Dimerization in quantum spin chains with O(n) symmetry

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joint work with

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Related recent work with Robert Sims (Arizona) and Amanda Young (TU Munich).

Outline

- Spin chains
- The bilinear - biquadratic spin 1 chains
- Dimerization
- SPT phases and Stability
- Generalizing the AKLT chain
- Phase diagram of $O(n)$ invariant spin chains
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Spin chains, Hamiltonians, ground states

Finite spin chain on $[a, b] \subset \mathbb{Z}$, Hilbert space $\mathcal{H}_{[a,b]} = \bigotimes_{x=a}^{b} \mathbb{C}^n$, $n \geq 2$, spins of magnitude $S = 2n + 1$, $SU(2)$ spin matrices S^i_x, $i = 1, 2, 3$, $x \in [a, b]$.

Translation-invariant nearest neighbor interaction is given by $h = h^* \in M_n(\mathbb{C}) \otimes M_n(\mathbb{C}) = \mathcal{B}(\mathcal{H}_{[x,x+1]})$.

Hamiltonian: $H_{[a,b]} = \sum_{x=a}^{b-1} h_{x,x+1}$. Interested in ground states.

Heisenberg model: $h_{x,x+1} = \boldsymbol{S}_x \cdot \boldsymbol{S}_{x+1} = S^1_x S^1_{x+1} + S^2_x S^2_{x+1} + S^3_x S^3_{x+1}$, n-dimensional spin matrices.

AKLT model, $n = 3$:
$h_{x,x+1} = \frac{1}{2} \boldsymbol{S}_x \cdot \boldsymbol{S}_{x+1} + \frac{1}{6} (\boldsymbol{S}_x \cdot \boldsymbol{S}_{x+1})^2 + \frac{1}{3} \mathbb{1} = P^{(2)}_{x,x+1}$.

Most general isotropic nearest neighbor interaction for $n = 3$:
$h_{x,x+1} = \cos\phi \boldsymbol{S}_x \cdot \boldsymbol{S}_{x+1} + \sin\phi (\boldsymbol{S}_x \cdot \boldsymbol{S}_{x+1})^2$.

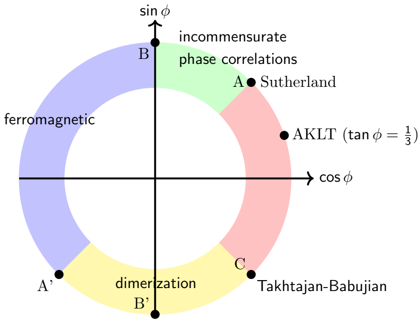
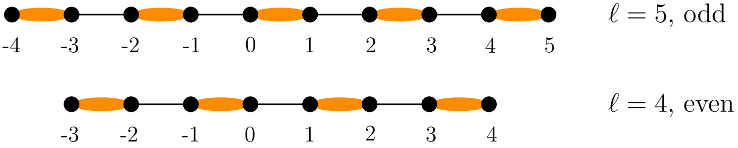


Figure: Ground state phase diagram for the $S = 1$ chain ($n = 3$) with nearest-neighbor interactions $\cos\phi \boldsymbol{S}_x \cdot \boldsymbol{S}_{x+1} + \sin\phi(\boldsymbol{S}_x \cdot \boldsymbol{S}_{x+1})^2$.

- $\phi = 0$ Heisenberg AF chain, Haldane phase (Haldane, 1983)
- $\tan\phi = 1/3$, AKLT point (Affleck-Kennedy-Lieb-Tasaki, 1987,1988), FF, MPS, gapped
- $\tan\phi = 1$, solvable, gapless, SU(3) invariant, (Sutherland, 1975)
- $\phi \in [\pi/2, 3\pi/2]$, ferromagnetic, FF, gapless
- $\phi = -\pi/2$, solvable, SU(3) invariant, Temperley-Lieb algebra, dimerized, gapped (Klümper; Affleck,1990)
- $\phi - = -\pi/4$ gapless, Bethe-ansatz, (Takhtajan; Babujian, 1982)

Dimerization

If a pair interaction favors a maximally entangled state (such as a spin singlet), monogamy of entanglement sets up a competition between pairings. In one dimension, this often leads to an instability and/or to spontaneous breaking of translation symmetry. In the family of $O(n)$ chains here, translation symmetry breaking occurs, called dimerization. For finite chains of 2ℓ spins the ground states can be viewed as chain of dimers:



The actual ground states need not consist of maximally entangled pairs. For the $O(n)$ chains maximally entangled pairs dominate for large n.

Gapped Symmetry Protected Topological (SPT) phases

For spin chains, gapped ground state can only have Short-Range Entanglement (SRE) (Chen-Gu-Wen, 2011; Ogata, 2019; Kapustin-Sopenko-Yang, 2021), meaning there is no non-trivial topologically order, and any two short range Hamiltonians with a unique gapped ground can be connected by a smooth path without closing the gap. There are non-topological orders such as dimerization.

This changes when a sufficient symmetry constraint is imposed: There exist SPT phases (Pollman-Turner-Berg-Oshikawa, 2010). Under the assumption of a gap and SRE, the SPT phases are classified by $H^2(G, U(1))$, where G is the imposed symmetry. $H^2(O(3), U(1)) = \mathbb{Z}_2$, and there is a non-trivial SPT phase, the Haldane phase. It turns out that a $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry is sufficient for this phase to be protected (Tasaki, 2018; Ogata, 2019).

The stability of gapped ground states

The gapped ground state phases are open regions in Hamiltonian space, not isolated special points, meaning they are stable.
For gapped, frustration-free models satisfying no-local order condition good general stability results exists:

Yarotsky 2006, Bravyi-Hastings-Michalakis 2010, Michalakis-Zwolak 2013, Szehr-Wolf 2015, Fröhlich-Pizzo 2018-20, N-Sims-Young 2020

These results prove the AKLT point is part of an open region on the red phase of the $n = 3$ phase diagram.
The uniqueness condition of the gapped ground state can be relaxed (N-Sims-Young 2020) but we have no general stability results yet that do not require frustration free property.

The point $\phi = -\pi/2$ with dimerization is not frustration free:

$$\langle h_{x,x+1} \rangle > \inf \operatorname{spec}(h_{x,x+1}).$$

$O(n)$ chains and generalizations of the AKLT model

Alternative way to represent the AKLT Hamiltonian in terms of 'swap' operator, T, and a rank-1 projection:

$$T = P^{(2)} - P^{(1)} + P^{(0)}.$$

Therefore, $h^{AKLT} = P^{(2)} = (T - 2P(0) + \mathbb{1})/2$ or, equivalently the AKLT model can be defined by the interaction

$$h_{x,x+1} = T - 2P^{(0)}.$$

The singlet state, in the usual basis of eigenvectors of S^3 is given by

$$\psi = \frac{1}{\sqrt{3}}(|1,-1\rangle - |0,0\rangle + |-1,1\rangle).$$

ψ is symmetric under T, therefore there is new o.n. basis e_1, e_0, e_{-1} such that

$$\psi = \frac{1}{\sqrt{3}}(e_1 \otimes e_1 + e_0 \otimes e_0 + e_{-1} \otimes e_{-1}).$$

Take $e_1 = (|1\rangle + |-1\rangle)/\sqrt{2}, e_0 = i|0\rangle, e_{-1} = i(|1\rangle - |-1\rangle)/\sqrt{2}$.

Equivalently, there is a local unitary change of basis in which the AKLT interaction is given by

$$h = T - 2Q,$$

where T is the swap operator and Q is the projection onto $\frac{1}{\sqrt{3}}(e_1 \otimes e_1 + e_0 \otimes e_0 + e_{-1} \otimes e_{-1})$.

This generalizes to n-dimensional spins and arbitrary coupling constants as follows

$$uT + vQ, \quad u, v \in \mathbb{R}$$

where Q is the projection to

$$\psi = \frac{1}{\sqrt{n}} \sum_{\alpha=1}^{n} |\alpha, \alpha\rangle.$$

Both T and Q commute with the natural action of $O(n)$ on the spins in this basis. It is the general $O(n)$ invariant nearest neighbor interaction for $n \geq 2$, which was studied by Tu & Zhang, 2008.

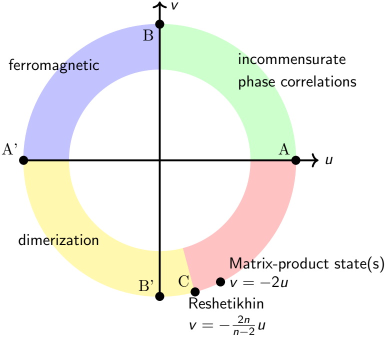


Figure: Ground state phase diagram for the chain with nearest-neighbor interactions $uT + vQ$ for $n \geq 3$.

- $v = -2nu/(n-2)$, $n \geq 3$, Bethe ansatz point (Reshetikhin, 1983)
- $v = -2u$: frustration free point, equivalent to $\perp$ projection onto symmetric vectors $\ominus$ one. Unique g.s. if n odd; two 2-periodic g.s. for even n; spectral gap in all cases and stable phase (N-Sims-Young, 2020).
- $u = 0$, $v = -1$. Equivalent to the $SU(n) - P^{(0)}$ models aka Temperley-Lieb chain; Affleck, 1990, Nepomechie-Pimenta 2016). Dimerized for all $n \geq 3$ (Aizenman, Duminil-Copin, Warzel, 2020). New result here: a proof of stability for large n (Björnberg-Mühlbacher-N-Ueltschi, arXiv:2101.11464).

Proving Stability

To date, there is no single approach for proving stability of gapped ground states that covers the generic situation, not even in one dimension.

Limiting property: frustration-freeness (FF) (classical configurations, AKLT chain, Toric Code Model)

Other special properties can sometimes be exploited, such as representation of $\mathrm{Tr} e^{-\beta H}$ as a classical partition function (aka Stoquastic Hamiltonians), with special monotonicity properties, this applies to $-P^{(0)}$ model (Aizenman, Duminil-Copin, Warzel 2020).

In our phase diagram the point $(0, -1)$ ($u = 0$) is not FF, but it has the special properties and this has allowed ADW to settle the dimerization question for all cases (all $n \geq 3$).

In (N-Ueltschi, 2017) we used a Peierls argument to prove dimerization for $n \geq 17$ for the models with $u = 0$.

The new result extends this to small $|u|$ and sufficiently large n by a cluster expansion, which also yields a spectral gap and exponential decay of correlations (in space and time).

Main Results (Björnberg-Mühlbacher-N-Ueltschi, arXiv:2101.11464)

Model: chain of n-dimensional spins with $O(n)$-invariant nearest neighbor interaction $h = uT + vQ$, $u, v \in \mathbb{R}$, T is the swap operator and Q projects onto $\psi = n^{-1/2} \sum_{\alpha=1}^{n} |\alpha, \alpha\rangle$.

Finite chains of 2ℓ spins, with Hamiltonian: $H_{[-\ell+1,\ell]} = \sum_{x=-\ell+1}^{\ell-1} h_{x,x+1}$.
Basic observables: generators of $O(n)$:

$$L^{\alpha,\alpha'} = |\alpha\rangle\langle\alpha'| - |\alpha'\rangle\langle\alpha|, 1 \leq \alpha < \alpha' \leq n.$$

Theorem (Dimerization)

There exist constants $n_0, c > 0$ (independent of ℓ) such that for $n > n_0$ and $|u| < n^{-4/3}$, we have that for all $1 \leq \alpha < \alpha' \leq n$,

$$\lim_{\beta\to\infty} \left[\langle L_0^{\alpha,\alpha'} L_1^{\alpha,\alpha'} \rangle_{\ell,\beta,u} - \langle L_{-1}^{\alpha,\alpha'} L_0^{\alpha,\alpha'} \rangle_{\ell,\beta,u} \right] > c \quad \text{for } \ell \text{ odd;}$$

$$\lim_{\beta\to\infty} \left[\langle L_0^{\alpha,\alpha'} L_1^{\alpha,\alpha'} \rangle_{\ell,\beta,u} - \langle L_{-1}^{\alpha,\alpha'} L_0^{\alpha,\alpha'} \rangle_{\ell,\beta,u} \right] < -c \quad \text{for } \ell \text{ even.}$$

Theorem (Exponential decay of correlations)

There exist constants $n_0, c_1, c_2, C > 0$ (independent of ℓ) such that for $n > n_0$ and $|u| < n^{-4/3}$, we have

$$\lim_{\beta\to\infty} \left| \langle L_x^{\alpha,\alpha'} e^{tH_\ell} L_y^{\alpha,\alpha'} e^{-tH_\ell} \rangle_{\ell,\beta,u} \right| \leq C e^{-c_1|x-y|-c_2|t|}$$

for all $\ell \in \mathbb{N}$, all $x, y \in \{-\ell+1, \ldots, \ell\}$, all $1 \leq \alpha < \alpha' \leq n$, and all $t \in \mathbb{R}$.

In fact, the decay of correlations between any two local observables is bounded by an exponential with a fixed rate.

Let $E_0^{(\ell)} < E_1^{(\ell)} < \dots$ be the eigenvalues of $H_{[-\ell+1,\ell]}$, and define the ground state gap $\Delta^{(\ell)}$ by

$$\Delta^{(\ell)} = E_1^{(\ell)} - E_0^{(\ell)}.$$

The gap is obviously positive but the question is whether there is a positive lower bound uniformly in ℓ.

Theorem (Spectral gap)

There exist constants $n_0, c > 0$ (independent of ℓ) such that for $n > n_0$ and $|u| < n^{-4/3}$, we have

(a) *$E_0^{(\ell)}$ is non-degenerate. That is, ground state is unique.*

(b) *$\Delta^{(\ell)} \geq c$ for all ℓ.*

'Random' loop representation (Toth 1993, Aizenman-N 1994, Ueltschi 2013)

First, the case $(u, v) = (0, -1)$.

Consider intervals of the form $[-\ell+1, \ell]$ (2ℓ spins), and denote the Hamiltonian by H_ℓ, and let ψ_ℓ be a normalized eigenvector of its smallest eigenvalue, which turns out to be simple. Then

$$|\psi_\ell\rangle\langle\psi_\ell| = \lim_{\beta\to\infty} \frac{e^{-2\beta H_\ell}}{\mathrm{Tr} e^{-2\beta H_\ell}},$$

and therefore, with $A = Q_{x,x+1}$, or any other observable,

$$\langle\psi_\ell, A\psi_\ell\rangle = \mathrm{Tr}|\psi_\ell\rangle\langle\psi_\ell|A = \lim_{\beta\to\infty} \frac{\mathrm{Tr} e^{-\beta H_\ell} A e^{-\beta H_\ell}}{\mathrm{Tr} e^{-2\beta H_\ell}}.$$

Both the numerator and the denominator can be given a nice representation by writing (for integer β)

$$e^{-\beta H_\ell} = \lim_{N\to\infty}(\mathbb{1} - \frac{1}{N}H_\ell)^{\beta N} = \lim_{N\to\infty}\left(\mathbb{1} + \frac{1}{N}\sum_{x=-\ell+1}^{\ell-1} Q_{x,x+1}\right)^{\beta N}.$$

The $(2\ell)^{\beta N}$ terms in the RHS resulting from expanding the product are labeled by a set $\Omega_{\ell,N}$ of diagrams we call random loop configurations, which are helpful to calculate the trace of each term using the matrix representation of each factor $Q_{x,x+1}$:

$$Q = \frac{1}{n}\sum_{\alpha,\beta=1}^{n} |\alpha,\alpha\rangle\langle\beta,\beta|.$$

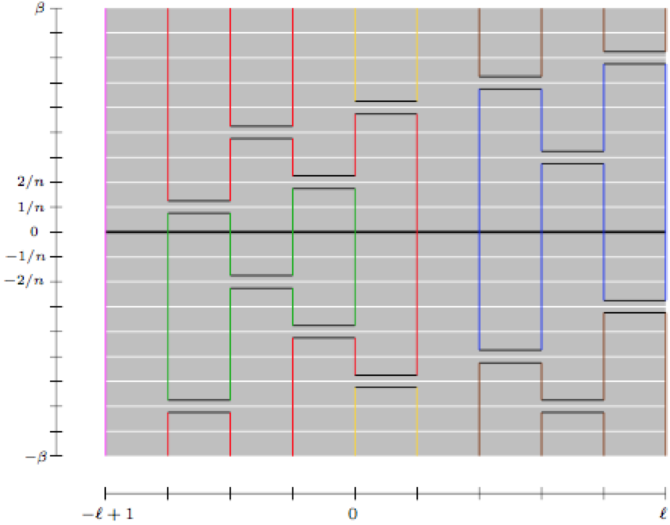


FIGURE 2. Loop representation of the $SU(2S+1)$-invariant quantum spin chains.

The trace of each term, labeled by $\omega \in \Omega_{\ell,N}$, is positive and depends only on the number of factors Q, denoted by $|\omega|$, and the number of loops in ω, denoted by $\mathcal{L}(\omega)$. This allows us to define a probability measure on $\Omega_{\ell,N}$. It is given by

$$\mu_{\beta,\ell,N}(\omega) = \frac{1}{Z_N(\beta,\ell)} \left(\tfrac{1}{N}\right)^{|\omega|} n^{\mathcal{L}(\omega)-|\omega|},$$

with

$$Z_N(\beta,\ell) = \sum_{\omega\in\Omega_{\ell,N}} \left(\tfrac{1}{N}\right)^{|\omega|} n^{\mathcal{L}(\omega)-|\omega|}.$$

For fixed $|\omega|$, the limit $N \to \infty$ is described by Lebesgue measure $dx^{\otimes|\omega|}$ on the family of time-intervals labeled by edges, $(-\beta, \beta]^{\times(2\ell-1)}$, and it is convenient to include a normalization factor so we get a probability measure on the configurations of loops:

$$d\rho_0(\omega) = e^{2\beta(2\ell-1)} dx^{\otimes|\omega|}.$$

The partition function then becomes

$$\lim_{N\to\infty} Z_N(\beta, \ell) = Z(\beta, \ell) = \int_{\Omega_{\ell,\beta}} d\rho_0(\omega) n^{\mathcal{L}(\omega)-|\omega|}.$$

Generalizing the representation to the spins with nearest-neighbor interaction $-uT - Q$, $u \in \mathbb{R}$ is straightforward.
Graphically we represent the two types of terms by crosses and double bars:

$$T = \asymp, \quad Q = \between$$

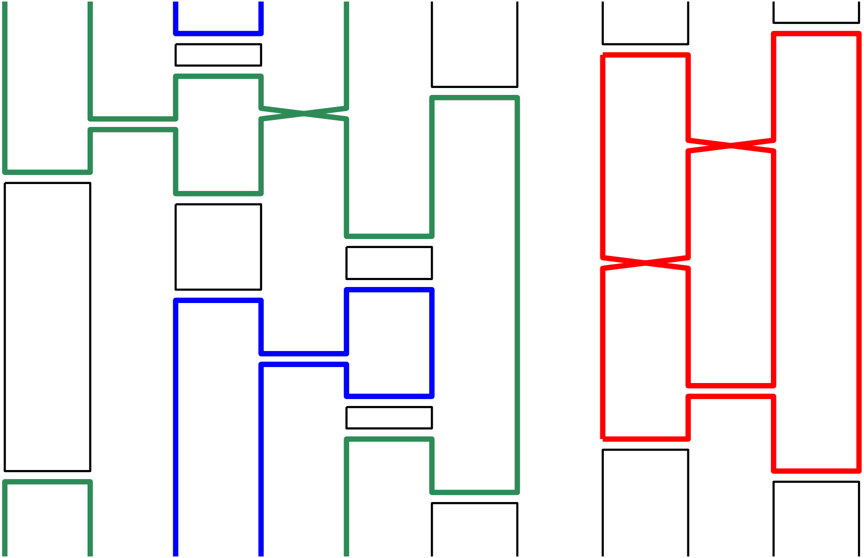
The trace of a product of T's and Q's at different nearest neighbor pairs is again easy to compute and the result has again a simple relationship to a space-time picture of loops:

$$Z(\beta, \ell, u) = \int_{\Omega_{\ell,\beta}} d\rho_u(\omega) n^{\mathcal{L}(\omega) - |\omega_{\between}|},$$

with

$$d\rho_u(\omega) = e^{(1+u)2\beta(2\ell-1)} u^{|\omega_{\asymp}|} dx^{\otimes|\omega|}.$$

Two important differences: (i) when $u < 0$ we now have a signed measure on the configuration of loops; (ii) the loops intersect and the time orientation of the lines is not ‘bipartite’. The latter reflects the presence of both ferro- and antiferromagnetic interactions.



Correlations

The basic correlation functions are integrals of indicator functions of 'events' for loop configurations.

$x \overset{+}{\longleftrightarrow} y$: the set of configurations ω where the top of $(x, 0)$ is connected to the bottom of $(y, 0)$;

$x \overset{-}{\longleftrightarrow} y$: the set of configurations ω where the top of $(x, 0)$ is connected to the top of $(y, 0)$

Proposition

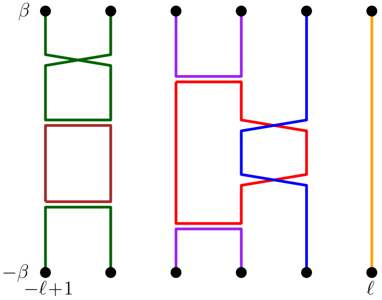
For the spin chain of length 2ℓ with interaction $h_{x,x+1} = -uT_{x,x+1} - Q_{x,x+1}$, we have:

(a) $Tr e^{-2\beta H_\ell} = e^{2\beta(1+u)(2\ell|-1)} Z(\beta, \ell, u)$.

(b) *For all $1 \leq \alpha < \alpha' \leq n$, we have*

$$Tr \;\; L_x^{\alpha,\alpha'} L_y^{\alpha,\alpha'} e^{-2\beta H_\ell}$$
$$= \tfrac{2}{n} e^{2\beta(1+u)(2\ell|-1)} \int_{\Omega_{\ell,\beta}} d\rho_u(\omega)\, n^{\mathcal{L}(\omega)-|\omega_{\boxminus}|} \left(\mathbb{1}[x \overset{-}{\longleftrightarrow} y] - \mathbb{1}[x \overset{+}{\longleftrightarrow} y]\right).$$

short loops, long loops, winding loops



- the winding loop are those that are not contractible (blue and orange)

- the long loops are those that are winding or visit 3 or more sites (red, blue, orange)

- short loops are those that are not long (green, brown, purple)

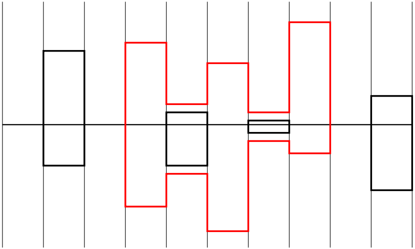
For large β, winding loops become negligible.

If there were only short loops, the measure would clearly be dominated by a perfectly dimerized state.

The challenge is to show that dimerization survives in spite of the non-vanishing contributions of long loops.

Contours

In the case $u = 0$, long loops can serve as contours separating one dimerized phase from the other:



The short loops outside and inside the contour are out of phase.
A Peierls argument using such contours was used to prove dimerization for $n \geq 17$ (N-Ueltschi, 2017).
Later, special properties of the random loop measure were used to prove dimerization for all $n \geq 3$ (Aizenman, Duminil-Copin, Warzel, 2020).

Clusters

For $u \neq 0$, configurations contain crosses ($\bowtie$), which may be crossings of different loops or self-crossings. Similarly, the top and bottom part of a double bar ($\vDash\!\dashv$), may belong to the same loop or to different loops. Since these distinction are non-local, we define clusters of long loops that share a $\bowtie$ or a $\vDash\!\dashv$.

As in the case $u = 0$, the short loops describe the reference dimerized states. A convergent cluster expansion of the partition function is the tool that allows us to prove that short loops dominate (for large n and small $|u|$).

Other spin chains

What if we kept the basis where the dominating term is $-P^{(0)}$ (the $SU(n)$ chain, the Temperley-Lieb chain)?
For odd n the the singlet state on which $P := P^{(0)}$ projects, and the model is unitarily equivalent, including the term $-uT$.
For even n, the singlet state is anti-symmetric. There is no translation invariant change of basis that will transform into something of the form Q we used so far, but there is an alternating one:

$$(\mathbb{1} \otimes V)P(\mathbb{1} \otimes V^*) = Q, \text{ and } (V \otimes \mathbb{1})P(V^* \otimes \mathbb{1}) = Q$$

with

$$V|\alpha\rangle = (-1)^{S-\alpha}|-\alpha\rangle.$$

Therefore the chains with interactions $uT + vP$ are unitarily equivalent to chains with interactions $u\tilde{T} + vQ$. It turns that $\tilde{T}$ satisfies

$$\tilde{T} = (\mathbb{1} \otimes V)T(\mathbb{1} \otimes V^*) = (\mathbb{1} \otimes V)(V^* \otimes \mathbb{1})T = -(V \otimes V)T.$$

In comparison to T, $\tilde{T}$ introduces additional signs associated with crosses in the definition of the measure.

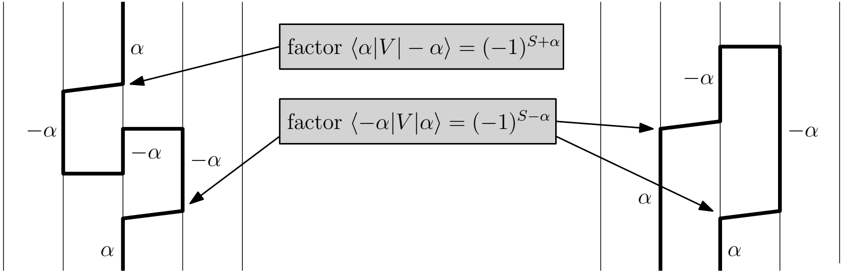


Figure: Left: the crosses are separated by an even number of double bars which yields the factor $(-1)^{S-\alpha}(-1)^{S+\alpha} = -1$. Right: the crosses are separated by an odd number of double bars which yields the factor 1.

This changes the measure and the ground states but, fortunately, no requires no change in the analysis to prove all the analogous results for this family of spin chains.

Does the story end here?