Lowest-energy states in $SO(N)$ spin chain

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Motivation

Spin and fermion systems with higher symmetries attract much attention due to

- Experiments in ultracold atoms;
- Hidden antiferromagnetic order characterized by a nonlocal string order parameter;
- Use for the classification of symmetry protected topological phases and study of the entanglement spectrum;
- Application in spin ladder systems.

Some results on nongenenerацy and quantum numbers of relative ground states of finite-size quantum antiferromagnets:

- For spin system on a bipartite lattice, the lowest-energy multiplet among spin-S states is nondegenerate [Lieb, Mattis (1962)].
- For open $SU(N)$ chain, the lowest-energy multiplet among all $SU(N)$-equivalent states is nondegenerate [T.H. (2004) (2010)].

Problem:

- What can be set for $SO(N)$ chains?

$SO(N)$ symmetric chain

The Hamiltonian of the $SO(N)$ open spin chain in vector representation:

$$\mathcal{H} = \sum_l \big(J_l\, \boldsymbol{L}_{l+1} \cdot \boldsymbol{L}_l + K'_l(\boldsymbol{L}_{l+1} \cdot \boldsymbol{L}_l)^2\big),$$

The local interactions

$$\boldsymbol{L}_i \cdot \boldsymbol{L}_j = \sum_{a<b} L_i^{ab} L_j^{ab}, \qquad a, b = 1, \ldots, N$$

are expressed via on-site $SO(N)$ rotation generators

$$L_l^{ab} = i(T_l^{ab} - T_l^{ba}), \qquad T^{ab} = |a\rangle\langle b|.$$

The range of couplings is:

$$0 < K'_l < \frac{1}{N-2} J_l.$$

Previous studies

The region includes some special points considered before. In particular, it contain:

- The integrable translationally invariant model [Reshetikhin (1985)], which generalized Babujian-Takhtajan spin-1 integrable chain at
$$K' = \frac{N-4}{(N-2)^2} J.$$
- The model with exact VBS ground state [Tu, Zhang, Xiang (2008)], [Tu, Zhang, Xiang, Liu, Ng (2009)] at
$$K' = \frac{1}{N} J.$$
- The $SU(N)$-invariant spin chain [Affleck, Lieb (1986); T.H. (2004)]
$$K'_l = \frac{1}{N-2} J_l : \qquad \mathcal{H} = \sum_{l,a,b} J_l T^{ab}_{l+1} T^{ba}_l .$$

The low-energy effective field theory has been studied [Tu, Ors, PRL (2011)].

Enhancing the symmetry from $SO(N)$ to $O(N)$

The Hamiltonina does not preserve the total number of each species,

$$[\mathcal{H}, \hat{N}_a] \neq 0 : \qquad \hat{N}_a = \sum_l T_l^{aa},$$

but preserves the parity

$$\hat{\sigma}_a = (-1)^{\hat{N}_a} : \qquad [\mathcal{H}, \hat{\sigma}_a] = 0.$$

The reflections $\hat{\sigma}_a$ expand $SO(N)$ symmetry of the Hamiltonian to $O(N)$ including improper rotations.

Evidently, $\sum_a N_a = L$. So, the parities are subjected to the rule

$$\sigma_1 \sigma_2 \ldots \sigma_N = (-1)^L.$$

This restricts the number of independent parities to $N-1$, giving rise to the group

$$G = Z_2^{\times(N-1)}.$$

Structure of $G = Z_2^{\times(N-1)}$ group

Focus on chains with even number of sites L. Then

$$\sigma_1 \dots \sigma_N = 1 \qquad \text{and} \qquad G = Z_2^{\times(N-1)} = \frac{Z_2^{\times N}}{Z_2}$$

with Z_2 in the denominator generated by $\hat{\sigma}_1 \dots \hat{\sigma}_N$.

- In case of $SO(2n+1)$ symmetry, G is generated by π-rotations of (a,b) planes

$$\hat{\sigma}_a \hat{\sigma}_b.$$

- For example, π-rotations in $N = 3$ case are

$$\hat{\sigma}_1 = \hat{\sigma}_2\hat{\sigma}_3, \qquad \hat{\sigma}_2 = \hat{\sigma}_3\hat{\sigma}_1, \qquad \hat{\sigma}_3 = \hat{\sigma}_1\hat{\sigma}_2.$$

- For $SO(2n)$ chains, the π-rotations form the subgroup $G_\pi = Z_2^{\times(N-2)}$. A single Z_2 reflection (for instance, $\hat{\sigma}_1$) complements it to G group.

For $SO(2n+1)$ chains with even number of sites L, the generators of reflection (G) and π-rotation (G_π) groups differ by sign. In $SO(3)$ case,

$$\hat{\sigma}_1 = -\hat{\sigma}_2\hat{\sigma}_3, \qquad \text{etc.}$$

σ-subspaces and N_--subspaces

- $G = Z_2^{\times(N-1)}$ symmetry splits the space of states into 2^{N-1} invariant σ-subspaces, parameterised by reflection quantum numbers (parities) $\sigma_a = \pm 1$:

$$V^L_{\sigma_1 \dots \sigma_N} = \{\psi \,|\, \hat{\sigma}_a \psi = \sigma_a \psi\}.$$

- Permutation symmetry maps between σ-subspaces with N_- negative parities ($\sigma_i = -1$)

$$s\hat{\sigma}_a s^{-1} = \hat{\sigma}_{s(a)}, \qquad sV^L_{\sigma_1 \dots \sigma_N} = V^L_{\sigma_{s(1)} \dots \sigma_{s(N)}}, \qquad s \in \mathcal{S}_N \subset O(N)$$

- All such σ-subspaces have the same spectrum and form the $\binom{N}{N_-}$-fold degenerate N_--subspace:

$$V^L_{N_-} = V^L_{\underbrace{- \dots -}_{N_-}\underbrace{+ \dots +}_{N_+}} \oplus V^L_{\underbrace{- \dots -}_{N_- -1}+-\underbrace{+ \dots +}_{N_+ -1}} \oplus \dots\dots \oplus V^L_{\underbrace{+ \dots +}_{N_+}\underbrace{- \dots -}_{N_-}}$$

- V^L_0 and V^L_N are nondegenerate.

Decomposition into N_- subspaces

The total space of states V^L splits into degenerate N_--subspaces $V^L_{N_-}$ with even/odd dependence on the spin rank N and chain length L.

For sufficiently long chains, $L \geq N$,

$$V^L = \begin{cases} V^L_N \oplus V^L_{N-2} \oplus \ldots \oplus V^L_0 & \text{even } N, \text{ even } L, \\ V^L_N \oplus V^L_{N-2} \oplus \ldots \oplus V^L_1 & \text{odd } N, \text{ odd } L, \\ V^L_{N-1} \oplus V^L_{N-3} \oplus \ldots \oplus V^L_1 & \text{even } N, \text{ odd } L, \\ V^L_{N-1} \oplus V^L_{N-3} \oplus \ldots \oplus V^L_0 & \text{odd } N, \text{ even } L. \end{cases}$$

Rule: The parities of N_- and L must coincide.

Main result

The lowest energy level in σ-subspace $V^L_{\sigma_1 \dots \sigma_N}$ is nondegenerate. It is a component of N_--th order antisymmetric $O(N)$ tensor, described by one-column Young tableau $\mathbb{Y}_{N_-} = \mathbb{Y}[\underbrace{1, 1, \dots, 1}_{N_-}]$.

Its components belong to the equivalent σ-subspaces so that:

The lowest-level states in the subspace $V^L_{N_-}$ form a unique $O(N)$ tensor $\mathbb{Y}_{N_-}$ It gathers the relative ground states of all σ-subspaces.

As a consequence, for the ground state we have:

The total ground state may be, at most, 2^{N-1}-fold degenerate combining the lowest-level $\mathbb{Y}_{N_-}$-multiplets from N_--subspaces.

Tensors and pseudotensors in the lowest states

The conjugate $SO(N)$ multiplets are distinguished by the sign under improper rotations, which maps tensor to pseudotensor. Therefore:

- The lowest state in the subspace V_0^L is a scalar $\mathbb{Y}_0$ while in the subspace in V_N^L it is a pseudoscalar $\mathbb{Y}_N \sim \mathbb{Y}'_0$.
- The lowest level state in V_1^L is a vector $\mathbb{Y}_1$, and in V_{N-1}^L it is a pseudovector $\mathbb{Y}_{N-1} \sim \mathbb{Y}'_1$, etc.

The distribution on k of the lowest-level multiplets $\mathbb{Y}_k$ in V_k^L depends sharply on parity of N:

- N is odd: the tensors and pseudotensors alternate each other with the growth of k:

$$\mathbb{Y}_0, \mathbb{Y}'_1, \mathbb{Y}_2, \mathbb{Y}'_3, \ldots .$$

- N is even: the tensors and pseudotensors appear together:

$$\mathbb{Y}_0, \mathbb{Y}'_0, \mathbb{Y}_2, \mathbb{Y}'_2, \ldots .$$

  The self-conjugate representation $\mathbb{Y}_{N/2}$ emerges only once for N being a multiple of 4.

Simplest example: $SO(3)$ chain

Consider the $N = 3$ case of $SO(3)$ chain

$$\mathcal{H} = \sum_l \left(J_l\, \boldsymbol{S}_{l+1} \cdot \boldsymbol{S}_l + K_l' (\boldsymbol{S}_{l+1} \cdot \boldsymbol{S}_l)^2 \right).$$

The σ-subspaces are unified into four degenerate subspaces,

even L: $\quad V_0^L = V_{+++}^L, \quad V_2^L = V_{+--}^L \oplus V_{-+-}^L \oplus V_{--+}^L, \quad V^L = V_0^L \oplus V_2^L,$

odd L: $\quad V_3^L = V_{---}^L, \quad V_1^L = V_{++-}^L \oplus V_{+-+}^L \oplus V_{-++}^L, \quad V^L = V_1^L \oplus V_3^L$

The lowest state is:

$$\text{singlet} = \begin{cases} \text{scalar in } V_0^L, \\ \text{pseudoscalar in } V_3^L, \end{cases} \qquad \text{triplet} = \begin{cases} \text{vector in } V_1^L, \\ \text{pseudovector in } V_2^L. \end{cases}$$

The total ground state is either a unique spin-singlet for $K_l' \leq 0$, [Murno, PRB (1976)], a unique spin-triplet, or their superposition at the AKLT point $K_l' = \frac{1}{3} J_l$ [Affleck, Kennedy, Lieb, Tasaki, PRL (1987)]. So, it may be at most fourfold degenerate [Kennedy, JPC (1990)].

Exact valence-bond solid (VBS) point

The $SO(N)$ open chain has an exact 2^{N-1}-fold degenerate valence-bond solid (VBS) ground state [Tu, Zhang, Xiang, PRB (2008); Tu, *et al.*, PRB (2009)] at

$$K'_l = \frac{1}{N} J_l.$$

In the matrix product form,

$$\Omega_{\alpha\beta} \sim \sum_{a_1, a_2, \ldots, a_L} (\Gamma^{a_1} \Gamma^{a_2} \ldots \Gamma^{a_L})_{\alpha\beta} |a_1 a_2 \ldots a_L\rangle,$$

$$1 \leq a_i \leq N, \qquad 1 \leq \alpha, \beta \leq 2^n, \qquad n = [\tfrac{N}{2}],$$

where $\Gamma^a = \Gamma^a_{\alpha\beta}$ are Dirac matrices defining $SO(N)$ spinor representation Δ:

$$L^{ab} = -\frac{i}{2}[\Gamma^a, \Gamma^b], \qquad \{\Gamma^a, \Gamma^b\} = 2\delta_{ab}.$$

Then $\Omega_{\alpha\beta}$ belongs to $\Delta \otimes \Delta^*$ since under finite rotations,

$$\mathbf{\Omega} \to U \mathbf{\Omega} U^+, \qquad U = \exp\left(\frac{i\omega_{ab}}{2} L_{ab}\right).$$

The Clebsch-Gordan decomposition depends on whether N is even or odd.

VBS degenerate ground state for $N = 2n$

For $O(2n)$, the Clebsch-Gordan decomposition is [Brauer, Weyl (1935)]:

$$\Delta \otimes \Delta^* = \bigoplus_{k=0}^{N} \mathbb{Y}_k = \bigoplus_{k=0}^{n-1} (\mathbb{Y}_k \oplus \mathbb{Y}'_k) \oplus \mathbb{Y}_n .$$

- $\hat{\sigma}_a = \Gamma^a \Gamma^0, \qquad \Gamma^0 \sim \Gamma^1 \Gamma^2 \dots \Gamma^N, \qquad \{\Gamma^0, \Gamma^a\} = 0.$
- The 2^{N-1}-fold degenerate ground state $\mathbf{\Omega}$ is split into antisymmetric tensors

  $$\Omega_{\mathbb{Y}_k}^{b_1 \dots b_k} = \mathrm{Tr}(\mathbf{\Omega} \Gamma^{[b_1} \dots \Gamma^{b_k]}), \qquad \Omega_{\mathbb{Y}'_k}^{b_1 \dots b_k} = \mathrm{Tr}(\mathbf{\Omega} \Gamma^0 \Gamma^{[b_1} \dots \Gamma^{b_k]})$$

  as follows:

  $$\mathbf{\Omega} = \begin{cases} \bigoplus_{i=0}^{n} \mathbf{\Omega}_{\mathbb{Y}_{2i}} = \mathbf{\Omega}_{\mathbb{Y}_0} \oplus \mathbf{\Omega}_{\mathbb{Y}'_0} \oplus \mathbf{\Omega}_{\mathbb{Y}_2} \oplus \mathbf{\Omega}_{\mathbb{Y}'_2} \oplus \dots : & \text{even } L \\ \bigoplus_{i=1}^{n} \mathbf{\Omega}_{\mathbb{Y}_{2i-1}} = \mathbf{\Omega}_{\mathbb{Y}_1} \oplus \mathbf{\Omega}_{\mathbb{Y}'_1} \oplus \mathbf{\Omega}_{\mathbb{Y}_3} \oplus \mathbf{\Omega}_{\mathbb{Y}'_3} \oplus \dots : & \text{odd } L \end{cases}$$

- π-rotation symmetry $= Z_2^{\times(N-2)}$ is broken partially,
  reflection symmetry $= Z_2^{\times(N-1)}$ is broken completely.

VBS degenerate ground state for $N = 2n + 1$

For $O(2n+1)$, the Clebsch-Gordan decomposition is [Brauer, Weyl (1935)]:

$$\Delta \otimes \Delta^* = \bigoplus_{i=0}^{n} \mathbb{Y}_{2i} = \mathbb{Y}_0 \oplus \mathbb{Y}'_1 \oplus \mathbb{Y}_2 \oplus \mathbb{Y}'_3 \oplus \ldots,$$

- $[\Gamma^0, \Gamma^a] = 0: \qquad \Gamma^0 = \text{const.}$
- We have alternate tesor-pseudotensor decomposition of 2^{N-1}-fold degenerate ground state:

$$\mathbf{\Omega} = \begin{cases} \bigoplus_{i=0}^{n} \mathbf{\Omega}_{\mathbb{Y}_{2i}} = \mathbf{\Omega}_{\mathbb{Y}_0} \oplus \mathbf{\Omega}_{\mathbb{Y}'_1} \oplus \mathbf{\Omega}_{\mathbb{Y}_3} \oplus \ldots : & \text{even } L, \\ \bigoplus_{i=0}^{n} \mathbf{\Omega}_{\mathbb{Y}'_{2i}} = \mathbf{\Omega}_{\mathbb{Y}'_0} \oplus \mathbf{\Omega}_{\mathbb{Y}_1} \oplus \mathbf{\Omega}_{\mathbb{Y}'_3} \oplus \ldots : & \text{odd } L. \end{cases}$$

- π-rotation symmetry = reflection symmetry = $Z_2^{\times(N-1)}$: are broken completely.

Sketch of proof: Nonpositive basis

Here off-diagonal elements of Hamiltonian are nonpositive: $\langle a|\mathcal{H}|b\rangle \leq 0$ if $a \neq b$.

- Nonpositivity implies the nondegeneracy of the lowest-energy levels [Marshall (1955)], [Lieb & Mattis (1962)].
- Such basis has no minus sign problem and can be used for Monte Carlo simulations.

The $SU(N)$ and $SO(N)$ chains have the same nonpositive basis. It equips the Ising basis with the sign factor

$$\overline{|a_1 \dots a_L\rangle} = \theta_{a_1 \dots a_L} |a_1 \dots a_L\rangle,$$

which counts the number of all inversely ordered pairs of flavors and returns its parity [Affleck & Lieb (1986)]:

$$\theta_{a_1 \dots a_L} = (-1)^{\{\#(i<j)|a_i>a_j\}}.$$

Properties of θ:

$$\theta_{\dots ab \dots} = -\theta_{\dots ba \dots} \qquad \text{[Hakobyan, NPB (2004)]},$$
$$\theta_{\dots aa \dots} = \theta_{\dots bb \dots} \qquad \text{[Okunishi \& Harada, PRB (2014)]}.$$

Sketch of proof: Hamiltonian is connected in σ-subspaces

The matrix of Hamiltonian $\mathcal{H}$ is connected in $V^L_{\sigma_1 \ldots \sigma_N}$, i.e. any $|n\rangle$ and $|m\rangle$ are connected by a chain of states so that

$$\langle n|\mathcal{H}|k_1\rangle\langle k_1|\mathcal{H}|k_2\rangle\langle k_2|\mathcal{H}|k_3\rangle \ldots \langle k_r|\mathcal{H}|m\rangle \neq 0.$$

This can be shown by following steps:

1. Set the spins in nondecreasing order by local $SU(N)$ exchange: $|\ldots ba \ldots\rangle \to |\ldots ab \ldots\rangle$ with $a < b$.
2. Replace a pair aa by 11 using the local $SO(N)$ exchange: $|\ldots aa \ldots\rangle \to |\ldots 11 \ldots\rangle$.
3. In this way $\mathcal{H}$ connects any state in $V^L_{\sigma_1 \ldots \sigma_N}$ to the state

$$|a_1^- \ldots a_{N_-}^- \underbrace{1 \ldots 1}_{L-N_-}\rangle, \qquad a_1^- < \cdots < a_{N_-}^- .$$

Sketch of proof: The lowest state

As a result:

- The lowest-energy state in σ-subspace is nondegenerate (Perron-Frobenius theorem),

$$\Omega_{\sigma_1\ldots\sigma_N} = \sum_{(-1)^{N_{a_i}}=\sigma_{a_i}} \omega_{a_1\ldots a_L} \overline{|a_1\ldots a_L\rangle}, \qquad \omega_{a_1\ldots a_L} > 0.$$

- It has a nonzero overlap with trial state, $\langle\Psi|\mathcal{H}|\Omega\rangle \neq 0$:

$$\Psi = \sum_{s\in\mathcal{S}_{N_-}} \epsilon_{s_1\ldots s_{N_-}} |a^-_{s_1}\ldots a^-_{s_{N_-}}\rangle \otimes \psi \otimes \cdots \otimes \psi, \qquad \psi = \sum_b |bb\rangle$$

- So, both states Ψ and Ω are in the same $O(N)$ multiplet.

Summary

We expanded the symmetry of the open finite-size $SO(N)$ symmetric spin chain to $O(N)$.

1. We partitioned its space of states into the eigenspaces of the parity transformations in spin space, generating the subgroup $G = Z_2^{\times(N-1)}$.
2. It is proven that the lowest-energy states in these eigenspaces are nondegenerate and assemble in antisymmetric tensors or pseudotensors.
3. At the valence-bond-solid point, they constitute the 2^{N-1}-fold degenerate ground state with fully broken by the G-symmetry.