries $U_x(u)$ depend on a parameter, called spectral parameter, that has some special points of physical interest:

- for $u \to 0$ we have $U^l_j(u) = 1 + iuh_{j,\dots,j+l-1} + \mathcal{O}(u^2)$ where $h_{j,\dots,j+l-1}$ is an Hermitian

operator acting on the cells $j, \ldots, j+l-1$ that we will identify as the Hamiltonian density

- for some models there exists a $u = u_0$ such that $U_j^l(u_0) \sim \mathcal{P}$ is a permutation (with a possible phase), so the unitary operator becomes deterministic and the QCA reduces to a classical cellular automaton

In the first case the global Hamiltonian is obtained by Taylor expanding the global evolution operator around zero

$$\mathcal{V} = 1 + iucH + \mathcal{O}(u^2) \tag{3.4}$$

such that $H = \sum_j h_{j,\ldots,j+l-1}$.
Let's consider an explicit example.

Folded XXZ quantum CA We consider a one dimensional QCA with $\mathcal{H}_j = \mathbb{C}^2$ with basis elements indicated by $|\circ>$ and $|\bullet>$ and length $L = 3k$. The Floquet period is $\tau = 3$.
The local unitary gate acts on three sites and is given by

$$U^{(3)}_{j,j+1,j+2}(u) = P^{\circ}_{j+1} + P^{\bullet}_{j+1} U^{(2)}_{j,j+2}(u) \tag{3.5}$$

where $U^{(2)}$ comes from the R-matrix of the XXZ spin chain at the free fermion point, that is

$$U^{(2)}_{j,j+2}(u) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \operatorname{sech}(u) & i\tanh(u) & 0 \\ 0 & i\tanh(u) & \operatorname{sech}(u) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{3.6}$$

and $P^{\circ,\bullet}$ are projectors on the basis.

It can be proven by direct computation that

$$U^{(3)}_{j,j+2}(u)U^{(3)}_{j,j+2}(-u) = 1, \quad \left(U^{(3)}_{j,j+2}(u)\right)^{\dagger} = U^{(3)}_{j,j+2}(-u) \tag{3.7}$$

so the local operator is actually unitary and it defines a family of quantum cellular automata.

The global evolution operator is given by

$$\mathcal{V}(u) = \mathcal{V}_3(u)\mathcal{V}_2(u)\mathcal{V}_1(u) \tag{3.8}$$

where

$$\mathcal{V}_t(u) = \prod_{j=1}^{k} U^{(3)}_{3j+t} \prod_{j=1}^{k} U^{(3)}_{3j+1+t} \prod_{j=1}^{k} U^{(3)}_{3j+2+t} \tag{3.9}$$

where we can see that, in this case, $\Delta_t = t$.

In the limit $u \to 0$ the local unitaries become trivial

$$U^{(3)}_{j,j+1,j+2} = 1 \tag{3.10}$$

so the total model becomes trivial. If we then consider also what happens at first order we find the expected form

$$U^{(2)}_{j,j+1}(u) = 1 + iu\left(\sigma^-_j\sigma^+_{j+1} + \sigma^+_j\sigma^-_{j+1}\right) + \mathcal{O}\left(u^2\right) \tag{3.11}$$

that leads to

$$U^{(3)}_{j,j+1,j+2}(u) = 1 + iuh_{j,j+1,j+2} + \mathcal{O}\left(u^2\right) \tag{3.12}$$

where

$$h_{j,j+1,j+2} = \sigma^-_j P^{\bullet}_{j+1}\sigma^+_{j+2} + \sigma^+_j P^{\bullet}_{j+1}\sigma^-_{j+2} \tag{3.13}$$

is an Hermitian operator density. Then the global evolution operator gives the global Hamiltonian:

$$\mathcal{V}(u) = 1 + iuH + \mathcal{O}\left(u^2\right) \tag{3.14}$$

This Hamiltonian is the Hamiltonian of the folded XXZ model.

The inverse procedure, starting from a spin chain to obtain a QCA is called Trotterization.

Instead in the $u \to \infty$ limit we get a permutation matrix plus a phase i

$$\lim_{u\to\infty} U^{(2)}_{j,j+2}(u) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & i & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \propto \mathcal{P}_{j,j+2} \tag{3.15}$$

and so the evolution operator of the corresponding classical CA is given by

$$U^{(3)}_j = P^{\circ}_{j+1} + P^{\bullet}_{j+1}\mathcal{P}_{j,j+2} \tag{3.16}$$

Brickwork Elementary CA

Since the update rule for elementary CAs depends on three sites, it will be useful to re-express the rules in the brickwork construction, to make a connection with spin chains [23].

First we need to transform the light-cone lattice in a rectangular lattice by adding new sites to the center of the light-cone plaquettes. Then we impose a local, three-sites update rule $U^{(3)}_{j,j+1.j+2}$ such that it is only the identity or a permutation.

Then the global update rule will have a Floquet period of $\tau = 2$ and it will act alternatively on the odd and even sites under time evolution. So the global rule is given by

$$\mathcal{V} = \mathcal{V}_2\mathcal{V}_1 \tag{3.17}$$

where

$$\mathcal{V}_t = \prod_{j=1}^{L/2} U^{(3)}_{2j+t}, \quad t = 1, 2 \tag{3.18}$$

Since the rule of elementary CAs evolves only the central bit and uses the other two as control bits we can write the local operator as

$$U^{(3)}_{j,j+1,j+2} = \sum_{a,b=\circ,\bullet} P^a_j f^{ab}_{j+1} P^b_{j+2} \tag{3.19}$$

where P^a_j is the projector to the basis state a acting on j and f^{ab}_{j+1} is a collection of four matrices acting on $j+1$.

We note that the local operators overlap at one site in $\mathcal{V}_t$ but, since they act diagonally on the boundary site, the local operators still commute.

The dynamics of the models are determined by the structure of the four matrices f^{ab} but we must impose the same restriction as we did for elementary CAs: up-down symmetry (time reversal) and left-right symmetry (space reflection). This leaves us with two possibilities for the matrices:

$$f^{ab} = 1 \text{ or } f^{ab} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \sigma^x \tag{3.20}$$

Then, in total, there are eight possible elementary CAs. Of these, two are trivial and two are related to the others by an exchange of basis states so we are left with four possibilities:

- Rule 54 $f^{00} = 1, \quad f^{01} = f^{10} = f^{11} = \sigma^x$
- Rule 105 $f^{00} = f^{11} = \sigma^x, \quad f^{01} = f^{10} = 1$
- Rule 105 $f^{00} = f^{11} = 1, \quad f^{01} = f^{10} = \sigma^x$
- Rule 201 $f^{00} = \sigma^x, \quad f^{01} = f^{10} = f^{11} = \sigma^x$

The relation between Rule 150 and 105 is a bit more involved in this formulation. Indeed, their matrices f^{ab} are obtained from each other by a multiplication by σ^x, so

$$\mathcal{V}_t^{(150)} = X_t \mathcal{V}_t^{(105)} = \mathcal{V}_t^{(105)} X_t \tag{3.21}$$

where

$$X_t = \prod_{j=1}^{L/2} \sigma_{2j+t}^x \tag{3.22}$$

and since

$$\left[\mathcal{V}_1^{(105/150)}, X_2\right] = \left[\mathcal{V}_2^{(150)}, X_1\right] = 0 \tag{3.23}$$

we get that the global update operators of the two rules are related by

$$\mathcal{V}^{(150)} = X\mathcal{V}^{(105)}, \quad X = X_2 X_1 = \prod_{j=1}^{L} \sigma_j^x \tag{3.24}$$

and it follows that

$$\left(\mathcal{V}^{(150)}\right)^2 = \left(\mathcal{V}^{(105)}\right)^2 \tag{3.25}$$

We expect that the physical behaviour of the two rules will be the same, up to a staggered global spin reflection.

Following the brickwork approach we found the same results as in the standard classification and we will be able to use this new formulation to connect elementary cellular automata to quantum spin chains.

Chapter 4

Medium Range Spin Chains

The spin chain is a very general setting in which many properties of more complex quantum systems can be studied in a controlled setting, like integrability and topological phases.

We want to focus our study to spin chains with interactions that can span multiple sites, in particular three and four. We will build systems that are integrable by design and we will make a connection between spin chains, quantum cellular automata and classical cellular automata [24].

A medium range integrable spin chain is a model which has an infinite set of commuting local charges $\{Q_\alpha\}$, where $\alpha \in \mathcal{S},\ S \in \mathbb{Z}^+$, such that the lowest dynamical charge, that we suppose is the Hamiltonian, has a range $l \geq 3$. By local operator we mean an operator that has a finite support that does not grow with the length of the system.

We need to require that the charge be dynamical because medium range models can have one and two-site conserved charges, but they will not be able to generate a dynamic on the chain.

A chain with L sites will have a total Hilbert space $\mathcal{H} = \otimes_{j=1}^{L} V_j$ given by the tensor products of the local Hilbert spaces at each site V_j; we will focus on chains with spin $\frac{1}{2}$ and periodic boundary conditions so $V_j = \mathbb{C}^2$, but the framework can accommodate any

spin.

The basis for spin $\frac{1}{2}$ Hilbert space is the standard one with spin up and spin down but we will use the notation $|\circ\rangle$ for spin down (empty site) and $|\bullet\rangle$ for spin up (occupied site). We will use the standard Pauli matrices $\sigma^{x,y,z}$ and ladder operators $\sigma^{\pm}$. We will indicate the projectors onto the basis as

$$P^{\circ} = P^{0} = \frac{1+\sigma^{z}}{2}, \quad P^{\bullet} = P^{1} = \frac{1-\sigma^{z}}{2} \tag{4.1}$$

Further, we will indicate with $\mathcal{O}(j)$ a local operator $\mathcal{O}$ that has finite support starting from the site j, with its range given by $|\mathcal{O}(j)| = l$ if the support is on the sites $[j, \dots, j+l-1]$.

Finally, we will consider Hamiltonians that are translationally invariant.

4.1 Nearest neighbour

First we want to see how integrability structures develop naturally for nearest neighbor chains. We focus only on Hamiltonians given by local Hamiltonian densities

$$H = \sum_{j} h(j) \tag{4.2}$$

where $h(j)$ is a local operator with some range l.

The tower of conserved charges is given by a set of operators $\{Q_{\alpha}\}$ such that it's extensive and composed by local charge densities

$$Q_{\alpha} = \sum_{j} q_{\alpha}(j) \tag{4.3}$$

Notice that it's not the only possibility, we could also construct integrable chains with quasi-local charges.

We require that $H = Q_\alpha$ for some α and that all the charges must commute

$$[Q_\alpha, Q_\beta] = 0 \tag{4.4}$$

If these conditions are met we can normally choose the label of the charge as the support of the charge density:

$$|q_\alpha(j)| = \alpha \tag{4.5}$$

In the case of the nearest neighbour (n.n.) models then we have

$$Q_2 = H, \quad Q_\alpha \neq 0 \ \forall \alpha > 2 \tag{4.6}$$

If the chain is also symmetric under $U(1)$ then also Q_1 is allowed.
A complete classification already exists, see [25], so we will only show the most common examples:

- $H = \sum_j \left(J_x \sigma_j^x \sigma_{j+1}^x + J_y \sigma_j^y \sigma_{j+1}^y + J_z \sigma_j^z \sigma_{j+1}^z\right)$ is the XYZ model
- $H = \sum_j \left(J_x \sigma_j^x \sigma_{j+1}^x + J_x \sigma_j^y \sigma_{j+1}^y + J_z \sigma_j^z \sigma_{j+1}^z + h_z \sigma_j^z\right)$ is the XXZ model, special point $J_x = J_y$ of XYZ, with magnetic field h_z (symmetric under $U(1)$)
- $H = J \sum_j \left(\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \sigma_j^z \sigma_{j+1}^z + h_z \sigma_j^z + h_x \sigma_j^x + h_y \sigma_j^y\right)$ is the Heisenberg model, special point $J_x = J_y = J_z$ of XYZ, with magnetic field h_x, h_y, h_z (symmetric under $SU(2)$)
- $H = \sum_j \left(J_x \sigma_j^x \sigma_{j+1}^x + J_y \sigma_j^y \sigma_{j+1}^y + h_z \sigma_j^z\right)$ is the XYh model
- $H = \sum_j \left(J_x \sigma_j^x \sigma_{j+1}^x + h_z \sigma_j^z\right)$ is the Ising chain

N.n. models satisfy a property called the Reshetikhin condition on integrability, here reported in a general formulation:

Theorem 4.1.1 *Reshetikhin Conjecture 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*

$$q_3(j) = [h(j), h(j+1)] + \tilde{h}(j) \tag{4.7}$$

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

The conjecture is very restrictive, since it requires that a three-site operator must be built only from two-site operators, but, unfortunately, it does not have a proof, we can only prove the reverse implication.

We further conjecture that, when the R-matrix is of difference form, $\tilde{h} = 0$.

4.1.1 Integrability

As we outlined earlier we need an auxiliary space $V_a = \mathbb{C}^2$ and a Lax operator $\mathcal{L}_{a,j}$ that acts on the tensor product $V_a \otimes \mathcal{H}_j$ of an auxiliary space and a physical space. We will also need an R-matrix $R_{a,b}(u, v)$ that satisfies a Yang-Baxter equation and a regularity property:

$$R_{ab}(u, u) \sim \mathcal{P}_{ab} \tag{4.8}$$

where $\mathcal{P}_{ab}$ is the permutation operator acting on $V_a \otimes V_b$.

If the R-matrix satisfies then regularity condition the it also satisfies the following relation

$$R_{ab}(\lambda, \mu) R_{ba}(\mu, \lambda) \sim 1 \tag{4.9}$$

called inversion property, where

$$R_{ba}(\mu, \lambda) = \mathcal{P} R_{ab}(\mu, \lambda) \mathcal{P} \tag{4.10}$$

Since we can always use the R-matrix as a Lax operator we impose

$$\mathcal{L}_{a,j}(\mu) = R_{a,j}(\mu, \xi_0) \tag{4.11}$$

where ξ_0 is a fixed parameter.

The regularity condition of the R-matrix then implies the initial condition

$$t(\xi_0) = \mathcal{U} \tag{4.12}$$

If the R-matrix is of difference form

$$R(u, v) = R(u - v) \tag{4.13}$$

then the parameter ξ_0 is irrelevant and it can be set to zero.

Let's compute the first two charges, to verify if the Reshetikin condition holds. We will use the log formula:

$$Q_\alpha = \partial_u^{(\alpha-1)} \log(t(u))|_{u=\xi_0} \tag{4.14}$$

We find that the second charge Q_2, the Hamiltonian, is given by

$$H = Q_2 = \sum_j h_{j,j+1} = \sum_j (\partial_u \tilde{\mathcal{L}}_{j,j+1}(u)|_{u=\xi_0}) \tag{4.15}$$

where

$$\tilde{\mathcal{L}}_{j,j+1}(u) = \mathcal{P}_{j,j+1}\mathcal{L}_{j,j+1}(u) \tag{4.16}$$

is the braided Lax operator.

The third charge is given by

$$Q_3 = \sum_j [h_{j,j+1}, h_{j+1,j+2}] + \tilde{\mathcal{L}}''_{j,j+1}(\xi_0) - h^2_{j,j+1} \tag{4.17}$$

We see that the first term is the commutator and the second is composed by two-sites operators, thereby verifying the Reshetikinn conjecture. Further, if the R-matrix is of difference form, the Lax braided Lax operator satisfies

$$\tilde{\mathcal{L}}(u)\tilde{\mathcal{L}}(-u) = 1 \tag{4.18}$$

and so the third charge reduces to

$$Q_3 = \sum_j [h_{j,j+1}, h_{j+1,j+2}] \tag{4.19}$$

4.2 Three site models

4.2.1 Integrability

First let's focus on models with $l = 3$, in which case

$$H = Q_3 = \sum_j h_{j,j+1,j+2}$$

where $h_{j,j+1,j+2}$ is a three site Hamiltonian density. To help us classify these Hamiltonian we use a generalization of the Reshetikhin condition:

Theorem 4.2.1 *A three site Hamiltonian is integrable iff the charge* $Q_5 = \sum_j q_5(j)$ *defined by*

$$q_5(j) = [h_{j,j+1,j+2}, h_{j+1,j+2,j+3} + h_{j+2,j+3,j+4}] + \tilde{h}_{j,j+1,j+2}$$

commutes with the Hamiltonian in every volume $L \geq 5$

This result is very restrictive since we use just two three-site operators to construct a five-site charge.

So to classify three-site models we can make an Ansatz for $h, \tilde{h}$ by also including some free parameters, then we construct Q_5 and we impose the commutation relation $[H, Q_5]$.

Since the most general form of h has 64 free parameters we will just check the subspaces of parameter space that appear to be most physically relevant.

Since we already know how to build the integrable structure for a nearest neighbour chain the best way forward is to map a three site chain to a nearest neighbour chain and we do this by grouping together every two spins into blocks. To make this process possible we consider chains with even length $L = 2k$. Then we pair the spin and we label then using the original coordinates thereby obtaining:

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

where, for example

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

This new model has k sites with dimension d^2 since each n.n. site is the tensor product of two spaces $j \otimes j+1$. In the same way we can construct local n.n. charges by using the charges of the original model, obtaining an integrable n.n. chain.

Let's focus on the n.n. chain: it has a set of commuting local charges so it is reasonable to assume that it's Yang-Baxter integrable and so it will have an R-matrix (and an auxiliary space V_A) which generates the charges. The auxiliary space will have the same dimensions of the physical spaces so $V_A = V_a \otimes V_b$ where V_a, V_b are isomorphic to the physical spaces of the original chain.

In this way we obtain a commuting set of transfer matrices

$$t(u) = \mathrm{Tr}_A \, R_{A,(L-1,L)}(u,0) \dots R_{A,(3,4)}(u,0) R_{A,(1,2)}(u,0) \tag{4.20}$$

Notice that the R-matrices act on the n.n. spaces and we can expect for it to be regular:

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

The transfer matrix that we built will act as a non local operator on the original Hilbert space but its Taylor expansion will still give us the charges of the original model, by design even though the grouping procedure explicitly breaks translational invariance. Further, given $\mathcal{U}$ the cyclic shift operator of the original chain, that translates the chain to the right by one site, the transfer matrix 4.20 will be invariant under a two-site shift by construction so

$$t(u) = \mathcal{U}^{-2} t(u) \mathcal{U}^2 \tag{4.21}$$

However we know that the original charges are one-site invariant and they are the Taylor coefficients of $t(u)$ so the transfer matrix must also be translationally invariant

$$t(u) = \mathcal{U}^{-1} t(u) \mathcal{U} \tag{4.22}$$

This implies that two different grouping procedures must lead to the same transfer matrix:

$$\mathrm{Tr}_{a,b}\, R_{(a,b),(L-1,L)}(u,0) \dots R_{(a,b),(1,2)}(u,0) = \mathrm{Tr}_{a,b}\, R_{(a,b),(L,1)}(u,0) \dots R_{(a,b),(2,3)}(u,0) \tag{4.23}$$

This, in turn, implies the existence of a Lax matrix for the original chain:

Theorem 4.2.2 *If the condition 4.23 holds in every volume L then the R-matrix of the n.n. chain factorizes as*

$$R_{(a,b),(j,j+1)}(u,0) = \mathcal{L}_{a,b,j+1}(u) \mathcal{L}_{a,b,j}(u) \tag{4.24}$$

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

$$R_{AB}(u,v) \mathcal{L}_{A,j}(u) \mathcal{L}_{B,j}(v) = \mathcal{L}_{B,j}(v) \mathcal{L}_{A,j}(u) R_{AB}(u,v) \tag{4.25}$$

It follows that, if the n.n. R-matrix is regular then

$$\begin{aligned} R_{(1,2),(3,4)}(0,0) =& \mathcal{P}_{2,4}P_{1,3} = \\ =& \mathcal{P}_{2,4}\mathcal{P}_{1,2}\mathcal{P}_{1,2}\mathcal{P}_{1,3} = \qquad (4.26) \\ =& (\mathcal{P}_{1,4}\mathcal{P}_{2,4})(\mathcal{P}_{1,3}\mathcal{P}_{2,3}) = \mathcal{L}_{1,2,4}(0)\mathcal{L}_{1,2,3}(0) \qquad (4.27) \end{aligned}$$

and so the Lax operator satisfies the equivalent regularity condition for three sites:

$$\mathcal{L}_{ab,j}(0) = \mathcal{P}_{a,j}\mathcal{P}_{b,j} \tag{4.28}$$

The RLL equations do not have unique solutions, up to normalization, if the R-matrix is gauge invariant with respect to a spectral parameter dependent $d \times d$ matrix $G_A(u)$

$$[R_{A,B}(u,v), G_A(u)G_B(v)] \tag{4.29}$$

This is due to the fact that, given a gauge invariant R-matrix, the transformed Lax operator $G_A(u)\mathcal{L}_{A,j}(u)$ is also a solution of the RLL equations.

We will focus on R-matrix with no gauge invariance.

So now we can factorize 4.20 as

$$t(u) = \mathrm{Tr}_{a,b}\, \mathcal{L}_{a,b,L}(u) \cdot \mathcal{L}_{a,b,1}(u) \text{ with } t(0) = \mathcal{U}^2 \tag{4.30}$$

and, as we expect, this representation is manifestly translationally invariant.

Now we can define a new operator $\tilde{\mathcal{L}}_{a,b,j}(u)$ such that $\tilde{\mathcal{L}}(0) = 1$ so

$$\mathcal{L}_{a,b,j} = \mathcal{P}_{a,j}\mathcal{P}_{b,j}\tilde{\mathcal{L}}_{a,b,j}(u) \tag{4.31}$$

So if we compute the logarithmic derivative of the transfer matrix

$$H = t^{-1}(0)\partial_u t(u)|_{u=0} = \sum_j h_{j,j+1,j+2} \tag{4.32}$$

$$h_{j,j+1,j+2} = \partial_u \tilde{\mathcal{L}}_{j,j+1,j+2}(u)|_{u=0} \tag{4.33}$$

We can formalize this ideas in the following conjecture:

Theorem 4.2.3 *Every integrable three-site Hamiltonian has a three-site Lax operator of the form*

$$\mathcal{L}_{1,2,3}(u) = \mathcal{P}_{1,3}\mathcal{P}_{2,3}(1 + uh_{123} + \mathcal{O}(u^2)) \tag{4.34}$$

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

$$R_{AB}(u,v)\mathcal{L}_{A,j}(u)\mathcal{L}_{B,j}(v) = \mathcal{L}_{B,j}(v)\mathcal{L}_{A,j}(u)R_{AB}(u,v) \tag{4.35}$$

such that the R-matrix factorizes as 4.24.

We can find immediately two trivial solution of the RLL relation that connect it directly with a n.n. chain:

- $\mathcal{L}_{a,b,j}(u) = \mathcal{L}_{a,j}(u)\mathcal{L}_{b,j}(u)$ where $\mathcal{L}_{a,j}(u)$ is the Lax operator of a n.n. chain. The transfer matrix obtained from this operator is the square of the n.n. transfer matrix
- $\mathcal{L}_{a,b,j}(u) = \mathcal{P}_{a,b}\mathcal{L}_{a,j}(u)$ this leads to two decoupled spin chains in the even and odd sub-lattices with n.n. interaction in each sub-lattice

This examples lead us to believe that the source of the three-site interaction comes from a coupling of the auxiliary spaces which can not be factorized in a trivial way.
To check if theorem 4.2.1 actually holds in this construction we compute the next conserved charge, Q_5. To do this we need to calculate

$$(\partial_u)^2 \log(t(u)) = t^{-1}(u)t''(u) - (t^{-1}(u)t'(u))^2 \tag{4.36}$$

and then substituting $u = 0$. We obtain a five-site operator

$$Q_5 = \sum_j [h_{j,j+1,j+2}, h_{j+1,j+2,j+3} + h_{j+2,j+3,j+4}] - (h_{j,j+1,j+2})^2 + \tilde{\mathcal{L}}''_{j,j+1,j+2}(0) \tag{4.37}$$

This is a generalization of 4.17 to a three-site Hamiltonian. We see that the first term, in the charge, is the commutator and the second is composed of two three-sites operators. This last term cancels if the Lax operator obeys the inversion relation:

$$\tilde{\mathcal{L}}_{a,b,j}(u)\tilde{\mathcal{L}}_{a,b,j}(-u) = 1 \tag{4.38}$$

4.2.2 Classification

We can perform a partial classification of three-site spin chains with spin 1/2 by following these steps:

- make an Ansatz for $h_{j,j+1,j+2}, \tilde{h}_{j,j+1,j+2}$
- compute Q_5 using 4.2.1
- impose the commutation relation $[H, Q_5] = 0$
- make an Ansatz for a three site operator $\mathcal{L}_{a,b,j}(u)$ and compute 4.20
- impose the commutation relation $[H, t(u)] = 0$
- check that $\mathcal{L}_{a,b,j}(0) = \mathcal{P}_{a,j}\mathcal{P}_{b,j}$ and $h_{j,j+1,j+2} = \partial_u \tilde{\mathcal{L}}_{j,j+1,j+2}(u)\Big|_{u=0}$
- solve the RLL equation for the R-matrix
- check if R solves the Yang-Baxter equation

By choosing the initial Ansatz correctly we can follow this procedure and find all the informations about the integrability structure of three-site chains. However we must first eliminate solutions that lead us to n.n. chains; this can happen by choosing, for example,

$h_{j,j+1,j+2} = h^{(nn)}_{j,j+1}$, with $h^{(nn)}_{j,j+1}$ Hamiltonian density of a n.n. chain.

The first non-trivial models can be found by imposing a global $U(1)$ symmetry, i.e. requiring that the Hamiltonian commutes with the charge $Q_1 = S_z$, and also requiring space reflection invariance. We find two families of spin chains.

The Bariev Model The Hamiltonian is

$$H = \sum_j \left(\sigma^-_j \sigma^+_{j+2} + \sigma^+_j \sigma^-_{j+2}\right) \frac{1 - U\sigma^z_{j+1}}{2}, \quad U \in \mathbb{R} \tag{4.39}$$

This model was described as a zig-zag spin ladder, a spin chain made up of two independent sub-lattices such that the particles cannot move between them but such that they can influence one another (see, for example [26]).

When $U = \pm 1$ we find the folded XXZ model in the bond picture.

The hard rod deformation of XXZ The Hamiltonian is

$$H = \sum_j \left[\sigma^-_j P^\bullet_{j+1} \sigma^+_{j+2} + \sigma^+_j P^\bullet_{j+1} \sigma^-_{j+2} - \Delta \left(P^\circ_j P^\bullet_{j+1} P^\bullet_{j+2} + P^\bullet_j P^\bullet_{j+1} P^\circ_{j+2}\right)\right], \quad \Delta \in \mathbb{R} \tag{4.40}$$

At the point $\Delta = 0$ we find again the folded XXZ model in the bond picture.

IRF models The last class of models is given by an Hamiltonian density $h_{j,j+1,j+2}$ that acts diagonally on the site j and $j+2$, so they act as control bits that can only influence the action on the site $j+1$. The most general form for the density is

$$h_{j,j+1,j+2} = \sum_{a,b=0,1} P^a_j h^{ab}_{j+1} P^b_{j+2} \tag{4.41}$$

where h^{ab} is a collection of four Hermitian matrices.

4.3 IRF models

We want to focus our attention on the interaction-round-a-face models since they have a very close relation with elementary cellular automata, as we will see. This models are characterized by a Lax operator that acts non-trivially only on one of the spins:

$$\tilde{\mathcal{L}}_{j,j+1,j+2}(u) = \sum_{a,b=0,1} P_j^a f_{j+1}^{ab}(u) P_{j+2}^b \tag{4.42}$$

where $f^{ab}(u)$ are four matrices that depends on the spectral parameter.

4.3.1 Integrability

Due to 4.42 the Lax operators satisfy the following condition

$$\left[\tilde{\mathcal{L}}_{123}(u), \tilde{\mathcal{L}}_{345}(v)\right] = 0 \tag{4.43}$$

so we can rewrite the RLL relation as

$$\tilde{\mathcal{L}}_{345}(u)^{-1} \tilde{R}_{23,45}(u,v) \tilde{\mathcal{L}}_{345}(v) = \tilde{\mathcal{L}}_{123}(v) \tilde{R}_{12,34}(u,v) \tilde{\mathcal{L}}_{123}(u)^{-1} \tag{4.44}$$

The l.h.s acts trivially on the space 1 while the r.h.s acts trivially on 5 so they have to be equal to a three-site operator $\tilde{\mathcal{G}}_{234}(u,v)$ such that

$$\tilde{\mathcal{G}}_{234}(u,v) = \tilde{\mathcal{L}}_{345}(u)^{-1} \tilde{R}_{23,45}(u,v) \tilde{\mathcal{L}}_{345}(v) \tag{4.45}$$

$$\tilde{\mathcal{G}}_{234}(u,v) = \tilde{\mathcal{L}}_{123}(v) \tilde{R}_{12,34}(u,v) \tilde{\mathcal{L}}_{123}(u)^{-1} \tag{4.46}$$

Then we can invert these relations to find the R-matrix

$$\tilde{R}_{12,34}(u,v) = \tilde{\mathcal{L}}_{123}(v)^{-1}\tilde{\mathcal{G}}_{234}(u,v)\tilde{\mathcal{L}}_{123}(u) \tag{4.47}$$

$$\tilde{R}_{23,45}(u,v) = \tilde{\mathcal{L}}_{345}(u)\tilde{\mathcal{G}}_{234}(u,v)\tilde{\mathcal{L}}_{345}(v)^{-1} \tag{4.48}$$

or equivalently

$$\tilde{R}_{12,34}(u,v) = \tilde{\mathcal{L}}_{234}(u)\tilde{\mathcal{G}}_{123}(u,v)\tilde{\mathcal{G}}_{234}(v)^{-1} \tag{4.49}$$

To have a consistent relation for the R-matrix we require that

$$\tilde{\mathcal{G}}_{234}(u,v)\tilde{\mathcal{L}}_{123}(u)\tilde{\mathcal{L}}_{234}(v) = \tilde{\mathcal{L}}_{123}(v)\tilde{\mathcal{L}}_{234}(u)\tilde{\mathcal{G}}_{123}(u,v) \tag{4.50}$$

This relation is similar to the standard RLL relation but in this one the supports for the Lax operators overlap at two spaces instead of just one. We call this equation the GLL relation.

Using the regularity of the R-matrix and 4.47 we get that

$$\tilde{\mathcal{G}}_{123}(v,v) = 1 \tag{4.51}$$

Further, using the factorization property of the R-matrix, 4.49 and 4.47, we get that

$$\tilde{\mathcal{G}}_{123}(u,0) = \tilde{\mathcal{L}}_{123}(u) \tag{4.52}$$

$$\tilde{\mathcal{G}}_{123}(0,v) = \tilde{\mathcal{L}}_{123}(v)^{-1} \tag{4.53}$$

We can also derive the inversion property from 4.47

$$\tilde{\mathcal{G}}_{123}(u,v)\tilde{\mathcal{G}}_{123}(v,u) = 1 \tag{4.54}$$

Finally it's easy to prove by substitution that the G-operator also satisfies a Yang-Baxter-like equation

$$\tilde{\mathcal{G}}_{234}(u_1,u_2)\,\tilde{\mathcal{G}}_{123}(u_1,u_3)\,\tilde{\mathcal{G}}_{234}(u_2,u_3) = \tilde{\mathcal{G}}_{123}(u_2,u_3)\,\tilde{\mathcal{G}}_{234}(u_1,u_3)\,\tilde{\mathcal{G}}_{123}(u_1,u_2) \tag{4.55}$$

4.3.2 Classification

Following the same steps as described for the general three-sites models we can obtain a partial classification of these IRF models. From the construction we just outlined we expect an Hamiltonian density of the form 4.41 with

$$h^{ab} = \partial_u f^{ab}(u)|_{u=0} \tag{4.56}$$

We require further that the inversion property hold, so we exclude the possibility of having a non-zero $\tilde{h}_{j,j+1,j+2}$ in Q_5.

Since h^{ab} are four 2×2 hermitean matrices we have 16 real free parameters, that can be brought down to 14 by subtracting the identity and performing a $U(1)$ rotation, but they were considered too many to do a full classification so a more restrictive Ansatz was chosen, that contains 6 free real parameters:

$$h_{123} = A\sigma_2^x + B\sigma_2^z + C\sigma_1^z\sigma_2^x + D\sigma_2^x\sigma_3^z + E\sigma_1^z\sigma_2^z\sigma_3^z + F\sigma_1^z\sigma_2^x\sigma_3^z + G\sigma_1^z\sigma_3^z \tag{4.57}$$

Three non-trivial models were found.

Bond-site transformed XYZ model (bXYZ) The Hamiltonian density is

$$h_{123} = J_x\sigma_2^x - J_y\sigma_1^z\sigma_2^x\sigma_3^z + J_z\sigma_1^z\sigma_3^z \tag{4.58}$$

It can be seen as the bond-site transformation of the XYZ model [27], thus it describes the interacting dynamics of domain walls. with creation and annihilation of pairs allowed.

When $J_x = J_y$ the model reduce to the bond-site transformation of XXZ and the Hamiltonian commutes with

$$Q_2 = \sum_j \sigma_j^z \sigma_{j+1}^z \tag{4.59}$$

which is the $U(1)$ charge that represent the number of domain walls.

Another special case is found at $J_y = 0$ when the model decouples in two Ising chains on the even and odd sublattices.

We can write explicitly the Lax operator for this family:

$$\tilde{\mathcal{L}}_{1,2,3}(u) = \frac{1}{2}\frac{\mathrm{sn}(\eta) + \mathrm{sn}(u)\sigma_2^x}{\mathrm{sn}(\eta) + \mathrm{sn}(u)}\,(1 - \sigma_1^z\sigma_3^z) + \frac{1}{2}\frac{\mathrm{sn}(u+\eta) + k\,\mathrm{sn}(\eta)\,\mathrm{sn}(u)\,\mathrm{sn}(u+\eta)\sigma_2^x}{\mathrm{sn}(\eta) + \mathrm{sn}(u)}\,(1 + \sigma_1^z\sigma_3^z) \tag{4.60}$$

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

$$\frac{J_y}{J_x} = \frac{1 - k\,\mathrm{sn}^2(\eta)}{1 + k\,\mathrm{sn}^2(\eta)} \quad \frac{J_z}{J_x} = \frac{\mathrm{cn}(\eta)\,\mathrm{dn}(\eta)}{1 + k\,\mathrm{sn}^2(\eta)} \tag{4.61}$$

where sn, cn, dn are Jacobi's elliptic functions.

The Lax operator for this model satisfies the inversion relation

$$\tilde{\mathcal{L}}_{1,2,3}(u)\tilde{\mathcal{L}}_{1,2,3}(-u) = 1 \tag{4.62}$$

and it has a very simple relation with the G-operator

$$\tilde{\mathcal{G}}_{123}(u,v) = \tilde{\mathcal{L}}_{123}(u-v) \tag{4.63}$$

To obtain the Lax operator in the XXZ limit we take $k \to 0$ so

$$\tilde{\mathcal{L}}_{1,2,3}(u) = (P_1^\circ P_3^\circ + P_1^\bullet P_3^\bullet)\frac{\sin(u+\eta)}{\sin(u)+\sin(\eta)} + (P_1^\circ P_3^\bullet + P_1^\bullet P_3^\circ)\frac{\sin(u)\sigma_2^x + \sin(\eta)}{\sin(u)+\sin(\eta)} \quad (4.64)$$

Instead, for $\eta \to 0, u = \eta v$, we get the XXX Lax operator

$$\tilde{\mathcal{L}}_{1,2,3}(u) = (P_1^\circ P_3^\circ + P_1^\bullet P_3^\bullet) + (P_1^\circ P_3^\bullet + P_1^\bullet P_3^\circ)\frac{u\sigma_2^x + 1}{u+1} \quad (4.65)$$

Twisted XX model For this model the Hamiltonian density is

$$h_{123} = \sigma_1^z\sigma_2^x + k\sigma_2^x\sigma_3^z + G\sigma_1^z\sigma_3^z \quad (4.66)$$

where $k = \pm 1, G \in \mathbb{R}$. To find the connection to the XX model, in the case $k = -1$, we can write the global Hamiltonian with the Pauli matrices cyclically changed such that

$$H = \sum_j 2i(\sigma_j^+\sigma_{j+1}^- - \sigma^-\sigma_{j+1}^+) + G\sigma_j^x\sigma_{j+2}^x \quad (4.67)$$

which can be seen as a twisted XX model with a next-to-nearest neighbor interaction. The Lax operator for the model is given by

$$\tilde{\mathcal{L}}_{123}(u) = G\frac{e^{2u}-1}{(e^u-1)^2 - 4G^2} \times \left(\frac{2G\kappa}{e^u-1} + (\sigma_1^z\sigma_2^x + \kappa\sigma_2^x\sigma_3^z) + \frac{e^u - 1 + 2G^2}{G\,(e^u+1)}\sigma_1^z\sigma_3^z\right) \quad (4.68)$$

and it satisfies the inversion relation but it's unitary only for $u \in i\mathbb{R}$.

The G-operator is more complex this time, given by

$$\tilde{\mathcal{G}}_{123}(u,v) = \kappa\frac{(4G^2-1)\,e^v - e^u + e^ue^v + 1}{2G\,(e^u - e^v)} + (\sigma_1^z\sigma_2^x + \kappa\sigma_2^x\sigma_3^z) + G\frac{(4G^2-3)\,e^v + e^u + e^ue^v + 1}{(2G^2-1)\,(e^u+e^v) + e^ue^v + 1}\sigma_1^z\sigma_3^z \quad (4.69)$$

Deformation of PXP model The Hamiltonian density is

$$h_{123} = \sigma_2^x + k(\sigma_1^z\sigma_2^x + \sigma_2^x\sigma_3^z) + \sqrt{2}\sigma_1^z\sigma_2^z\sigma_3^z - \sigma_1^z\sigma_2^x\sigma_3^z \tag{4.70}$$

with $k = \pm 1$.

Even though there is no tunable parameter this model can be seen as an integrable deformation of the PXP model, and it's probably a particular case of a continuous family of models that goes beyond the initial Ansatz.

The Lax operator for this model is

$$\tilde{\mathcal{L}}_{123}(u) = \frac{1 + uh_{123}}{1 + \sqrt{6}u} \tag{4.71}$$

4.4 Four site models

To find the integrability structure of four-site models we can follow the same strategy as before: by grouping some sites together, in this case three, we obtain a n.n. chain. Then, since the n.n. chain is integrable, we can find a regular R-matrix $R_{(a,b,c)(j,j+1,j+2)}(u,0)$ that will act on the three spin sites and on three auxiliary spaces.

Since we want translationally invariant charges for the original chain we can expect also a translationally invariant transfer matrix and so we conjecture that the R-matrix factorizes in

$$R_{(a,b,c)(j,j+1,j+2)}(u,0) = \mathcal{L}_{a,b,c,j+2}(u)\mathcal{L}_{a,b,c,j+1}(u)\mathcal{L}_{a,b,c,j}(u) \tag{4.72}$$

where $\mathcal{L}_{a,b,c,j}(u)$ is the Lax operator that acts on three auxiliary spaces and one physical space.

The transfer matrix is then given by

$$t(u) = \mathrm{Tr}_{a,b,c}\, \mathcal{L}_{a,b,c,L}(u) \dots \mathcal{L}_{a,b,c,1} \tag{4.73}$$

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

$$\mathcal{L}_{a,b,c,j}(0) = \mathcal{P}_{a,j}\mathcal{P}_{b,j}\mathcal{P}_{c,j} \longrightarrow t(0) = \mathcal{U}^3 \tag{4.74}$$

Given the braided Lax operator, defined as

$$\mathcal{L}_{a,b,c,j}(u) = \mathcal{P}_{a,j}\mathcal{P}_{b,j}\mathcal{P}_{c,j}\tilde{\mathcal{L}}_{a,b,c,j}(u) \tag{4.75}$$

with the inversion property

$$\tilde{\mathcal{L}}_{a,b,c,j}(u)\tilde{\mathcal{L}}_{a,b,c,j}(-u) = 1 \tag{4.76}$$

we can compute the Hamiltonian density of the four-site model

$$h_{1,2,3,4} = \partial_u \tilde{\mathcal{L}}_{1,2,3,4}(u)|_{u=0} \tag{4.77}$$

and also the next conserved charge density, a seven-site operator $q_7(j)$ such that

$$q_7(1) = \left[h_{1,2,3,4}, \sum_{k=1}^{3} h_{1+k,2+k,3+k,4+k} \right] \tag{4.78}$$

As before, we can use the fact that H and Q_7 commutes as a criterion for integrability, to classify four-site interacting models.

As an example, the only new, non-trivial model with $SU(2)$ and space reflection symmetry found is

$$h_{1,2,3,4} = 2(\mathcal{P}_{1,4} - 1)(\mathcal{P}_{2,3} - 1) - \mathcal{P}_{1,3} - \mathcal{P}_{2,4} \tag{4.79}$$

4.5 Quantum Automata

We're now ready to flesh out the connection between spin chains and quantum cellular automata.

To this end we will use the brickwork formulation, that is we want to build QCA with Floquet cycles with time period τ with global evolution operator given by

$$\mathcal{V} = \mathcal{V}_\tau \dots \mathcal{V}_1 \tag{4.80}$$

where the update at time t is

$$\mathcal{V}_t = \prod_j U^{(l)}(x_j + \Delta_t) \tag{4.81}$$

There are multiple ways to connect an integrable spin chain with a QCA so we will focus on the Trotterization procedure, introduced in [28] for n.n. chains and on a more general method for medium range chains.

4.5.1 Integrable Trotterization

This procedure creates a time-discretized version of an interacting lattice model with nearest neighbours interactions. In particular, we want to obtain a QCA with Floquet period $\tau = 2$ and $\Delta_t = 2$ given a regular R-matrix $R(u, v)$ of a n.n. spin chain. Since we deal with n.n. chains the unitary operator $U_j^{(l)}$ will have support on two sites, so $l = 2$, and the length of the chain must be an even number $L = 2k$.

On the chain we build an inhomogeneous transfer matrix with alternating inhomogeneities μ, ν:

$$t(u) = \mathrm{Tr}_a \left[R_{a,L}(u, \nu) R_{a,L-1}(u, \mu) \dots R_{a,2}(u, \nu) R_{a,1}(u, \mu) \right] \tag{4.82}$$

Using the regularity condition we obtain two special points of the transfer matrix when the spectral parameter assumes the values μ and ν

$$\begin{aligned} t(\mu) &= \mathcal{U}\tilde{R}_{L-1,L}(\mu,\nu)\dots\tilde{R}_{1,2}(\mu,\nu) \\ t(\nu) &= \mathcal{U}\tilde{R}_{L,1}(\nu,\mu)\dots\tilde{R}_{2,3}(\nu,\mu) \end{aligned} \tag{4.83}$$

where $\tilde{R}_{a,b}$ is the braided R-matrix.

Then we can use the inversion relation to compute the inverse of the transfer matrix $t(\nu)$ as follows

$$t(\nu)^{-1} = \tilde{R}_{L,1}(\mu,\nu)\dots\tilde{R}_{2,3}(\mu,\nu)\mathcal{U}^{-1} \tag{4.84}$$

And so the operator product

$$t(\nu)^{-1}t(\mu) \tag{4.85}$$

can be interpreted as a brickwork QCA with period $\tau = 2$ and with local unitary given by

$$U^{(2)}_{j,j+1} = \tilde{R}_{j,j+1}(\mu,\nu) \tag{4.86}$$

Since $U^{(2)}$ must be unitary not all R-matrices are compatible; indeed, using the inversion property, we find that the braided R-matrix must satisfy the following condition:

$$\left(\tilde{R}_{a,b}(\mu,\nu)\right)^{\dagger} = \tilde{R}_{a,b}(\nu,\mu) \tag{4.87}$$

4.5.2 Three site QCA

There are two ways to create the correct QCA from the R-matrix of a three site spin chain: the first is an extension of the Trotterization scheme that is straightforward but it does not generate a true brickwork QCA since it leaves some site untouched at every discrete timestep; the second method leads to the expected brickwork QCA but it has a more complex integrability structure.

Extended Trotterization

We want to use the grouped chain, as in 4.2.1, to write the inhomogeneous transfer matrix 4.82. So we obtain a QCA with four-site local evolution operators that, for special values of the spectral parameter, can be written as a three-site operator using the factorization 4.24.

Let's consider a chain of length $L = 4k$ and a four-site R-matrix $R_{(a,b)(j,j+2)}$, we can define the inhomogeneous transfer matrix as

$$t(u) = \mathrm{Tr}_{ab}\left[R_{(a,b)(4k-1,4k)}(u,\nu)R_{(a,b)(4k-3,4k-2)}(u,\mu)\dots R_{(a,b)(3,4)}(u,\nu)R_{(a,b)(2,1)}(u,\mu)\right] \tag{4.88}$$

The special points of the family of the transfer matrix is found for $u = \nu, \mu$:

$$\begin{aligned} t(\mu) &= \mathcal{U}^2\tilde{R}_{(4k-3,4k-2)(4k-1,4k)}(\mu,\nu)\dots\tilde{R}_{(1,2)(3,4)}(\mu,\nu), \\ t(\nu) &= \mathcal{U}^2\tilde{R}_{(4k-1.4k)(1,2)}(\nu,\mu)\dots\tilde{R}_{(3,4)(5.6)}(\nu,\mu) \end{aligned} \tag{4.89}$$

As before, we take the inverse of the second transfer matrix

$$t(\nu)^{-1} = \tilde{R}_{(4k-1,4k)(1,2)}(\mu,\nu)\dots\tilde{R}_{(3,4)(5,6)}(\mu,\nu)\mathcal{U}^{-2} \tag{4.90}$$

and so we define the global evolution operator as

$$\mathcal{V} = t^{-1}(\nu)t(\mu) = \tilde{R}_{(4k-1,4k)(1,2)}(\mu,\nu)\dots\tilde{R}_{(3,4)(5,6)}(\mu,\nu)\tilde{R}_{(4k-3,4k-2)(4k,4k-1)}(\mu,\nu)\dots\tilde{R}_{(1,2)(3,4)}(\mu,\nu) \tag{4.91}$$

This can be seen as a QCA with Floquet cycle with period $\tau = 2$ and with unitary with support $l = 4$ and expression:

$$U^{(4)}_{j,j+1,j+2,j+3} = \tilde{R}_{(j,j+1)(j+2,j+3)}(\mu,\nu) \tag{4.92}$$

The coordinates of the local operator are $x_j = 4j$ with a time delay $\Delta_t = 2t$.

For the special value $\nu = 0$ the braided R-matrix factorizes as

$$\tilde{R}_{j,j+1,j+2,j+3}(\mu, 0) = \tilde{\mathcal{L}}_{j+1,j+2,j+3}(\mu)\tilde{\mathcal{L}}_{j,j+1,j+2}(\mu) \tag{4.93}$$

where $\tilde{\mathcal{L}}$ is the braided Lax operator. Substituting this expression in 4.91 we obtain a QCA with Floquet period $\tau = 4$ and unitaries of support $l = 3$:

$$U^{(3)}_{j,j+1,j+2} = \tilde{\mathcal{L}}_{j,j+1,j+2}(\mu) \tag{4.94}$$

with coordinates $x_j = 4j$ and time displacement $\Delta_t = t$.

This construction as two issues: the QCA is not symmetric under left-right symmetry and it's not tightly packed (the fourth spin is untouched for every time step).

Five-site construction

This time, instead, we want to build a QCA with period $\tau = 3$, coordinates $x_j = 3j$ and time delay $\Delta_t = t$ using as a unitary the three-site, braided, Lax matrix

$$U^{(3)}_{j,j+1,j+2} = \tilde{\mathcal{L}}_{j,j+1,j+2}(\mu) \tag{4.95}$$

as in 4.94. This Lax matrix has a corresponding R-matrix given by $\tilde{R}_{(a,b),(j,j+1)}$.

We build a new, five-site operator $\tilde{\mathcal{R}}_{1,2,3,4,5}(\theta, \mu)$:

$$\begin{aligned} \tilde{\mathcal{R}}_{1,2,3,4,5}(\theta, u) &= \tilde{\mathcal{L}}^{-1}_{1,2,3}(u)\tilde{R}_{2,3,4,5}(\theta, u)\tilde{\mathcal{L}}_{1,2,3}(\theta) \\ &= \tilde{\mathcal{L}}_{3,4,5}(\theta)\tilde{R}_{1,2,3,4}(\theta, u)\tilde{\mathcal{L}}^{-1}_{3,4,5}(u) \end{aligned} \tag{4.96}$$

We also need to define another operator $\mathcal{R}_{(1,2,3),(4,5,6)}$ that acts on six sites using permutation operators on $\tilde{\mathcal{R}}$

$$\mathcal{R}_{(1,2,3)(4,5,6)}(\theta,u) = \mathcal{P}_{1,4}\mathcal{P}_{2,5}\mathcal{P}_{3,6}\tilde{\mathcal{R}}_{1,2,3,4,5}(\theta,u) \tag{4.97}$$

This operator satisfies the Yang-Baxter equation

$$\mathcal{R}_{(1,2,3),A}(\theta,u)\mathcal{R}_{(1,2,3),B}(\theta,v)\mathcal{R}_{A,B}(u,v) = \mathcal{R}_{A,B}(u,v)\mathcal{R}_{(1,2,3),B}(\theta,v)\mathcal{R}_{(1,2,3),A}(\theta,u) \tag{4.98}$$

where $A = (4,5,6), B = (7,8,9)$ are two triplets of auxiliary spaces.
Then we can group together triplets of physical spaces to build the transfer matrix

$$t(u) = \mathrm{Tr}_A\left[\mathcal{R}_{(1,2,3),A}(\theta,u)\mathcal{R}_{(4,5,6),A}(\theta,u)\ldots\mathcal{R}_{(L-5,L-4,L-3),A}(\theta,u)\mathcal{R}_{(L-2,L-1,L),A}(\theta,u)\right] \tag{4.99}$$

where $A = (a,b,c)$ are a triplet of auxiliary spaces. Note that the ordering of the product of the sites is the inverse of the usual one.
The family of transfer matrix commutes, if we take θ as a fixed parameter. Further, at the point $u = \theta$ the transfer matrix reduces to the shift operator

$$t(\theta) = \mathcal{U}^{-3} \tag{4.100}$$

Instead, at the point $u = 0$ the operator $\tilde{\mathcal{R}}$ factorizes as

$$\tilde{\mathcal{R}}_{1,2,3,4,5}(\theta,0) = \tilde{\mathcal{L}}_{3,4,5}(\theta)\tilde{\mathcal{L}}_{2,3,4}(\theta)\tilde{\mathcal{L}}_{1,2,3}(\theta) \tag{4.101}$$

The, the global evolution operator of the corresponding QCA is given by

$$\mathcal{V} = t(\theta)^{-1}t(0) = \mathcal{V}_3\mathcal{V}_2\mathcal{V}_1 \tag{4.102}$$

with

$$\mathcal{V}_t = \prod_j U^{(3)}_{3j+t,3j+1+t,3j+2+t} \tag{4.103}$$

So we obtained an actual brickwork QCA from the Lax operator of a three-site spin chain.

4.5.3 Interaction-round-a-face QCA

Since we would like to describe a QCA that, in the classical limit, gives back an elementary CA we need a different method than the one developed in the previous section, since the unitaries found there do not overlap at a single time step [29].

This time we want a QCA with Floquet period $\tau = 2$ and so we consider a three-site unitary such that

$$U^{(3)}_{j,j+1,j+2} = \tilde{\mathcal{L}}_{j,j+1,j+2}(\theta) \tag{4.104}$$

where θ will be a fixed parameter.

The two fixed time operators are given by

$$\begin{aligned} \mathcal{V}_1 &= \tilde{\mathcal{L}}_{1,2,3}(\theta)\tilde{\mathcal{L}}_{3,4,5}(\theta)\dots\tilde{\mathcal{L}}_{L-3,L-2,L-1}(\theta)\tilde{\mathcal{L}}_{L-1,L,1}(\theta) \\ \mathcal{V}_2 &= \tilde{\mathcal{L}}_{2,3,4}(\theta)\tilde{\mathcal{L}}_{4,5,6}(\theta)\dots\tilde{\mathcal{L}}_{L-2,L-1,L}(\theta)\tilde{\mathcal{L}}_{L,1,2}(\theta) \end{aligned} \tag{4.105}$$

Notice that neighbouring Lax operators overlap at one site.

Then we can write the global update operator as

$$\mathcal{V} = \mathcal{U}^2 \,\mathrm{Tr}_{ab}\left[\mathcal{L}_{1,2,b}\mathcal{L}_{1,2,a}\mathcal{L}_{3,4,b}\mathcal{L}_{3,4,a}\dots\mathcal{L}_{L-1,L,b}\mathcal{L}_{L-1,L,a}\right] \tag{4.106}$$

We use the factorization property of the R-matrix, written as

$$R_{(1,2),(3,4)}(\theta,0) = \mathcal{L}_{1,2,4}(\theta)\mathcal{L}_{1,2,3}(\theta) \tag{4.107}$$

to reexpress 4.106 using the R-matrix as

$$\mathcal{V} = \mathcal{U}^2 \operatorname{Tr}_A \left[R_{(1,2),A}(\theta,0) R_{(3,4),A}(\theta,0) \dots R_{(L-1,L),A}(\theta,0) \right] \tag{4.108}$$

where $A = (a,b)$ is a pair of auxiliary spaces.

We can define the transfer matrix $t(u)$, with the opposite order of products, as

$$t(u) = \operatorname{Tr}_A \left[R_{(1,2),A}(\theta,u) R_{(3,4),A}(\theta,u) \dots R_{(L-1,L),A}(\theta,u) \right], \quad [t(u),t(v)] = 0 \tag{4.109}$$

with initial condition

$$t(\theta) = \mathcal{U}^{-2} \tag{4.110}$$

so that the global update rule can assume the standard form

$$\mathcal{V} = t(\theta)^{-1} t(0) \tag{4.111}$$

As a trick to compute the fourth charge we can define a spectral parameter dependent global rule

$$\mathcal{V}(u) = t(\theta)^{-1} t(u) \tag{4.112}$$

This family of operators commutes with itself and so with $\mathcal{V}(0) = \mathcal{V}$. Then the charge is given by

$$Q_4 = \partial_u \mathcal{V}(u)|_{u=\theta} \tag{4.113}$$

Since the transfer matrix is not translationally invariant, but only two-site invariant, the charge will also be two-site invariant.

Let's consider a few examples from the IRF models found in 4.3.2.

The bonded XXX model has a three-site unitary given by the Lax operator 4.65 so

$$U^{(3)}_{1,2,3}(u) = (P^{\circ}_1 P^{\circ}_3 + P^{\bullet}_1 P^{\bullet}_3) + (P^{\circ}_1 P^{\bullet}_3 + P^{\bullet}_1 P^{\circ}_3) \frac{v\sigma^x_2 + 1}{v+1} \tag{4.114}$$

with $u = \eta v$. In the limit $v \to \infty$ the unitary operator reduces to

$$U^{(3)}_{1,2,3} = P^{\circ}_1 P^{\circ}_3 + P^{\bullet}_1 P^{\bullet}_3 + (P^{\circ}_1 P^{\bullet}_3 + P^{\bullet}_1 P^{\circ}_3)\sigma^x_2 \tag{4.115}$$

that is a classical update rule and coincides with the parametrization given for the Rule 150, proving that it's Yang-Baxter integrable. Further, we found an entire family of integrable QCAs connected to the bonded XYZ model.

If instead we focus on the twisted XX model, in the limit $k = 1$ and $G = 1$, we have a Lax operator, and so a three-site unitary, given by

$$\tilde{\mathcal{L}}_{1,2,3}(u) = \frac{e^u - 1}{e^u - 3}\left(\frac{2}{e^u - 1} + \sigma^z_1\sigma^x_2 + \sigma^x_2\sigma^z_3 + \sigma^z_1\sigma^z_3\right) \tag{4.116}$$

that follows from 4.68. The classical limit is found for $u = i\pi$ where the classical CA is given by

$$U^{(3)}_{1,2,3} = \frac{1}{2}\left(-1 + \sigma^z_1\sigma^x_2 + \sigma^x_2\sigma^z_3 + \sigma^z_1\sigma^z_3\right) \tag{4.117}$$

The f matrices of this CA can be easily found to be equal to

$$f^{00} = -f^{11} = \sigma^x, \quad f^{01} = f^{10} = -1 \tag{4.118}$$

These, up to phases, are equal to the one of Rule 105.

4.5.4 Four-Site QCA

Let's consider a Lax operator for a four-site model with the condition:

$$\left[\tilde{\mathcal{L}}_{1234}(u), \tilde{\mathcal{L}}_{4567}(v)\right] = 0 \tag{4.119}$$

We're asking for the first and last site to be control bits.

Then there exists a five site operator $\tilde{\mathcal{G}}$ such that the R-matrix factorizes as

$$\begin{aligned}\tilde{R}_{123456}(u,v) &= \tilde{\mathcal{L}}_{1234}(v)^{-1}\tilde{\mathcal{G}}_{23456}(u,v)\tilde{\mathcal{L}}_{1234}(u) = \\ &= \tilde{\mathcal{L}}_{3456}(u)\tilde{\mathcal{G}}_{12345}(u,v)\tilde{\mathcal{L}}_{3456}(v)^{-1}\end{aligned} \tag{4.120}$$

For this factorization to be consistent the following GLL relation must be satisfied

$$\tilde{\mathcal{G}}_{23456}(u,v)\tilde{\mathcal{L}}_{1234}(u)\tilde{\mathcal{L}}_{3456}(v) = \tilde{\mathcal{L}}_{1234}(v)\tilde{\mathcal{L}}_{3456}(u)\tilde{\mathcal{G}}_{12345}(u,v) \tag{4.121}$$

The update rule for a single step can be constructed then as

$$\mathcal{V}_1 = \tilde{\mathcal{L}}_{1234}(\theta)\tilde{\mathcal{L}}_{4567}(\theta)\dots\tilde{\mathcal{L}}_{L-2,L-1,L,1}(\theta) \tag{4.122}$$

where θ is a fixed parameter. The full update rule is

$$\begin{aligned}&\mathcal{V} = \mathcal{V}_3\mathcal{V}_2\mathcal{V}_1 = \\ &= \mathcal{U}^3\,\mathrm{Tr}_{abc}\left[\mathcal{L}_{123c}(\theta)\mathcal{L}_{123b}(\theta)\mathcal{L}_{123a}(\theta)\dots\mathcal{L}_{L-2,L-1,L,c}(\theta)\mathcal{L}_{L-2,L-1,L,b}(\theta)\mathcal{L}_{L-2,L-1,L,a}(\theta)\right]\end{aligned} \tag{4.123}$$

Then, applying the factorization formula

$$\tilde{R}_{123456}(\theta,0) = \tilde{\mathcal{L}}_{3456}(\theta)\tilde{\mathcal{L}}_{2345}(\theta)\tilde{\mathcal{L}}_{1234}(\theta) \tag{4.124}$$

we can build the transfer matrix

$$t(u) = \mathrm{Tr}_a\left[R_{(123)A}(\theta,u)R_{(456)A}(\theta,u)\dots R_{(L-2,L-1,L)A}(\theta,u)\right] \tag{4.125}$$

where the auxiliary space $A = (abc)$. This family of transfer matrices commutes and it generates the time evolution of the QCA as

$$\mathcal{V} = t^{-1}(\theta)t(0) \tag{4.126}$$

So the update rule of the QCA is a member of the family of transfer matrices at the special point $u = 0$.

Chapter 5

RSOS spin chains

The models the we studied until now all have the property that the total Hilbert space $\mathcal{H} = \otimes\mathcal{H}_i$ factorizes over the sites of the chain. There are more complex models where this property doesn't hold, such as Restricted-Solid-On-Solid lattice models.

RSOS models are a class of two-dimensional lattice models such that each site can assume an integer value $l_i \leq m'$ called height, subject to the condition $|j - j'| = 1$, i.e. neighbouring sites can assume values according to a given Dynkin diagram of the A family[30]. Near criticality, these models correspond to the $\phi_{1,3}$ perturbation of the $\mathcal{M}(m, m')$ minimal models of 2D conformal field theory.

Even though RSOS models are two dimensional models it was possible to find an equivalent spin chain Hamiltonian using the elliptic Boltzmann face weights of the RSOS models and face transfer matrices. Since the Hamiltonian that was found in [31] has a very similar structure as the one for IRF quantum cellular automata we want to study if RSOS chains can be included in the same framework and, consequently, if there exists a classical limit of the corresponding quantum CA.

5.1 RSOS spin chain

The RSOS models are two dimensional models defined on a squared lattice of dimension N such that each lattice site can assume as a value an integer $j = 1, 2, ..., m' - 1$ such that the nearest neighibours on the edges of the square differ by ± 1; the heights then live on the $A_{m'-1}$ Dynkin diagram. The corresponding minimal model is $\mathcal{M}(m, m'; t)$, where $2 \leq m < m'$, m, m' coprime and $t = q^2$ is a temperature-like parameter.

The possible Boltzmann weights given the restriction are three and they are given by:

$$\begin{aligned}
\omega_{1,j}(u) &= W\begin{pmatrix} j \pm 1 & j \\ j & j \mp 1 \end{pmatrix} = \frac{s(\lambda - u)}{s(\lambda)} \\
\omega^{\pm}_{2,j}(u) &= W\begin{pmatrix} j & j \pm 1 \\ j \mp 1 & j \end{pmatrix} = \frac{g_{j\mp 1}}{g_{j\pm 1}} \frac{s((j \pm 1)\lambda)}{s(j\lambda)} \frac{s(u)}{s(\lambda)} \\
\omega^{\pm}_{3,j}(u) &= W\begin{pmatrix} j & j \pm 1 \\ j \pm 1 & j \end{pmatrix} = \frac{s(j\lambda \pm u)}{s(j\lambda)}
\end{aligned} \tag{5.1}$$

where u is the spectral parameter, $s(u) = \theta_1(u, q)$ is a standard elliptic theta function

$$\theta_1(u, q) = 2q^{1/4} \sin u \prod_{n=1}^{\infty} (1 - 2q^{2n} \cos 2u + q^{4n})(1 - q^{2n}) \tag{5.2}$$

and λ is the crossing parameter, given by

$$\lambda = \frac{(m' - m)\pi}{m'} \tag{5.3}$$

As we can see the elliptic nome q of the theta function is the square root of the temperature parameter of the minimal models and thus it measures the departure from criticality corresponding to the $\varphi_{1,3}$ integrable perturbation. To find the critical models we will send $q \to 0$.

The function g_j is a gauge factor and so is an arbitrary function of j; for convenience we

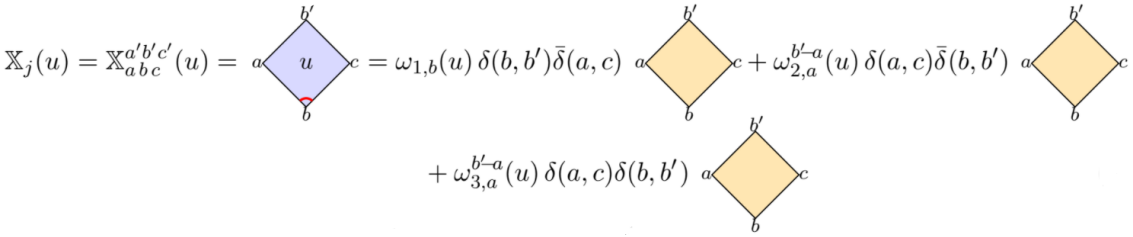

Fig. 5.1. Face transfer matrix as linear sum of elementary tiles

set $g_j = 1$ thereby breaking the $\mathbb{Z}_2$ reflection symmetry about the SE-NW diagonal.

In the article the face transfer matrix $\mathbb{X}_j(u)^{\sigma'}_{\sigma}$ is built as an operator acting on a lower row configuration of the lattice $\sigma = \sigma_1, \ldots, \sigma_N$ that adds a single face at position j to the upper row σ'. The explicit expression of the operator $\mathbb{X}_j$ in terms of the Boltzmann weights is given in a diagrammatic form using a planar algebra decomposition, as in figure 5.1.

We can write the face transfer operator as

$$\mathbb{X}_j(u) = \mathbb{X}^{\sigma'_j}_{\sigma_{j-1}\sigma_j\sigma_{j+1}}(u) = \omega_{1,\sigma_j}(u)\delta(\sigma_j,\sigma'_j)\bar{\delta}(\sigma_{j-1},\sigma_{j+1}) + \omega^{\sigma'_j-\sigma_{j-1}}_{2,\sigma_{j-1}}(u)\delta(\sigma_{j-1},\sigma_{j+1})\bar{\delta}(\sigma_j,\sigma'_j) + \\ + \omega^{\sigma'_j-\sigma_{j-1}}_{3,\sigma_{j-1}}(u)\delta(\sigma_{j-1},\sigma_{j+1})\delta(\sigma_j,\sigma'_j) \tag{5.4}$$

Notice that the symbol $\bar{\delta}(a,b) = 1 - \delta(a,b)$.

The face operators satisfy an inversion relation

$$\mathbb{X}_j(u)\mathbb{X}_j(-u) = \frac{s(\lambda-u)s(\lambda+u)}{s(\lambda)^2} \tag{5.5}$$

and the Yang-Baxter equation

$$\mathbb{X}_j(u)\mathbb{X}_{j+1}(u+v)\mathbb{X}_j(v) = \mathbb{X}_{j+1}(v)\mathbb{X}_j(u+v)\mathbb{X}_{j+1}(u) \tag{5.6}$$

Further, the Hamiltonian of the chain is given by

$$\mathcal{H} = \sum_{j=1}^{N} \left(\frac{s'(0)}{s(\lambda)} F_j + X_j \right) \tag{5.7}$$

where

$$F^{\sigma'_j}_{\sigma_{j-1}\sigma_j\sigma_{j+1}} = \frac{s(\sigma'_j\lambda)}{s(\sigma_{j+1}\lambda)}\delta(\sigma_{j-1},\sigma_{j+1}) \tag{5.8}$$

$$X^{\sigma'_j}_{\sigma_{j-1}\sigma_j\sigma_{j+1}} = \frac{s'(\lambda)}{s(\lambda)} - \frac{s'(0)s(\sigma'_j\lambda)}{s(\lambda)s(\sigma_{j+1}\lambda)} + (\sigma'_j - \sigma_{j+1})\frac{s'(\sigma_{j+1}\lambda)}{s(\sigma_{j+1}\lambda)}\delta(\sigma_{j-1},\sigma_{j+1})\delta(\sigma'_j,\sigma_j) \tag{5.9}$$

The face transfer operator 5.4 is a three site operator that, depending on the values of the $j-1$ and $j+1$ cells, evolves the j cell only while leaving untouched all the other cells. The action of this operator reminds us of the Lax operator for IRF spin chains; further it satisfies a Yang-Baxter equation, an inversion relation and it can be used to derive an Hamiltonian so we want to check if these properties are equivalent to the one found in the IRF chains.

Let's assume that we can identify $\mathbb{X}_j(u) = \tilde{\mathcal{L}}_{j-1,j,j+1}(u)$, then the Yang Baxter equation 5.6 becomes

$$\tilde{\mathcal{L}}_{j-1,j,j+1}(u)\tilde{\mathcal{L}}_{j,j+1,j+2}(u+v)\tilde{\mathcal{L}}_{j-1,j,j+1}(v) = \tilde{\mathcal{L}}_{j,j+1,j+2}(v)\tilde{\mathcal{L}}_{j-1,j,j+1}(u+v)\tilde{\mathcal{L}}_{j,j+1,j+2}(u) \tag{5.10}$$

The presence of the sum between two spectral parameters tells us that the underlying R-matrix is of difference form so $\tilde{\mathcal{G}}(u,v) = \tilde{\mathcal{G}}(u-v)$.

Let's write equation 4.55 choosing as the value of the spectral parameters $u_1 = v, u_3 = -u$ and $u_2 = 0$, a parameterization that we can always make for R-matrices of difference form:

$$\tilde{\mathcal{G}}^{-1}_{j-1,j,j+1}(-u)\tilde{\mathcal{G}}_{j,j+1,j+2}(u+v)\tilde{\mathcal{G}}_{j-1,j,j+1}(v) = \tilde{\mathcal{G}}_{j,j+1,j+2}(v)\tilde{\mathcal{G}}_{j-1,j,j+1}(u+v)\tilde{\mathcal{G}}^{-1}_{j,j+1,j+2}(-u) \tag{5.11}$$

where we used the relations 4.52.

Since the $\tilde{\mathcal{G}}(u,v)$ operator satisfies the inversion relation 4.54 while the operator $\mathbb{X}_j(u)$ does not we need to normalize the latter. We define a new face transfer operator as

$$\mathbb{Z}_j(u) = \frac{\mathbb{X}_j(u)s(\lambda)}{\sqrt{s(\lambda-u)s(\lambda+u)}} \tag{5.12}$$

Then the relation 5.5 becomes

$$\mathbb{Z}_j(u)\mathbb{Z}_j(-u) = 1 \tag{5.13}$$

and so the Lax given as $\tilde{\mathcal{L}}_{j-1,j,j+1}(u) = \mathbb{Z}_j(u) = \tilde{\mathcal{G}}_{j-1,j,j+1}(u,0)$ satisfies the correct inversion relation.

We can now use this relation in 5.11 to find

$$\tilde{\mathcal{G}}_{j-1,j,j+1}(u)\tilde{\mathcal{G}}_{j,j+1,j+2}(u+v)\tilde{\mathcal{G}}_{j-1,j,j+1}(v) = \tilde{\mathcal{G}}_{j,j+1,j+2}(v)\tilde{\mathcal{G}}_{j-1,j,j+1}(u+v)\tilde{\mathcal{G}}_{j,j+1,j+2}(u) \tag{5.14}$$

We have proven that the normalized face transfer operator satisfies the same Yang-Baxter equation as the IRF models.

Another property of $\tilde{\mathcal{G}}$ operators that is easily checked is the regularity condition that, for operators in difference form, simplifies to $\tilde{\mathcal{G}}_{j-1,j,j+1}(0) = 1$. By doing a simple calculation is easy to see that this is true also for the operator $\mathbb{Z}_j(0)$.

As our last test we want to check if the Hamiltonian density can be recovered as the derivative of the $\mathbb{X}$ operator computed in $u = 0$; in the article there is a different convention so we do not put the minus sign in the derivative. First we derive the Boltzmann

weights:

$$\frac{d\omega^{\sigma'_j}_{1,\sigma_{j-1}\sigma_j\sigma_{j+1}}(u)}{du}|_{u=0} = -\frac{s'(\lambda)}{s(\lambda)} \tag{5.15}$$

$$\frac{d\omega^{\pm,\sigma'_j}_{2,\sigma_{j-1}\sigma_j\sigma_{j+1}}u)}{du}|_{u=0} = \frac{s'(0)s(\sigma'_j\lambda)}{s(\lambda)s(\sigma_{j+1}\lambda)} \tag{5.16}$$

$$\frac{d\omega^{\pm,\sigma'_j}_{\sigma_{j-1}\sigma_j\sigma_{j+1}}(u)}{du}|_{u=0} = (\sigma'_j - \sigma_{j-1})\frac{s'(\sigma_{j+1}\lambda)}{s(\sigma_{j+1}\lambda)} \tag{5.17}$$

Adding these derivatives in 5.4 we find

$$\frac{d\mathbb{X}^{\sigma'_j}_{\sigma_{j-1}\sigma_j\sigma_{j+1}}(u)}{du}|_{u=0} = -\frac{s'(\lambda)}{s(\lambda)}\delta(\sigma_j,\sigma'_j)\bar{\delta}(\sigma_{j-1},\sigma_{j+1}) + \frac{s'(0)s(\sigma'_j\lambda)}{s(\lambda)s(\sigma_{j+1}\lambda)}\delta(\sigma_{j-1},\sigma_{j+1})\bar{\delta}(\sigma_j,\sigma'_j) + \\ + (\sigma'_j - \sigma_{j-1})\frac{s'(\sigma_{j+1}\lambda)}{s(\sigma_{j+1}\lambda)}\delta(\sigma_{j-1},\sigma_{j+1})\delta(\sigma_j,\sigma'_j) \tag{5.18}$$

Using the definition of $\bar{\delta}$

$$= -\frac{s'(\lambda)}{s(\lambda)}\delta(\sigma_j,\sigma'_j) + \frac{s'(0)s(\sigma'_j\lambda)}{s(\lambda)s(\sigma_{j+1}\lambda)}\delta(\sigma_{j-1},\sigma_{j+1}) + \\ + \left[\frac{s'(\lambda)}{s(\lambda)} - \frac{s'(0)s(\sigma'_j\lambda)}{s(\lambda)s(\sigma_{j+1}\lambda)} + (\sigma'_j - \sigma_{j-1})\frac{s'(\sigma_{j+1}\lambda)}{s(\sigma_{j+1}\lambda)}\right]\delta(\sigma_{j-1},\sigma_{j+1})\delta(\sigma_j,\sigma'_j))$$

In this equation we recognize the F_j and X_j operators of equation 5.8 and 5.9 so

$$\frac{d}{du}\mathbb{X}^{\sigma'_j}_{\sigma_{j-1}\sigma_j\sigma_{j+1}}(u)|_{u=0} = -\frac{s'(\lambda)}{s(\lambda)}\delta(\sigma_j,\sigma'_j) + \frac{s'(0)}{s(\lambda)}F_j + X_j \tag{5.19}$$

Then the total Hamiltonian is given by

$$\mathcal{H}^{\sigma'_j}_{\sigma_{j-1}\sigma_j\sigma_{j+1}} = \sum_{j=1}^{N}\left[-\frac{s'(\lambda)}{s(\lambda)}\delta(\sigma_j,\sigma'_j)\right] + \sum_{j=1}^{N}\left[\frac{s'(0)}{s(\lambda)}F_j + X_j\right] \tag{5.20}$$

We can shift the energy by an amount given by the first term to finally obtain the expected result of 5.7.

Since we need to use the normalized face transfer operator let's check if the normalization

spoils this result. By putting

$$\alpha(u) = \frac{s(\lambda)}{\sqrt{s(\lambda-u)s(\lambda+u)}} \tag{5.21}$$

we have

$$\tilde{h}_j = \frac{d}{du}(\alpha(u)\mathbb{X}_j(u))|_{u=0} = \alpha(0)\frac{d\mathbb{X}_j(u)}{du}|_{u=0} + \mathbb{X}_j(0)\frac{d\alpha(u)}{du}|_{u=0} = 1h_j + 0 = h_j \tag{5.22}$$

So the normalization does not spoil the previous result.

In the IRF models we wrote the Lax operator using f matrices as

$$\tilde{\mathcal{L}}_{j-1,j,j+1}(u) = \sum_{a,b=1}^{m'-1} P^a_{j-1} f^{ab}_j(u) P^b_{j+1} \tag{5.23}$$

so we want translate the face transfer operator 5.4 in this IRF form. As we can see from 5.23 a and b relates to the height of the $j-1$ and $j+1$ cell and so the term $P^a_j f^{ab}_{j+1}(u) P^b_{j+2}$ is different from zero if and only if $\sigma_{j-1} = a$. $\sigma_{j+1} = b$ and $f^{ab} \neq 0$. Then we can rewrite 5.23 as

$$\tilde{\mathcal{L}}_{j-1,j,j+1}(u) = \sum_{a,b=1}^{m'-1} \mathbb{I}_{j-1}\delta(\sigma_{j-1}, a) f^{ab}_j(u) \mathbb{I}_{j+1}\delta(\sigma_{j+1}, b) \tag{5.24}$$

However in RSOS models the heights of j and $j-1$ are not independent but must follow the nearest neighbours constraint; this strongly reduces the number of possible non-zero f matrices. We are left with two possibilities:

- a and b differs by 2 so $f^{ab,1} = f^{ab}\delta(|a-b|, 2)$
- a and b are the same so $f^{ab,2} = f^{ab}\delta(a, b)$

There are $2(m'-3)$ of the first kind of f matrices and $m'-1$ of the second kind for a total of $3m'-7$ f matrices in the IRF representation of the RSOS spin chains. As we can see the number of non-zero f matrices is much smaller than in the standard case, where is simply $(m'-1)^2$.

As we can see from the Boltzmann weights 5.1 the first weight give the elements for the first class of f matrices while the second and the third for the second class:

- $(f^{ab,1})_{cd} = \omega_{1,c}(u)\alpha(u)$ if $c = d = \frac{a+b}{2}$, otherwise $(f^{ab,1})_{cd} = 0$
- $(f^{ab,2})_{cd} = \omega^{\pm}_{2,b}(u)\alpha(u)$ if $c = b \mp 1, 0 < c < m'$ and $d = b \pm 1, 0 < d < m'$, otherwise $(f^{ab,2})_{cd} = 0$
- $(f^{ab,2})_{cd} = \omega^{\pm}_{3,b}(u)\alpha(u)$ if $c = b \pm 1, 0 < c < m'$ and $d = b \pm 1, 0 < d < m'$, otherwise $(f^{ab,2})_{cd} = 0$

Notice that the first class of f matrices contains a single non-zero value on the diagonal while, in the second class, there are four elements in a square pattern centered on the diagonal.

We report the non-zero matrices for the simple case of $m' = 4, m = 3$:

$$f^{00}(u) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \frac{s(\lambda+u)}{\sqrt{s(\lambda-u)s(\lambda+u)}} & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad f^{02}(u) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \frac{s(\lambda-u)}{\sqrt{s(\lambda-u)s(\lambda+u)}} & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$f^{11}(u) = \begin{pmatrix} \frac{s(\lambda)s(2\lambda-u)}{s(2\lambda)\sqrt{s(\lambda-u)s(\lambda+u)}} & 0 & \frac{s(3\lambda)s(u)}{s(2\lambda)\sqrt{s(\lambda-u)s(\lambda+u)}} \\ 0 & 0 & 0 \\ \frac{s(\lambda)s(u)}{s(2\lambda)\sqrt{s(\lambda-u)s(\lambda+u)}} & 0 & \frac{s(\lambda)s(2\lambda+u)}{s(2\lambda)\sqrt{s(\lambda-u)s(\lambda+u)}} \end{pmatrix}$$

$$f^{20}(u) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \frac{s(\lambda-u)}{\sqrt{s(\lambda-u)s(\lambda+u)}} & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad f^{22}(u) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \frac{s(3\lambda-u)s(\lambda)}{s(3\lambda)\sqrt{s(\lambda-u)s(\lambda+u)}} & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

If we call Ω^i_{ab} the f matrices generated by the Boltzmann weights ω_i we obtain the following Lax operator

$$\tilde{\mathcal{L}}_{j-1,j,j+1}(u) = \sum_{a,b=1}^{m'-1} P^a_{j-1} \left[\Omega^1_{ab}(u)\delta(|a-b|,2) + (\Omega^2_{ab}(u) + \Omega^3_{ab}(u))\delta(a,b)\right]_j P^b_{j+1} \qquad (5.25)$$

Since the theta function $s(0) = 0$, the Boltzmann weights computed in zero are equal to

$$\omega_{1,j}(0) = 1$$
$$\omega^{\pm}_{2,j}(0) = 0$$
$$\omega^{\pm}_{3,j}(0) = 1$$

and so the f matrices are of diagonal form with only ones on the diagonals; they do not become the identity due to the constraints of the RSOS models.
Then we need to check if $\mathbb{Z}_j(u)$ are actually unitary in the IRF sense, since we will need this operator as the three-site unitary. Due to the inversion property of $\mathbb{Z}_j(u)$ we just need the following property

$$(\mathbb{Z}_j(u)^*)^T = \mathbb{Z}_j(-u) \tag{5.26}$$

Since at first we will use real values of the spectral parameter the property reduces to

$$\mathbb{Z}_j(u)^T = \mathbb{Z}_j(-u) \tag{5.27}$$

Further, due to 5.25, we can verify this directly for the f matrices:

- since ω_1 is on the diagonal of Ω^1_{ab} we require that $\omega_1(u) = \omega_1(-u)$ and this is true only for $u^* = \pi k,\ k \in \pm\mathbb{N}$
- since ω_3 are on the diagonal of Ω^3_{ab} we require that $\omega_3(u) = \omega_3(-u)$ and this is true only for $u^* = \pi k,\ k \in \pm\mathbb{N}$
- since ω_2 are in a position of Ω^2_{ab} symmetrical w.r.t the diagonal we require that $\omega^{\pm}_2(u) = \omega^{\mp}_2(-u)$ and this is true only for $u^* = \pi k,\ k \in \pm\mathbb{N}$, but only because the term $s(u)$ becomes zero for $u = u^*$

So the only values of the spectral parameter for which the Lax operator is unitary are those for which $\omega^{\pm}_2(u) = 0$ and $\omega^{\pm}_3 = \omega_1 = \pm 1$ and so the operator reduces to a diagonal

form.

This is clearly an issue, since any non-trivial Lax operator is not unitary.

Now let's consider instead a purely imaginary spectral parameter iu, where $u \in \mathbb{R}$. First we want to understand how the theta function behaves under complex conjugation with a purely imaginary variable.

By substituting $x \to ix$

$$\begin{aligned} s(iu)^* = \theta_1(iu,q)^* &= 2q^{1/4}\sin(iu)^* \prod_{n=1}^{\infty}(1-2q^{2n}\cos(2iu)^*+q^{4n})(1-q^{2n}) = \\ &= 2q^{1/4}\sin(-iu)\prod_{n=1}^{\infty}(1-2q^{2n}\cos(-2iu)+q^{4n})(1-q^{2n}) = \\ &= -s(iu) \end{aligned} \tag{5.28}$$

$$\begin{aligned} s(\lambda-iu)^* = \theta_1(\lambda-iu,q)^* &= 2q^{1/4}\sin(\lambda-iu)^* \prod_{n=1}^{\infty}(1-2q^{2n}\cos(\lambda-2iu)^*+q^{4n})(1-q^{2n}) = \\ &= 2q^{1/4}\sin(\lambda+iu)\prod_{n=1}^{\infty}(1-2q^{2n}\cos(\lambda+2iu)+q^{4n})(1-q^{2n}) = \\ &= s(\lambda+iu) \end{aligned} \tag{5.29}$$

where we used the properties of the trigonometric functions.

Since now the spectral parameter is complex we have to check if the f matrices respect 5.26 so let's first compute the complex conjugate of the Boltzmann weights:

$$\omega_1(iu)^* = \left(\frac{s(\lambda-iu)}{s(\lambda)}\right)^* = \frac{s(\lambda+iu)}{s(\lambda)} = \omega_1(-iu) \tag{5.30}$$

$$\omega_2^{\pm}(iu)^* = \left(\frac{s((j\pm1)\lambda)}{s(j\lambda)}\frac{s(iu)}{s(\lambda)}\right)^* = -\frac{s((j\pm1)\lambda)}{s(j\lambda)}\frac{s(iu)}{s(\lambda)} = \frac{s((j\mp1)\lambda)}{s(j\lambda)}\frac{s(iu)}{s(\lambda)} = \omega_2^{\mp}(iu) \tag{5.31}$$

$$\omega_3^{\pm}(iu)^* = \left(\frac{s(j\lambda\pm iu)}{s(j\lambda)}\right)^* = \frac{s(j\lambda\mp u)}{s(j\lambda)} = \omega_3^{\pm}(-iu) \tag{5.32}$$

Now we can see that

- since ω_1 is on the diagonal of Ω^1_{ab} we require that $\omega_1(iu)^* = \omega_1(-iu)$ and this is true $\forall u \in \mathbb{R}$
- since ω_3 are on the diagonal of Ω^3_{ab} we require that $\omega_3(iu)^* = \omega_3(-iu)$ and this is true $\forall u \in \mathbb{R}$
- since ω_2 are in a position of Ω^2_{ab} symmetrical w.r.t the diagonal we require that $\omega_2^{\mp}(iu)^* = \omega_2^{\pm}(-iu)$ but, given 5.32, $\omega_2^{\mp}(iu)^* = \omega_2^{\pm}(iu)$ and so the requirement is fulfilled only for $u^* = \pi k,\ k \in \pm\mathbb{N}$, but only because the term $s(u)$ becomes zero for $u = u^*$

-It appears that there are no non-trivial values of the spectral parameter such that we obtain a unitary Lax operator.

Further, even if the Lax operator was unitary, there is no clear value of the spectral parameter such that the QCA becomes classical for that value. This is mostly due to the fact that the elements of the f matrices depends on the heights of the cells, adding complexity to the model.

This can be seen more clearly by considering the operator $\mathbb{X}_j(u)$ at criticality, i.e. when $q = 0$. In that case then

$$\mathbb{X}_j(u) = \frac{\sin(\lambda - u)}{\sin(\lambda)}\mathbb{I} + \frac{\sin(u)}{\sin(\lambda)}e_j \tag{5.33}$$

were e_j are generators for the Temperley-Lieb algebra with $\beta = 2\cos\lambda$.

A Temperley-Lieb algebra $TL_N(\beta)$ is a unital associative algebra generated by $N-1$ elements that satisfy the following properties:

- $e_j^2 = \beta e_j$ where β is a constant
- $e_j e_{j\pm1} e_j = e_j$
- $e_i e_j = e_j e_i$ for $|i - j| > 1$

We know that a classical cellular automaton is characterized by f matrices that are elements of the permutation group, since permutations are the only operations that we can do on the cells while keeping the system classical.

As we can see the matrices e_j are not compatible with elements of the permutation groups due do the second property.

By looking at the structure of 5.33 we recognize that it's an element of a class of spin chains called Temperley-Lieb spin chains. This spin chains are defined on an Hilbert space $\mathcal{H}_N$ and the Hamiltonian is given by

$$H = \sum_i b_i \tag{5.34}$$

where b_i is given by a representations of the generators e_i on $\mathcal{H}_N$ [32].

Due do the properties of the Temperley-Lieb algebra the related spin chains are generally integrable, with R-matrices having the form

$$\tilde{R}_i(u) = f(u)\mathbb{I} + g(u)e_i \tag{5.35}$$

Inserting this R-matrix in the Yang-Baxter equation, the trigonometric solution was found to be

$$f(u) = \sin(\lambda - u), \quad g(u) = \sin(u) \tag{5.36}$$

for $\beta = 2\cos\lambda$. We can then identify that critical RSOS chains are Temperley-Lieb chains for a specific choice of the total Hilbert space of the chain.

We've encountered another Temperley-Lieb chain already, the XXZ chain. As we saw it was not possible to find the quantum cellular automata directly from the XXZ chain but first it was necessary to transform it using the bond-site transformation.

It is natural to ask if an IRF chain is the correct choice of QCA for the RSOS chain or if it's first necessary to consider some kind of higher-spin generalization of the bond-

site transformation to be able to obtain an higher-range unitary RSOS quantum cellular automata.

Chapter 6

Conclusions

In this work we studied the connection between two very different systems: cellular automata and spin chains. This connection, in turn, will simplify the study of quantum integrable systems by giving access to a class of new integrable quantum cellular automata.

To fully understand this connection first we explored the meaning of integrability in a classical and quantum setting; then we proposed a few constructions for classical and quantum cellular automata; finally we described a framework that allows us to build different classes of quantum spin chains with an interaction range of three or more sites and spin S. This construction is also capable of finding, given a spin chain, the corresponding time-discretized model, i.e. a quantum cellular automaton, and, in some cases, its classical limit.

We focused on spin $\frac{1}{2}$ chains with an interaction range of three and four sites since two models were found with a well defined classical cellular automaton, thereby proving the integrability of the latter: the bond-site XXX model with the related rule 150 and the twisted XX model with rule 105.

We wanted then to study a more complex class of spin chains, the RSOS quantum chains, using this framework due to the structure of the face transfer operator that closely re-

sembled the Lax operator of a interaction-round-a-face cellular automata. After a careful examination we found that, despite the similarities, the IRF quantum chain cannot be used to describe the CA related to the RSOS models since the evolution operator is not unitary.

We propose two possible interpretations for this incongruence: the first possibility is that the issue is related to the presence of a more complex Braid symmetry behind the model such that the corresponding total Hilbert space of the chain is not decomposable as the tensor product of the spaces of the single sites, therefore making the system deeply non-local; the second and more intriguing possibility is that, even though the RSOS chain has a three site interaction, the CA do not. This is due to the fact the the critical RSOS chain is an element of a large class of models based on the Temperley-Lieb algebra, like the XYZ model. This algebra is incompatible with a QCA directly but it was possible to build avoid the issue by transforming the XYZ chain, a nearest neighbour chain, in a new model with a three site interaction through the bond-site transformation.

So, as the next step, it would be necessary to adapt the bond-site transformation to work on the RSOS chain, a highly non-trivial task due to the nature of RSOS models.

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