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Topological Phases in Quantum Systems with Quantum Group Symmetries

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Abstract

We investigate the symmetry protection of topological phases in the q-deformed Affleck-Kennedy-Lieb-Tasaki model, providing evidence that the $\mathbb{Z}_2$-classification is maintained in the deformation. We also propose a q-analogue of Rényi entropy and demonstrate its ability to encode the full q-deformed entanglement spectrum of a spin chain with $\mathcal{U}_q[sl(2)]$ symmetry.

Acknowledgements

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Statement of Authorship

This report contains a mixture of new and existing results in the area of quantum spin chains. The new results, which I discovered with regular guidance from my supervisor, are incorporated into Sections 3.2 and 4.3. Some of the mathematical arguments used in Section 2.2 are known to the community working on quantum spin chains, but were discovered independently. Throughout the report, results of non-original nature are accompanied by references to their original sources as appropriate.

Contents

1. Introduction

One of the key ways to understand a physical system is to classify its states by their qualitative physical properties, or in other words, to identify *phases* of the system. The consideration of symmetries is a useful tool for this classification task: a familiar example would be the distinction between solids and liquids, which possess discrete and continuous translational symmetries in their molecular arrangements respectively. Indeed, characterising phase transitions by how symmetries form and break underpins the highly-successful Landau theory of phase transitions. One often refers to Landau theory as identifying phase transitions by the presence of 'spontaneous symmetry breaking'.

However, it was discovered that in some physical systems, there exist multiple phases with exactly the same symmetries. This prompted an exploration into alternative origins of phase transitions outside of the Landau symmetry-breaking paradigm. One of the novel concepts that sprung up was that of *symmetry-protected topological (SPT) phases* [Gu and Wen, 2009]. In this setting, whether or not two states belong to the same phase rests on the question of whether they are path-connected by intermediate states satisfying certain properties.

In this project, we study one particular type of physical system: a one-dimensional infinite lattice with a quantum spin on each site, also known as a *quantum spin chain*. The goals of this project are twofold, and extend the recent work of Quella [2020]. Firstly, we address the question of whether the *q-deformed AKLT ground states*, a specific family of states on quantum spin chains, can be classified into SPT phases. Secondly, we explore the entanglement aspect of q-deformed spin chains and propose a q-analogue of the Rényi entanglement entropy, a powerful quantifier of entanglement in a quantum system. These two avenues of the project encompass Sections 3 and 4 of this report. Prior to this, we devote Section 2 to preliminary matters on the AKLT model and SPT phases.

This report assumes a rudimentary knowledge of quantum mechanics and in particular the theory of spin angular momentum, which is reviewed in Appendix A. The formalism of matrix product states is also relied on heavily; we give a surface-level overview of this in Appendix B.

2. Topological Phases in the AKLT Model

2.1. The AKLT Model

The Affleck-Kennedy-Lieb-Tasaki (AKLT) model, introduced by Affleck et al. [1987], is a model of great importance in one-dimensional quantum spin chains. It is a spin-1 chain (i.e. each site of the lattice contains a quantum spin of total spin 1), and for a chain of length L its Hamiltonian is a sum of nearest-neighbour interactions,

$$H_{\mathrm{AKLT}} = \sum_{\ell=1}^{L-1} \mathbf{S}_\ell \cdot \mathbf{S}_{\ell+1} + \frac{1}{3}(\mathbf{S}_\ell \cdot \mathbf{S}_{\ell+1})^2, \tag{1}$$

where ℓ indexes sites of the lattice. The ground state $|\mathrm{AKLT}_1\rangle$ of H_{AKLT} is unique and gapped.[1] Here, 'gapped' refers to an energy gap between the ground state and the first excited state of H_{AKLT} that remains strictly positive in the thermodynamic limit $L \to \infty$. Such a gap was conjectured by Haldane [1983] to exist for all integer-spin Heisenberg chains, the AKLT model being one such instance. The AKLT model is perhaps most well-known for being one of the first constructions to exhibit the 'Haldane gap', and its peculiar properties characterise it as belonging to the so-called 'Haldane phase'. In addition, it is also celebrated for admitting convenient analytic computations of physical

[1] The subscript 1 refers to the spin; we will soon generalise to arbitrary spin S.

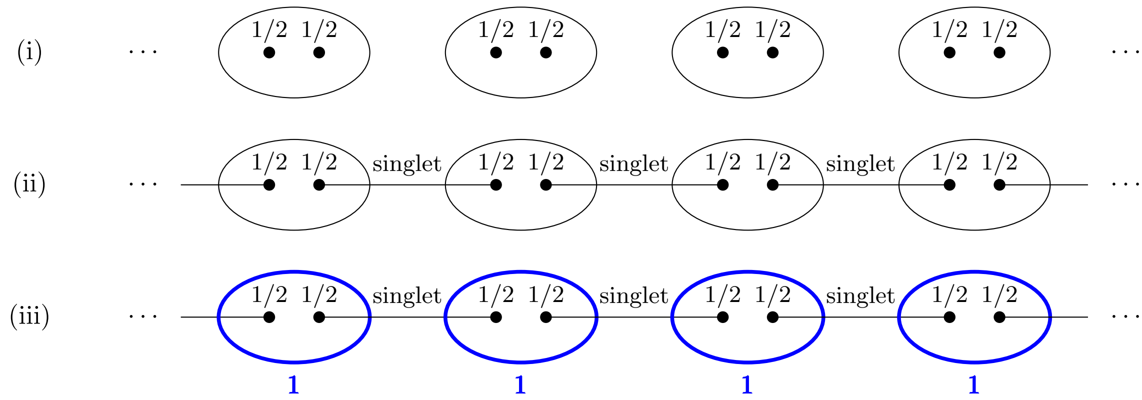

Figure 1: Construction of $|\mathrm{AKLT}_1\rangle$.

parameters, as well as exemplifying the concept of symmetry-protected topological (SPT) phases, as we shall see soon.

The state $|\mathrm{AKLT}_1\rangle$ is obtained by a simple construction, illustrated in Figure 1. First divide each site of the lattice ('physical site') into left and right subsites ('auxiliary sites'), and place a spin-$\frac{1}{2}$ on each auxiliary site. Next, induce a singlet coupling between the right auxiliary spin on each physical site ℓ and the left auxiliary spin on its right-hand physical site $\ell+1$. The physical spin, made of the two auxiliary spin-$\frac{1}{2}$s, is now a spin-$(0 \oplus 1)$ by the coupling rules for spin angular momenta (Theorem A.11). To make the chain a spin-1 chain, the final step is therefore to project each physical spin to the spin-1 sector.

The state $|\mathrm{AKLT}_1\rangle$ is also a matrix product state (MPS), with the MPS tensor for each site given by

$$\mathcal{A}_{(S=1)} = \frac{1}{\sqrt{3}} \begin{bmatrix} -|0\rangle & \sqrt{2}\,|1\rangle \\ -\sqrt{2}\,|-1\rangle & |0\rangle \end{bmatrix}, \tag{2}$$

where $(|1\rangle, |0\rangle, |-1\rangle)$ is the orthonormal spin-1 basis [Schollwöck, 2011]. The scalar coefficients are related to $\mathsf{SU}(2)$ Clebsch-Gordan coefficients; see Example B.4 in Appendix B for a derivation. In general, an MPS is a state that can be specified by rank-3 tensors like the above. These tensors encode the data of the state and are particularly useful for computations of the state's physical properties. For this reason, we will only consider states that are MPSes, and will refer to states by their MPS tensors where appropriate. The reader is welcome to refer to Appendix B for a brief introduction to MPS representations.

Provided some injectivity condition is satisfied, every MPS $|\psi\rangle$ has a *parent Hamiltonian*, i.e. a Hamiltonian having $|\psi\rangle$ as its unique ground state [Fernández-González et al., 2015]. For $|\mathrm{AKLT}_1\rangle$, this parent Hamiltonian is given by (1) [Affleck et al., 1987].

2.2. Symmetry-Protected Topological Phases in Generalised AKLT States

The construction of $|\mathrm{AKLT}_1\rangle$ outlined in Section 2.1 can be easily generalised to arbitrary spin-S chains, where S is an integer [Affleck et al., 1988]. Specifically, we place a spin-$\frac{S}{2}$ on each auxiliary site, establish singlet bonds between auxiliary spin-$\frac{S}{2}$s on neighbouring sites, and project each physical site to the spin-S sector. The result is a spin-S AKLT state, denoted $|\mathrm{AKLT}_S\rangle$. Diagrammatically, this is just Figure 1(iii) with $1/2$ replaced by S and 1 replaced by

S. By the method of Example B.4, the MPS tensor for $|\mathrm{AKLT}_S\rangle$ has (vector-valued) matrix entries

$$[\mathcal{A}_S]^\alpha_\beta = (-1)^{\beta+S/2}\sqrt{\frac{S+1}{2S+1}}\left\langle \frac{S}{2},\alpha\,;\frac{S}{2},-\beta \;\middle|\; S,\alpha-\beta\right\rangle |S,\alpha-\beta\rangle\,, \tag{3}$$

where

- $\langle\, j_1, m_1\,; j_2, m_2 \mid J, M\,\rangle$ denotes an $\mathsf{SU}(2)$ Clebsch-Gordan coefficient;
- the final term $|S,\alpha-\beta\rangle$ is a spin-S basis state with spin-z eigenvalue $\alpha-\beta$;
- upper and lower indices label rows and columns respectively;
- the indices α and β each run across $\frac{S}{2}, \frac{S}{2}-1, \dots, -\frac{S}{2}$ in that order.

In essence, the states $|\mathrm{AKLT}_S\rangle$, $S = 1, 2, \dots$ are distinguished by a degree of freedom for the dimension of the physical spin, which mathematically translates into a choice of dimension for the representation of $\mathsf{SU}(2)$, and influences other parameters such as the size of the MPS tensor. However, once a dimension has been chosen, the states $|\mathrm{AKLT}_S\rangle$ are constructed identically. It is then natural to ask whether these states are equivalent in some physical sense, and if not, whether a classification of these states into phases can be carried out.

Whilst the states $|\mathrm{AKLT}_S\rangle$ are all constructed to be $\mathsf{SO}(3)$ (i.e. rotationally) symmetric, the story of Section 1 demonstrates that we cannot immediately conclude that they all belong to the same phase. In fact, it has been shown that $|\mathrm{AKLT}_S\rangle$ exhibits different physical properties depending on the parity of S, and the difference can be captured by a topological invariant [Chen et al., 2013]. This traces back to the emergence of leftover spin-$\frac{S}{2}$s at the boundary, which features among the AKLT states. The behaviour of a spin-$\frac{S}{2}$ in the bosonic case (when S is even) vastly differs from the behaviour in the fermionic case (when S is odd), and the difference propagates throughout the bulk of the chain. Thus there exist at least two phases among the states $|\mathrm{AKLT}_S\rangle$, and no phase contains both even-S and odd-S AKLT states.

There is now abundant evidence supporting the position that the above $\mathbb{Z}_2$-classification is terminal [Pollmann et al., 2012]. That is to say, there are exactly two phases among the AKLT states and no more; all even-S AKLT states belong to a phase called the *trivial phase* and all odd-S AKLT states belong to a distinct phase called the *Haldane phase*. Furthermore, these phases are examples of *symmetry-protected topological phases* [Gu and Wen, 2009], protected by $\mathsf{SO}(3)$ symmetry. We now define this term.

Definition 2.1. *A* ***symmetry-protected topological (SPT) phase*** $\mathcal{P}$*, protected by a symmetry group* G*, is a collection of matrix product states for a physical system such that for all* $|\psi_0\rangle, |\psi_1\rangle \in \mathcal{P}$*, their MPS tensors (*$\mathcal{M}(0)$ *and* $\mathcal{M}(1)$ *respectively) are connected by a continuous path of MPS tensors* $\mathcal{M}(t), 0 \le t \le 1$*, satisfying the following:*

(SPT1) *For all* t*, the state* $|\psi_t\rangle$ *represented by* $\mathcal{M}(t)$ *possesses* G*-invariance. That is, for every* $g \in G$ *there exists a phase* θ *with* $g\,|\psi_t\rangle = e^{i\theta}\,|\psi_t\rangle$*.*

(SPT2) *The path incurs no phase transition: the dominant eigenvalue of the transfer matrix* $\mathbb{E}_t = \sum_\sigma \mathcal{M}(t)^\sigma \otimes \overline{\mathcal{M}(t)^\sigma}$*, i.e. the eigenvalue with largest modulus, is nondegenerate for all* t*.*

Remark. Condition (SPT2) is exactly the statement that a finite correlation length must be maintained during the path. Exactly why this translates into the absence of a phase transition is discussed in Wolf et al. [2006]. We elaborate on the transfer matrix in the latter half of Appendix B. The need for (SPT1) is due to the fact that without imposing a symmetry, all states are connected to each other in the sense of (SPT2), and all states would belong to a single phase [Chen et al., 2011]. Therefore the imposition of a symmetry in (SPT1) 'protects' physical phases from blending into one another.

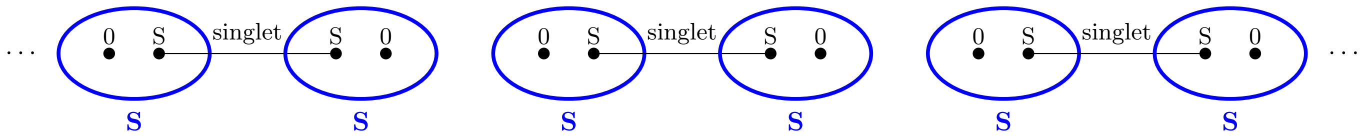

Figure 2: The trivial state $|\mathrm{triv}_S\rangle$.

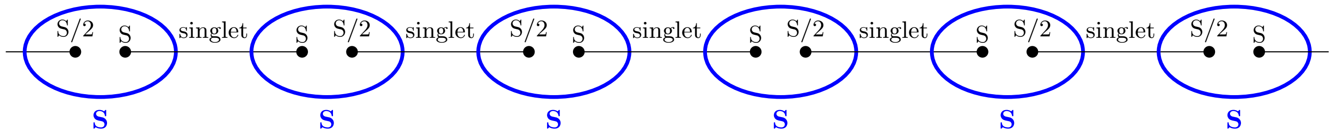

Figure 3: The blended state $|\mathrm{blend}_S\rangle$.

We present the approach of Pollmann et al. [2012] in showing that the even-S AKLT states belong to a so-called 'trivial' SPT phase. This involves constructing an interpolating path, satisfying (SPT1) and (SPT2), from any even-S AKLT state to a certain separable state $|\mathrm{triv}_S\rangle$ on the spin-S chain, the *trivial spin-S state*. This suffices because all separable states are connected by such paths regardless of any imposed symmetry.[2] One then has a continuous path

$$|\mathrm{AKLT}_{S_1}\rangle \to |\mathrm{triv}_{S_1}\rangle \to |\mathrm{triv}_{S_2}\rangle \to |\mathrm{AKLT}_{S_2}\rangle$$

on the level of MPS representations, satisfying (SPT1) and (SPT2) for any even S_1, S_2. Below we define $|\mathrm{triv}_S\rangle$, as well as a third state $|\mathrm{blend}_S\rangle$ which will be used to construct the path.

The trivial spin-S state $|\mathrm{triv}_S\rangle$

The state $|\mathrm{triv}_S\rangle$ is a dimerised state depicted in Figure 2. Each dimer comprises two sites with auxiliary spins $(0, S, S, 0)$, and neighbouring pairs of spin-S auxiliary spins are coupled into singlets. As each physical site contains a spin-0 and a spin-S, the total physical spin is S, making $|\mathrm{triv}_S\rangle$ a valid state on the spin-S chain. Because all entanglement is localised to disjoint pairs of sites, the state is separable (when viewing every pair of sites as a two-site unit), hence is 'trivial' in this sense. The MPS tensors for $|\mathrm{triv}_S\rangle$ are

$$\mathcal{T}_{S,L} = \frac{1}{\sqrt{2S+1}} \begin{bmatrix} |{-S}\rangle & -|{-S+1}\rangle & |{-S+2}\rangle & \cdots & |S-2\rangle & -|S-1\rangle & |S\rangle \end{bmatrix}, \quad \mathcal{T}_{S,R} = \begin{bmatrix} |S\rangle \\ |S-1\rangle \\ \cdots \\ |{-S}\rangle \end{bmatrix}. \tag{4}$$

where the kets are spin-S eigenstates labelled by their spin-z eigenvalue. Again these are derived using the method of Example B.4. There are two tensors since $|\mathrm{triv}_S\rangle$ is two-site translationally invariant.

The blended spin-S state $|\mathrm{blend}_S\rangle$

The state $|\mathrm{blend}_S\rangle$ is also two-site translationally invariant, but unlike $|\mathrm{triv}_S\rangle$ each pair of sites consists of auxiliary spins $(S/2, S, S, S/2)$; see Figure 3. The remainder of the construction is identical to that of $|\mathrm{AKLT}_S\rangle$: singlet bonds are established between neighbouring pairs of auxiliary spins with same total spin, then the auxiliary spins $S/2$ and S belonging to each physical site are projected to the spin-S sector. The MPS tensors for $|\mathrm{blend}_S\rangle$ are given by matrix

[2] It is easy to see this when defining SPT phases using Hamiltonians; see e.g. Tasaki [2020].

entries

$$
\begin{aligned}
[\mathcal{B}_{S,L}]^{\alpha}_{\beta} &= (-1)^{\beta+S}\sqrt{\frac{S+1}{2S+1}}\left\langle \frac{S}{2},\alpha\,;S,\beta\,\middle|\,S,\alpha-\beta\right\rangle |S,\alpha-\beta\rangle \\
[\mathcal{B}_{S,R}]^{\gamma}_{\delta} &= (-1)^{\delta+S/2}\left\langle S,\gamma\,;\frac{S}{2},-\delta\,\middle|\,S,\gamma-\delta\right\rangle |S,\gamma-\delta\rangle
\end{aligned} \tag{5}
$$

where we adopt the same notational conventions as in (3). Here the indices α and δ run across $S, S-1, \ldots, -S$ in that order, while the indices β and γ run across $\frac{S}{2}, \frac{S}{2}-1, \ldots, -\frac{S}{2}$ in that order. Therefore $\mathcal{B}^{S,L}$ is an $(S+1)\times(2S+1)$ matrix, while $\mathcal{B}_{S,R}$ is a $(2S+1)\times(S+1)$ matrix. For instance, if $S=2$ then the MPS tensors for $|\text{blend}_2\rangle$ are

$$
\mathcal{B}_{2,L} = \begin{bmatrix}
\frac{1}{\sqrt{5}}|-1\rangle & -\sqrt{\frac{3}{10}}|0\rangle & \sqrt{\frac{3}{10}}|1\rangle & -\frac{1}{\sqrt{5}}|2\rangle & 0 \\
\sqrt{\frac{2}{5}}|-2\rangle & -\frac{1}{\sqrt{10}}|-1\rangle & 0 & \frac{1}{\sqrt{10}}|1\rangle & -\sqrt{\frac{2}{5}}|2\rangle \\
0 & \frac{1}{\sqrt{5}}|-2\rangle & -\sqrt{\frac{3}{10}}|-1\rangle & \sqrt{\frac{3}{10}}|0\rangle & -\frac{1}{\sqrt{5}}|1\rangle
\end{bmatrix}, \quad
\mathcal{B}_{2,R} = \begin{bmatrix}
\frac{1}{\sqrt{3}}|1\rangle & -\sqrt{\frac{2}{3}}|2\rangle & 0 \\
\frac{1}{\sqrt{2}}|0\rangle & -\frac{1}{\sqrt{6}}|1\rangle & -\frac{1}{\sqrt{3}}|2\rangle \\
\frac{1}{\sqrt{2}}|-1\rangle & 0 & -\frac{1}{\sqrt{2}}|1\rangle \\
\frac{1}{\sqrt{3}}|-2\rangle & \frac{1}{\sqrt{6}}|-1\rangle & -\frac{1}{\sqrt{2}}|0\rangle \\
0 & \sqrt{\frac{2}{3}}|-2\rangle & -\frac{1}{\sqrt{3}}|-1\rangle
\end{bmatrix}. \tag{6}
$$

An interpolating path from $|\text{AKLT}_S\rangle$ to $|\text{triv}_S\rangle$ for any even S

As mentioned above, we will construct a path of MPS tensors $\mathcal{M}_S(t)$, $0 \le t \le 1$, satisfying (SPT1) and (SPT2). Given the one-site and two-site translational invariance of $|\text{AKLT}_S\rangle$ and $|\text{triv}_S\rangle$ respectively, we use a two-site translationally invariant MPS ansatz. In other words, for each t we specify two tensors $\mathcal{L}_S(t)$ and $\mathcal{R}_S(t)$ for the repeating two-site unit, and set $\mathcal{M}_S(t) = \mathcal{L}_S(t)\mathcal{R}_S(t)$.

First consider what happens on the left physical spin of each two-site unit as t increases from 0 to 1. When $t=0$ (the AKLT state), the auxiliary spins on this site both have total spins $\frac{S}{2}$. When $t=1$ (the trivial state), the total spins are 0 and S. Therefore the auxiliary spins must be able to coexist in different representations of $\mathsf{SU}(2)$ during the path. More specifically, let us denote by $\mathcal{V}_j$ the spin-j representation of $\mathfrak{su}(2)$ (i.e. the $(2j+1)$-dimensional irreducible representation). For all t, the left auxiliary spin should belong to $\mathcal{V}_{\frac{S}{2}} \oplus \mathcal{V}_0$, while the right auxiliary spin should belong to $\mathcal{V}_{\frac{S}{2}} \oplus \mathcal{V}_S$. Fix ordered bases for these two vector spaces:[3]

$$
\begin{gathered}
\left(\left|\frac{S}{2},\frac{S}{2}\right\rangle, \left|\frac{S}{2},\frac{S}{2}-1\right\rangle, \ldots, \left|\frac{S}{2},-\frac{S}{2}\right\rangle, |0,0\rangle\right) \text{ for } \mathcal{V}_{\frac{S}{2}} \oplus \mathcal{V}_0, \\
\left(\left|\frac{S}{2},\frac{S}{2}\right\rangle, \left|\frac{S}{2},\frac{S}{2}-1\right\rangle, \ldots, \left|\frac{S}{2},-\frac{S}{2}\right\rangle, |S,S\rangle, |S,S-1\rangle, \ldots, |S,-S\rangle\right) \text{ for } \mathcal{V}_{\frac{S}{2}} \oplus \mathcal{V}_S.
\end{gathered} \tag{7}
$$

We will then express the left MPS tensor $\mathcal{L}(t)$ in terms of these ordered bases:

$$
\mathcal{L}_S(t) = \begin{array}{c} \\ \left|\frac{S}{2},\frac{S}{2}\right\rangle \\ \left|\frac{S}{2},\frac{S}{2}-1\right\rangle \\ \vdots \\ \left|\frac{S}{2},-\frac{S}{2}\right\rangle \\ |0,0\rangle \end{array}
\begin{array}{c}
\begin{array}{cccc|cccc} \left|\frac{S}{2},\frac{S}{2}\right\rangle & \left|\frac{S}{2},\frac{S}{2}-1\right\rangle & \cdots & \left|\frac{S}{2},-\frac{S}{2}\right\rangle & |S,S\rangle & |S,S-1\rangle & \cdots & |S,-S\rangle \end{array} \\
\left[\begin{array}{cccc|cccc}
? & ? & \cdots & ? & ? & ? & \cdots & ? \\
? & ? & \cdots & ? & ? & ? & \cdots & ? \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\
? & ? & \cdots & ? & ? & ? & \cdots & ? \\
\hline
? & ? & \cdots & ? & ? & ? & \cdots & ?
\end{array}\right]
\end{array} \tag{8}
$$

where the question marks are vector-valued entries specified below. This is a $(S+2)\times[(S+1)+(2S+1)]$ matrix,

[3] Since the basis vectors are now labelled with their total spin $|j,m\rangle$ instead of just $|m\rangle$, we choose to omit the otherwise-necessary '$\mathbf{0}\oplus$' and '$\oplus\mathbf{0}$' terms.

and by the exact same reasoning $\mathcal{R}(t)$ is an $[(S+1)+(2S+1)]\times(S+2)$ matrix. We set

$$\mathcal{L}_S(t) = \begin{array}{c} \\ |\frac{S}{2},\frac{S}{2}\rangle \\ |\frac{S}{2},\frac{S}{2}-1\rangle \\ \vdots \\ |\frac{S}{2},-\frac{S}{2}\rangle \\ |0,0\rangle \end{array} \begin{array}{c} \begin{array}{cccccc} |\frac{S}{2},\frac{S}{2}\rangle & |\frac{S}{2},\frac{S}{2}-1\rangle & \cdots & |\frac{S}{2},-\frac{S}{2}\rangle & |S,S\rangle & |S,S-1\rangle \; \cdots \; |S,-S\rangle \end{array} \\ \left[\begin{array}{c|c} (1-t)\mathcal{A}_S & t(1-t)\mathcal{B}_{S,L} \\ \hline \mathbf{0} & t\mathcal{T}_{S,L} \end{array}\right] \end{array}, \tag{9}$$

$$\mathcal{R}_S(t) = \begin{array}{c} \\ |\frac{S}{2},\frac{S}{2}\rangle \\ |\frac{S}{2},\frac{S}{2}-1\rangle \\ \vdots \\ |\frac{S}{2},-\frac{S}{2}\rangle \\ |S,S\rangle \\ |S,S-1\rangle \\ \vdots \\ |S,-S\rangle \end{array} \begin{array}{c} \begin{array}{ccccc} |\frac{S}{2},\frac{S}{2}\rangle & |\frac{S}{2},\frac{S}{2}-1\rangle & \cdots & |\frac{S}{2},-\frac{S}{2}\rangle & |0,0\rangle \end{array} \\ \left[\begin{array}{c|c} (1-t)\mathcal{A}_S & \mathbf{0} \\ \hline t(1-t)\mathcal{B}_{S,R} & t\mathcal{T}_{S,R} \end{array}\right] \end{array}, \tag{10}$$

where the submatrices are defined in (3), (4) and (5). It follows that the two-site MPS tensor is

$$\mathcal{M}_S(t) = \mathcal{L}_S(t)\mathcal{R}_S(t) = \begin{array}{c} \\ |\frac{S}{2},\frac{S}{2}\rangle \\ |\frac{S}{2},\frac{S}{2}-1\rangle \\ \vdots \\ |\frac{S}{2},-\frac{S}{2}\rangle \\ |0,0\rangle \end{array} \begin{array}{c} \begin{array}{ccccc} |\frac{S}{2},\frac{S}{2}\rangle & |\frac{S}{2},\frac{S}{2}-1\rangle & \cdots & |\frac{S}{2},-\frac{S}{2}\rangle & |0,0\rangle \end{array} \\ \left[\begin{array}{c|c} (1-t)^2(\mathcal{A}_S)^2 + t^2(1-t)^2\mathcal{B}_{S,L}\mathcal{B}_{S,R} & t^2(1-t)\mathcal{B}_{S,L}\mathcal{T}_{S,R} \\ \hline t^2(1-t)\mathcal{T}_{S,L}\mathcal{B}_{S,R} & t^2\mathcal{T}_{S,L}\mathcal{T}_{S,R} \end{array}\right] \end{array}. \tag{11}$$

When $t=0$, only the upper-left submatrix is nonzero, and the two-site MPS tensor is $\mathcal{M}_S(0) = \mathcal{L}_S(0)\mathcal{R}_S(0) = (\mathcal{A}_S)^2 \oplus \mathbf{0}$. This precisely corresponds to the two-site MPS tensor for $|\mathrm{AKLT}_S\rangle$, as the trailing zero matrix has no effect on the induced state. When $t=1$, only the bottom-right submatrix is nonzero, and the two-site MPS tensor is $\mathcal{M}_S(1) = \mathbf{0} \oplus (\mathcal{T}_S^L\mathcal{T}_S^R)$, which represents $|\mathrm{triv}_S\rangle$. For $0<t<1$, the MPS tensors for $|\mathrm{blend}_S\rangle$ are embedded into (9) and (10), which roughly corresponds to the state being mixed into the path. Note that this is not a true mix in terms of a superposition because there exist off-diagonal interactions between $|\mathrm{blend}_S\rangle$ and $|\mathrm{triv}_S\rangle$ in (11). Rather, this serves as a heuristic argument to justify this particular choice of $\mathcal{M}_S(t)$.

We now verify that the path $\mathcal{M}_S(t)$ satisfies (SPT1) and (SPT2). For (SPT1), one can check that for the tensors $\mathcal{C} \in \{\mathcal{A}_S, \mathcal{B}_{S,L}, \mathcal{B}_{S,R}, \mathcal{T}_{S,L}, \mathcal{T}_{S,R}\}$, the equivariance properties

$$\mathbb{S}^z \triangleright \mathcal{C} = \mathbb{S}^z\mathcal{C} - \mathcal{C}\mathbb{S}^z, \quad \mathbb{S}^\pm \triangleright \mathcal{C} = \mathbb{S}^\mp\mathcal{C} - \mathcal{C}\mathbb{S}^\mp \tag{12}$$

are satisfied. Here $\mathbb{S}^z$, $\mathbb{S}^+$ and $\mathbb{S}^-$ are the generators of the Lie algebra $\mathfrak{su}(2)$. The symbol $\triangleright$ denotes an action on the physical spins, while matrix multiplication on MPS tensors acts using the appropriate representation for the auxiliary spins. It follows by a simple calculation that these equivariance properties also hold for $\mathcal{C} \in \{\mathcal{L}_S(t), \mathcal{R}_S(t)\}$, $0 \le t \le 1$.

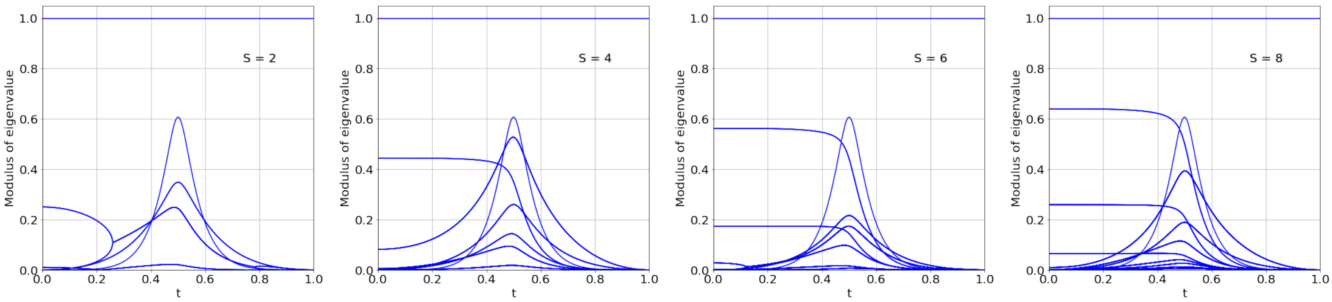

Figure 4: Eigenvalues (by modulus) of the transfer matrices along the path for $S = 2, 4, 6, 8$, normalised so that the dominant eigenvalue has constant modulus 1. The AKLT state is at $t = 0$; the trivial state is at $t = 1$. The dominant eigenvalue is always nondegenerate. Note that at $t = 0$, the spectral gap narrows for increasing values of S.

Using the coproduct

$$\Delta : \mathbb{S}^z \mapsto \mathbb{S}^z \otimes \mathbb{I} + \mathbb{I} \otimes \mathbb{S}^z, \quad \mathbb{S}^\pm \mapsto \mathbb{S}^\pm \otimes \mathbb{I} + \mathbb{I} \otimes \mathbb{S}^\pm \tag{13}$$

which lifts the representations to the tensor product space (i.e. the state space for multipartite spin systems) iteratively, the properties (12) are also met for $\mathcal{C} = (\mathcal{M}_S(t))^L$, $0 \le t \le 1$, $L \in \mathbb{N}$. If we denote by $|\mathrm{path}_S(t)\rangle$ the state on a length-L chain represented by the MPS tensors $\mathcal{M}_S(t)$, then the above implies that

$$\mathbb{S}^z \triangleright |\mathrm{path}_S(t)\rangle = \mathrm{tr}\left[\mathbb{S}^z \triangleright (\mathcal{M}_S(t))^L\right] = \mathrm{tr}\left[\mathbb{S}^z (\mathcal{M}_S(t))^L - (\mathcal{M}_S(t))^L \mathbb{S}^z\right] = 0, \tag{14}$$

which translates into invariance under the action of $\mathbb{S}^z$. Replacing $\mathbb{S}^z$ with $\mathbb{S}^\pm$ yields the same calculation, so $|\mathrm{path}_S(t)\rangle$ is $\mathsf{SO}(3)$-invariant. This shows that (SPT1) holds.

The situation for (SPT2) is somewhat different; to our knowledge, analytic expressions of the transfer matrix spectrum of $\mathcal{M}_S(t)$ for generic even-valued S and $t \in [0, 1]$ have yet to be discovered. Nevertheless, existing evidence points towards the affirmative. Figure 4 plots the eigenvalue moduli along the path $\mathcal{M}_S(t)$ for $S = 2, 4, 6, 8$, normalised so that the dominant eigenvalue has constant modulus 1. In all cases, the dominant eigenvalue has multiplicity one, and is separated by a spectral gap from the second-largest eigenvalue by modulus at all points along the path. This confirms, at least at a numeric level, that (SPT2) is satisfied for small values of even S. For general even-valued S, the graphs in Figure 4 do not preclude the possibility that this spectral gap ceases to exist, especially since there is a clear pattern of the second-largest eigenvalue at $t = 0$ approaching the dominant eigenvalue as S increases. However, we note the following analytical result regarding the $t = 0$ transfer matrix.

Proposition 2.2. *For all positive integers S, the transfer matrix for the state $|\mathrm{AKLT}_S\rangle$ has real eigenvalues*

$$\lambda_j = (-1)^j \binom{S+1}{j+1} \binom{S+j+1}{S}^{-1}, \quad j = 0, 1, \ldots, S, \tag{15}$$

where $\binom{n}{k}$ is a binomial coefficient. Each λ_j has multiplicity $2j+1$. In particular, the eigenvalues satisfy $|\lambda_0| > |\lambda_1| > \cdots > |\lambda_S|$, so the dominant eigenvalue λ_0 is nondegenerate.

A proof can be found in [Santos et al., 2012b], which gives the result in terms of Wigner $6j$-symbols. In view of the decreasing second-largest eigenvalue with respect to t near the beginning of the path (as seen in Figure 4), Proposition 2.2 suggests that the spectral gap remains positive as long as S is finite, and hence (SPT2) should hold true for generic even S.

3. Topological Phases in the q-deformed AKLT Model

We begin to consider a q-deformation of the AKLT model (or the qAKLT model for short), which is based on a $\mathcal{U}_q[sl(2)]$ quantum group symmetry. We will first outline the mathematical details of $\mathcal{U}_q[sl(2)]$, then turn to the question of whether a $\mathbb{Z}_2$-classification of qAKLT states can also be achieved, as with the undeformed case (i.e. in the limit $q \to 1$).

3.1. The Quantum Group $\mathcal{U}_q[sl(2)]$

There are plenty of comprehensive accounts on quantum groups and their representations. The interested reader may refer to Klimyk and Schmüdgen [1997], for example. We only present the essentials here.

If x is a number or an operator, the q-number (resp. q-operator) corresponding to x is

$$[x]_q = \frac{q^x - q^{-x}}{q - q^{-1}}, \tag{16}$$

where $q \in \mathbb{C}\backslash\{-1, 0, 1\}$. Note that $[x]_q \to x$ as $q \to 1$. We define the quantum group $\mathcal{U}_q[sl(2)]$, following the convention of Quella [2020]. First recall that $\mathfrak{su}(2)$ is generated by three elements $\mathbb{S}^+, \mathbb{S}^-, \mathbb{S}^z$ satisfying the commutation relations

$$[\mathbb{S}^z, \mathbb{S}^\pm] = \pm\mathbb{S}^\pm \quad \text{and} \quad [\mathbb{S}^+, \mathbb{S}^-] = 2\mathbb{S}^z. \tag{17}$$

We obtain $\mathcal{U}_q[sl(2)]$ by deforming the right-hand relation to

$$[\mathbb{S}^+, \mathbb{S}^-] = [2\mathbb{S}^z]_q. \tag{18}$$

The resulting structure is a Hopf algebra, and the Lie algebra $\mathfrak{su}(2)$ is recovered in the limit $q \to 1$. Being a Hopf algebra, $\mathcal{U}_q[sl(2)]$ is endowed with the structure maps of unit $\eta : \mathbb{C} \to \mathcal{U}_q[sl(2)]$, counit $\varepsilon : \mathcal{U}_q[sl(2)] \to \mathbb{C}$, coproduct $\Delta : \mathcal{U}_q[sl(2)] \to \mathcal{U}_q[sl(2)] \otimes \mathcal{U}_q[sl(2)]$ and antipode $S : \mathcal{U}_q[sl(2)] \to \mathcal{U}_q[sl(2)]$. These are defined by

$$\begin{gathered} \eta(1) = \mathbb{I}, \\ \varepsilon(\mathbb{S}^z) = \varepsilon(\mathbb{S}^\pm) = 0, \\ \Delta(\mathbb{S}^z) = \mathbb{S}^z \otimes \mathbb{I} + \mathbb{I} \otimes \mathbb{S}^z, \quad \Delta(\mathbb{S}^\pm) = \mathbb{S}^\pm \otimes q^{\mathbb{S}^z} + q^{-\mathbb{S}^z} \otimes \mathbb{S}^\pm, \\ S(\mathbb{S}^z) = -\mathbb{S}^z, \quad S(\mathbb{S}^\pm) = -q^{\pm 1}\mathbb{S}^\pm, \end{gathered} \tag{19}$$

where $\mathbb{I}$ is the multiplicative identity in $\mathcal{U}_q[sl(2)]$. As seen for $\mathfrak{su}(2)$ in (13), Δ lifts the operators and defines the actions of $\mathbb{S}^\pm$ and $\mathbb{S}^z$ in the tensor product space. We further define an involution $* : \mathcal{U}_q[sl(2)] \to \mathcal{U}_q[sl(2)]$ by setting

$$(\mathbb{S}^z)^* = \mathbb{S}^z, \quad (\mathbb{S}^\pm)^* = \mathbb{S}^\mp. \tag{20}$$

This gives a notion of the adjoint of an operator, and turns $\mathcal{U}_q[sl(2)]$ into a Hopf-$*$ algebra.

When q is not a root of unity, the representation theory of $\mathcal{U}_q[sl(2)]$ mimics that of $\mathfrak{su}(2)$.[4] For every nonnegative integer or half-integer S there exists, up to isomorphism, one irreducible representation of $\mathcal{U}_q[sl(2)]$ with dimension $2S+1$. As in the case for $\mathfrak{su}(2)$, the number S is referred to as the 'spin'. The Casimir element of $\mathcal{U}_q[sl(2)]$ is given by

$$C = \mathbb{S}^+\mathbb{S}^- + [\mathbb{S}^z]_q[\mathbb{S}^z - 1]_q, \tag{21}$$

[4]The representation theory becomes much subtler when q is a root of unity.

which can be checked to commute with the generators. The $(2S+1)$-dimensional representation of $\mathcal{U}_q[sl(2)]$ has an orthonormal eigenbasis $(|S,S\rangle_q, |S,S-1\rangle_q, \ldots, |S,-S\rangle_q)$ with respect to the operators $\mathbb{S}^z$ and C. We have

$$\mathbb{S}^z\,|S,m\rangle_q = m\,|S,m\rangle_q \quad \text{and} \quad C\,|S,m\rangle_q = [S]_q[S+1]_q\,|S,m\rangle_q\,. \tag{22}$$

In terms of physics, there is an additional complication. We would like to think of $\mathbb{S}^z$ and C as being analogues of the spin-z and total spin operators from the representation theory of $\mathfrak{su}(2)$, which means the eigenvalues appearing in (22) should ideally be real-valued. We will therefore only consider positive real values of q, where this is guaranteed.[5]

3.2. Symmetry-Protected Topological Phases in Generalised qAKLT States

The AKLT states $|\mathrm{AKLT}_S\rangle$ from Section 2.2 were constructed using $\mathsf{SU}(2)$ singlets between adjacent auxiliary spins on neighbouring physical sites. By using $\mathcal{U}_q[sl(2)]$ singlets in the construction of the ground state instead, one obtains the *q-deformed AKLT (qAKLT) model* [Batchelor et al., 1990, Klümper et al., 1993]. The qAKLT states $|\mathrm{AKLT}_S\rangle_q$ have an identical pictorial representation as Figure 1(iii), although the singlets are now from $\mathcal{U}_q[sl(2)]$. For any S, the MPS tensor for $|\mathrm{AKLT}_S\rangle_q$ is given by matrix entries

$$[\mathcal{A}_S^{(q)}]^\alpha_\beta = (-1)^{\beta+S/2}q^{-\beta}\sqrt{\frac{[S+1]_q}{[2S+1]_q}}\left\langle \frac{S}{2},\alpha\,;\frac{S}{2},-\beta\,\middle|\, S,\alpha-\beta\right\rangle_q |S,\alpha-\beta\rangle_q\,, \tag{23}$$

where $\langle\, j_1,m_1\,;j_2,m_2 \mid J,M\,\rangle_q$ is a $\mathcal{U}_q[sl(2)]$ Clebsch-Gordan coefficient (which generally depends on q), and $\alpha,\beta = \frac{S}{2},\frac{S}{2}-1,\ldots,-\frac{S}{2}$ in that order. Observe that (23) reduces to (3) as $q\to 1$.

Quella [2020] showed that despite the q-deformation, the $S=1$ qAKLT state retains all properties of the undeformed $S=1$ AKLT state, and by extension the Haldane phase. We will see an example of this in Section 4.3. It was then put forward as a natural conjecture that the qAKLT states also admit a $\mathbb{Z}_2$-classification into SPT phases, now protected by $\mathcal{U}_q[sl(2)]$ symmetry, similar to what we have seen in Section 2.2 for the undeformed case. We address this conjecture below by giving numerical evidence that the even-S qAKLT states belong to the trivial SPT phase. To this end, we construct an MPS path $\mathcal{M}_S^{(q)}(t)$, $0\le t\le 1$, which starts from an even-S qAKLT state $|\mathrm{AKLT}_S\rangle_q$, ends at a trivial state $|\mathrm{triv}_S\rangle_q$, preserves $\mathcal{U}_q[sl(2)]$ symmetry, and satisfies (SPT1) and (SPT2) for all t (Definition 2.1). The construction is exactly the same as that from Section 2.2, except all $\mathsf{SU}(2)$ singlets are replaced with $\mathcal{U}_q[sl(2)]$ singlets. The final MPS tensor for the path is

$$\mathcal{M}_S^{(q)}(t) = \begin{array}{c} \\ \left|\frac{S}{2},\frac{S}{2}\right\rangle_q \\ \left|\frac{S}{2},\frac{S}{2}-1\right\rangle_q \\ \vdots \\ \left|\frac{S}{2},-\frac{S}{2}\right\rangle_q \\ |0,0\rangle_q \end{array} \begin{array}{c} \begin{array}{cccc|c} \left|\frac{S}{2},\frac{S}{2}\right\rangle_q & \left|\frac{S}{2},\frac{S}{2}-1\right\rangle_q & \cdots & \left|\frac{S}{2},-\frac{S}{2}\right\rangle_q & |0,0\rangle_q \end{array} \\ \left[\begin{array}{c|c} (1-t)^2(\mathcal{A}_S^{(q)})^2 + t^2(1-t)^2\mathcal{B}_{S,L}^{(q)}\mathcal{B}_{S,R}^{(q)} & t^2(1-t)\mathcal{B}_{S,L}^{(q)}\mathcal{T}_{S,R}^{(q)} \\ \hline t^2(1-t)\mathcal{T}_{S,L}^{(q)}\mathcal{B}_{S,R}^{(q)} & t^2\mathcal{T}_{S,L}^{(q)}\mathcal{T}_{S,R}^{(q)} \end{array}\right] \end{array}, \tag{24}$$

[5]It is also guaranteed for $q=e^{i\theta}$ where $\theta\in\mathbb{R}$, but since the representation theory becomes subtle at roots of unity, which are dense in the unit circle, we shall omit complex-valued q from our discussion altogether.

where the inner matrices are given by

$$[\mathcal{B}_{S,L}^{(q)}]_\beta^\alpha = (-1)^{\beta+S} q^{-\beta} \sqrt{\frac{[S+1]_q}{[2S+1]_q}} \left\langle \frac{S}{2}, \alpha\,; S, -\beta \,\middle|\, S, \alpha-\beta \right\rangle_q |S, \alpha-\beta\rangle_q$$

$$[\mathcal{B}_{S,R}^{(q)}]_\gamma^\delta = (-1)^{\delta+S/2} q^{-\beta} \left\langle S, \gamma\,; \frac{S}{2}, -\delta \,\middle|\, S, \gamma-\delta \right\rangle_q |S, \gamma-\delta\rangle_q$$

$$[\mathcal{T}_{S,L}^{(q)}] = \frac{1}{\sqrt{[2S+1]_q}} \begin{bmatrix} |-S\rangle_q & -|-S+1\rangle_q & |-S+2\rangle_q & \cdots & |S-2\rangle_q & -|S-1\rangle_q & |S\rangle_q \end{bmatrix} \tag{25}$$

$$[\mathcal{T}_{S,R}^{(q)}] = \begin{bmatrix} |S\rangle_q \\ |S-1\rangle_q \\ \cdots \\ |-S\rangle_q \end{bmatrix}.$$

Like in (5), the indices α and δ run across $S, S-1, \ldots, -S$ in that order, while the indices β and γ run across $\frac{S}{2}, \frac{S}{2}-1, \ldots, -\frac{S}{2}$ in that order. To check that the path $\mathcal{M}_S^{(q)}(t)$ satisfies (SPT1), we may use the equivariance properties

$$\mathbb{S}^z \triangleright \mathcal{C} = \mathbb{S}^z \mathcal{C} - \mathcal{C}\mathbb{S}^z, \quad \mathbb{S}^\pm \triangleright \mathcal{C} = \mathbb{S}^\mp \mathcal{C} q^{-\mathbb{S}^z} - q^{\mp 1} q^{-\mathbb{S}^z} \mathcal{C} \mathbb{S}^\mp \tag{26}$$

in place of (12) for $\mathcal{C} \in \{\mathcal{A}_S^{(q)}, \mathcal{B}_{S,L}^{(q)}, \mathcal{B}_{S,R}^{(q)}, \mathcal{T}_{S,L}^{(q)}, \mathcal{T}_{S,R}^{(q)}\}$. The remaining steps follow similarly as above, although we need to use the fact that for q-deformed systems the MPS tensors are related to their corresponding state vectors by

$$|\psi\rangle_q = \operatorname{tr}\left[q^{2\mathbb{S}^z} \mathcal{C}_1 \mathcal{C}_2 \cdots \mathcal{C}_L\right]. \tag{27}$$

The property (SPT2) is again verified numerically. Figure 5 shows the eigenvalue spectrum for different values of even S and $q \in (0,1)$ along the path.[6] It is again seen in each case that a positive spectral gap is maintained between the dominant eigenvalue and the one beneath it. This confirms (SPT2) numerically for small even values of S. As in the undeformed case, there is a pattern in which the spectral gap for $t = 0$ (the qAKLT state) narrows for increasing values of S. The following proposition, which is the q-analogue of Proposition 2.2, suggests that the spectral gap never closes completely. See [Santos et al., 2012b] for a proof.

Proposition 3.1. *For all positive integers S and for all $q \in (0,1)$, the transfer matrix for the state $|\mathrm{AKLT}_S\rangle_q$ has real eigenvalues*

$$\lambda_j = (-1)^j \binom{S+1}{j+1}_q \binom{S+j+1}{S}_q^{-1}, \quad j = 0, 1, \ldots, S, \tag{28}$$

and each λ_j has multiplicity $2j+1$. Here $\binom{n}{k}_q$ is a q-binomial coefficient, defined by

$$\binom{n}{k}_q = \frac{[n]_q [n-1]_q \cdots [n-k+1]_q}{[k]_q [k-1]_q \cdots [1]_q}.$$

In particular, the eigenvalues satisfy $|\lambda_0| > |\lambda_1| > \cdots > |\lambda_S|$, so the dominant eigenvalue λ_0 is nondegenerate.

It follows from these experiments that the q-deformed AKLT states likely permit a $\mathbb{Z}_2$-classification into SPT phases, like what we have seen in the undeformed case. However, a formal proof has yet to be discovered.

[6] It suffices to consider $q \in (0,1)$ instead of the entire positive real line since q-numbers are invariant under the substitution $q \mapsto q^{-1}$.

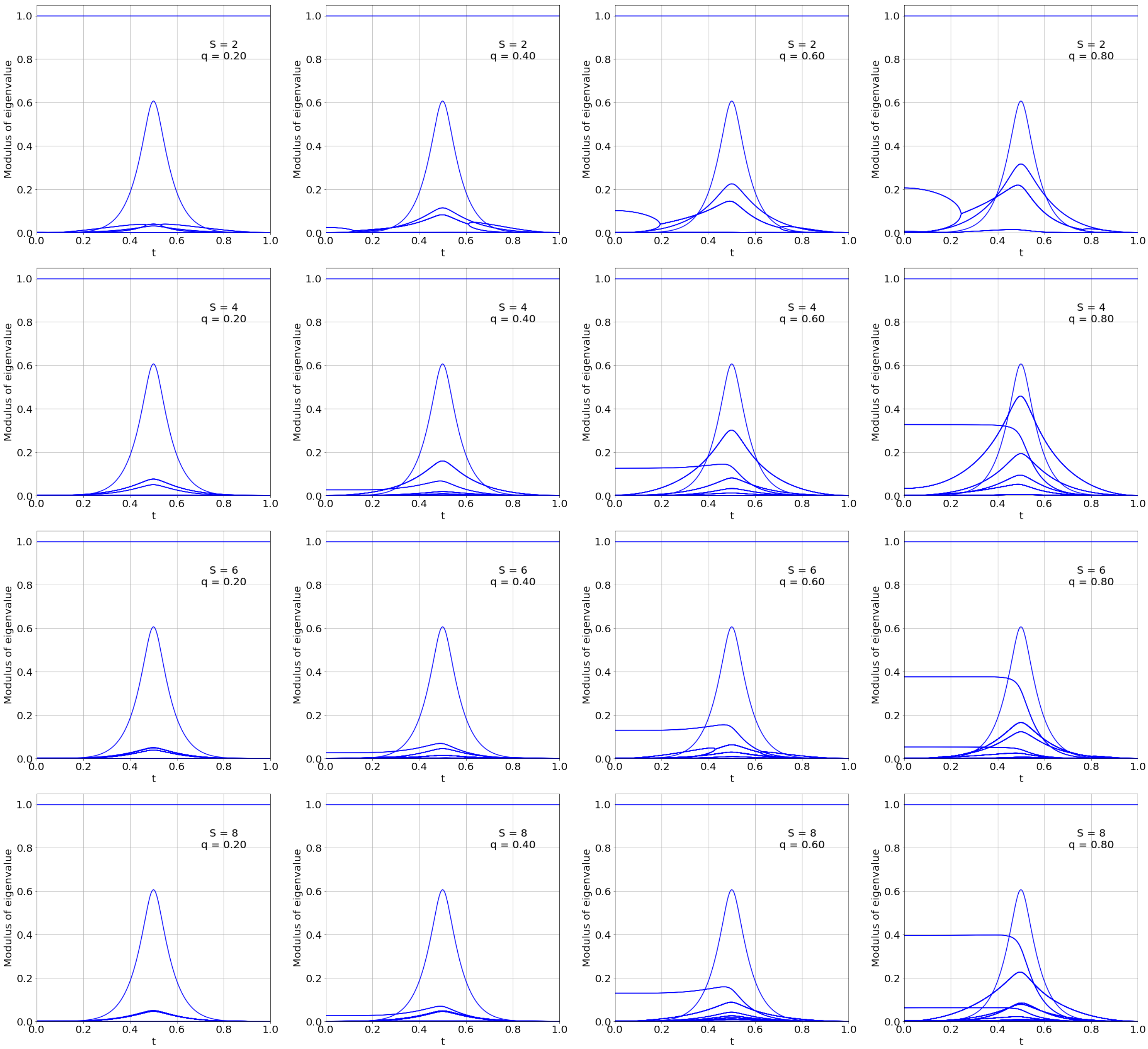

Figure 5: Eigenvalues (by modulus) of the transfer matrices along the path for $S = 2, 4, 6, 8$ (rows) and $q = 0.2, 0.4, 0.6, 0.8$ (columns), normalised so that the dominant eigenvalue has constant modulus 1. The qAKLT state is at $t = 0$; the trivial state is at $t = 1$. The dominant eigenvalue is always nondegenerate. For larger values of S, Proposition 3.1 suggests that the nondegeneracy remains.

4. A q-deformed Rényi Entropy

4.1. Overview of Entanglement Entropies

Quantifying the entanglement of a state is a task of central importance in quantum information science. We review how this is done in a bipartite system with subsystems R and L (standing for right and left, but this applies to any bipartite system). If the combined system is in a pure state $|\psi\rangle$, then its density matrix is given by $\rho = |\psi\rangle\langle\psi|$. One then obtains the reduced density matrix $\rho_R = \mathrm{tr}_L(\rho)$ for subsystem R by taking the partial trace over subsystem L. We state two well-known measures of quantum entanglement.

Definition 4.1. *The* ***von Neumann entanglement entropy*** *of subsystem R with respect to subsystem L is*

$$S(\rho_R) = -\mathrm{tr}_R(\rho_R \log \rho_R).$$

Definition 4.2. *The* ***Rényi entanglement entropy*** *of subsystem R with respect to subsystem L is a family of entropies defined in terms of a parameter α by*

$$S_\alpha(\rho_R) = \frac{1}{1-\alpha} \log \mathrm{tr}_R(\rho_R^\alpha), \quad \alpha > 0,\ \alpha \neq 1.$$

Rényi entanglement entropy is a one-parameter generalisation of the von Neumann entanglement entropy, in the sense that the latter is recovered from the former in the limit $\alpha \to 1$. These entropies are readily calculable if a Schmidt decomposition of the state into its subsystems' states is available:

Proposition 4.3. *Let $\{|u_j\rangle_R\}_{j=1}^m$ and $\{|v_k\rangle_L\}_{k=1}^n$ be orthonormal bases for the state spaces of subsystems R and L respectively, and assume without loss of generality that $m \le n$. If*

$$|\psi\rangle = \sum_{j=1}^m \lambda_j |u_j\rangle_R \otimes |v_j\rangle_L, \quad \lambda_j > 0, \quad \sum_{j=1}^m \lambda_j^2 = 1$$

is a Schmidt decomposition of the system's state, then the von Neumann and Rényi entanglement entropies are given respectively by

$$S(\rho_R) = -\sum_{j=1}^m \lambda_j^2 \log(\lambda_j^2) \quad \text{and} \quad S_\alpha(\rho_R) = \frac{1}{1-\alpha}\log\left(\sum_{j=1}^m \lambda_j^{2\alpha}\right).$$

Proof. We compute

$$\begin{aligned} \rho &= \sum_{j=1}^m \sum_{k=1}^m \lambda_j \lambda_k |u_j\rangle_R |v_j\rangle_L \langle u_k|_R \langle v_k|_L, \\ \rho_R &= \sum_{j=1}^m \lambda_j^2 |u_j\rangle_R \langle u_j|_R. \end{aligned} \tag{29}$$

So the λ_j^2 are the eigenvalues of ρ_R, and the result follows from Definitions 4.1 and 4.2. □

From the above calculation, it is apparent that $S(\rho_R) = S(\rho_L)$ and $S_\alpha(\rho_R) = S_\alpha(\rho_L)$, so we will simply refer to von Neumann and Rényi entanglement entropies of the bipartite system as a whole. We make one more definition:

Definition 4.4. *Let the Schmidt decomposition for $|\psi\rangle$ be as in Proposition 4.3. The* ***entanglement spectrum*** *is the set of numbers $\{-\log(\lambda_j^2)\}_{j=1}^m$, i.e. the negative logarithm of the eigenvalues of ρ_R.*

As the entanglement spectrum corresponds directly to the Schmidt decomposition coefficients λ_j, it controls exactly how the state is entangled. While the von Neumann entanglement entropy is convenient as a single-number measure of entanglement, it cannot be used to recover the entanglement spectrum and therefore does not encode the full entanglement structure. However, this is possible for the Rényi entanglement entropy, making it a powerful measure:

Proposition 4.5. *If the Rényi entanglement entropies $S_\alpha(\rho_R)$ are known for all α, then the entanglement spectrum can be fully recovered.*

Proof. [Riedel, 2019] Suppose the entanglement spectrum is $\{-\log(\lambda_j^2)\}_{j=1}^m$. Then the eigenvalues of ρ_R are λ_j^2 by definition. Since $S_\alpha(\rho_R)$ is known for all α, we have a known function

$$f(\alpha) := \exp\{(1-\alpha)S_\alpha(\rho_R)\} = \sum_{j=1}^m \lambda_j^{2\alpha}, \tag{30}$$

using Definition 4.2 in the second equality. Applying the inverse Fourier transform, we get

$$\hat{f}(\omega) := \int_{-\infty}^{\infty} f(it)e^{-i\omega t}dt = \sum_{j=1}^m \int_{-\infty}^{\infty} e^{i(\log(\lambda_j^2)-\omega)t}dt = \sum_{j=1}^m \delta(\log(\lambda_j^2)-\omega). \tag{31}$$

Hence the entanglement spectrum $\{-\log(\lambda_j^2)\}_{j=1}^m$ can be read off the peaks of $\hat{f}$ with their degeneracies encoded in the coefficients of the Dirac delta functions. $\square$

4.2. Measuring Entanglement in Quantum Spin Chains

For one-dimensional infinite quantum spin chains, the standard procedure is to make an imaginary cut in the chain between two physical sites, splitting the chain into two semi-infinite halves. The entanglement between the halves is measured. This is easily done in the MPS framework for spin chains with one-site translational invariance, so long as the MPS is written in *canonical form*:

Definition 4.6. *Let $\mathcal{M}$ be an MPS tensor. We say that $\mathcal{M}$ is **right-canonical** if $\sum_\sigma \mathcal{M}^\sigma(\mathcal{M}^\sigma)^\dagger = \mathbb{I}$. We say that $\mathcal{M}$ is **left-canonical** if $\sum_\sigma (\mathcal{M}^\sigma)^\dagger\mathcal{M}^\sigma = \mathbb{I}$.*

Definition 4.7. *Let $|\psi\rangle$ be a state in a one-site translationally invariant infinite spin chain. The state $|\psi\rangle$ is said to be written in **canonical form** if there exists a rank-3 tensor Γ (represented as a vector-valued matrix) and a diagonal scalar matrix Λ such that $\Gamma\Lambda$ is right-canonical, $\Lambda\Gamma$ is left-canonical, $\mathrm{tr}(\Lambda^2)=1$, and $|\psi\rangle = \cdots\Lambda\Gamma\Lambda\Gamma\Lambda\Gamma\Lambda\cdots$.*

It can be shown that the entries λ_i of Λ are precisely the Schmidt decomposition coefficients of $|\psi\rangle$ when thinking of the chain as two semi-infinite halves [Vidal, 2007]. Thus we can obtain the entanglement spectrum using the definition, and the von Neumann and Rényi entanglement entropies using Proposition 4.3. For instance, it is easy to check that the MPS tensor $\mathcal{A}_{(S=1)}$ for the spin-1 AKLT state, defined in (2), is right-canonical. We can turn this into canonical form by finding Γ and Λ that satisfy $\Gamma\Lambda = \mathcal{A}_{(S=1)}$ as well as the above properties. This is done by setting

$$\Gamma = \sqrt{2}\mathcal{A}_{(S=1)}, \quad \Lambda = \mathrm{diag}\left(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right). \tag{32}$$

It follows that there is a two-fold degeneracy in the entanglement spectrum. The von Neumann entangement entropy is $\log 2$, while the Rényi entropy is also a constant value of $\log 2$ with respect to the parameter α. The same computations may be repeated for any generalised AKLT state $|\mathrm{AKLT}_S\rangle$, defined in (3). This reveals a $(2S+1)$-fold degeneracy in the entanglement spectrum, and the von Neumann and Rényi entanglement entropies evaluate to $\log(2S+1)$.

Equations (30) and (31) enable recovering the entanglement spectrum from Rényi entropies. Let us make another comment regarding this formula in the context of quantum spin chains and MPS. A generic spin state is a vector in $\mathcal{V}_0 \oplus \mathcal{V}_{\frac{1}{2}} \oplus \mathcal{V}_1 \oplus \cdots \oplus \mathcal{V}_S$, where $\mathcal{V}_j$ is the spin-j representation of $\mathfrak{su}(2)$ and S is finite. A basis for this space is $|0,0\rangle, |\frac{1}{2},-\frac{1}{2}\rangle, |\frac{1}{2},\frac{1}{2}\rangle, \ldots, |S,-S\rangle, \ldots, |S,S\rangle$. Now consider a spin chain state $|\psi\rangle$ where on each physical site the auxiliary spins belong to this space. Then the MPS tensor should be expressed in the basis just stated, and in canonical form we write the matrix Λ as $\Lambda = \mathrm{diag}(\lambda_{|0,0\rangle}, \lambda_{|\frac{1}{2},-\frac{1}{2}\rangle}, \lambda_{|\frac{1}{2},\frac{1}{2}\rangle}, \ldots, \lambda_{|S,-S\rangle}, \ldots, \lambda_{|S,S\rangle})$. Once a cut in the chain is made into left and right halves, Λ induces the Schmidt decomposition

$$|\psi\rangle = \sum_{j=0}^{S}{}' \sum_{m=-j}^{j} \lambda_{|j,m\rangle} |j,m\rangle_L \otimes |j,m\rangle_R \,, \tag{33}$$

where $|j,m\rangle_L$ and $|j,m\rangle_R$ are orthonormal basis states on the left and right halves labelled by the states of auxiliary spins adjacent to the cut, and the primed sum $\sum'$ indicates increments by $1/2$ instead of 1 in the index. Now suppose the Rényi entropies $S_\alpha(\rho_R)$ are known. To recover the entanglement spectrum $\{-\log(\lambda^2_{|j,m\rangle})\}$, we would follow (30) and (31) by computing

$$\begin{aligned} f(\alpha) &:= \exp\{(1-\alpha)S_\alpha(\rho_R)\} = \sum_{j=0}^{S}{}' \sum_{m=-j}^{j} \lambda^2_{|j,m\rangle}, \\ \hat{f}(\omega) &= \sum_{j=0}^{S}{}' \sum_{m=-j}^{j} \delta\left(\log\left(\lambda^2_{|j,m\rangle}\right) - \omega\right). \end{aligned} \tag{34}$$

For each value of total spin $j = 0, \frac{1}{2}, 1, \ldots, S$, there are $2j+1$ delta functions in the inner sum. This number coincides with the dimension of $\mathcal{V}_j$. Although not a particularly astute observation, this will resurface in the setting of a q-deformed Rényi entropy we propose in Section 4.3.

4.3. q-deformed Entanglement Entropies

Full degeneracy in the entanglement spectrum is characteristic to the AKLT states, but the results of Santos et al. [2012a] show that the deformation into qAKLT states does not preserve this degeneracy. On the other hand, Couvreur et al. [2017] suggested that the classical definitions of reduced density matrices and entanglement entropies are not suitable for systems with quantum symmetries in the first place, and proposed more general definitions applicable to systems with $\mathcal{U}_q[sl(2)]$ symmetry in particular:

Definition 4.8. *Given a density matrix $\rho^{(q)} = |\psi\rangle_q \langle\psi|_q$ representing a pure state $|\psi\rangle_q$ in a spin chain with $\mathcal{U}_q[sl(2)]$ symmetry, the q-**deformed reduced density matrix** is*

$$\rho_R^{(q)} = \mathrm{tr}_L(q^{-2\mathbb{S}_L^z}\rho^{(q)}),$$

where $\mathbb{S}_L^z$ is the action of $\mathbb{S}^z$ on the left part of the chain, with respect to a virtual cut made in the chain.

Definition 4.9. *The q-**deformed von Neumann entanglement entropy** of the state $|\psi\rangle_q$ is the number*

$$S^{(q)}(\rho_R^{(q)}) = -\mathrm{tr}_R(q^{2\mathbb{S}_R^z}\rho_R^{(q)} \log \rho_A^{(q)}).$$

Definition 4.10. *The q-**deformed entanglement spectrum** of $|\psi\rangle_q$ is the negative logarithm of the eigenvalues of the q-deformed reduced density matrix $\rho_R^{(q)}$.*

Using these definitions, Quella [2020] showed that each q-deformed spin-S AKLT state $|q\mathrm{AKLT}\rangle_S$, where S is a positive integer, exhibits full $(2S+1)$-fold degeneracy of the value $\log(q^{2S} + q^{2(S-1)} + \ldots + q^{-2S}) = \log([2S+1]_q)$ in its q-deformed entanglement spectrum. The q-deformed von Neumann entanglement entropy was also shown to equal $\log([2S+1]_q)$. This mirrors exactly the situation for the undeformed case as we saw in Section 4.2.

We now propose a definition of *q-deformed Rényi entanglement entropy* to complete the picture:

Definition 4.11. *Given a q-deformed reduced density matrix $\rho_R^{(q)}$, we define the* ***q-deformed Rényi entanglement entropies*** *to be the parametrised family of entropies given by*

$$S_\alpha^{(q)}(\rho_R^{(q)}) = \frac{\mathrm{tr}_R\left[q^{2\mathbb{S}_R^z}\rho_R^{(q)}\right]}{1-\alpha}\log\left(\mathrm{tr}_R\left[q^{2\mathbb{S}_R^z}\left(\rho_R^{(q)}\right)^\alpha\right]\right), \quad \alpha>0, \alpha\neq 1.$$

The following proposition, which is analogous to Proposition 4.5, establishes the above definition as a viable q-analogue of Rényi entropy.

Proposition 4.12. *If the q-deformed Rényi entanglement entropies $S_\alpha^{(q)}(\rho_R^{(q)})$ are known for all α, then the q-deformed entanglement spectrum can be recovered modulo degeneracies.*

Proof. The extra $\mathbb{S}^z$-dependent terms appearing in the above definitions force us to specify our physical system in order to understand the effect of such terms. The physical system at hand is a q-deformed quantum spin chain, so in general the auxiliary spin on each site belongs to the representation

$$\mathcal{V}_0^{(q)} \oplus \mathcal{V}_{\frac{1}{2}}^{(q)} \oplus \mathcal{V}_1^{(q)} \oplus \cdots \oplus \mathcal{V}_S^{(q)} \tag{35}$$

of $\mathcal{U}_q[sl(2)]$ for some S, where $\mathcal{V}_j^{(q)}$ is the spin-j irreducible representation of $\mathcal{U}_q[sl(2)]$. Make an imaginary cut in the chain, as one does to measure entanglement. As in (33), there exists a Schmidt decomposition

$$|\psi\rangle_q = {\sum_{j=0}^{S}}' \sum_{m=-j}^{j} \lambda_{|j,m\rangle_q} (|j,m\rangle_q)_L \otimes (|j,m\rangle_q)_R, \tag{36}$$

where $(|j,m\rangle_q)_L$ and $(|j,m\rangle_q)_R$ are orthonormal basis states for the left and right halves labelled by the states of auxiliary spins adjacent to the cut, and the primed sum $\sum'$ indicates increments by $1/2$ instead of 1 in the index. This expression is the q-deformed version of (33). Now we only work in these basis states, which are ordered as

$$|0,0\rangle_q, \left|\frac{1}{2},-\frac{1}{2}\right\rangle_q, \left|\frac{1}{2},\frac{1}{2}\right\rangle_q, \ldots, |S,-S\rangle_q, \ldots, |S,S\rangle_q. \tag{37}$$

In this basis, $\mathbb{S}^z$ is acts as a diagonal matrix:

$$\mathbb{S}^z = \mathrm{diag}\left(0,-\frac{1}{2},\frac{1}{2},-1,0,1,\ldots,-S,-S+1,\ldots,S\right). \tag{38}$$

Using this fact while applying the definition of q-deformed reduced density matrix gives

$$\rho_R^{(q)} = \mathrm{tr}_L(q^{-2\mathbb{S}_L^z}|\psi\rangle_q\langle\psi|_q) = \cdots = {\sum_{j=0}^{S}}' \sum_{m=-j}^{j} q^{-2m}\lambda^2_{|j,m\rangle_q}(|j,m\rangle_q)_R(\langle j,m|_q)_R. \tag{39}$$

Therefore, from the definition, the q-deformed entanglement spectrum is

$$\left\{-\log(\xi_{|j,m\rangle_q}) : j=0,\frac{1}{2},1,\ldots,S;\ m=-j,-j+1,\ldots,j\right\}, \tag{40}$$

where $\xi_{|j,m\rangle_q} := q^{-2m}\lambda^2_{|j,m\rangle_q}$. Now suppose we know all q-deformed Rényi entropies $S^{(q)}_\alpha(\rho^{(q)}_R)$ and we wish to recover (40). From (38) and (39), we compute

$$\begin{aligned}\mathrm{tr}_R\left[q^{2\mathbb{S}^z}\left(\rho^{(q)}_R\right)^\alpha\right] &= {\sum_{j=0}^{S}}' \sum_{m=-j}^{j} q^{2m}\left(\xi_{|j,m\rangle_q}\right)^\alpha, \\ \mathrm{tr}_R\left[q^{2\mathbb{S}^z}\rho^{(q)}_R\right] &= {\sum_{j=0}^{S}}' \sum_{m=-j}^{j} \lambda^2_{|j,m\rangle_q} = 1,\end{aligned} \tag{41}$$

since the $\lambda_{|j,m\rangle_q}$ are Schmidt decomposition coefficients. We proceed as in the proof of Proposition 4.5. Write

$$f(\alpha) := \exp\left\{(1-\alpha)S^{(q)}_\alpha\left(\rho^{(q)}_R\right)\right\} = {\sum_{j=0}^{S}}' \sum_{m=-j}^{j} q^{2m}\left(\xi_{|j,m\rangle_q}\right)^\alpha, \tag{42}$$

which is known because $S^{(q)}_\alpha(\rho^{(q)}_R)$ is. Analytically continue f to the complex plane and write

$$\begin{aligned}\hat{f}(\omega) &= \int_{-\infty}^{\infty} f(it)e^{-i\omega t}dt \\ &= {\sum_{j=0}^{S}}' \sum_{m=-j}^{j} q^{2m}\int_{-\infty}^{\infty}\exp\left\{i\left[\log\left(\xi_{|j,m\rangle_q}\right)-\omega\right]t\right\}dt \\ &= {\sum_{j=0}^{S}}' \sum_{m=-j}^{j} q^{2m}\delta\left(\log\left(\xi_{|j,m\rangle_q}\right)-\omega\right),\end{aligned} \tag{43}$$

which is also known. The entanglement spectrum (40) can be read off the peaks of the Dirac delta functions. □

Unlike the undeformed case (Proposition 4.5), the degeneracies of the q-deformed entanglement spectrum cannot be read off due to the q^{2m} prefactors. Nevertheless, this feature has been deformed away in a somewhat orderly manner. The final expression in (43) is a weighted sum of delta functions, and the weights for each spin sector (i.e. each j) sum to $q^{2j}+q^{2j-2}+\ldots+q^{-2j} = [2j+1]_q$. This is known as the *quantum dimension* of j which is an important invariant associated with the representation $\mathcal{V}_j$. We had already discussed this observation for the undeformed case towards the end of Section 4.2, in which the quantum and standard dimensions coincide.

5. Conclusion

We have developed evidence supporting a classification of q-deformed AKLT ground states into two distinct symmetry-protected topological phases depending on the spin parity, in analogy to the undeformed case. We have also put forward a notion of q-deformed Rényi entropy. In view of the vast amount of current research on quantum spin systems, what we have studied here admits natural generalisations that warrant further exploration. The q-deformed AKLT model is a special case of the q-deformed bilinear-biquadratic spin chain, and it would be interesting to investigate SPT phases in that setting. There is also the ambition of studying two- or three-dimensional quantum systems, as well as those with more general quantum group symmetries. Of course, proving the existence of SPT phases analytically remains an important task from the mathematical standpoint.

Appendix A Theory of Spin Angular Momentum

Mathematically, the theory of spin angular momentum in quantum mechanics is the representation theory of the Lie group $\mathsf{SU}(2)$ (equivalently, that of the Lie algebra $\mathfrak{su}(2)$). We motivate and introduce the theory while borrowing notation commonly seen in the physics literature. An excellent reference for further reading is Hall [2013].

Definition A.1. *The orientation-preserving group of 3D rotations, or* $\mathsf{SO}(3)$*, is the group of* 3×3 *orthogonal matrices with determinant 1. Since it is a closed subgroup of* $\mathsf{GL}(3,\mathbb{C})$*, it is a three-dimensional matrix Lie group.*

A *spin* is a state vector in a Hilbert space $\mathcal{H}$ on which rotations act. Hence we are compelled to find a unitary representation $(\pi,\mathcal{H})$ of the Lie group $\mathsf{SO}(3)$.[7] However, instead of stipulating that the representation is linear (as one usually means by a representation), we only impose a weaker condition that the representation be *projective*, i.e.

$$\pi : \mathsf{SO}(3) \to \mathsf{U}(\mathcal{H}), \quad \pi(g_1 g_2) = e^{i\theta}\pi(g_1)\pi(g_2),$$

where $\mathsf{U}(\mathcal{H})$ is the group of unitary transformations on $\mathcal{H}$, and $\theta \in \mathbb{R}$ is a phase which may depend on g_1 and g_2. This is because two vectors in $\mathcal{H}$ which only differ by a phase are deemed to be physically equivalent in quantum mechanics. That said, we still prefer the convenience of linear representations, so the following facts are incredibly useful.

Lemma A.2. *If G is a finite-dimensional matrix Lie group with universal cover $\tilde{G}$, there is a one-to-one correspondence*

$$\left\{\begin{array}{c}\textit{irreducible, projective, unitary}\\ \textit{representations of } G\end{array}\right\} \overset{\sim}{\leftrightarrow} \left\{\begin{array}{c}\textit{irreducible, linear, unitary}\\ \textit{representations of } \tilde{G}\\ \textit{with determinant 1}\end{array}\right\}.$$

Lemma A.3. *The Lie group* $\mathsf{SO}(3)$ *is a finite-dimensional matrix Lie group, and its universal cover is the Lie group* $\mathsf{SU}(2)$ *of* 2×2 *unitary matrices with determinant 1.*

Thus the projective unitary representations of $\mathsf{SO}(3)$ are studied by looking at the *linear* unitary representations of $\mathsf{SU}(2)$. This is the premise of using representations of $\mathsf{SU}(2)$ to study spin angular momentum. From here on, a *spin* will be a state vector in a unitary representation of $\mathsf{SU}(2)$, and we will drop the descriptor 'linear'. Let us now look at the irreducible unitary representations of $\mathsf{SU}(2)$. It is well-known that Lie group representations are conveniently studied via representations of its Lie algebra. For the $\mathsf{SU}(2)$ case we have the following.

Lemma A.4. *There are one-to-one correspondences*[8]

$$\left\{\begin{array}{c}\textit{irreducible unitary}\\ \textit{representations of } \mathsf{SU}(2)\end{array}\right\} \overset{\sim}{\leftrightarrow} \left\{\begin{array}{c}\textit{irreducible hermitian}\\ \textit{representations of the}\\ \textit{real Lie algebra } \mathfrak{su}(2)\end{array}\right\} \overset{\sim}{\leftrightarrow} \left\{\begin{array}{c}\textit{irreducible}\\ \textit{representations of the}\\ \textit{complex Lie algebra } \mathfrak{su}(2)\end{array}\right\}.$$

We are therefore instructed to look at the representations falling into the right-hand set. In the following, we define the complex Lie algebra $\mathfrak{su}(2)$ and classify its irreducible representations.

Definition A.5. *The Lie algebra* $\mathfrak{su}(2)$ *is the complex algebra generated by the elements* $\mathbb{S}^z$*,* $\mathbb{S}^+$ *and* $\mathbb{S}^-$ *which satisfy the commutation relations*

$$[\mathbb{S}^z, \mathbb{S}^\pm] = \pm\mathbb{S}^\pm \quad \textit{and} \quad [\mathbb{S}^+, \mathbb{S}^-] = 2\mathbb{S}^z.$$

It is also endowed with a $*$-structure by setting $(\mathbb{S}^z)^* = \mathbb{S}^z$ *and* $(\mathbb{S}^\pm)^* = \mathbb{S}^\mp$*.*

[7] The unitarity requirement is due to Wigner's Theorem.
[8] The complexified Lie algebra $\mathfrak{su}(2)$ is often denoted $\mathfrak{sl}(2,\mathbb{C})$ in the mathematical literature.

Remark. The physics convention is used here; the mathematics convention differs by some multiplicative factors (but is nevertheless equivalent). We could have also defined $\mathfrak{su}(2)$ as the set of 2×2 hermitian traceless matrices, but we prefer to picture $\mathfrak{su}(2)$ as an abstract Lie algebra with matrix representations of various dimensions.

Theorem A.6. *Up to unitary equivalence, there is exactly one irreducible representation of the complex Lie algebra $\mathfrak{su}(2)$, and hence one irreducible unitary representation of $\mathsf{SU}(2)$, for each finite dimension $d \geq 1$.*

Having classified the irreducible representations of $\mathsf{SU}(2)$, we now infuse some physics terminology.

Definition A.7. *Let s be a nonnegative integer or half-integer. The $(2s+1)$-dimensional irreducible representation of $\mathfrak{su}(2)$ is referred to as the **spin-s representation**. A state vector in this representation is said to have **(total) spin s**, or simply called a **spin-s**.*

Definition A.8. *The **(quadratic) Casimir element** of $\mathfrak{su}(2)$ is the element*

$$\mathbb{S}^2 = \mathbb{S}^+\mathbb{S}^- + \mathbb{S}^z(\mathbb{S}^z - 1),$$

and can be checked to commute with all generators of $\mathfrak{su}(2)$.

The Casimir element finds use in determining an orthonormal basis for the spin-s representation. We state the result below:

Theorem A.9. *A basis of spin-s states for the spin-s representation is given by $|s, m\rangle$, where $m = -s, -s+1, \ldots, s$. These are defined by the requirement that they are unit vectors (hence making an orthonormal basis), and that*

$$\mathbb{S}^2 |s, m\rangle = s(s+1) |m\rangle , \quad \mathbb{S}^z |s, m\rangle = m |m\rangle .$$

We then also have

$$\mathbb{S}^\pm |s, m\rangle = \sqrt{(s \mp m)(s \pm m + 1)}\, |s, m \pm 1\rangle .$$

Definition A.10. *We say that the z-component of the spin state $|s, m\rangle$ is equal to m.*

Denote the spin-j representation of $\mathfrak{su}(2)$ by $\mathcal{V}_j$. Let us now consider the tensor product of two representations of $\mathfrak{su}(2)$, say $\mathcal{V}_j \otimes \mathcal{V}_k$. This corresponds to the coupling of two spin angular momenta, and the space $\mathcal{V}_j \otimes \mathcal{V}_k$ is again a representation of $\mathfrak{su}(2)$ (although not an irreducible one). The operators are lifted the obvious way:

$$A \in \mathsf{End}(\mathcal{V}_j), B \in \mathsf{End}(\mathcal{V}_k) \quad \Rightarrow A \otimes B = A \otimes \mathbb{I} + \mathbb{I} \otimes B, \tag{A1}$$

where $\mathbb{I}$ is the identity map. It turns out that the tensor product has a nice decomposition into irreducibles:

Theorem A.11. *With the above notation, $\mathcal{V}_j \otimes \mathcal{V}_k$ decomposes as a direct sum of irreducible representations of $\mathfrak{su}(2)$ by*

$$\mathcal{V}_j \otimes \mathcal{V}_k = \mathcal{V}_{|j-k|} \oplus \mathcal{V}_{|j-k|+1} \oplus \cdots \oplus \mathcal{V}_{j+k}.$$

Definition A.12. *In the context of a decomposition into irreducibles as above, we call each $\mathcal{V}_s$ the **spin-s sector**.*

Finally, to make this workable we must know how to actually project a coupled spin state into its spin sectors. This is taken care of by the *Clebsch-Gordan coefficients*, defined below.

Definition A.13. *Let $|j_1, m_1\rangle \in \mathcal{V}_{j_1}$ and $|j_2, m_2\rangle \in \mathcal{V}_{j_2}$ be spin-j_1 and spin-j_2 basis states respectively. By Theorem A.11, we have a decomposition*

$$\mathcal{V}_{j_1} \otimes \mathcal{V}_{j_2} = \mathcal{V}_{|j_1-j_2|} \oplus \mathcal{V}_{|j_1-j_2|+1} \oplus \cdots \oplus \mathcal{V}_{j_1+j_2},$$

and by Theorem A.9 this has an orthonormal basis

$$\begin{gathered} \left| |j_1 - j_2|, -|j_1 - j_2| \right\rangle, \left| |j_1 - j_2|, -|j_1 - j_2| + 1 \right\rangle, \ldots, \left| |j_1 - j_2|, |j_1 - j_2| \right\rangle, \\ \vdots \\ \left| j_1 + j_2, -(j_1 + j_2) \right\rangle, \left| j_1 + j_2, -(j_1 + j_2) + 1 \right\rangle, \ldots, \left| j_1 + j_2, j_1 + j_2 \right\rangle, \end{gathered}$$

where we have omitted the '$\mathbf{0}\oplus$' and '$\oplus\mathbf{0}$' terms for brevity. The projection of the state $|j_1, m_1\rangle \otimes |j_2, m_2\rangle \in \mathcal{V}_{j_1} \otimes \mathcal{V}_{j_2}$ onto one of these basis vectors, say $|J, M\rangle$, is called an $(\mathsf{SU}(2))$ ***Clebsch-Gordan coefficient*** *and is denoted*

$$\langle\, j_1, m_1\,; j_2, m_2 \mid J, M\,\rangle = \mathrm{proj}_{|J,M\rangle}\left(|j_1, m_1\rangle \otimes |j_2, m_2\rangle\right).$$

The Clebsch-Gordan coefficients are all real-valued.

The Clebsch-Gordan coefficients have no simple closed form in general. However they are tabulated for small values of the j's and m's, and in any case there are many symmetry and recursion relations between them.

For the quantum group $\mathcal{U}_q[sl(2)]$, the Clebsch-Gordan coefficients are different due to the modified commutation relations and coproduct; see equations (18) and (19) in the main text. The procedure of obtaining the coefficients is unchanged, and many of the recursion and symmetry relations admit q-analogues. We denote the $\mathcal{U}_q[sl(2)]$ Clebsch-Gordan coefficients by $\langle\, j_1, m_1\,; j_2, m_2 \mid J, M\,\rangle_q$.

Appendix B Matrix Product States

The matrix product state formalism is extremely useful but rather technical. For an elaborate non-technical introduction, we recommend Orús [2014]. Otherwise, Schollwöck [2011] provides a comprehensive walkthrough. In what follows, take our physical system to be a spin chain on a one-dimensional lattice, where each site has state space $\mathcal{V}$.

Definition B.1. *Suppose the length of the spin chain is L with periodic boundary conditions. Practically, we think of the lattice as infinite with a repeating unit of L sites. A **matrix product state** (MPS) is a quantum state $|\psi\rangle$ on the lattice that can be written as*

$$|\psi\rangle = \mathrm{tr}\left[\mathcal{M}^{[1]}\mathcal{M}^{[2]}\cdots\mathcal{M}^{[L]}\right]$$

*where each $\mathcal{M}^{[i]}$ is a tensor of rank 3, and is viewed as a matrix whose entries are vectors in $\mathcal{V}$. We call the $\mathcal{M}^{[i]}$ the **MPS tensors** for the state.*

Remark. In this definition, the multiplication of rank-3 tensors is ordinary matrix multiplication except where multiplication of vectors is replaced by the tensor product. The tensor $\mathcal{M}^{[i]}$ is associated to the ith site of the lattice.

Remark. For states with $\mathcal{U}_q[sl(2)]$ symmetry, we may relate state vectors to MPS tensors by

$$|\psi\rangle_q = \mathrm{tr}\left[q^{2\mathbb{S}^z}\mathcal{M}^{[1]}\mathcal{M}^{[2]}\cdots\mathcal{M}^{[L]}\right],$$

where $\mathbb{S}^z$ is the spin-z operator, one of the generators of $\mathcal{U}_q[sl(2)]$.[9]

Definition B.2. *A state on the lattice is **one-site translationally invariant** if all the $\mathcal{M}^{[i]}$ are equal.*

Remark. In this case, the single MPS tensor $\mathcal{M}$ describes the entire system, up to the length of the spin chain. If the period L is specified, then Definition B.1 can be used to recover the state vector. In many applications, like in this report, it is customary to think of the length as infinite and to ignore specifying the length of the period altogether.

[9]The implication of this are subtle and we will mostly be ignoring them, given that we are mainly concerned with infinite chains.

Example B.3. *The spin-1 AKLT ground state is specified by the single MPS tensor*

$$\mathcal{M} = \frac{1}{\sqrt{3}} \begin{bmatrix} -\left|0\right\rangle & \sqrt{2}\left|1\right\rangle \\ -\sqrt{2}\left|-1\right\rangle & \left|0\right\rangle \end{bmatrix},$$

since it is translationally invariant. Here the one-site state space $\mathcal{V}$ is the spin-1 representation of $\mathsf{SU}(2)$ with orthonormal basis $\{\left|1\right\rangle, \left|0\right\rangle, \left|-1\right\rangle\}$. If the length of the chain is 2 with periodic boundary conditions, then the spin-1 AKLT ground state has state vector

$$\begin{aligned}\left|\psi\right\rangle &= \operatorname{tr}\left[\mathcal{M}^2\right] \\ &= \frac{1}{3}\operatorname{tr}\begin{bmatrix} \left|0\right\rangle \otimes \left|0\right\rangle - 2\left|1\right\rangle \otimes \left|-1\right\rangle & -\sqrt{2}\left|0\right\rangle \otimes \left|1\right\rangle + \sqrt{2}\left|1\right\rangle \otimes \left|0\right\rangle \\ \sqrt{2}\left|-1\right\rangle \otimes \left|0\right\rangle - \sqrt{2}\left|0\right\rangle \otimes \left|-1\right\rangle & -2\left|-1\right\rangle \otimes \left|1\right\rangle + \left|0\right\rangle \otimes \left|0\right\rangle \end{bmatrix} \\ &= \frac{2}{3}(\left|0\right\rangle \otimes \left|0\right\rangle - 2\left|1\right\rangle \otimes \left|-1\right\rangle - 2\left|-1\right\rangle \otimes \left|1\right\rangle).\end{aligned}$$

Example B.4 (Obtaining MPS tensors from state constructions)**.** *We demonstrate, without proof, how the derivation of an MPS tensor can be performed in conjunction with the physical construction of a state on the lattice using auxiliary spins. Indeed this is how the MPS tensors in the main text were obtained. As an example, we derive the MPS tensor for the spin-1 AKLT ground state $\left|\mathrm{AKLT}_1\right\rangle$ whose physical construction is illustrated in Figure 1 of the main text.*

Consider the two auxiliary spin-$\frac{1}{2}$s on a physical site together with the left auxiliary spin-$\frac{1}{2}$ on its right-hand physical site. Of the three auxiliary spins, the two on the right are coupled into a singlet:

$$\left|\mathrm{singlet}_1\right\rangle = \frac{1}{\sqrt{2}}(\left|\uparrow\right\rangle\left|\downarrow\right\rangle - \left|\downarrow\right\rangle\left|\uparrow\right\rangle). \tag{B1}$$

This induces two orthonormal states for the three-auxiliary-site unit, labelled by the leftmost auxiliary spin:

$$\left|\hat{\alpha}\right\rangle := \frac{1}{\sqrt{2}}(\left|\alpha\uparrow\right\rangle\left|\downarrow\right\rangle - \left|\alpha\downarrow\right\rangle\left|\uparrow\right\rangle), \quad \left|\alpha\right\rangle \in \{\left|\uparrow\right\rangle, \left|\downarrow\right\rangle\}. \tag{B2}$$

To complete the construction, we project the two left auxiliary spins to the spin-1 sector. The projection operator is

$$\mathrm{proj}_1 = \left|1\right\rangle\left\langle\uparrow\uparrow\right| + \left|0\right\rangle\frac{\left\langle\uparrow\downarrow\right| + \left\langle\downarrow\uparrow\right|}{\sqrt{2}} + \left|-1\right\rangle\left\langle\downarrow\downarrow\right|, \tag{B3}$$

which is derived from the $\mathsf{SU}(2)$ Clebsch-Gordan coefficients. Applying this to (B2) *yields the two states*

$$\mathrm{proj}_1|\hat{\uparrow}\rangle = \frac{1}{\sqrt{2}}\left|1\right\rangle\left|\downarrow\right\rangle - \frac{1}{2}\left|0\right\rangle\left|\uparrow\right\rangle, \quad \mathrm{proj}_1|\hat{\downarrow}\rangle = \frac{1}{2}\left|0\right\rangle\left|\downarrow\right\rangle - \frac{1}{\sqrt{2}}\left|-1\right\rangle\left|\uparrow\right\rangle.$$

Writing these states in the basis $B = \{\left|\uparrow\right\rangle, \left|\downarrow\right\rangle\}$ for the rightmost auxiliary spin as rows of a matrix directly gives the MPS tensor:

$$\mathcal{M} = \begin{array}{c c} & \begin{array}{cc} \left|\uparrow\right\rangle & \left|\downarrow\right\rangle \end{array} \\ \begin{array}{c} \left|\uparrow\right\rangle \\ \left|\downarrow\right\rangle \end{array} & \begin{bmatrix} [\mathrm{proj}_1|\hat{\uparrow}\rangle]_B \\ [\mathrm{proj}_1|\hat{\downarrow}\rangle]_B \end{bmatrix} \end{array} = \begin{array}{c c} & \begin{array}{cc} \left|\uparrow\right\rangle & \left|\downarrow\right\rangle \end{array} \\ \begin{array}{c} \left|\uparrow\right\rangle \\ \left|\downarrow\right\rangle \end{array} & \begin{bmatrix} -\frac{1}{2}\left|0\right\rangle & \frac{1}{\sqrt{2}}\left|1\right\rangle \\ -\frac{1}{\sqrt{2}}\left|-1\right\rangle & \frac{1}{2}\left|0\right\rangle \end{bmatrix} \end{array}.$$

Right-normalising the tensor (see Definition 4.6) yields a tensor that agrees with (2) *in the main text. This procedure* *was used to obtain all MPS tensors appearing in the report, with* (B1) *and* (B3) *generalised to arbitrary spins:*

$$|\text{singlet}_S\rangle = \frac{1}{\sqrt{2S+1}} \sum_{M=-S}^{S} (-1)^{M+S} |S,-M\rangle |S,M\rangle ,$$
$$\text{proj}_S = \sum_{M=-S}^{S} |S,M\rangle \left(\sum_{(m_1,m_2)} \langle\, j_1, m_1 \,; j_2, m_2 \mid S, M \,\rangle \langle j_1, m_1| \langle j_2, m_2| \right),$$

where j_1 *and* j_2 *are the total spins of the auxiliary spins, and the inner sum is taken over pairs* (m_1, m_2) *satisfying the triangle condition* $m_1 + m_2 = -M$*. For states with* $\mathcal{U}_q[sl(2)]$ *symmetry, we use*

$$|\text{singlet}_S\rangle_q = \frac{1}{\sqrt{[2S+1]_q}} \sum_{M=-S}^{S} (-1)^{M+S} q^{-M} |S,-M\rangle_q |S,M\rangle_q ,$$
$$\text{proj}_S^{(q)} = \sum_{M=-S}^{S} |S,M\rangle_q \left(\sum_{(m_1,m_2)} \langle\, j_1, m_1 \,; j_2, m_2 \mid S, M \,\rangle_q \langle j_1, m_1|_q \langle j_2, m_2|_q \right).$$

Definition B.5. *Given an MPS tensor* $\mathcal{M}$*, the* ***transfer matrix*** *is the matrix given by*

$$\mathbb{E} = \sum_{\sigma} \mathcal{M}^{\sigma} \otimes \overline{\mathcal{M}^{\sigma}},$$

where σ *indexes the basis states of the physical state space* $\mathcal{V}$*, and* $\otimes$ *is the Kronecker product of matrices.*

Example B.6. *Let us compute the transfer matrix for the spin-1 AKLT ground state to clear up this mysterious definition. The notation* $\mathcal{M}^{\sigma}$ *involves 'shifting the view' of an MPS tensor, interpreting it as a collection of scalar matrices rather than a single matrix with vector-valued entries. In our example, we have the single MPS tensor*

$$\mathcal{M} = \frac{1}{\sqrt{3}} \begin{bmatrix} -|0\rangle & \sqrt{2}\,|1\rangle \\ -\sqrt{2}\,|-1\rangle & |0\rangle \end{bmatrix},$$

which can be deconstructed into three separate scalar matrices:

$$\mathcal{M}^1 = \frac{1}{\sqrt{3}} \begin{bmatrix} 0 & \sqrt{2} \\ 0 & 0 \end{bmatrix}, \quad \mathcal{M}^0 = \frac{1}{\sqrt{3}} \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \mathcal{M}^{-1} = \frac{1}{\sqrt{3}} \begin{bmatrix} 0 & 0 \\ -\sqrt{2} & 0 \end{bmatrix}.$$

The transfer matrix is therefore calculated by

$$\mathbb{E} = \sum_{\sigma\in\{1,0,-1\}} \mathcal{M}^{\sigma} \otimes \overline{\mathcal{M}^{\sigma}} = \underbrace{\frac{1}{3}\begin{bmatrix} 0 & 0 & 0 & 2 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}}_{\mathcal{M}^1\otimes\overline{\mathcal{M}^1}} + \underbrace{\frac{1}{3}\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}}_{\mathcal{M}^0\otimes\overline{\mathcal{M}^0}} + \underbrace{\frac{1}{3}\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 2 & 0 & 0 & 0 \end{bmatrix}}_{\mathcal{M}^{-1}\otimes\overline{\mathcal{M}^{-1}}} = \frac{1}{3}\begin{bmatrix} 1 & 0 & 0 & 2 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 2 & 0 & 0 & 1 \end{bmatrix}.$$

The transfer matrix is a central object in the computation of many physical parameters associated with a state. Many computations can be executed by taking iterated powers and/or traces of the transfer matrix. For this reason, one would like to diagonalise the transfer matrix and solve for its spectrum. The following is one example.

Definition B.7. *The* ***spin-spin correlation*** *between two spins at sites* a *and* b *of a periodic spin chain with length* L *is the number*

$$\langle S_a^z S_b^z \rangle = E[S_a^z S_b^z],$$

where S^z is the component of spin angular momentum along the z-axis, and $E[\cdot]$ denotes an expectation value.

This corresponds to a shifted covariance of S_a^z and S_b^z, and measures the signed interaction between the spins at distance $|a-b|$. The transfer matrix makes this computation quite handy:

Proposition B.8. *Assume that the spin chain is one-site translationally invariant with MPS tensor $\mathcal{M}$. Using the transfer matrix $\mathbb{E}$, the spin-spin correlation between sites a and b (assuming $a < b$) can be computed using the formula*

$$\langle S_a^z S_b^z \rangle = \mathrm{tr}[\mathbb{E}^{L+a-b-1} C \mathbb{E}^{(b-a-1)} C]$$

for some matrix C (which is easily derived, but omitted here to keep to the point).

Related to the spin-spin correlation is the following quantity which finds widespread use in the study of one-dimensional spin chains.

Definition B.9. *The **correlation length** of a state in a spin chain is the number ξ such that*

$$\lim_{|a-b|\to\infty} \langle S_a^z S_b^z \rangle \sim e^{-\frac{|a-b|}{\xi}},$$

if it exists.

Proposition B.10. *For a one-site translationally invariant MPS with MPS tensor $\mathcal{M}$, the correlation length is*

$$\xi = \frac{1}{\ln |\lambda_0/\lambda_1|},$$

where λ_i are the eigenvalues of the transfer matrix $\mathbb{E}$ labelled by the requirement that $|\lambda_0| \geq |\lambda_1| \geq \ldots \geq |\lambda_n|$. If $|\lambda_0| = |\lambda_1|$, then we say the correlation length is infinite.

Remark. Heuristically, the correlation length is the largest distance on the chain at which two spins are interacting with one another. The correlation length is intimately related to continuous phase transitions, in that an infinite correlation length marks a critical point in the state diagram of a system, i.e. a point on the boundary between two phases.

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