Two dimerized gapped ground state phases of O(n) spin chains?

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Main questions regarding gapped ground state phases

- 1. Existence of a gap for specific Hamiltonians.
- 2. Stability of the gap under perturbations (existence of a 'phase').
- 3. Classification of equivalence classes of gapped phases, for example, those defined by gapped curves of Hamiltonians (Chen-Gu-Wen 2011).

Outline

- 1. AKLT chain
- 2. Ground state phase diagram
- 3. O(n) spin chains
- 4. Answer the question of the title

Spin chains, Hamiltonians, ground states

Finite spin chain on $[a, b] \subset \mathbb{Z}$, Hilbert space $\mathcal{H}_{[a,b]} = \bigotimes_{x=a}^{b} \mathbb{C}^{n}$, $n \ge 2$, spins or qdits of dimension n = 2J + 1.

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: $h_{x,x+1} = \mathbf{S}_x \cdot \mathbf{S}_{x+1} = S_x^1 S_{x+1}^1 + S_x^2 S_{x+1}^2 + S_x^3 S_{x+1}^3$, where S_x^i , $i = 1, 2, 3, x \in [a, b]$, are *n*-dimensional spin matrices.

AKLT model, n = 3: $h_{x,x+1} = \frac{1}{2} \mathbf{S}_x \cdot \mathbf{S}_{x+1} + \frac{1}{6} (\mathbf{S}_x \cdot \mathbf{S}_{x+1})^2 + \frac{1}{3} \mathbb{1} = P_{x,x+1}^{(2)}$. Most general isotropic nearest neighbor interaction for n = 3: $h_{x,x+1} = \cos \phi \mathbf{S}_x \cdot \mathbf{S}_{x+1} + \sin \phi (\mathbf{S}_x \cdot \mathbf{S}_{x+1})^2$.



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

- ▶ φ = 0: Heisenberg antiferromagnet, Haldane phase (Haldane, 1983)
- ► tan φ = 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
- ▶ φ = −π/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.

The AKLT chain

The AKLT chain (Affleck-Kennedy-Lieb-Tasaki 1987-88) is the spin-1 chain with nearest neighbor interaction given by the projection onto the spin-2 states:

$$H_{[a,b]} = \sum_{x \in [a,b]} P_{x,x+1}^{(2)}, \quad P_{x,x+1}^{(2)} = \frac{1}{3}\mathbb{1} + \frac{1}{2}\mathbf{S}_x \cdot \mathbf{S}_{x+1} + \frac{1}{6}(\mathbf{S}_x \cdot \mathbf{S}_{x+1})^2.$$

 $[a,b] \in \mathbb{Z}$, $H_{[a,b]}$ is the Hamiltonian, acts on $\bigotimes_{x \in [a,b]} \mathbb{C}^3$, self-adjoint.

Ground state space is 4-dimensional and given by ker $H_{[a,b]}$, for all $b > a \in \mathbb{Z}$. AKLT proved that the infinite chain has a unque ground state with a spectral gap and exponential decay of correlations (Haldane's Conjecture).

- ▶ $\lim_{n} \langle \psi_n, A\psi_n \rangle = \omega(A)$, independent of the sequence of unit vectors $\psi_n \in \ker H_{[a_n, b_n]}$, $a_n \to -\infty$, $b_n \to \infty$.
- ► There exists $\gamma > 0$ such that spec ker $H_{[a,b]} \subset \{0\} \cup [\gamma,\infty)$, for all $b > a \in \mathbb{Z}$.

•
$$|\omega(A_x B_y)| \le 4 ||A_x|| ||B_y||_{\frac{1}{3}}^{|x-y|}$$

The exact ground state is a Matrix Product State (MPS) (Fannes-N-Werner 1989-1992).

AKLT settled Q1 (existence of the gap).

Q2 (stability) was first addressed by Yarotsky (2004), who proved that translation-invariant, finite-range perturbations of the AKLT chain do not close the gap for sufficiently small coupling constants.

$$H(s) = \sum_{x} P_{x,x+1}^{(2)} + s \sum_{X \subset \mathbb{Z}} \Phi(X).$$

 $\Phi(X) = \Phi(X)^*$ acts non-trivially only on spins at $x \in X \subset \mathbb{Z}$. Finite range $R: \Phi(X) = 0$ if diam X > R.

Other proofs and generalizations of stability for the AKLT chain by Michalakis-Zwolak 2013, Szehr-Wolf 2015, Moon-N 2018, Sims-N-Young 2021,

and for other models by Bravyi-Hastings-Michalakis 2010-11, Sims-N-Young 2018, De Roeck-Salmhofer 2019, Hastings 2019, Fröhlich-Pizzo 2018-2020, Del-Vecchio-Fröhlich-Pizzo-Rossi 2020-2022.

Q3 (classification of phases)

One can construct a C^1 -curve of projections P(s) such that $P(1) = P^{(2)}$ and the model with nn interaction P(0) has a unique product ground state (for the infinite chain) and prove a uniform positive lower bound for the gap for $s \in [0, 1]$ (Bachmann-N 2014).

This implies that the AKLT chain belongs to the same phase as the model with a unique product ground state (the trivial phase).

In contrast, if we one restricts to interpolations P(s) that respect spin rotation symmetry about 1 axis and an additional \mathbb{Z}_2 symmetry, an index argument shows that any curve connecting the AKLT model with a model in the trivial phase, must pass through a phase transition where the gap closes (Tasaki 2018, Ogata 2019-20).

This implies that the AKLT chain belongs to a SPT phase distinct from the trivial phase.

Gapped ground state phases

Gapped phase

Def: two interactions, Φ_0 and Φ_1 , with a (unique) gapped ground state belong to the same gapped phase if there exists a (piecewise) differentiable interpolation $[0,1] \ni s \mapsto \Phi_s$, that is uniformly gapped (Chen-Gu-Wen 2011).

Symmetry Protected / Enhanced gapped phase

Def: Given a symmetry G, defined as 'gapped phase' above, but with G-symmetric Φ_s , for all $s \in [0, 1]$ (Pollman-Turner-Berg-Oshikawa, 2010).

There are other definitions in the literature which, under suitable conditions, are equivalent to those above.

See From Lieb-Robinson bounds to automorphic equivalence, in Rupert L. Frank, Ari Laptev, Mathieu Lewin, and Robert Seiringer (eds), The Physics and Mathematics of Elliott Lieb, vol. 2, pp. 79–92, European Mathematical Society Press, 2022, arXiv:2205.10460.

O(n) chains and generalizations of the AKLT model

There is a local unitary change of basis in which the AKLT interaction is given by

$$P^{(2)} = rac{1}{2}(T - 2Q + 1),$$

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 $n \ge 2$, which was studied by Tu & Zhang, 2008.



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

- v = −2nu/(n − 2), n ≥ 3, Bethe ansatz point (Reshetikhin, 1983)
- ▶ v = -2u: frustration free point, equivalent to \bot 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, 2022).
- ▶ u = 0, v = -1. Equivalent to the $SU(n) P^{(0)}$ models aka Temperley-Lieb chain; Affleck, 1990, Nepomechie-Pimenta 2016). Dimerized for all $n \ge 3$ (Aizenman, Duminil-Copin, Warzel, 2020). Proof of some stability for large n(Björnberg-Mühlbacher-N-Ueltschi, 2021).

Two distinct gapped phases for all $n \ge 3$

- MPS/FF point
 - odd n: unique gapped ground state
 - even n: two 2-periodic gapped ground states
- South Pole: two dimerized gapped ground states for all $n \ge 3$.

All these MPS/FF gapped phase are fully stable (N-Sims-Young 2022). The dimerized phase (South Pole) is also expected to be fully stable under translation-invariant short-range perturbations, but only specific stability has been proved (Björnberg-Mühlbacher-N-Ueltschi 2021).

New results (N-Ragone, in prep)

- the MPS/FF point and the South Pole always belong to distinct phases.
- the two ground states for even n at the MPS/FF point have identical entanglement properties

Phase structure of the MPS states (N-Ragone, in prep) An equivalent parent Hamiltonian is given by

$$h=\frac{1}{2}(T+1)-Q,$$

which is the projection on the symmetric states in ker Q.

Case of odd *n*: up to a local unitary basis transformation this is the following SU(2)-invariant interaction for a spin-*J* chain with 2J + 1 = n:

$$h = P^{(2)} + P^{(4)} + \dots + P^{(2J)}.$$

These spin chains have a unique gapped ground state.

The case n = 3 is the well-known Haldane SPT phase with string order (den Nijs-Rommelse 1989), a hidden $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry (Kennedy-Tasaki 1992) and characterized by a non-trivial index Pollmann-Berg-Turner-Oshikawa 2012, Tasaki 2018, Ogata 2020.

Tu-Zhang 2008 found this model has a unique matrix product state ground state with several string order parameters and a hidden $(\mathbb{Z}_2 \times \mathbb{Z}_2)^J$ symmetry.

Clifford MPS (Tu-Zhang 2008, Fannes-N-Werner, 2010 unpub notes)

Case of odd *n*:

The unique MPS ground states is given by

$$\psi^{(\ell)}(B) = \sum_{i_1,\ldots,i_\ell=1}^n (\operatorname{Tr} B \gamma_{i_\ell} \cdots \gamma_{i_1}) | i_1 \ldots i_\ell \rangle.$$

where the γ_i are an irrep of the Clifford algebra:

$$\gamma_i\gamma_j+\gamma_j\gamma_i=2\delta_{ij}.$$

Up to unitary equivalence, there is a unique irrep given by *n* traceless Hermitian $2^{(n-1)/2} \times 2^{(n-1)/2}$ matrices.

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Case of even *n*:

The MPS ground states are also given by

$$\psi^{(\ell)}(B) = \sum_{i_1,\ldots,i_\ell=1}^n (\operatorname{Tr} B \gamma_{i_\ell} \cdots \gamma_{i_1}) | i_1 \ldots i_\ell \rangle.$$

where the γ_i are an irrep of the Clifford algebra:

$$\gamma_i \gamma_j + \gamma_j \gamma_i = 2\delta_{ij}.$$

Again, there is a unique irrep, now given by $2^{n/2} \times 2^{n/2}$ matrices. In contrast to the odd *n* case, the transfer matrix

$$\mathbb{E}(B) := \sum_{i=1}^n \gamma_i B \gamma_i$$

has an eigenvalue -1, and two projections $P_\pm\in M_{2^{n/2}}$ such that $P_++P_-=1\!\!1$, and

$$\mathbb{E}(P_{\pm})=P_{\mp}.$$

This implies the existence of two 2-periodic gapped ground states.

Entanglement structures

For the infinite chain we have two pure ground states ω_+ and $\omega_-,$ in FCS form given by

$$\omega_{\pm}(A_1 \otimes \cdots \otimes A_{\ell}) = \frac{2}{n} \operatorname{Tr} \mathbb{E}_{A_1} \circ \mathbb{E}_{A_2} \circ \mathbb{E}_{A_3} \circ \cdots \circ \mathbb{E}_{A_{\ell-1}} \circ \mathbb{E}_{A_{\ell}}(P_{\pm}).$$

where, for $A \in M_n$, $\mathbb{E}_A(B) = \sum_{ij} A_{ij}\gamma_i B\gamma_j$. ω_+ and ω_- are selected by different b.c.. Define automorphisms α on $M_{2^{n/2}}$, and σ on M_n by

$$\alpha(B) = \gamma_1 B \gamma_1, \quad \sigma(A) = RAR,$$

with

$$R = \begin{pmatrix} -1 & & & \\ & 1 & & \\ & & \ddots & \\ & & & 1 \end{pmatrix}.$$

Then

$$\alpha(\mathbb{E}_{A}(B)) = \mathbb{E}_{\sigma(A)}(\alpha(B)), \quad \alpha(P_{+}) = P_{-}.$$

One finds two MPS states with primitive transfer matrices by defining $\mathbb{F}_{A}^{(i)}: P_{+}M_{2^{n/2}}P_{+} \to P_{+}M_{2^{n/2}}P_{+}$, i = 1, 2, as follows:

$$\mathbb{F}_{A}^{(1)} = \alpha \circ \mathbb{E}_{\sigma(A)}, \quad \mathbb{F}_{A}^{(2)} = \alpha \circ \mathbb{E}_{A}.$$

In terms of these, we have

$$\begin{split} \omega_+(A_1\otimes\cdots\otimes A_\ell) &= \frac{2}{n}\mathrm{Tr}\mathbb{F}_{A_1}^{(2)}\circ\mathbb{F}_{A_2}^{(1)}\circ\mathbb{F}_{A_3}^{(2)}\circ\cdots\circ\mathbb{F}_{A_{\ell-1}}^{(2)}\circ\mathbb{F}_{A_\ell}^{(1)}(P_+)\\ \omega_-(A_1\otimes\cdots\otimes A_\ell) &= \frac{2}{n}\mathrm{Tr}\mathbb{F}_{A_1}^{(1)}\circ\mathbb{F}_{A_2}^{(2)}\circ\mathbb{F}_{A_3}^{(1)}\circ\cdots\circ\mathbb{F}_{A_{\ell-1}}^{(1)}\circ\mathbb{F}_{A_\ell}^{(2)}(P_+). \end{split}$$

This shows ω_+ and ω_- are translates of each other. But also

$$\omega_+(A_1\otimes\cdots\otimes A_\ell)=\omega_-(\sigma(A_1)\otimes\cdots\otimes\sigma(A_\ell)).$$

Hence, ω_+ and ω_- are related by a local unitary transformation and have the same entanglement.

The two-fold degeneracy of the ground state turns out to be breaking of this local symmetry of the Hamiltonian, $R \in O(n)$. Since the O(n) symmetry is fully preserved in the dimerized ground state of the South Pole model, this suffices to show that the two 2-periodic phases are distinct (N-Sims-Young 2022).

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Properties of the South Pole phase

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 $\psi = n^{-1/2} \sum_{\alpha=1}^{n} |\alpha, \alpha\rangle$. South Pole means u = 0, v = -1.

Finite chains of 2ℓ spins, with Hamiltonian: $H_{\ell} = \sum_{x=-\ell+1}^{\ell-1} h_{x,x+1}$. Consider ground states as limits of Gibbs states:

$$\langle A \rangle_{\ell,\beta,u} = rac{\operatorname{Tr} A e^{-\beta H_{\ell}}}{\operatorname{Tr} e^{-\beta H_{\ell}}}.$$

Basic observables: generators of O(n):

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

Theorem (Dimerization, Björnberg-Mühlbacher-N-Ueltschi 2021) There exist constants n_0 , u_0 , c > 0 (independent of ℓ) such that for $n > n_0$, v = -1, and $|u| < u_0$, we have that for all $1 \le \alpha < \alpha' \le n$,

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

Theorem (Exponential decay of correlations, Björnberg-Mühlbacher-N-Ueltschi 2021)

There exist constants n_0 , u_0 , c_1 , c_2 , C > 0 (independent of ℓ) such that for $n > n_0$, v = -1, and $|u| < u_0$, we have

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

for all $\ell \in \mathbb{N}$, all $x, y \in \{-\ell + 1, \dots, \ell\}$, all $1 \le \alpha < \alpha' \le n$, 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 is there is a positive lower bound independent of ℓ ?

Theorem (Spectral gap, Björnberg-Mühlbacher-N-Ueltschi 2021) There exist constants $n_0, u_0, c > 0$ (independent of ℓ) such that for $n > n_0, v = -1$, and $|u| < u_0$, we have (a) $E_0^{(\ell)}$ is non-degenerate. (b) $\Delta^{(\ell)} \ge c$ for all ℓ .

These results are proved using a 'random' loop representation of the partition function and the Gibbs states (Toth 1993, Aizenman-N 1994, Ueltschi 2013).

Some corollaries of the previous results and the random loop representation:

Consider the case (u, v) = (0, -1), and 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 turn out to be simple. Then

$$|\psi_{\ell}\rangle\langle\psi_{\ell}| = \lim_{eta
ightarrow\infty}rac{e^{-2eta H_{\ell}}}{\mathsf{Tr}e^{-2eta H_{\ell}}},$$

and therefore, with $A = L_0^{\alpha, \alpha'} L_1^{\alpha, \alpha'}$, or $Q_{x, x+1}$, or any other observable,

$$\langle \psi_{\ell}, A\psi_{\ell} \rangle = \mathsf{Tr}[|\psi_{\ell}\rangle\langle\psi_{\ell}|A] = \lim_{\beta \to \infty} \frac{\mathsf{Tr}e^{-\beta H_{\ell}}Ae^{-\beta H_{\ell}}}{\mathsf{Tr}e^{-2\beta H_{\ell}}}$$

One can define weak limits over even and odd (sub-)sequences of ℓ :

$$\omega_{e}(A) = \lim_{\ell, \text{even}} \langle \psi_{\ell}, A\psi_{\ell} \rangle, \quad \omega_{o}(A) = \lim_{\ell, \text{odd}} \langle \psi_{\ell}, A\psi_{\ell} \rangle.$$

 ω_o and ω_e are the pure ground states with dimerization. For example:

$$\omega_o(\mathcal{Q}_{0,1}) > \omega_e(\mathcal{Q}_{0,1})$$

and for any observable A:

 $\omega_o(A) = \omega_e(\tau(A)) = \omega_o(\tau^2(A)), \tau$ is translation by one site.



Both states are O(n) invariant.

Conclusion

At and near the South Pole we have:

- ω_e and ω_o have full O(n) invariance.
- ω_e and ω_o are 2-period, distinct, and translates of each other.
- ω_e and ω_o are dimerized: 2-periodic nearest neighbor entanglement.

In contrast, at and near the MPS/FF point, for even n, we have a 2-periodic phase with

- ▶ In ω_+ and ω_- the O(n) symmetry is broken down to SO(n).
- $\blacktriangleright \ \omega_e$ and ω_o are 2-periodic, distinct, and are translates of each other.
- ω_e and ω_o have translation invariant nearest neighbor entanglement; not dimerized.

Of the two 2-periodic gapped phases only the South Pole phase is dimerized. Of course, but there may well be other dimerized phases...