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The Fredkin spin chain

Master's Thesis in Condensed Matter Physics

Olof Salberger

Department of Physics & Engineering Physics
Condensed Matter Physics
Chalmers University of Technology & Gothenburg University
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Abstract

We introduce a new model of interacting spin 1/2. It describes interaction of three nearest neighbors. The Hamiltonian can be expressed in terms of Fredkin gates. The Fredkin gate (also known as the CSWAP gate) is a computational circuit suitable for reversible computing. Our construction generalizes the work of Ramis Movassagh and Peter Shor. Our model can be solved by means of Catalan combinatorics in the form of random walks on the upper half of a square lattice [Dyck walks]. Each Dyck path can be mapped to a wave function of the spins. The ground state is an equally weighted superposition of Dyck walks [instead of Motzkin walks]. We can also express it as a matrix product state. We further construct the model of interacting spins 3/2 and greater half-integer spins. The models with higher spins require coloring of Dyck walks. We construct SU(k) symmetric model [here k is the number of colors]. The leading term of the entanglement entropy is then proportional to the square root of the length of the lattice [like in Shor-Movassagh model]. The gap closes as a high power of the length of the lattice.

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Introduction

The Fredkin model is a continuation of several different traditions. The first of these is that of spin chains with local interactions, which aim to construct very simple but reasonably realistic models for magnetism.

1.0.1 The Heisenberg model

The closest analogies in that direction would be to the Ising model and the Heisenberg model. These are one-dimensional models with two-site interactive Hamiltonians:

$$H_I = \sum_{j=1}^{N} J\sigma_j^z\sigma_{j+1}^z$$

for the Ising model and

$$H_H = \sum_{j=1}^{N} J_x\sigma_j^x\sigma_{j+1}^x + J_y\sigma_j^y\sigma_{j+1}^y + J_z\sigma_j^z\sigma_{j+1}^z$$

for the general, anisotropic Heisenberg model [9] (sometimes called the XYZ model), where σ_j^i are the familiar Pauli matrices acting on site j. Special cases of the general Heisenberg model include the Isotropic XXX case (with $J_x = J_y = J_z$), the XXZ case (with $J_x = J_y$), the XY case (with $J_z = 0$), and the Ising model ($J_x = J_y = 0$).

The general Heisenberg model is solved using the Algebraic Bethe Ansatz [9] (ABA) which is beyond the scope of this summary. However, the basic idea involves making use of the large family of Invariants that is available. We will focus on the XXX and XXZ cases. Then we can observe that the commutator $[\sigma_j^x\sigma_{j+1}^x + \sigma_j^y\sigma_{j+1}^y, \sigma_j^z + \sigma_{j+1}^z]$ vanishes. This can be seen by observing that $\frac{1}{2}(1 + \vec{\sigma}_j \cdot \vec{\sigma}_{j+1})$ is equal to the permutation operator

which permutes site j and site j+1.

The consequence is that the Hamiltonian commutes with the invariant $Z = \sum_{j=1}^{N} \sigma_j^z$. In other words, it preserves the number of spins pointing up minus the number of spins pointing down. We can compare this to a reference state where all spins point up, where a given number of spins have been flipped, corresponding to quasiparticles which we call Magnons whose total number is conserved. We then observe that for a fixed number of magnons, the size of the Hilbert space scales polynomially as opposed to the exponential scaling of the full Hilbert space, which demonstrate the conceptual simplification that this brings us. The dynamics of the model can then be analyzed using properties of the magnon-magnon interaction such as the Yang-Baxter equation [9].

However, in the ferromagnetic XXX model where $J_x = J_z = J$ is negative, we have a property called the Frustration Free property: the total ground state is a ground state of each individual term. Hence, we can immediately get the ground state "for free" without considering the Dynamics. Any ground state must be a maximally symmetric state. Then the ground state in the subspace corresponding to any given magnon number is the uniform superposition of all possible positions of the magnons, or a sum of all permutations of any fixed basis state.

Both the conservation of Z and the Frustration Free property generalizes directly to our model, while the Yang-Baxter equation used in the ABA does not seem to generalize. Hence the Fredkin model is harder to solve than the Heisenberg model due to more complicated magnon-magnon interactions, but we can still obtain a significant amount of information about it. In particular, it turns out that the single-magnon dispersion relation is exactly the same.

1.0.2 Frustration-Free models

The other tradition that the Fredkin model originates from is that of models with highly entangled ground states. This consisits of finding fine-tuned Hamiltonians such that they have a unique highly entangled ground state. This was the way in which the model was found, and it was essentially a miraculous coincidence that the two overlapped.

One line of research has been to find natural frustration free Hamiltonian with dynamics that are hard to solve, but with an interesting and nontrivial solvable ground state. Examples of this include the Heisenberg chain, valence bond solids (VBS) such as the AKLT model [1] and the Majumdar–Ghosh [5] chain, and any parent Hamiltonian of a Tensor product state. However, one common trend among these is that the entanglement which is present is short-ranged rather than long ranged. For example, looking at the AKLT ground state, tracing over the center of the lattice and considering the edges gives us a product state with no entanglement between the edges. Furthermore, the entanglement between two blocks is constant. This corresponds to a rule known as

the Area law which puts strong restrictions on the kinds of entanglement that may exist.

Another line of research is then to find counterexamples to the Area law, which essentially corresponds to "Easy" systems to solve. It was expected that all physically reasonable local models conform to some variants of it, and hence the counterexamples that were initially constructed relied on long-range interactions that decayed polynomially [3]. In particular, B. Swingle and T. Senthil [8], based on scaling arguments, argued that "physically reasonable" local Hamiltonians with unique ground states can violate the area law by at most a $log(n)$ factor, which for a spin chain implies that $log(n)$ is the maximum expected entanglement entropy scaling. Physically reasonable essentially means not fine-tuned; for example, translational invariance or robustness against perturbations qualify as physically reasonable.

Fine-tuned counterexamples were presented in two papers, [2] by Sergei Bravyi et al which found a local example of a spin-1 chain based on Motzkin paths which saturated the $log(n)$ limit, and in [6] by Peter Shor and Ramis Movassagh which generalized the first model to a colored version corresponding to higher-integer spin chains. The generalized model then allows for a square root scaling of the entanglement entropy. The general idea in both models is that basis states of the Hilbert space can be identified with Motzkin words: sequences of symbols "(","),"0" such as "(0)0(()0)" such that all parentheses are matched, where the parenthesis matching condition is what gives rise to entanglement within the model. The correspondence to basis states in a spin chain in the spin-1 case is made by identifying $|\uparrow\rangle$ with $|(\rangle$, $|0\rangle$ with $|0\rangle$ and $|\downarrow\rangle$ with $|)\rangle$.

1.0.3 The origin of the Fredkin model

Our approach was initially to find a three-site (next-nearest neighbour) interaction hamiltonian which reproduced the result of the first paper for spin-1/2 chains. This was thought to be a hard task because of a no-go theorem for 2-site interaction spin 1/2 models which forces any unique ground state to have only two-site entanglement with no multipartite entanglement allowed, which for a translation invariant system forces the ground state to conform to the Area law.

However, it turned out that for three site interactions, there existed a counterexample. This could be found by observing that the Bravyi et al model from [2] was obtained by considering three rules for Motzkin words $0(= (0,\ 0) =)0$, $() = 00$ and making projectors (such as $(|()\rangle - |00\rangle)(\langle()| - \langle 00|)$) out of them. Our approach was then to "weaken" them by considering their consequences. One such set of consequences is $()(= (()$ and $)() = ())$, which corresponds to a spin-1/2 model (identifying $|\uparrow\rangle$ with $|(\rangle$ and $|\downarrow\rangle$ with $|)\rangle$) with a local three site interaction given by

$$H = (|()(\rangle - |(())\rangle)(\langle()(| - \langle(()|) + (|())\rangle - |)()\rangle)(\langle())| - \langle)()|)$$

Miraculously however, this Hamiltonian that was initially given as a hard to read expression in terms of projectors onto Dyck/Motzkin words (Dyck words are Motzkin words with no "0" symbol) turned out to have a simple expression in terms of standard Pauli matrices. This expression is:

$$H_j = (1 + \sigma_j^z)(1 - \vec{\sigma}_{j+1} \cdot \vec{\sigma}_{j+2}) + (1 - \vec{\sigma}_j \cdot \vec{\sigma}_{j+1})(1 - \sigma_{j+2}^z) \tag{1.1}$$

which has a close relationship to the Heisenberg XXX model and unifies the two schools of model-building. Further investigation of the model found that it saturated the $\log n$ bound just like the spin-1 model and that it could also be generalized to a colored model with a $\sqrt{N}$ scaling of the entanglement entropy. The findings relating to the explicit construction of the ground states, the Entanglement entropies of the ground states, along with a general introduction to the model and a comparison to the Heisenberg model, were then published in [7] (paper I in this thesis). Furthermore, a general survey of correlation functions was made along with a thorough numerical analysis of the gap and of propagation of information using the DMRG method was published in [4] (paper II in this thesis).

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A

Paper I: Fredkin Spin Chain

Fredkin Spin Chain

Olof Salberger and Vladimir Korepin

June 22, 2016

Abstract

We introduce a new model of interacting spin 1/2. It describes interactions of three nearest neighbors. The Hamiltonian can be expressed in terms of Fredkin gates. The Fredkin gate (also known as the CSWAP gate) is a computational circuit suitable for reversible computing. Our construction generalizes the model presented in [5] to half-integer spins.

Our model can be solved by means of Catalan combinatorics in the form of random walks on the upper half plane of a square lattice [Dyck walks]. Each Dyck path can be mapped on a wave function of spins. The ground state is an equally weighted superposition of Dyck walks [instead of Motzkin walks]. We can also express it as a matrix product state. We further construct a model of interacting spins 3/2 and greater half-integer spins. The models with higher spins require coloring of Dyck walks. We construct a SU(k) symmetric model [where k is the number of colors]. The leading term of the entanglement entropy is then proportional to the square root of the length of the lattice [like in the Shor-Movassagh model].

A.1 Introduction

Entanglement is a feature separating the classical and quantum worlds. It was discovered 80 years ago, but it becomes increasingly important in modern contexts for building quantum devices. Entanglement is used in quantum communication and computation. A good measure of entanglement is the so called entanglement entropy [1]. It has previously been studied in various models of interacting spins. Quantum fluctuations in spin models are enhanced as the number of spatial dimensions decreases. Spin chains provide good models for the experimental realization of quantum devices such as quantum computers [8] [4] [6] [7]. Entanglement entropy in spin chains was studied intensely. Recently Peter Shor and Ramis Movassagh constructed an spin chain describing local interaction of integer spins [5], [2]. It display abnormally high levels of entanglement. We generalize their results to half-integer spins.

One challenge when generalizing this construction of entangled ground states to spin 1/2 chains is the no-go theorem proven by Chen et al in [3], which proves that unfrustrated spin 1/2 chains with Hamiltonians that can be reduced to two-site interactions (including all models with nearest neighbour interactions) must have at least one ground state which is a product of two-qbit state, which eliminates the possibility of *unique* entangled ground states. However, it turns out that we can circumvent this limitation by looking at chains with irreducible three-site (next nearest neighbour) interactions. Thus, the model that we present belongs to the simplest possible spin 1/2 case which may exhibit a unique, unfrustrated, and non-trivially entangled ground state.

A.2 The Hamiltonian and ground state

Our bulk Hamiltonian is given by an interaction between singlet pairs with neighbouring sites. Specifically, the Hamiltonian can be written as

$$H = H_{bulk} + H_{\partial} = H_{\partial} + \sum_j H_j \tag{A.1}$$

where we have the boundary term $H_{\partial} = |{\downarrow_1}\rangle \langle{\downarrow_1}| + |{\uparrow_N}\rangle \langle{\uparrow_N}|$, and where the bulk term is given by the following three-site interaction between singlet pairs and neighbouring sites:

$$H_j = |{\uparrow_j}\rangle \langle{\uparrow_j}| \otimes |S_{j+1,j+2}\rangle \langle S_{j+1,j+2}| + |S_{j,j+1}\rangle \langle S_{j,j+1}| \otimes |{\downarrow_{j+2}}\rangle \langle{\downarrow_{j+2}}| \tag{A.2}$$

where $|S_{i,j}\rangle$ is the familiar singlet state $\frac{1}{\sqrt{2}}(|{\uparrow_i}\rangle |{\downarrow_j}\rangle - |{\downarrow_i}\rangle |{\uparrow_j}\rangle)$. In other words, we have an interaction term for a spin up on the left of a singlet, and a term for a spin down on the right of a singlet.

Despite its simplicity, this seemingly innocent Hamiltonian turns out to have a highly entangled ground state with a very rich combinatorial structure, as we will see in the following section which introduces the necessary formalism to write down the ground state.

Before we move on however, we allow ourselves to rewrite the bulk Hamiltonian in a few alternate ways. The first is in terms of Pauli spin operators, where it can be written as:

$$H_j = (1 + \sigma_j^Z)(1 - \vec{\sigma}_{j+1} \cdot \vec{\sigma}_{j+2}) + (1 - \vec{\sigma}_j \cdot \vec{\sigma}_{j+1})(1 - \sigma_{j+2}^Z) \tag{A.3}$$

finally, we have yet another way to write down the bulk terms of the Hamiltonian, by noting their relationship to Fredkin (Controlled-Swap) gates:

$$H_j = (1 - F_{j,j+1,j+2}) + (1 - \sigma_{j+2}^x F_{j+2,j+1,j} \sigma_{j+2}^x) \tag{A.4}$$

Where $F_{i,j,k}$ is the Fredkin gate acting on three qbits, which is both Hermitian and unitary. It swaps j,k if site i is in state $|\uparrow\rangle$ and does nothing if it is in state $|\downarrow\rangle$.

A.2.1 Combinatorial prerequisites: Dyck Words

In this section we consisely describe the of combinatorics necessary to describe the ground state and its relation to the Hamiltonian.

The central idea for defining our model is to think of the basis states of our length N chain of two-state systems as the set of N-symbol words in a two-letter alphabet. Depending on context, the letters would then be called $\uparrow$ and $\downarrow$ for the basis states $|\uparrow\rangle$ and $|\downarrow\rangle$, 0 and 1 for $|0\rangle$ and $|1\rangle$, or more suggestively for our purposes, (and) for $|($ $\rangle$ and $|$ $)\rangle$.

Among generic two-letter words, we may single out the set of Dyck words. *These are precisely the set of words consisting of an equal number of left and right parentheses, such that every left parenthesis has a matching right parenthesis further right along the word.* That is, there are no right or left parentheses that are unmatched on either side of the word.

For example, ()(()) and (()()) are both valid six-letter Dyck words, while)(()() or ())(() are not.

Clearly, a word can only be Dyck if N = 2n is even, however since splitting up a word into pieces that may be odd is a useful operation we will still consider words of odd length.

The Dyck-ness of a word is thus a global feature which forces symbols at different places in the word to be correlated. For example, if we slice up the word along the middle the number of unmatched left parentheses in the left half must be equal to the number of unmatched right parentheses in the right half. These correlations will be the key source of entanglement in the physical model that we propose below.

Dyck words as an equivalence class

Having defined Dyck words and observed that their definition is global, we then observe that they do admit a local description.

To do this, we consider the larger set of arbitrary words and introduce the following moves, which in analogy to Reidemeister moves we call the Fredkin moves:

$$()) \leftrightarrow)() \tag{A.5}$$
$$(() \leftrightarrow ()(\tag{A.6}$$

where we allow a matched pair of adjacent parentheses to be moved anywhere. The reason why we call these the Fredkin moves is that when viewed as bit strings, the involution that takes one side to the other is a three-bit reversible logic gate known as the Fredkin gate, up to a flipped control bit. We will sometimes also refer to these as Fredkin relations.

We now consider how these relations divide up the set of words of length N into equivalence classes. We immediately observe that the relations preserve the matchings of the parentheses, and as such map Dyck words to Dyck words only and non-Dyck words to non-Dyck words only.

A full classification of the equivalence classes may be performed fairly straightforwardly by observing that:

1) If any given word has at least one pair of adjacent matched parentheses, we may use the Fredkin relation to move it to the front of the word. This allows us to focus on a subword of length N-2

2) The only words that have no matched pair of adjacent parentheses are of the form , i.e. consist of a left parentheses followed by b right parentheses.

Together, these observations imply that every word of length N is equivalent to exactly one word consisting of 2k matched parentheses, followed by a unmatched right parenthese, followed by b left parentheses. That is, of the form ()()...k times () ())))... a times ...)) ((((... b times...(((, where $a+b+2k=N$. We call this the *standard form* of the word. Since clearly none of these words are equivalent to each other this completes our classification. We may denote these equivalence classes $C_{a,b}(N)$, and observe that $C_{0,0}(N)$, which is non-empty for even N, is exactly the set of Dyck words of length N = 2n.

We finish off by stating that the number of words in each equivalence class $C_{a,b}(N)$

is given by:

$$|C_{a,b}(N)| = \begin{cases} \binom{N}{\frac{N+a+b}{2}} - \binom{N}{\frac{N+a+b}{2}+1} & \text{if } N-a-b \text{ is even and positive} \\ 1 & \text{if N = a + b} \\ 0 & \text{otherwise} \end{cases} \tag{A.7}$$

which in the nonzero cases match the numbers in the Catalan triangle (where each number is the sum of the numbers above it and the one to its left). We note that in the special case where N = 2n and a = b = 0, we recover the famous Catalan numbers $C_N = \frac{1}{n+1}\binom{2n}{n}$.

We may prove this by constructing an explicit bijection between $C_{a,b}$ and $C_{0,a+b}$, which incidentally is also a symmetry of the bulk Hamiltonian. This simply consists of exchanging each unmatched right parenthesis in a member of $C_{a,b}$ with an unmatched left parenthesis. Since the subword between one unmatched parenthesis of a word and the next must be a Dyck word, this must map matched parentheses to matched parentheses and unmatched parentheses to unmatched parentheses, which makes the inverse of the map trivial to find.

The number of elements in $C_{0,a+b}$ can then be obtained directly from Bertrand's ballot theorem with ties allowed [9], or by using the combinatorial definition of the numbers in Catalan's triangle.

Dyck words reinterpreted as Dyck paths

In this section, we introduce the path notation to describe Dyck words. This notation is particularly useful in handwritten work and has the advantage of being easier to parse. The path formalism is also generally the most convenient to use for counting the number of elements in a given Fredkin equivalence class.

The key observation is that two-letter words can also be interpreted as paths on the upper half plane of a lattice. Specifically, all words in the equivalence class $C_{a,b}(N)$ can be viewed as a path from the lattice point (0,a) to the lattice point (N,b) such that on each step the path can only travel diagonally from (x,y) to $(x+1, y \pm 1)$, and such that it is always stays in the upper half plane $y \geq 0$. The bijection is given simply by associating left parentheses with a step up and right parentheses with a step down.

Parenthesis matching can be obtained in the following way: for any word of the form $W = w_1(w_2)w_3$, we have that w_2 must be a Dyck word if and only if the two parentheses we have written out are matched, since otherwise, either the left or right parentheses would instead be matched with an unmatched parenthesis of w_2.

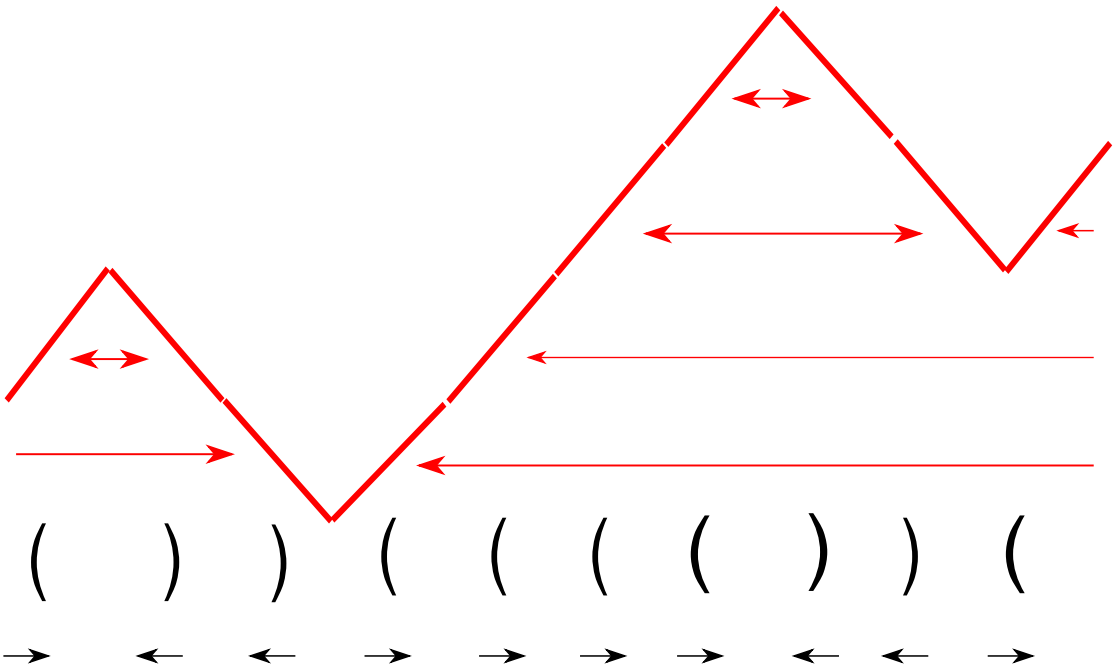

Figure A.1: In this figure we show the different ways in which our basis states can be expressed: as a sequence of spins up or down, as Dyck words, or as paths. It also shows the relation between matched parentheses and matched steps.

As a result, the path corresponding to w_2 never goes further down than its starting point. The matching of parentheses can then be translated into matching steps in the following way: for a given up step from $y = y_0$ to $y = y_0 + 1$, the first down step after it which goes from $y = y_0 + 1$ to $y = y_0$, if it exists, is the *matching down step* which corresponds to the matching right parenthesis. The two-dimensional nature of paths make matchings significantly easier to parse, at the expense of using a less compact notation.

A.2.2 The ground state

The ground state of our model with 2n sites $|D_n\rangle$ can be written as a uniform superposition of the basis states corresponding to Dyck words(or paths).

To give some low-n examples, using the bracket notation where $|\uparrow\rangle = |($ and $|\downarrow\rangle = |)\rangle$, we have:

$$|D_1\rangle = |()\rangle$$
$$|D_2\rangle = |()()\rangle + |(())\rangle$$
$$|D_3\rangle = |((()))\rangle + |(()())\rangle + |()(())\rangle + |(())()\rangle + |()()()\rangle$$

and

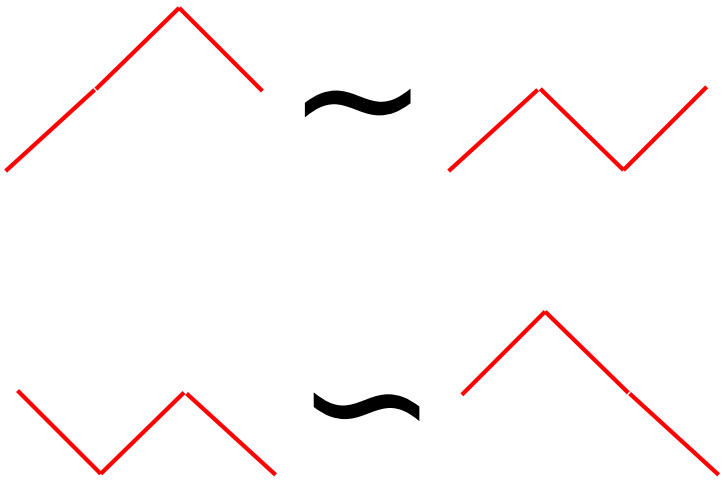

Figure A.2: The Fredkin moves in path notation.

$$
\begin{aligned}
|D_4\rangle = |(((\,)(\,))(\,))\rangle + \\
|(((\,)(\,))(\,))\rangle + |(((\,)(\,))(\,))\rangle + |((\,)((\,))(\,))\rangle + \\
|(\,)(((\,))(\,))\rangle + |(((\,))(\,))(\,)\rangle + |((\,))((\,))\rangle + \\
+ |((\,)(\,)(\,))\rangle + |\,)(((\,)(\,))\rangle + |((\,)(\,))(\,)\rangle \\
+ |((\,))(\,)(\,)\rangle + |(\,)((\,))(\,)\rangle + |(\,)(\,)((\,))\rangle \\
+ |(\,)(\,)(\,)(\,)\rangle
\end{aligned}
$$

which have 1, 2, 5, and 14 terms, respectively.

To see that it is the unique ground state, we do the following: first, we show that $|D_n\rangle$ is indeed a zero eigenstate of all individual terms in the Hamiltonian. Next, we observe that this implies frustration freeness: each term is positive semidefinite, therefore any other eigenstate with zero eigenvalues must be a zero eigenstate of all individual terms. Finally, we show that any state with that last property must be equal to $|D_n\rangle$. Alternatively, one can simply apply the orbit theorem in the appendix to the bulk Hamiltonian, and check which ground states are also ground states of the boundary terms.

We start with the boundary terms. Since every Dyck word must start with an opening parenthesis and end with a closing parenthesis(for walks, start with a step up and end with a step down), $|D_n\rangle$ is indeed a ground state of the boundary terms.

Next, we consider the bulk terms. Consider the term

$$|\uparrow_j\rangle\langle\uparrow_j| \otimes |S_{j+1,j+2}\rangle\langle S_{j+1,j+2}| = \left[\,|(\,)\rangle_j - |\,)(\,\rangle_j\,\right]\left[\,\langle(\,)|_j - \langle\,)(\,|_j\,\right]$$

, where the index j denotes the position of the first site.

This term is a projector onto the state $|(\,)\rangle_j - |\,()\rangle_j$. We then observe that we may generically write the Dyck state as $|\psi_1\rangle \otimes |(\,)\rangle_j \otimes |\psi_2\rangle + |\chi_1\rangle \otimes |\,()\rangle_j \otimes |\chi_2\rangle + |\psi\rangle$, where $|\psi\rangle$ is orthogonal to both $|(\,)\rangle_j$ and $|\,()\rangle_j$. By definition, the last term is annihilated by our projector, so we may focus on the first two.

However, we note that the invariance of the set of Dyck words under the Fredkin moves (A.5) give us that if $w_1 w_2$ is a Dyck word, so is $w_1(\,)(w_2$ and vice versa. Therefore, in our expression above we must have $|\psi_1\rangle = |\chi_1\rangle$ and $|\psi_2\rangle = |\chi_2\rangle$, and we have $|D_n\rangle = |\psi_1\rangle \otimes \big[\, |(\,)\rangle_j + |\,()\rangle_j \,\big] \otimes |\psi_2\rangle + |\psi\rangle$. Both terms are orthogonal to $|(\,)\rangle_j - |\,()\rangle_j$ and will be annihilated by our projector. The process is analogous for the second bulk term.

Therefore, the Dyck state is indeed a ground state of all individual terms of our Hamiltonian. Since such a state exists, any other ground state of the Hamiltonian must also be a ground state of all individual terms.

Now, we consider the possible ground states of the bulk terms. We now know that it must be a ground state of each individual term. We may then perform the above calculation in reverse: we break up an arbitrary ground state candidate $|\psi\rangle$ into $|\Psi\rangle = |\psi_1\rangle \otimes |(\,)\rangle_j \otimes |\psi_2\rangle + |\chi_1\rangle \otimes |\,()\rangle_j \otimes |\chi_2\rangle + |\psi\rangle$, where $|\psi\rangle$ is orthogonal to both $|(\,)\rangle_j$ and $|\,()\rangle_j$. If this is annihilated by the projector $\big[\, |(\,)\rangle_j - |\,()\rangle_j \,\big]\big[\, \langle(\,)|_j - \langle\,()|_j \,\big]$, we must have $\big[\, \langle(\,)|_j - \langle\,()|_j \,\big]\, |\Psi\rangle = 0$. Expanding this, we get $|\psi_1\rangle \otimes \langle(\,)|_j\, |(\,)\rangle_j \otimes |\psi_2\rangle - |\chi_1\rangle \otimes \langle\,()|_j\, |\,()\rangle_j \otimes |\chi_2\rangle$, so we come to the conclusion that for any such ground state $|\chi_1\rangle = |\chi_2\rangle$ and $|\psi_1\rangle = |\psi_2\rangle$. In other words, the parts of the ground state containing $|\,()\rangle_j$ and $|(\,)\rangle_j$ are exactly equal. We can then simply repeat this for all bulk terms in the hamiltonian.

This is the key observation we needed to make. Writing out the ground state as $|\Psi\rangle = \sum_i c_i\, |w_i\rangle$, we have just proven that if the words w_i and w_j are related by a Fredkin move, then $c_i = c_j$.

To formulate this in terms of an explicit orthogonal basis for our ground states, we can use our discussion of equivalence classes under Fredkin moves in section A.2.1 to define the states $|C_{a,b}(N)\rangle = \sum_{w_i \in C_{a,b}(N)} |w_i\rangle$ which are direct superpositions of all states in the equivalence class $C_{a,b}(N)$. Then, we see that any ground state $|\Psi\rangle$ of the bulk terms can be written as $|\Psi\rangle = \sum_{a,b} |C_{a,b}(N)\rangle$, so the states $|C_{a,b}(N)\rangle$ form a complete basis for the space of bulk term ground states.

Among these, for even N = 2n, only $|C_{0,0}(N)\rangle = |D_n\rangle$ which has no unpaired parentheses/steps is also a ground state of the boundary terms, which finally proves that the Dyck state is indeed the unique ground state of our Hamiltonian when the boundary terms are introduced.

Schmidt decomposition and measures of entanglement

The Dyck state is highly entangled. If we break up the chain into two halves with lengths L and N-L, where without loss of generalization we may assume that $L < N - L$. The Schmidt rank will then be $\xi = \lfloor \frac{L}{2} \rfloor$, while the the entanglement entropy will scale as

$$S = \frac{1}{2}\log(L) + O(1)$$

.

Our primary tool to study the entanglement between blocks will be the the Schmidt decomposition. The Dyck state can be decomposed into the states

$$|D_n\rangle = \sum_{m=0}^{L} \sqrt{p_m}\, |C_{0,m}(L)\rangle \otimes |C_{m,0}(N-L)\rangle \tag{A.8}$$

where we define the states $|C_{a,b}(L)\rangle$ as a direct generalization of the Dyck state, which is a direct superposition of the basis states corresponding to the equivalence classes $C_{a,b}(N)$ that we defined in section A.2.1.

In particular, we note that $C_{a,b}(L)$ is non-empty if and only if $a + b < L$ and the parity of $a + b$ matches that of L. As a result, the nonzero terms $|C_{0,m}(L)\rangle \otimes |C_{m,0}(L)\rangle$ will be those with even $m < L$ if L is even, or odd $m < L$ if L is odd.

This leads to our above expression for the Schmidt rank, since the number of even integers $\leq$ L if L is even is given by $\frac{L}{2}$, and the number of odd integers less than L if L is odd is given by $\frac{L-1}{2}$. The two expressions may be combined concisely with the floor function.

Now we may move on to compute the entanglement entropy. We start by deriving a useful expression for p_m, which must be the product of the normalization factors of $|C_{0,m}(L)\rangle$ and $|C_{m,0}(L)\rangle$ divided by the normalization factor of $|D_n\rangle$. This gives us $p_m = \frac{|C_{0,m}(L)||C_{0,m}(N-L)|}{|C_{0,0}(N)|}$.

To find a useful expression for the p_m, we will start by cleaning up our notation a bit. We have already written $N = 2n$. We will split the expression into two cases where L is odd or even.

For the even case, we write $L = 2l$, and $m = 2h, h \in [0,l]$ as the p_m will be zero for odd m. Then for the $h < l$ case we may simplify:

$$|C_{0,m}(L)| = \binom{2l}{l+h} - \binom{2l}{l+h+1} = \frac{2h+1}{l+h+1}\binom{2l}{l+h}$$
$$|C_{m,0}(N-L)| = \binom{2(n-l)}{n-l+h} - \binom{2(n-l)}{n-l+h+1} = \frac{2h+1}{n-l+h+1}\binom{2(n-l)}{n-l+h}$$

while in the odd case we write $L = 2l + 1$ and $m = 2h + 1, h \in [0,l]$ which gives us

$$|C_{0,m}(L)| = \binom{2l+1}{l+h+1} - \binom{2l+1}{l+h+2} = \frac{2h+2}{l+h+2}\binom{2l+1}{l+h+1}$$
$$|C_{m,0}(N-L)| = \binom{2(n-l)-1}{(n-l)+h} - \binom{2(n-l)-1}{(n-l)+h+1}$$

which in the even case gives us:

$$p_h = \frac{1}{Cat(n)}\frac{(2h+1)^2}{(h+1+\frac{n}{2})^2-(l-\frac{n}{2})^2}\binom{2l}{l+h}\binom{2(n-l)}{n-l+h}$$

Our next step is then simply to use the Gaussian approximation for binomials $\binom{2n}{n+k} \approx \frac{4^n}{\sqrt{\pi n}}\exp(-\frac{k^2}{n})$, which gives us:

$$p_h \approx \frac{4^n}{\pi Cat(n)\sqrt{l(n-l)}}\frac{(2h+1)^2}{(h+1+\frac{n}{2})^2-(l-\frac{n}{2})^2}\exp\left[-h^2(\frac{1}{l}+\frac{1}{n-l})\right]$$

Which is a good approximation when n is large, and peaks when $\frac{h^2 n}{l(n-l)} \approx 1$. Since the Gaussian factor will suppress the parts where h is comparable to $\frac{n}{2}$, our final approximation becomes

$$p_h \approx \frac{h^2}{Z}\exp\left[-h^2\frac{n}{l(n-l)}\right]$$

where Z is a normalization factor.

This expression is largely analogous to the one in [2], [5], and from here on we may proceed in a manner fully analogous to the method outlined in these publications. The key idea is to approximate sums with integrals, and performing a change of variables to isolate the $L(N-L)$ dependence. In particular, we have:

$$S = -\sum_h p_h log(h) \approx -\int_0^\infty p_x log(p_x)dx = \left[\sqrt{\frac{l(n-l)}{l}}d\alpha = dx\right] =$$
$$-\int_0^\infty \sigma\rho_\alpha \log(\sigma\rho_\alpha)\sigma^{-1}d\alpha = -\int_0^\infty \rho_\alpha[\log(\sigma)+\log(\rho_\alpha)]d\alpha =$$
$$-\log(\sigma) - \int_0^\infty \rho_\alpha \log(\rho_\alpha)d\alpha = \frac{1}{2}\log\left[\frac{l(n-l)}{l}\right] - \int_0^\infty \rho_\alpha \log(\rho_\alpha)d\alpha$$

Where $p_x = \frac{x^2}{\tilde{Z}}\exp\left[-x^2\frac{n}{l(n-l)}\right]$, $\tilde{Z}$ is a normalization factor so that $\int p_x dx = 1$ and $\alpha = \sigma x$ and $\sigma = \sqrt{\frac{N}{L(N-L)}}$. Furthermore, we define $\rho_\alpha = \frac{1}{Z'}\alpha^2\exp[-\alpha^2]$ where Z' is a constant such that $\int \rho_\alpha = 1$, which gives us $p_x = \sigma\rho_\alpha$ (with a factor σ^3 from the normalization factor and a σ^{-2} from $x^2 = \sigma^{-2}\alpha^2$), which we used to insert the correct

sigma factors. Thus, when N and L are large enough for the integral approximation to be valid, we have:

$$S = \frac{1}{2} \log \left[\frac{L(N-L)}{N} \right] + O(1)$$

Matrix product state definition

To find the MPS formulation we let ourselves be guided by the form of the Fredkin moves (A.5). We would like the product $A^(A^)$ to commute with $A^($ and $A^)$, or at least have a commutator which can easily be projected out, while having a more nontrivial expression for $A^)A^($. Here A is a local matrix in matrix state represettation of the ground state. It can be compared with L operator of quantum inverse scattering method.

We can do this by setting $A^(_{ij} = \delta^{i+1,j}$ and $A^)_{ij} = \delta i,j+1$ for $\infty > i,j \geq 1$ and 0 otherwise. In that case, before we truncate to a finite bond dimension, we have $A^(A^) = 1$ while $A^)A^($ is a projector that does not commute with $A^($ or $A^)$.

To obtain the Dyck state, we introduce the boundary (basis) vector $v_i = \delta^{i,1}$. Then we have that a the matrix element $v^T A^{k_1} A^{k_2} ... A^{k_{N-1}} A^{k_N} v$ of the product will be nonzero if and only if the indices $k_1 k_2 ... k_{N-1} k_N$, which each are) or (-valued, together form a Dyck word.

This is true because for any index values we can remove $A^(A^) = 1$ without changing the value of the product until we are left with an expression of the form $v^T [A^)]^a [A^(]^b v$. Hence the matrix product depends only on to which equivalence class of the word formed by the indices belongs to under the Fredkin moves, and using the boundary vector $v_i = \delta^{i,1}$ the relevant matrix element this will yield zero if the word belongs to any equivalence class other than that of Dyck words. Hence, the matrices above do indeed give a matrix product state description of the Dyck state.

We now only have to check whether we can truncate our infinite-dimensional matrices to finite-dimensional matrices to obtain an MPS description that is actually useful. This can be done by observing that the entries of A_{ij} with i or j larger than N do not affect the product [ground state]

$$v^T A^{i_1} A^{i_2} ... A^{i_{N-1}} A^{i_N} v$$

, meaning that we can simply truncate it to an N-dimensional MPS (which can be refined to N/2 exactly, and to $O(\sqrt{N})$ with arbitrarily small errors as N becomes large).

A.2.3 Spin wave solutions

The Fredkin model is closely related to the XXX Heisenberg model. In particular, since it commutes with z-component of total spin $Z = \sum_j \sigma^z_j$, we can straightforwardly apply

the coordinate Bethe ansatz analyze the 1-magnon sector of the model.

In fact, since our model has two invariants a and b, we can obtain a slightly stronger result, namely that all sectors with $a + b = N - 2$ have a spectrum fully isomorphic to the 1-Magnon sector of a ferromagnetic Heisenberg XXX chain of length N-1.

The key insight is that when viewed as a path, these equivalence classes consist of a long dip with a single /\ peak that may be moved around. The N-1 basis states of this class, which we call $|\psi_j\rangle$, correspond to the path where the single peak has an up-step at site j and the down-step at site $j + 1$.

For each j, the only terms in the Fredkin Hamiltonian that can affect $|\psi_j\rangle$ non-trivially will be the three-site terms that act on both site j and j+1, which leads to four candidates. By brute force consideration of all cases, we will see that up to constants there will be exactly two terms remaining, one which maps $|\psi_j\rangle$ to $-|\psi_{j+1}\rangle$ and one which maps $|\psi_j\rangle$ to $-|\psi_{j-1}\rangle$. Therefore, the restriction of the Fredkin model Hamiltonian with open boundary conditions to this sector is isomorphic to the ferromagnetic Heisenberg XXX Hamiltonian with open boundary conditions restricted to the one-magnon sector, on a chain of length N-1.

A.2.4 Ground states with alternative boundary conditions

While we have been focusing on the ground states with boundary terms $H_\partial = |\downarrow_1\rangle\langle\downarrow_1| + |\uparrow_N\rangle\langle\uparrow_N|$, our model does exhibit some rather surprising properties with other boundary conditions.

The first generalization we could make is to vary the boundary terms in the following way:

$$H_\partial(\alpha, \beta) = (1 - \alpha\sigma_0^z) + (1 + \beta\sigma_N^z)$$

,which yields our previous boundary terms for $\alpha = \beta = 1$. For $\alpha = -\beta$, the bulk ground states $|C_{N,0}\rangle$ and $|C_{0,N}\rangle$ will be ground states of the case where $\alpha = 1$ and $\alpha = -1$, respectively. For $\alpha = \beta = -1$, we have an $N - 2$ degeneracy as all the domain wall states $|C_{a,b}\rangle$ with $a + b = N$ and a,$b \geq 1$ are ground states. Since in call cases we have bulk ground states which are also boundary ground states, the model stays frustration free meaning these are the only possible ground states for these boundary conditions.

Furthermore, since the model is frustration free for all possible sign combinations of α, β, the ground state depends *only* on the signs of α, β and not on their magnitude. In other words, phase transitions may happen only when α or β is zero. These results may be combined into the phase diagram in figure A.3, which features four different phases separated by first order phase transitions where the energy levels become degenerate.

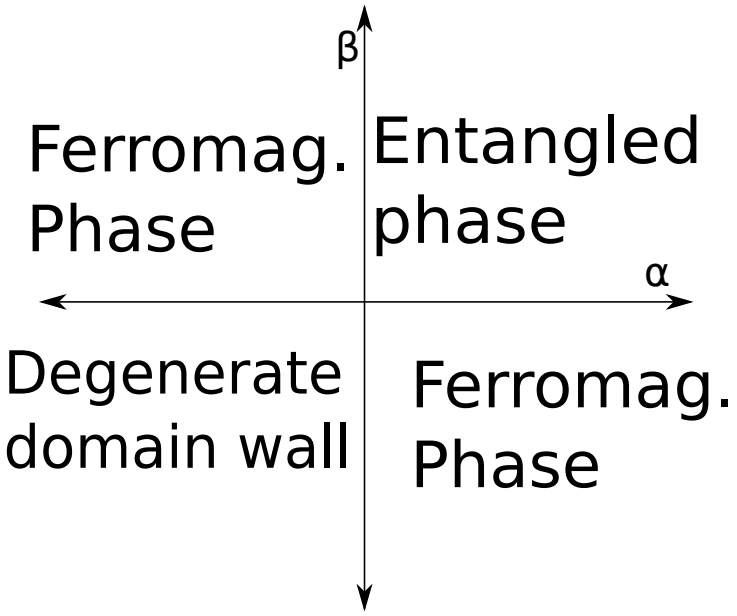

Figure A.3: A phase diagram describing the different phases of the model as we vary the boundary conditions.

Periodic boundary conditions

We get a somewhat more surprising result with periodic boundary conditions. Here, we note that the Hamiltonian commutes with $Z = \sum_j \sigma_j^z$ and with the cyclic shift operator Π which maps the site j to the site $j + 1$. We may use the eigenvalues of these two operators to index our ground states in the model with periodic boundary conditions.

For odd N, all ground states are eigenstates with eigenvalue 1 of Π, and can be indexed solely using the Z operator. In this case all ground states also happen to be eigenstates of the Heisenberg XXX model and are totally symmetric. The degeneracy in this case is N.

For even $N = 2n$, the situation is different, and we have a ground state degeneracy N+1. N of these are eigenvectors with unit eigenvalues of the shift operator Π and are also Heisenberg XXX ground states. However, there is one additional state, which we call the *anomalous state* $|D_{an}\rangle$, which is an eigenstate of Π with eigenvalue -1, and a zero eigenstate of Z. Is is given by:

$$|D_{an}\rangle = \frac{1}{\sqrt{\binom{2n}{n}}} \sum_{m=0}^{n} \sqrt{|C_{m,m}|}(-1)^m |C_{m,m}\rangle$$

To see why this is the case, we consider what happens to the equivalence classes as we add Fredkin moves that continue periodically across the edge.

We may define a periodic matching across the edge, which is most easily done by going back to the Dyck word formalism: two parentheses are periodically matched if they are matched in the usual sense for at least one cyclic permutation of the Dyck word. Two steps are periodically matched if their corresponding parentheses in the Dyck word formalism are periodically matched.

The key idea is then that we can use our previous algorithm that reduces any path to a series of down steps (right parentheses), followed by a series of /\ peaks (matched pairs), followed by a series of up steps (left parentheses). However, whenever we have a down-step at site 1 and an up step at site N, we have a peak wound across the edge.

If we have any unmatched step adjacent to it, we can move this peak away from the edge to join the other peaks. By repeating this process, we can then always reduce to the case where all matched steps are adjacent to their match, and we are left with Z unmatched up steps and no unmatched down steps if Z is positive, or $|Z|$ unmatched down steps and no unmatched upsteps if Z is negative.

At this point, we are left with two cases: Either there is a peak wound across the edge, or there isn't. If $Z > 0$, we can move an unmatched up-step to site N-1, move the peak past it, and we will be left with no peaks wound across the edge. For $Z < 0$, we may perform the mirror image of this algorithm. However, for Z = 0 there is no way to transform one case into the other.

Thus, for $Z \neq 0$ we are left with exactly one equivalence class for each value of Z:

$$C_Z = \begin{cases} \cup_k C_{Z+k,k} & \text{if } Z > 0 \\ \cup_k C_{k,Z+k} & \text{if } Z < 0 \end{cases}$$

which all just contain all basis states that satisfy $\sum_j \sigma_j^z = Z$. Using the orbit theorem we see that these all generate the same ground states as the Heisenberg XXX Hamiltonian.

In the the Z = 0 case, we have two equivalence classes that classify whether the number of pairs matched across the edge is odd or even. Each of these gives us a ground state. The symmetric sum of these is the $Z = 0$ ground state of Heisenberg XXX, while the difference yields the anomalous state above.

A.3 Generalizing to a colored SU(k)-symmetric model with a square root entanglement entropy leading term

It is possible to generalize the Fredkin model to exhibit a colored Dyck state as its ground state in a manner largely analogous to [5], which yields an exponentially increasing

Schmidt rank and entanglement entropy. However, since we consider Dyck paths rather than Motzkin paths the Hilbert space for each site will be of even dimension, which allows us to naturally write it as a tensor product of a two-dimensional Hilbert space and a k-dimensional "color" Hilbert space.

In particular our colored model has a manifest $U(1) \times SU(k)$ symmetry which generalizes the U(1) symmetry of the uncolored Fredkin model, where k is a positive integer giving the number of colors.

The expression for the Fredkin Hamiltonian above in terms of Pauli matrices can be generalized to an expression in terms of $SU(2) \otimes SU(c)$ matrices for each site j of the form $T_j^a = \sigma_j^z \otimes t_j^a$ where the t^a are the generators of SU(k) in the fundamental representation. For convenience we will also use the $SU(2)$ matrices that by abuse of notation we write $\sigma_j^i = \sigma_j^i \otimes 1_j$.

Finally, we define the projection operators $P_j^{\pm} = \frac{1 \pm \sigma_j^z}{2}$ and the cyclic permutation operator C_{j_1,j_2,j_3} which cyclically permutes the sites j_1, j_2, j_3.

This allows us to conveniently write the Hamiltonian in a manifestly SU(k)-invariant way as:

$$H = H_F + H_X + H_\partial \tag{A.9}$$

where

$$H_F = \sum_{j=1}^{N-2} P_j^+ P_{j+1}^+ P_{j+2}^- + P_j^+ P_{j+1}^- P_{j+2}^+ - P_j^+ P_{j+1}^+ P_{j+2}^- C_{j,j+1,j+2} - C_{j,j+1,j+2}^\dagger P_j^+ P_{j+1}^+ P_{j+2}^- +$$
$$+ P_j^+ P_{j+1}^- P_{j+2}^- + P_j^- P_{j+1}^+ P_{j+2}^- - P_j^+ P_{j+1}^- P_{j+2}^- C_{j,j+1,j+2}^\dagger - C_{j,j+1,j+2} P_j^+ P_{j+1}^- P_{j+2}^-$$

$$H_X = \sum_{j=1}^{N-1} P_j^+ P_{j+1}^- \left[\sum_a (T_j^a + T_{j+1}^a)^2 \right]$$

$$H_\partial = P_1^- + P_N^+$$

All three of these operators manifestly commute with the $SU(k)$ generators $T^a = \sum_{j=1}^N T_j^a$, and with the operator $Z = \sum_{j=1}^N \sigma_j^z$, which together generate the symmetry group $SU(k) \times U(1)$ of the model, which can naturally be viewed as a full $U(k)$ symmetry. The Hilbert space at each site is then most naturally viewed as a sum of two mutually conjugate fundamental representations of U(k).

To illustrate the Hamiltonian more clearly, we can expand it in the product state basis as a sum of projectors. In that case, we can naturally write:

$$H_F = \sum_{j=1}^{N-2} \sum_{c_1,c_2,c_3} (|\downarrow_j^{c_1}\uparrow_{j+1}^{c_2}\downarrow_{j+2}^{c_3}\rangle - |\uparrow_j^{c_2}\downarrow_{j+1}^{c_3}\downarrow_{j+2}^{c_1}\rangle)(\langle\downarrow_j^{c_1}\uparrow_{j+1}^{c_2}\downarrow_{j+2}^{c_3}| - \langle\uparrow_j^{c_2}\downarrow_{j+1}^{c_3}\downarrow_{j+2}^{c_1}|)+$$
$$(|\uparrow_j^{c_1}\uparrow_{j+1}^{c_2}\downarrow_{j+2}^{c_3}\rangle - |\uparrow_j^{c_2}\downarrow_{j+1}^{c_3}\uparrow_{j+2}^{c_1}\rangle)(\langle\uparrow_j^{c_1}\uparrow_{j+1}^{c_2}\downarrow_{j+2}^{c_3}| - \langle\uparrow_j^{c_2}\downarrow_{j+1}^{c_3}\uparrow_{j+2}^{c_1}|)$$

$$H_X = \sum_{j=1}^{N-1} \left[1 - \frac{1}{k}(\sum_{c_1} |\uparrow_j^{c_1}\downarrow_{j+1}^{c_1}\rangle)(\sum_{c_2} \langle\uparrow_j^{c_2}\downarrow_{j+1}^{c_2}|)\right] P_j^+ P_{j+1}^-$$
$$H_\partial = P_1^- + P_N^+ = \sum_{c_1} |\downarrow_1^{c_1}\rangle \langle\downarrow_1^{c_1}| + |\uparrow_N^{c_1}\rangle \langle\uparrow_N^{c_1}|$$

where c_1,c_2, c_3 are colour indices running from 1 to k.

This model can be shown to reduce to the Fredkin model when $k = 1$, and in general the ground states can be obtained in a fully analogous manner and described in terms of combinatorial objects. The extension we will need is colored Dyck paths.

A.3.1 Invariants of the Hamiltonian and characterization of the bulk ground states

The basic idea here is the same as before: identifying basis states with paths, where we generalize the k=1 case by considering colored paths.

Our first move should then be to identify invariants of H_F that may allow us to block diagonalize it. In the uncolored case, the only invariants were the number of unmatched up/down steps in the path notation or unmatched left/right parentheses in the word notation.

In the colored case, the Fredkin moves have more invariants, as we have already seen from the fact that the Hamiltonian commutes with the T^a operators.

The key observation here is that the Hamiltonian generates the colored Fredkin moves, which we have presented in path notation in figure A.4. We see that these must preserve the color and order of the unmatched steps, as well as the color of the matched pairs.

Since we can move any /\ peak to any point in the path, we may use our previous algorithm where we repeatedly move the last peak to the beginning of the path until we are left with a series of single peaks followed by a dip, which up to permutations of the peaks will give the same result for any member of an equivalence class. This allows us to clearly see what equivalence classes we will be left with.

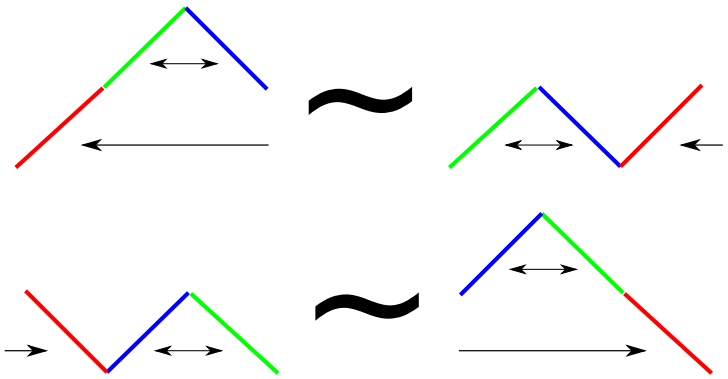

Figure A.4: The colored Fredkin moves in path notation. Note that the color of the matched pair and of the unmatched step is preseved, as well as the height of the unmatched step.

Specifically, the equivalence classes are fully specified by an ordered list of the colors of the unmatched up and down steps, along with the number of matched pairs corresponding to each color combination along the path.

To keep our approach SU(k)-covariant, it is convenient to work with basis states that are not quite product states when trying to use the orbit theorem. Since the colors of up and down steps form mutually conjugate fundamental representations of SU(k), they can combine into an SU(k) singlet or a member of the adjoint representation of SU(k). Our choice of basis states will thus correspond to paths(σ_j^z eigenstates), where the colors of each matched pair combine to either a color singlet $|0\rangle$, or to an element $|a\rangle$, $a \in [1,k^2-1]$ in the adjoint representation of SU(k).

Therefore, we may define the equivalence classes $C_{a,c_a,b,c_b,N^0,N^1\ldots N^{k^2-1}}$, where a,b are analogous to in the uncolored case, c_a, c_b are lists of length a,b, of the colors of the unmatched steps, N^0 is the number of matched pairs whose colors combine to singlets, and N^a is the number of matched pairs that combine into the adjoint representation state a, and where we have the additional relation $2(N^0 + \sum_{a=1}^{k^2-1} N^a) + a + b = N$.

The bulk ground states

The colored Fredkin moves generates a group that permute our chosen SU(k)-covariant basis vectors, preserve the equivalence classes, and can map any element of an equivalence class to any other. Therefore, as a consequence of the orbit theorem each equivalence class will have a unique ground state $|C_{a,c_a,b,c_b,N^0,N^1\ldots N^{N^2-1}}\rangle$ which is just the symmetric sum of all basis states in the class. These provide a nice orthogonal basis for all ground states of H_F.

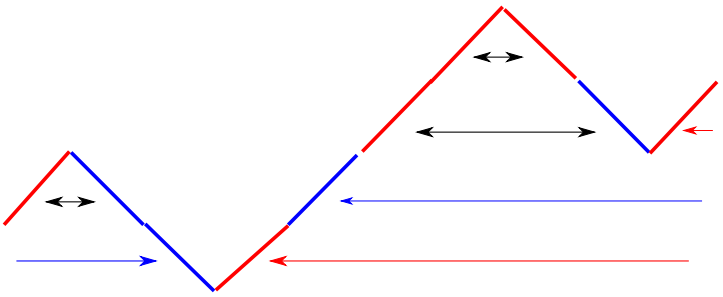

Figure A.5: An example of a path corresponding to a product state basis element.

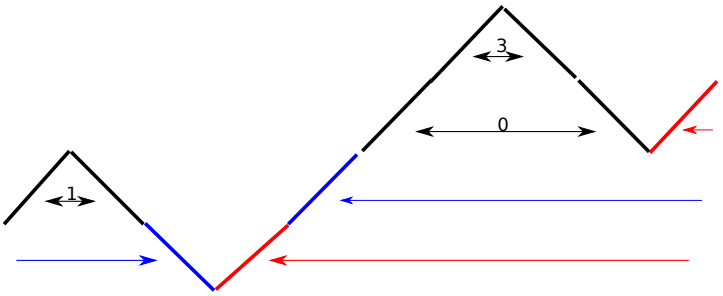

Figure A.6: An example of a path corresponding to a covariant basis element, with one SU(k) singlet pair and two pairs in the SU(k) adjoint representation.

This characterization is exactly what we will need to find out the combined ground state of $H_F + H_X + H_\partial$. The condition that the combined ground state is also a ground state of H_X leaves us with $N^a = 0$ for all a, and clearly the entire subspace that does not fulfill this can not have any common $H_F + H_X$ zero eigenstate. Since in that case $N^0 = N - (a + b)$, we can simply call the bulk $H_F + H_X$ ground states $|C_{a,c_a,b,c_b}\rangle$.

For an even number of sites $N = 2n$ this leaves us with the unique ground state $|C_{0,\emptyset,0,\emptyset}\rangle$ as we add in the boundary terms, which we call the colored Dyck state $|D_n^k\rangle$.

A.3.2 The colored Dyck state

We have now fully introduced the ground state $|D_n^k\rangle$. Depending on whether we use the covariant or the product state basis. In the nonlocal covariant basis that we used in the previous section to simultaneously block-diagonalize H_F and H_X, $|D_n^k\rangle$ is the symmetric sum of all paths colored such that all matched pairs form SU(k) singlets.

We may expand this expression as a sum of product states. In the local product state basis, $|D_n^k\rangle$ is instead the sum of all basis states corresponding to *properly colored paths*, i.e. colored paths such that matching parentheses have the same color. The number of basis states in the sum is given by $k^n Cat(n)$. For k = 2, we will give some low-n examples in bracket notation:

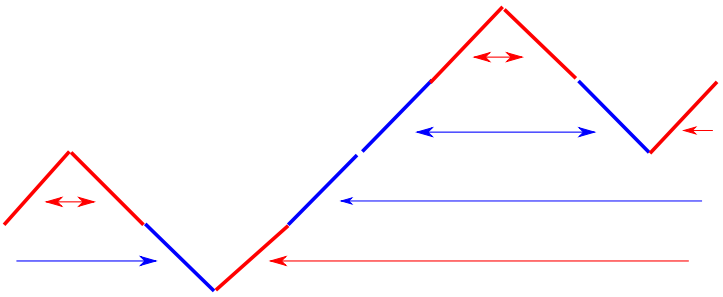

Figure A.7: An example of a properly colored path.

$$|D_2^2\rangle = \frac{1}{\sqrt{2}}\left(|()\rangle + |[]\rangle\right)$$
$$|D_2^2\rangle = \frac{1}{\sqrt{8}}(|()()\rangle + |[]()\rangle + |()[]\rangle + |[][]\rangle + |(())\rangle + |([])\rangle + |[()]\rangle + |[[]]\rangle)$$

The Schmidt decomposition and measures of entanglement

Just as before, our primary tool to analyze the entanglement of the colored Dyck state will be the Schmidt decomposition, which is given by

$$|D_n^k\rangle = \sum_{m=0}^{L} \sum_{c\in\mathbb{Z}_k^m} \sqrt{p_{m,c}}\,|C_{0,\emptyset,m,c}(L)\rangle \otimes |C_{m,c,0,\emptyset}(N-L)\rangle \tag{A.10}$$

where c is a list of length m consisting of the colors of the unmatched parentheses of $|C_{0,\emptyset,m,c}(L)\rangle$ and $|C_{m,c,0,\emptyset}(N-L)\rangle$. Since as before

$$p_{m,c} = \frac{|C_{0,\emptyset,m,c}(L)||C_{m,c,0,\emptyset}(N-L)|}{|C_{0,0,0,0}(N)|}$$

, and since $|D_n^k\rangle$ is an equally weighted sum of every coloring of each path, we get $p_{m,c}$ is independent of c. By inserting the correct powers of k to account for every possible color combination we obtain

$$p_{m,c} = p_m \frac{k^{\frac{L-m}{2}} k^{\frac{N-L-m}{2}}}{k^{\frac{N}{2}}} = k^{-m} p_m$$

where p_m are the Schmidt coefficients from the uncolored case.

This allows us to compute the Schmidt rank and the Entanglement entropy in the colored case. We will start with the Schmidt rank. The number of nonzero $p_{m,c}$ coefficient

is a geometric sum. In the case where L is even and $L = 2l$, the Schmidt rank is $\sum_{h=0}^{l} k^{2h} = \frac{k^{L+2}-1}{k^2-1}$. In the case where L is odd and equal to 2l+1, we have $\sum_{h=0}^{l} k^{2h+1} = k\frac{k^{L+1}-1}{k^2-1}$. The two may be combined into:

$$\xi = \begin{cases} \frac{k^{L+2}-1}{k^2-1} & \text{if L is even} \\ k\frac{k^{L+1}-1}{k^2-1} & \text{if L is odd} \end{cases}$$

Now we may move on to the entanglement entropy. By definition, we have:

$$S = \sum_{m,c} -p_{m,c}\log(p_{m,c}) = \sum_{m} -p_m \log(k^{-m}p_m) = \sum_{m} mp_m \log(k) - p_m \log(p_m)$$

which gives us

$$S = S_{1/2} + \log(k)\sum_{m=0}^{L} p_m m \tag{A.11}$$

where the first term is just the log-scaling entanglement entropy from the uncolored case. The second term however, is the expectation value of the height at L for a random Dyck walk, which scales as $O(\sqrt{L})$ and is thus the key term leading to our violation of the area law.

Computing the coefficient of the leading square root term in the entanglement entropy

We are interested in computing the expression $\sum_{m=0}^{L} p_m m$. We proceed much like in the uncolored case. We consider the even case $L = 2l$ with nonzero p_m when $m = 2h, h \in [0,l]$, and consider the coefficient $p_h \approx \frac{h^2}{Z}\exp\left[-h^2\frac{n}{l(n-l)}\right]$, so that we are left with $2\sum_h hp_h$. Replacing the sum with an integral gives us:

$$\sum_h hp_h = \int_0^\infty xp_x dx = \left[\sqrt{\frac{l(n-l)}{l}}d\alpha = dx\right] = \int_0^\infty \sigma\rho_\alpha\sigma^{-1}\alpha\sigma^{-1}d\alpha$$
$$= \sigma^{-1}\int_0^\infty \alpha\rho_\alpha d\alpha = \sqrt{\frac{l(n-l)}{n}}\int_0^\infty \frac{\alpha^3}{Z}\exp\left[-\alpha^2\right]d\alpha$$

where just like before, $p_x = \frac{x^2}{Z'}\exp\left[-x^2\frac{n}{l(n-l)}\right]$, $\int p_x dx = 1$, $\alpha = \sigma x$ and $\sigma = \sqrt{\frac{N}{L(N-L)}}$. We move to $\rho_\alpha = \frac{1}{Z'}\alpha^2\exp[-\alpha^2]$ where Z is a constant such that $\int \rho_\alpha = 1$, which gives us $p_x = \sigma\rho_\alpha$ (with a factor σ^3 from the normalization factor and a σ^{-2} from $x^2 = \sigma^{-2}\alpha^2$), which we used to insert the correct sigma factors.

The integral $\int_0^\infty \frac{\alpha^3}{Z} \exp\left[-\alpha^2\right] d\alpha$ is the third absolute central moment of the normal distribution, while in this formalism the constant $\frac{1}{Z}$ is chosen such that the second moment is one. Thus, we have:

$$S \approx S_{1/2} + \log(k) \frac{M_3}{M_2} \sqrt{2 \frac{L(N-L)}{L}}$$

where M_2 and M_3 are the second and third absolute moments of the normal distribution. Computing these gives us our final approximate expression:

$$S \approx S_{1/2} + \frac{2}{\sqrt{\pi}} \log(k) \sqrt{2 \frac{L(N-L)}{L}}$$

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Appendix: The orbit theorem

In this appendix, we will prove a useful theorem that we (implicitly or explicitly) repeatedly make use of throughout this paper. It is our main tool for classifying ground states by looking at equivalence classes. We chose to call it the orbit theorem. It reads as follows:

Theorem 1 *Let V be a Hilbert space of finite dimension, and let $v_1...v_n$ be an orthonormal basis of V. Let G be a finite group which acts on $B = \{v_1, v_2...v_n\}$ by permutations. Suppose that G is generated by the generators $g_1, g_2...g_n$ and let $P_1, P_2...P_n$ be the corresponding permutation matrices. Let H be a Hamiltonian defined by $H = \sum_{i=1}^{m}(1 - P_i^\dagger)(1 - P_i) = \sum_{i=1}^{m} 2 - P_i^\dagger - P_i$ and let $W \subset V$ be the zero eigenspace of H.*

Then H is positive semidefinite, is a frustration free Hamiltonian, and the dimension of the ground state space W is equal to the number of orbits under the action of G on B. Furthermore, The Hamiltonian can be block diagonalized into the different vector spaces V_i spanned by the elements of B_i, and each block has a unique ground state which is a zero eigenstate of H. The ground states of the different blocks form an orthogonal basis for W.

Proof 1 *H is clearly positive semidefinite since it is a sum of the form $\sum_i A_i^\dagger A_i$. Let $B_1, B_2...B_k$ be the orbits of G and V_i the spaces spanned by the elements of B_i. Then the linear representation of G on V decomposes into representations of G on the subspaces $V_1...V_k$ such that W is a direct sum of the spaces $W_i := W \cap V_i$. and $dim W = dim W_1 + dim W_2 + ... + dim W_k$. It is thus enough to show that $dim W_i = 1$ for all i, or after change of notation that $dim\ W = 1$ when G acts transitively on V (if G can map any element to any element). Suppose that $|v\rangle \in W$. Then we have $\sum_i [\langle v| (1 - P_i^\dagger)][(1 - P_i)|v\rangle] = \langle v| H |v\rangle = 0$ which implies that $(1 - P_i)|v\rangle = 0$, which finally gives us $P_i|v\rangle = |v\rangle$ for all i.*

Any $v \in W$ will therefore be fixed by all permutations generated by the P_i matrices, and since they can map any basis state to any other basis state (act transitively) the coordinates of v corresponding to any two basis states must coincide. So $dim\ W = 1$ as the equally weighted sum of all basis states is the only ground state of H in V, as desired. The last part of the theorem then simply follows by noticing that the sets B_i of basis vectors do not intersect, therefore their spanned vector spaces V_i are orthogonal to each other.

We note that in all cases where we apply this theorem, the permutation matrices (corresponding to Fredkin moves) happen to be involutions(and as such have eigenvalues ± 1), so $(1 - P_i^\dagger)(1 - P_i) = 2(1 - P_i)$, which we for convenience normalize as $1 - P_i$.

B

Paper II: Violation of Cluster Decomposition and Absence of Light-Cones in Local Integer and Half-Integer Spin Chains

Violation of Cluster Decomposition and Absence of Light-Cones in Local Integer and Half-Integer Spin Chains

L. Dell'Anna[1], O. Salberger[2], L. Barbiero[1,3], A. Trombettoni[3,4], V. E. Korepin[2]

Abstract

We compute the correlation functions of the exactly solvable chain of integer spins (recently introduced in Ref. [1]), whose ground-state can be expressed in terms of a uniform superposition of all colored Motzkin paths. Our analytical results show that for spin $s \geq 2$ there is a violation of the cluster decomposition property. This has to be contrasted with $s = 1$, where the cluster property holds. Correspondingly, for $s = 1$ one get a light-cone profile in the propagation of excitations after a local quench, while the cone is absent for $s = 2$, as shown by time dependent density-matrix-renormalization-group (t-DMRG). Moreover, we introduce an original solvable model of half-integer spins whose ground-state can be expressed in terms of superposition of all Dyck paths. For this model we exactly calculate the magnetization and correlation functions, finding that for $s = 1/2$, a cone-like propagation occurs while for higher spins, $s \geq 3/2$, the colors prevent any cone formation.

Locality plays a fundamental role in physical theories, with far reaching consequences, one of them being the cluster decomposition property (CDP) [2]. The CDP implies that

when computing at large distances expectation of products of operators the product factorizes in the product of expectation values, therefore, sufficiently distant regions behave independently. Of course, CDP requires that the ground-state is a pure state while in presence of a mixed or degenerate ground state the CDP can not be preserved.

Another fundamental consequence related to locality is given by the peculiar propagation of excitations. In particular once the system is subject to a local or global quench the time evolution of the correlations shows a well defined light cone-like propagation [3]. For general lattice models with short-range interactions locality and the presence of CDP imply a bound, called Lieb-Robinson bound [4], for the commutator of two operators defined in different points of the space. This result is, of course, equivalent to the existence of a finite speed for the propagation of excitations [5, 6, 7]. This gives rise to a light-cone defining causally connected regions up to exponentially small deviations. From the other side, the presence of long-range interaction causes the violation of the Lieb-Robinson bound and the presence of power-law tails outside the light-cone [8, 9, 10, 11, 12, 13]. In this direction experimental evidences of the absence of Lieb-Robinson bound have been provided by means of interacting trapped ions [14].

The appearence of non-exponentially small corrections outside the cone signals non-local effects, which are induced by the long-range interactions or couplings. Moreover quantum correlations are also signaled by entanglement. This lies at the heart of the area law violation of the von Neumann entropy for long-range interacting systems. Indeed a variety of cases [8, 15, 16, 17, 18], including a study of the nonlinear growth after quenches [19], have been theoretically investigated.

Due to the latter arguments the study of non-local properties and their consequences on the light-cone propagation in addition to the violation of the area law are certainly at the present date a very challenging field of research.

In this letter we intend to investigate if one can have violation of CDP and absence of a light-cone in the dynamics for a local quantum theory, which is translationally invariant in the bulk. Here we first consider the exactly solvable chain of integer spins introduced in [20] for $s = 1$ and recently generalized to larger-than-one integer spins [1]. The peculiarity of this spin chain is that the ground-state can be expressed in terms of a superposition of all Motzkin paths which are "colored" for $s > 1$ [22]. A (non-colored) Motzkin path is any path from the point (0,0) to $(0,L)$ with steps $(1,0),(1,1),(1,-1)$. The path is said to be colored when the steps can be drawn with more (than one) colors [23].

The following facts motivated us to investigate CDP and dynamics of correlations in this model: *i)* the model is local; *ii)* the ground-state is unique, it is a pure state made by a uniform superposition of all the Motzkin paths; *iii)* it exhibits a logarithmic deviation from the area law for $s = 1$ and a square root deviation for $s \geq 2$; *iv)* it can be written in terms of spins-s $S_\alpha(j)$ where $j = 1, \cdots, L$ (L then being interpreted as the number of spins) and $\alpha = x,y,z$. For $s = 1$ the one-point correlation functions were computed in Ref. [20], while the two-point correlation functions were reported in Ref. [24].

In this letter, instead, we present analytical results for one-point and two-point correlation functions for any integer spin s, also for $s \geq 2$. In particular we will focus our

attention to the connected correlation function

$$\langle\langle S_z(j)S_z(k)\rangle\rangle \equiv \langle S_z(j)S_z(k)\rangle - \langle S_z(j)\rangle\langle S_z(k)\rangle. \tag{B.1}$$

in order to see if CDP is preserved. Indeed, the unconnected correlation may tend, for large distances $|j-k|$, to a number different from zero (e.g., when there is off-diagonal long-range order [25]), but the connected one goes to zero in the presence of CDP.

From our analytical results we conclude that there is a violation of CDP: indeed, among others, we present a closed-form expression for $\langle\langle S_z(j)S_z(L-j+1)\rangle\rangle$ valid for $L\to\infty$, showing that it tends to a non-zero value for $s>1$, but to zero for $s=1$. We then correspondingly study by means of t-DMRG [26] the dynamical propagation of excitations [27]. We show that the evolution of the magnetization, once the ground state is perturbed by a local quench, exhibits a well defined light-cone profile for spin $s=1$. For $s=2$ instead the propagation is practically instantaneous and the cone formation is absent. In order to check the validity of our results we also calculate the magnetization spreading following the inverse path, namely by finding the ground state in presence of a local magnetic field and letting the system evolves once the latter is removed. Also in this configuration the colors, characteristic of the $s=2$ case, allow a practically instantaneous signal propagation.

In order to establish the generality of the previous results, we then proceed by introducing and solving a model for half-integer spins. This allows us to check if both the violation of the CDP and the absence of the light-cone for $s>1$ are related to the topological nature of the Motzkin paths and eventually to the integerness of the spins. This new model, which we may refer to as the *Fredkin* model, since its Hamiltonian can be expressed in terms of Fredkin gates [21], has as ground state a uniform superposition of all Dyck paths [22], as opposite to the integer case where the ground state is based on Motzkin paths. A (non-colored) Dyck path is any path from the point (0,0) to (0,L) (L here should be even) with steps (1,1),(1,$-$1). The path is colored when the steps can be drawn with more than one color with the same rule as in Ref. [1]. Deferring details to the Supplemental Material [23], one can write the Hamiltonian in terms of half-integer spins $s=1/2,3/2,\cdots$ and compute for general s the one-point and two-point correlation functions and the dynamics after a quantum quench. Our results show that the von Neumann entropy exhibits just a logarithmic violation of the area law for $s=1/2$, while a square root violation for $s\geq 3/2$. Furthermore for $s=1/2$ CDP is preserved together with the presence of light-cone in the dynamics, while for $s\geq 3/2$ CDP is violated and the light-cone is absent.

In what follows we start presenting our results for the integer Motzkin model (both non-colored and colored) and afterwards we will consider the half-integer Fredkin model.

The integer-spin Motzkin Hamiltonian [1, 20, 24] can be written as a local Hamilto-

nian made by a bulk contribution,

$$\begin{aligned} H_0 &= \frac{1}{2}\sum_{c=1}^{q}\sum_{j=1}^{L-1}\Big\{\mathcal{P}\left(\left|0_j \Uparrow_{j+1}^{c}\right\rangle - \left|\Uparrow_j^{c} 0_{j+1}\right\rangle\right) \\ &+\mathcal{P}\left(\left|0_j \Downarrow_{j+1}^{c}\right\rangle - \left|\Downarrow_j^{c} 0_{j+1}\right\rangle\right) \\ &+\mathcal{P}\left(|0_j 0_{j+1}\rangle - \left|\Uparrow_j^{c}\Downarrow_{j+1}^{c}\right\rangle\right)\Big\} \end{aligned} \tag{B.2}$$

plus a crossing term $H_X = \sum_{c\neq\bar{c}}^{q}\sum_{j=1}^{L-1}\mathcal{P}\left(\left|\Uparrow_j^{c}\Downarrow_{j+1}^{\bar{c}}\right\rangle\right)$ and a boundary term $H_\partial = \sum_{c=1}^{q}\left[\mathcal{P}\left(|\Downarrow_1^{c}\rangle\right)+\mathcal{P}\left(|\Uparrow_L^{c}\rangle\right)\right]$, where $\mathcal{P}(|.\rangle)$ denotes the projector $|.\rangle\langle.|$, and $|\Uparrow\rangle$ ($|\Downarrow\rangle$) the integer spin up (down), $c,\bar{c}$ the colors from 1 to $q\in\mathbb{Z}^+$ and the spin s being equal to the number of colors q.

The one-point and two-point correlation functions for $s=1$ have been computed in Ref. [1, 24]. Here, instead, we present explicit expressions for both $\langle S_z(i)\rangle$ and $\langle S_z(j)S_z(k)\rangle$, for very general colored case, namely for any $s\geq 1$ (see Ref. [23] for further details) determining, in this way, the connected correlation functions. In the rest of the paper we will adopt the following notation: we denote expectation values by $\langle.\rangle_M$ for the integer spin model with Motzkin ground state, and by $\langle.\rangle_D$ for the half-integer spin model with Dyck ground state.

Defining $\mathcal{M}_{hh'}^{(n)}$ as the number of colored Motzkin-like paths between two points at heights h and h' and linearly distant n steps, from combinatoric calculation, the magnetization as a function of the position is given by

$$\langle S_z(j)\rangle_M = \frac{(1+q)}{2\mathcal{M}^{(L)}}\sum_{h}\mathcal{M}_{0h}^{(j-1)}\left(q\,\mathcal{M}_{h+1,0}^{(L-j)}-\mathcal{M}_{h-1,0}^{(L-j)}\right) \tag{B.3}$$

where $\mathcal{M}^{(L)}\equiv\mathcal{M}_{00}^{(L)}$ is the colored Motzkin number (explicit expressions are given in Ref. [23]), the subscript $_M$ refers to the Motzkin model. Equation (B.3), which are valid for any positive integer s, has been plotted in Fig. B.1 (left side) and has been tested against Exact Diagonalization results for small sizes and DMRG for larger ones. $\langle S_z(j)\rangle$ is an odd function of the position as shown in Fig. B.1. The two-point correlation

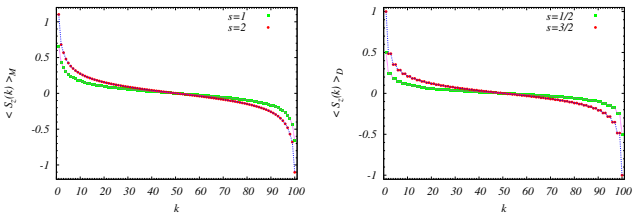

Figure B.1: Magnetization for integer (left) and half-integer (right) spin cases for a chain of lenght $L=100$.

function has been also analytically calculated and reads as it follows

$$\begin{aligned}\langle S_z(j)S_z(k)\rangle_M = &\frac{(1+q)^2}{4\mathcal{M}^{(L)}}\sum_{h,h'}\mathcal{M}_{0h}^{(j-1)}\\ &\left(q\,\mathcal{M}_{h+1,h'}^{(k-j-1)}-\mathcal{M}_{h-1,h'}^{(k-j-1)}\right)\left(q\,\mathcal{M}_{h'+1,0}^{(L-k)}-\mathcal{M}_{h'-1,0}^{(L-k)}\right)\\ &-\frac{\mathcal{M}^{(k-j-1)}}{\mathcal{M}^{(L)}}\frac{(q^3-q)}{12}\sum_{h}\mathcal{M}_{0h}^{(j-1)}\mathcal{M}_{h0}^{(L-k)}.\end{aligned} \tag{B.4}$$

The last term of the previous equation, which vanishes for $s = q = 1$, is actually responsible for the violation of the CDP.

Using Eqs. (B.1) and (B.4) we can compute the connected correlation function, shown for $j = 1$ as a function of k in the left part of Fig. B.2. Analytical results in closed form can be obtained for the boundary connected correlation functions:

$$\langle\langle S_z(1)S_z(k)\rangle\rangle_M \underset{k\gg 1}{\longrightarrow} \frac{(q-q^3)}{12}\frac{\mathcal{M}^{(L-k)}\mathcal{M}^{(k-2)}}{\mathcal{M}^{(L)}} \tag{B.5}$$

$$\langle\langle S_z(j)S_z(L-j+1)\rangle\rangle_M \underset{L\gg j}{\longrightarrow} \frac{(q-q^3)}{12}\frac{\mathcal{M}^{(L-2j)}\mathcal{M}^{(2j-2)}}{\mathcal{M}^{(L)}} \tag{B.6}$$

In particular for spin $s = q = 2$ we get

$$\lim_{L\to\infty}\langle\langle S_z(1)S_z(L)\rangle\rangle_M = \frac{1}{2}\lim_{L\to\infty}\frac{\mathcal{M}^{(L-2)}}{\mathcal{M}^{(L)}} \simeq -0.034 \tag{B.7}$$

These results show that CDP is violated for colored spin chains.

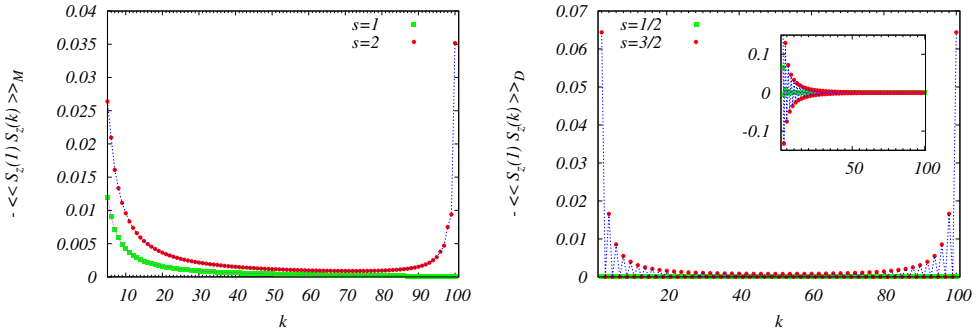

Figure B.2: Connected correlation functions, $-\langle\langle S_z(1)S_z(k)\rangle\rangle$, as a function of k for integer (left) (for $5 \leq k \leq L$), and half-integer (right) spins for a chain of length $L = 100$ (for $2 \leq k \leq L$). Inset: DMRG results for the same connected correlation functions for the Heisenberg XXX model with a boundary term H_∂, for $s = 1/2, 3/2$.

For the half-integer spin case, for generic spin $s = q - \frac{1}{2}$, we introduce the following

Fredkin model

$$\begin{aligned} H_0 &= \frac{1}{2}\sum_{c,\bar{c}=1}^{q}\Big\{\sum_{j=1}^{L-2}\Big[\mathcal{P}\left(\left|\downarrow_j^{\bar{c}}\uparrow_{j+1}^{c}\downarrow_{j+2}^{c}\right\rangle - \left|\uparrow_j^{c}\downarrow_{j+1}^{c}\downarrow_{j+2}^{\bar{c}}\right\rangle\right) \\ &\quad +\mathcal{P}\left(\left|\uparrow_j^{\bar{c}}\uparrow_{j+1}^{c}\downarrow_{j+2}^{c}\right\rangle - \left|\uparrow_j^{c}\downarrow_{j+1}^{c}\uparrow_{j+2}^{\bar{c}}\right\rangle\right)\Big] \\ &\quad +\sum_{j=1}^{L-1}\mathcal{P}\left(\left|\uparrow_j^{c}\downarrow_{j+1}^{c}\right\rangle - \left|\uparrow_j^{\bar{c}}\downarrow_{j+1}^{\bar{c}}\right\rangle\right)\Big\} \end{aligned} \tag{B.8}$$

with the inclusion of a crossing term, analogous to the previous one, $H_X = \sum_{c\neq\bar{c}}^{q}\sum_{j=1}^{L-1}\mathcal{P}\left(\left|\uparrow_j^{c}\downarrow_{j+1}^{\bar{c}}\right\rangle\right)$, and a boundary term $H_\partial = \sum_{c=1}^{q}\left[\mathcal{P}\left(|\downarrow_1^c\rangle\right) + \mathcal{P}\left(|\uparrow_L^c\rangle\right)\right]$, where $|\uparrow^c\rangle$ is the half-integer $(c-\frac{1}{2})$-spin up and $|\downarrow^c\rangle$ the half-integer $(c-\frac{1}{2})$-spin down.

We define $\mathcal{D}_{hh'}^{(n)}$ the number of colored Dyck-like paths between two points at heights h and h' and linearly distant n, such that $\mathcal{D}^{(2n)} \equiv \mathcal{D}_{00}^{(2n)} = q^n C(n)$, where $C(n)$ are the Catalan numbers. The magnetizations is, then, found to be

$$\langle S_z(j)\rangle_D = \frac{q}{2\mathcal{D}^{(L)}}\sum_h \mathcal{D}_{0h}^{(j-1)}\left(q\,\mathcal{D}_{h+1,0}^{(L-j)} - \mathcal{D}_{h-1,0}^{(L-j)}\right) \tag{B.9}$$

(the subscript $_D$refers to the Fredkin model). The result Eq. (B.9) is plotted in the right hand side of Fig. B.1, for spins $s = 1/2$ and $s = 3/2$. We can also calculate analytically the correlation functions getting

$$\begin{aligned} \langle S_z(j)S_z(k)\rangle_D &= \frac{q^2}{4\mathcal{D}^{(L)}}\sum_{h,h'}\mathcal{D}_{0h}^{(j-1)} \\ &\left(q\,\mathcal{D}_{h+1,h'}^{(k-j-1)} - \mathcal{D}_{h-1,h'}^{(k-j-1)}\right)\left(q\,\mathcal{D}_{h'+1,0}^{(L-k)} - \mathcal{D}_{h'-1,0}^{(L-k)}\right) \\ &- \frac{\mathcal{D}^{(k-j-1)}}{\mathcal{D}^{(L)}}\frac{(q^3-q)}{12}\sum_h \mathcal{D}_{0h}^{(j-1)}\mathcal{D}_{h0}^{(L-k)} \end{aligned} \tag{B.10}$$

Also in this case the last term which vanishes for $q = 1$, i.e. $s = 1/2$, is responsable for the violation of the cluster decomposition property. In particular, for $j = 1$, and $1 < k \leq L$, we get simply

$$\langle\langle S_z(1)S_z(k)\rangle\rangle_D = \frac{(1-q^2)}{12}p_k\frac{C(\frac{L-k}{2})C(\frac{k}{2}-1)}{C(\frac{L}{2})} \tag{B.11}$$

which for $q = 1$ (spin $s = 1/2$) is exactly zero, since the spin at the first site has to be $\uparrow$, no matter the rest of the chain. In Eq. (B.11) $p_k = 1$ for even k and $p_k = 0$ for odd k. Putting $k = L$ and sending $L \to \infty$ we have, however, a finite correlation

$$\lim_{L\to\infty}\langle\langle S_z(1)S_z(L)\rangle\rangle_D = \frac{(1-q^2)}{12}\frac{1}{4}. \tag{B.12}$$

More generally, the analytic expression for the correlators, in the long L limit, and $j \geq 1$, are

$$\lim_{L\to\infty} \langle\langle S_z(j)S_z(L)\rangle\rangle_D = \frac{(1-q^2)}{12}\frac{C(\frac{j-1}{2})}{2^{j+1}}p_{(j+1)} \tag{B.13}$$

$$\lim_{L\to\infty} \langle\langle S_z(j)S_z(L-j+1)\rangle\rangle_D = \frac{(1-q^2)}{12}\frac{C(j-1)}{4^j} \tag{B.14}$$

We show therefore that, also in the half-integer spin chains, for $s \geq 3/2$ the violation of the CDP occurs. The connected correlation functions for $s = 1/2$ and $s = 3/2$ are plotted in the right part of Fig. B.2. In the inset of the same figure we plot for comparison static DMRG results for the Heisenberg XXX Hamiltonian with a boundary magnetic term H_∂, for both spin 1/2 and 3/2. The result is that, as expected, in this model CDP is preserved.

Motivated by the violation of CDP we study the dynamics in order to ascertain what is the effect of such lack of clusteing decomposition property on the evolution in time. By means of t-DMRG, we study the evolution of the magnetization as a function of time. We can notice in Fig. B.3 that once the colors are present, both for ingeger and half-integer cases, the system is not able to exibit light cone propagation. On the contrary, for the non-colored cases, namely $s = 1/2$ and $s = 1$, a clear signature of the light-cone is visible in the evolution of the local magnetization, after switching on a local field. We also checked that similar results (presence or absence of a light-cone in the propagation respectively for $s > 1$ and $s \leq 1$) hold also after switching off the local field [23].

Finally, we report for completeness the results for the von Neumann entropy. We find that for both integer and half-integer chains the entanglement entropy do not follow the area law. We find that the entropies for the Motzkin and the Fredkin models, after a bipartition of the chain in two parts, [1,j] and [$j+1$,L], are gven by

$$\mathcal{S}_M = \log_2(q)\,\langle h_j\rangle_M + O(\log_2(j(L-j))) \tag{B.15}$$

$$\mathcal{S}_D = \log_2(q)\,\langle h_j\rangle_D + O(\log_2(j(L-j))) \tag{B.16}$$

namely, the leading contrbution, for colored cases ($q > 1$) is no longer a log-term. Remarkably we show that, in both cases, the entanglement entropy has a geometrical meaning, since the leading term is proportional to the average height of the Motzkin paths (for the integer case) and the average height of the Dyck paths (for the half-integer case), measured right at the bipartition position j. This quantity, in both cases, in the large L limit, is approximatelly given by

$$\langle h_j\rangle \sim \sqrt{\frac{j\,(L-j)}{L}}. \tag{B.17}$$

To conclude, we also report results for the finite-size scaling of the gap $\Delta E = E_1 - E_{GS}$ where E_{GS} is the ground state and E_1 is the energy of the first excited state. These energies are obtained by performing static DMRG simulations of systems with L up to 100 for the $s = 1/2$ and $s = 1$ case and up to $L = 60$ for $s = 3/2$,2. Here we kept

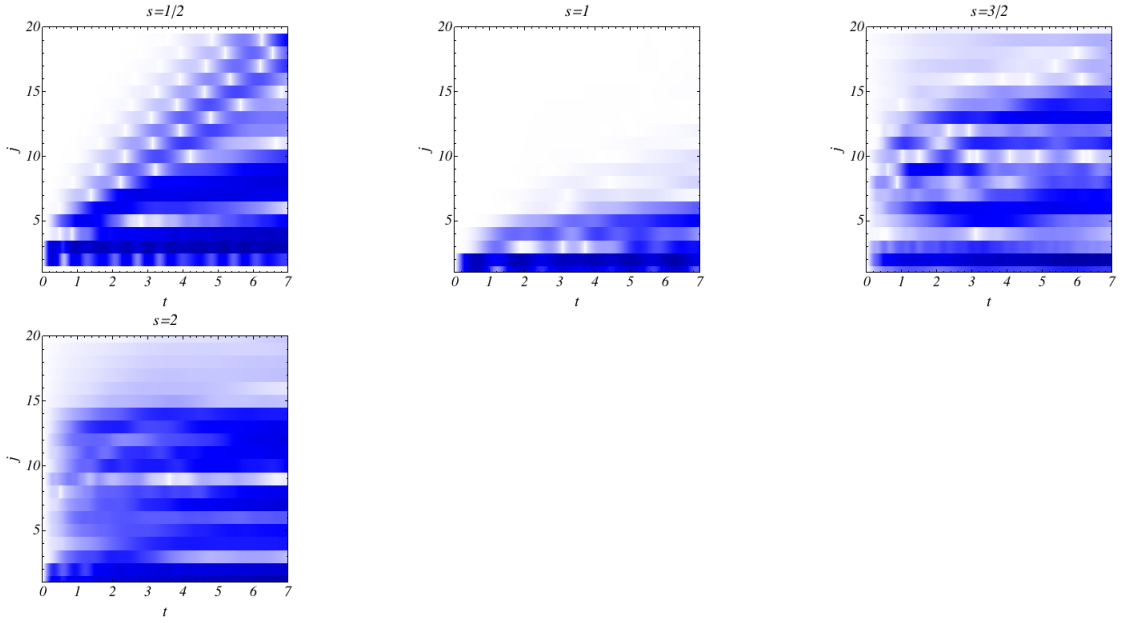

Figure B.3: Time evolution of $\langle S_z(j,t)\rangle - \langle S_z(j,0)\rangle$ after switching on a local field, $5\,S_z(j_0)$: a) on $j_0 = 2$ of a spin $s = 1/2$ chain, b) on $j_0 = 1$ of a spin $s = 1$ chain, c) on $j_0 = 2$ of a spin $s = 3/2$ chain, d) on $j_0 = 1$ of a spin $s = 2$ chain. The light-cones are absent for $s = 3/2$ and $s = 2$.

at most 2000 DMRG states and 5 finite size sweeps. We found that the gap scales as $\Delta \propto 1/L^c$ and, for the four considered s-values, we always get $c > 2$. In particular our estimates are $c = 2.91 \pm 0.05$ ($s = 1/2$), $c = 2.72 \pm 0.06$ ($s = 1$), $c = 3.8 \pm 0.4$ ($s = 3/2$) and $c = 3.3 \pm 0.3$ ($s = 2$). We think that the analytic expression for c is different for Motzkin and Fredkin cases. Still we conjecture that in both cases c increase as a linear function of logarithm of number of colors q.

Conclusions: We exactly computed the connected z-z correlation functions of a local quantum spin chain, for a general integer spin, whose ground-state can be represented by a uniform superposition of all colored Motzkin paths allowed by the length of the chain and the number of colors. Our analytical results show that, except for $s = 1$, for any $s \geq 2$ there is a violation of the cluster decomposition property and that the connected correlation function $\langle\langle S_z(j)S_z(L-j+1)\rangle\rangle$ tends to a finite value for $L \to \infty$. Motivated by the violation of the clustering, we then studied by t-DMRG numerical simulations the dynamics of the magnetization and two-point connected correlation functions after a quench. We showed that for $s = 1$ one has a light-cone for the propagation of the excitations, while the cone is absent for $s = 2$. We also introduced and determined the ground-state and correlation functions of a solvable chain of half-integer spins, which we called Fredkin spin chain, whose ground-state can be expressed in terms of a uniform superposition of all Dyck paths, colored for $s \geq 3/2$. Also in this case the cluster decomposition holds for $s = 1/2$, while is not preserved for $s \geq 3/2$. This result un-

ambiguously shows that the violation of cluster property does not depend on the spin integerness. Analogously to the integer spin case, numerical simulations indicate that there is a light-cone for $s = 1/2$, while the cone is absent for $s = 3/2$. We finally computed the von Neumann entropy of the Fredkin model, showing a (non-logarithmic) square root violation of the area law, and the scaling behavior of the first gap.

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[27] In all our dynamical simulations the ground state is found by keeping up to 1400 DMRG states and performing 5 finite size sweeps. The dynamics is computed by using up to 1024 DMRG states and a time step $\delta t = 0.01$.