Spin Gap in Chains with Hidden Symmetries

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We investigate the formation of spin gap in one-dimensional models characterized by the groups with hidden dynamical symmetries. A family of two-parametric models of isotropic and anisotropic Spin-Rotator Chains characterized by SU(2) × SU(2) and SO(2) × SO(2) × Z2 × Z2 symmetries is introduced to describe the transition from SU(2) to SO(4) antiferromagnetic Heisenberg chain. The excitation spectrum is studied with the use of the Jordan-Wigner transformation generalized for αl algebra and by means of bosonization approach. Hidden discrete symmetries associated with invariance under various particle-hole transformations are discussed. We show that the spin gap in SRC Hamiltonians is characterized by the scaling dimension 2/3 in contrast to dimension 1 in conventional Haldane problem.

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More than 20 years ago Haldane made a conjecture that the properties of spin S Heisenberg antiferromagnetic (AF) chains are different for integer and half-integer spins. Namely, the excitations in the Heisenberg AF chains with half-integer spins are gapless, whereas for integer spins there is a gap in the spectrum (Haldane gap). While the first part of Haldane conjecture has been proven long time ago (see [2, 3]), the second part, although being confirmed by many numerical studies and experimental studies and tested by some approximate analytical calculations [3, 17], remains a hypothesis. The problem of SU(2) Heisenberg chains has been attacked by the modern tools as e.g. bosonization (see also book [11]), various numerical methods [4, 12, 13] and recently proposed fermionization by means of Jordan-Wigner transformation for higher spins [14]. However, the main focus of interests has been put either on SU(2) symmetry or on N-leg antiferromagnetic Heisenberg chain. This family includes conventional two-leg ladder models and several models intermediate between the ladder chain and the AF interaction J∥ along the leg (Fig. 1). The model Hamiltonian is

\[ H = J∥ \sum_i \tilde{s}_{1,i} \tilde{s}_{1,i+1} - J_\perp \sum_i \tilde{s}_{1,i} \tilde{s}_{2,i}. \]

This model is a natural extension of the S = 1 chain model to a case where the states on a given rung form a triplet/singlet pair. We call the chain shown in Fig. 1 the Spin Rotator Chain (SRC) (in contrast to the spin rotor model [10]). Unlike earlier attempts to construct the representation of S = 1 state out of s = 1/2 ingredients [5, 8], we respect in this case the SO(4) symmetry of spin manifold on each rung [10]. As a result, the singlet state cannot be projected out. Moreover, it plays integral part in formation of the spin gap. We show that the hidden Z2 symmetries in this model are the intrinsic property of the local SO(4) group of spin rotator on the rung, and the symmetry breaking due to nonlocal (string) effects results in spin gap formation. These special symmetries distinguish our model from N ≥ 2-leg ladder models and SU(2) chains. In particular we show also that the scaling dimension of a spin gap in SRC differs from that in 2-leg ladder.

New variables on a rung are introduced to keep track on S = 1 properties. We define \( \tilde{S}_i = \tilde{s}_{1,i} + \tilde{s}_{2,i} \), \( \tilde{R}_i = \tilde{s}_{1,i} - \tilde{s}_{2,i} \), where \( \tilde{S}_i \) stands for a triplet S = 1 ground state and singlet S = 0 excited state. The operator \( \tilde{R} \) describes dynamical triplet/singlet mixing [17, 13]. Then

\[ H = \frac{J∥}{4} \sum_i \left[ \tilde{S}_i \tilde{S}_{i+1} + \tilde{S}_i \tilde{R}_{i+1} + (\tilde{S} \leftrightarrow \tilde{R}) \right] - \frac{J_\perp}{4} \sum_i \left( \tilde{S}_i^2 - \tilde{R}_i^2 \right), \]

FIG. 1: Spin Rotator Chain.
where the set of operators $\vec{S}_i, \vec{R}_i$ fully defines the $o_4$ algebra in accordance with the commutation relations

\[
[S^\alpha_i, S^\beta_j] = i\delta_{ij}\epsilon_{\alpha\beta\gamma}S^\gamma_i, \quad [R^\alpha_i, R^\beta_j] = i\delta_{ij}\epsilon_{\alpha\beta\gamma}R^\gamma_i,
\]

\[
[R^\alpha_i, S^\beta_j] = i\delta_{ij}\epsilon_{\alpha\beta\gamma}R^\gamma_i,
\]

where $\epsilon_{\alpha\beta\gamma}$ is the totally antisymmetric Levi-Civita tensor and Casimir constraints on each sites are given by

\[
(\vec{S}_i)^2 + (\vec{R}_i)^2 = 3, \quad (\vec{S}_i \cdot \vec{R}_i) = 0.
\]

In order to characterize low-lying excitations in SRC we propose a fermionization procedure, which extends Jordan-Wigner (JW) transformation to SO(4) group, and a bosonization formalism based on this procedure. Our method incorporates JW transformation for $S = 1$ proposed by Batista and Ortiz (BO) in \[14\]. The BO representation is however redundant and requires a constraint overlooked in \[14\]. The relationships between SO(4) JW representation and BO representation is discussed below in some detail.

We begin with a single-rung dimer problem. A two-component fermion $(a^\dagger b^\dagger)$ basis representing $\vec{S}$-operators is introduced as follows $(S^\pm = S^x \pm iS^y)$

\[
S^+ = a^\dagger + e^{i\pi a^\dagger}a^\dagger, \quad S^- = a + be^{-i\pi a^\dagger}a, \quad S^z = a^\dagger a + b^\dagger b - 1.
\]

The complementary representation for $\vec{R}$ generators is

\[
R^+ = a^\dagger - e^{-i\pi a^\dagger}a^\dagger, \quad R^- = a - be^{i\pi a^\dagger}a, \quad R^z = a^\dagger a - b^\dagger b.
\]

This representation satisfies commutation relations \[11\] for the SO(4) group and preserves Casimir operators \[11\]. The advantage of two-fermion formalism in comparison with two independent JW transformations for each $s = 1/2$ is that the latter requires an additional Majorana fermion to provide commutation of two spins on the same rung. Two-component spinless fermions may be combined into one spin fermion, which is most conveniently done by the definition

\[
f_\uparrow = (a - b)/\sqrt{2}, \quad f_\downarrow = (a + b)/\sqrt{2}.
\]

In order to generalize one-rung representation for a linear chain of rungs we introduce a "string" operator $K_j$

\[
K_j = \exp[i\pi \sum_{k<j} n_{sk}] = \prod_{k<j} (1 - 2n_{\uparrow k})(1 - 2n_{\downarrow k}),
\]

\[
(n_{\sigma} = f_\sigma^\dagger f_\sigma).
\]

As a result of JW transformation the SO(4) generators acquire the following form

\[
S^+_j = \sqrt{2} \left( f_\uparrow^\dagger (1 - n_{\uparrow j})K_j + K_j^\dagger f_\downarrow^\dagger (1 - n_{\downarrow j}) \right),
\]

\[
S^-_j = (S^+_j)^\dagger, \quad S^z_j = n_{\uparrow j} - n_{\downarrow j},
\]

\[
R^+_j = \sqrt{2} \left( f_\uparrow^\dagger n_{\uparrow j}K_j + K_j^\dagger f_\downarrow^\dagger n_{\downarrow j} \right),
\]

\[
R^-_j = (R^+_j)^\dagger, \quad R^z_j = f_\uparrow^\dagger f_\downarrow^\dagger n_{\downarrow j} + f_\downarrow^\dagger f_\uparrow^\dagger n_{\uparrow j}.
\]

Part of the representation \[7\] describing $S=1$ coincides with BO representation. Nevertheless, since $\vec{S}^2$ is no more a conserved quantity, being defined by $\vec{S}^2_{\uparrow j} = 2[1 - n_{\uparrow j}, n_{\downarrow j}]$, the projection of SO(4) group on $S=1$ representation of SU(2) group requires an additional Hubbard-like interaction responsible for the hidden constraint overlooked in BO paper \[14\]. When the $S=1$ sector is fixed, three states $(n_{\uparrow j}, n_{\downarrow j})$, namely $(1,0)$, $(0,1)$ and $(0,0)$ determine three-fold degenerate triplet state whereas the doubly occupied state $(1,1)$ stands for a singlet separated from the ground state by the gap $\Delta = J_\perp$.

The Hamiltonian \[2\] is fermionized by means of purely 1D string operator $K_j \[9\]$ in contrast to meanderings strings proposed for the theory of 2-leg ladders (see \[24\] and references therein).

The Hamiltonian of anisotropic XXZ SRC model is

\[
H = H_\parallel + \sum_i H_{\perp,i},
\]

where

\[
H_\parallel = J_\parallel \sum_i \left[ S^\uparrow_i S^\uparrow_{i+1} + S^\uparrow_i R^-_{i+1} + (S \leftrightarrow R) + h.c. \right]
\]

\[
+ \frac{J^z_\parallel}{4} \sum_i \left[ S^\uparrow_i S^\uparrow_{i} + S^\uparrow_i R^z_{i+1} + (S^z \leftrightarrow R^z) \right]
\]

\[
H_{\perp,i} = \frac{J^z_\parallel}{8} \left( R^z_i R^-_i + R^-_i R^z_i \right) - \frac{J^z_\parallel}{4} (R^z_i)^2 - (\vec{R}_i \leftrightarrow \vec{S}_i).
\]

There exists a set of discrete transformations keeping the Hamiltonians \[2\] and \[9\] intact and preserving commutation relations \[3\] and Casimir operators \[4\]. In general, these transformations are described by the matrix of finite rotations characterized by Euler angles $\theta, \psi, \phi$ for the case of SU(2) x SU(2) or SO(2) x SO(2) x $Z_2$ x $Z_2$ groups. An example of such transformation is

\[
S^+ \rightarrow R^+, \quad S^- \rightarrow R^-, \quad S^z \rightarrow S^z, \quad R^z \rightarrow R^z.
\]

being a $U(1) \times U(1)$ rotation in "$S^z - R^z"$ and "$S^\uparrow - R^\uparrow"$ subspaces. This is in fact a particle-hole flavor transformation $f_\uparrow \rightarrow f_\downarrow^\dagger$, $f_\downarrow \rightarrow f_\uparrow^\dagger$. On the other hand, it corresponds to replacement $b \rightarrow -b$ thus manifesting hidden $Z_2$ symmetry. This means that an additional gauge factor $\exp(i\theta)$ with $\theta = \pm \pi$ appears in a fermion operator characterizing "free ends" of rungs in SRC chain. Other examples are $(f_\uparrow \rightarrow f_\downarrow)$ and $(f_\downarrow \rightarrow f_\uparrow^\dagger, f_\downarrow \rightarrow f_\uparrow^\dagger)$. The latter one corresponds to a particle-hole transformation $(a \rightarrow a^\dagger, b \rightarrow b^\dagger)$ in the non-rotated fermion basis.

After JW transformation in $a - b$ basis \[3\] - \[9\] the Hamiltonian \[9\] is written as follows

\[
H_\parallel = J_\parallel \sum_i \left( a^\dagger_i a_{i+1} + a^\dagger_{i+1} a_i \cos(\pi n^z_i) \right)
\]

\[
+ \frac{J^z_\parallel}{4} \sum_i \left( n^z_i - \frac{1}{2} \right) \left( n^a_{i+1} - \frac{1}{2} \right)
\]

\[
(11)
\]

and $H_{\perp,i} = \sum_i H_{\perp,i}$ with

\[
H_{\perp,i} = -\frac{J^z_\parallel}{2} \left( a^\dagger_i b_i + b^\dagger_i a_i \right) - \frac{J^z_\parallel}{4} \left( n^a_i - \frac{1}{2} \right) \left( n^b_i - \frac{1}{2} \right).
\]

(12)
where the shorthand notations $n^a = a^\dagger a$, $n^b = b^\dagger b$ and $\cos(\pi n^b) = \text{Re } \exp(\pm i\pi n^b) = 1 - 2n^b$ are used. Below we consider the domain $J_\perp \ll J_\parallel$ where strongest deviations from conventional Haldane gap regime [11, 12] are anticipated. In the limit $J_\perp = 0$ our SRC model reduces to an $s = 1/2$ AF chain, the gauge factor $\cos(\pi n^b) = \pm 1$ is a fictitious random variable which can be eliminated by $S^x \rightarrow -S^x$ and $S^y \rightarrow -S^y$ on the corresponding site. This situation is similar to the so called Mattis disorder [21] where the randomness in interaction is removed by proper redefinition of spin variables.

The kinematic factor $\sim \cos(\pi n^i)$ in $H^F_{\perp}$ (11) can be eliminated by a unitary transformation $\hat{H} = U^\dagger H U$ with $U = \exp(\mp i\pi \sum_{j > i} n^a_j n^b_j)$. Then $H^\perp_{\perp}$ and $H^\parallel_{\perp}$ remain unchanged and $J^\perp_{\perp}$ term acquires the string form

$$\hat{H}^\perp_{\perp,i} = -\frac{1}{2} J^\perp_{\perp} \left(a^\dagger_i b_i e^{-\pi \sum_j [a^\dagger_j a_j + b^\dagger_j b_j]} + \text{h.c.}\right). \quad (13)$$

The $s = 1/2$ chain is represented in terms of a half-filled band of fermions. Since interactions (11) and (12) do not change the occupation numbers for each color, we expect that interacting case is also represented by two half-filled bands (see below). We note that the Hamiltonian $H_1$ in [9] possesses $U(1) \times U(1)$ symmetry whereas only one local $U(1)$ associated with $b$-fermions exists in (11) due to non-local character of JW transformation.

Let us consider the XY$|| - XY_\perp$ model ($J^\parallel_{\perp} = J^\perp_{\perp} = 0$). We split the first term in (11) into the bare hopping and the kinematic term $\sim J^\perp_{\perp} n^i (a^\dagger_i a_{i+1} + \text{h.c})$ playing part of effective interaction $H^{
abla XY}_{\perp}$. One gets after diagonalization of the hopping term

$$H_0 = \sum_{\lambda, \rho, \pm} \varepsilon_{\lambda}(p) c_{\lambda, \rho, \pm}^\dagger c_{\lambda, \rho, \pm} \quad (14)$$

with $c_+ = u_+ a + u_- b$, $c_- = u_+ b - u_- a$, $u^\pm_+(p) = \pm \varepsilon_+(p)/\varepsilon_+(p) - \varepsilon_-(p)$, $\varepsilon_{\pm}(p) = J^\perp_{\perp} \cos p \pm [J^\perp_{\perp} \cos p)^2 + (J^\parallel_{\perp})^2]^{1/2}. \quad (15)$

The chemical potential $\eta = 0$ is pinned in the gap. The mixing term fixes global phase difference for $a - b$ fields. The remaining symmetry is local $Z_2 \times Z_2$.

We represent $H^{
abla XY}_{\perp}$ in terms of new variables $c_\pm$ by expanding the Hamiltonian (11) in the vicinity of two Fermi points of non-hybridized system

$$H^{
abla XY}_{\perp} = \frac{1}{2} \sum_{\nu, \nu', \alpha} g^\nu_{\nu', \alpha}(q) \rho_{\nu, \nu', \alpha}(q) \Lambda_{\nu, \nu', \alpha}(-q) \quad (17)$$

where the operator $\rho_{\nu, \nu', \alpha}$ is given by

$$\rho_{\nu, \nu', \alpha}(q) = \sum_k c_{\alpha, \nu, k-q/2}^\dagger c_{\alpha, \nu', k+q/2}. \quad (18)$$

Its diagonal part is the quasiparticle density. The operator $\Lambda_{\nu, \nu', \alpha}$ is defined as

$$\Lambda^\nu_{\nu', \alpha}(q) = -\alpha \sum_k c_{\alpha, \nu, k-q/2}^\dagger c_{\alpha, \nu', k+q/2}. \quad (19)$$

while its diagonal part is $\Lambda_{\nu, \nu} = \text{div} \nu = -\partial \nu_{\nu, \nu}$. In expressions (15), (19) the index $\alpha = \pm$ stands for "old" Fermi surface points $k_\pm^R = \pm \pi/2$ (we take a unit lattice spacing), $k$ is measured from $k_F$. Indices $\mu, \mu', \nu, \nu' = \pm$ denote the branch of fermions $c_\pm$. We used the property of $u_\pm, \pm((\pi/2) \approx 1/2$. The tensor $g_{\nu, \nu', \alpha}^\nu$ for these scattering processes has the form

$$g_{\nu, \nu', \alpha}^\nu = J^\parallel_{\perp}(\delta_{\mu, \mu'} + \sigma^\nu_{\mu, \mu'}(\delta_{\nu, \nu'} - \sigma^\nu_{\nu, \nu'})). \quad (20)$$

We analyze (17) in terms of $g$-ology approach classifying various terms in $g_{\nu, \nu', \alpha}^\nu(q)$ as forward, backward scattering and Umklapp processes. We see, first, that if $|q| < \pi/2$, and $g \sim \pm J^\parallel_{\perp}$, both diagonal and off-diagonal matrix elements of $\Lambda_{\nu, \nu', \alpha}$ vanish in accordance with Adler’s principle [22]. Thus, the forward scattering processes leading to small renormalization of the coupling $\sim (J^\parallel_{\perp})^2/J^\parallel_{\perp}$ are irrelevant. The backward scattering processes $(\pm \pi/2 \rightarrow \mp \pi/2)$ result in a reduction $J_{\parallel} \rightarrow J_{\parallel}^\perp J^\perp_{\perp}$ of the effective coupling (0 < $\gamma < 1$ is a constant). To get this estimate we cut logarithmic corrections to the coupling constant by $\Delta_{\min} \sim (J^\perp_{\perp})^2/J^\parallel_{\perp}$ where $\Delta_{\min}$ determines the gap in the density of spin-fermion states $\varepsilon_\pm$. However there is yet another energy scale $\Delta \sim J^\perp_{\perp}$ associated with the gap in a two-point particle-hole correlator with zero total momentum of the pair. This energy scale is attributed to the gap separating $S = 0$ excited state on a rung from the triplet state. The crossover between two energy scales will be discussed elsewhere. The Hamiltonian (17) allows also ”inter-band” Umklapp processes determined by the off-diagonal elements of $\rho_{\nu, \nu'}$ and $\Lambda_{\nu, \nu'}$ and responsible for periodicity $Q = 2\pi$. These processes, associated with the transfer of pair of quasiparticles over the gap do not change the leading term in (16).

The above arguments are complemented by the bosonization calculations for the strongly asymmetric 2-leg ladder with finite Fermi velocity $u_0$ in the $b$ subsystem which may be turned to zero in the end of scaling procedure. The continuum representation for spin operators
\( s_1, s_2 \) in (1) reads (2) (we denote \( i=a(1), b(2) \))

\[
\begin{align*}
s_1^\pm(x) & \sim e^{\pm i \theta_i (\cos(\pi x) + \cos(2\phi_i))}, \\
s_2^\pm(x) & \sim \pi^{-1} \partial_x \phi_i + \cos(\pi x + 2\phi_i)
\end{align*}
\] (21)

with canonically conjugated variables \( \phi_i \) and \( \Pi_i = \partial_x \theta_i \). Keeping only most relevant terms in the rung interaction, \( J_{11} \), we arrive at the conventional equations of Abelian bosonization for the spin Hamiltonian (3)

\[
H = \sum_{i=a,b} \int dx \left[ \frac{\pi u_i K}{2} \Pi_i^2 + \frac{u_i}{2nK} (\partial_x \phi_i)^2 + J_{1i}^z \cos(\theta_i - \beta_b) + J_{1i}^z \cos 2\phi_a \cos 2\phi_b \right]
\] (22)

with \( K=1/2 \) and \( J_{1i} \ll u_i \ll u_a = \pi J_{1i}/2 \) for \( J_{1i}=J_{1i}^+=J_{1i}^- \).

To find the scaling dimension of the gap we start with the case \( J_{1i}^z = 0, J_{1i}^z = J_{1i} \neq 0 \). Using the scaling procedure \( (x \rightarrow \Lambda x, t \rightarrow \Lambda t) \), one has \( J_{1i} \rightarrow J_{1i} \Lambda^{2-\beta} \) where \( \beta/2 = K/2 \) is a scaling dimension of \( \cos 2\phi_a \). The renormalization of b-component stops when the renormalized \( J_{1i} \) becomes comparable with the lower scale of the energy \( u_a \). The corresponding scale \( \Lambda_0 \) defines the first correlation length \( \xi_a = (u_a/J_{1i})^{1/(2-\beta)} \) and the first energy gap \( \Delta_0 = u_b \xi_a^{-3} = u_b (J_{1i}/u_a)^{1/(2-\beta)} \). At the second stage of the renormalization, with frozen \( \cos 2\phi_a \sim \xi_b^{-\beta/2} \) the factor \( \cos 2\phi_a \) undergoes further enhancement. The procedure halts when the renormalized amplitude \( J_{1i} \) compares with \( u_a \) at \( J_{1i} \Lambda^{2-\beta} \sim u_a \), which defines a second correlation length \( \xi_a = (\xi_b^{3/2} u_a/J_{1i})^{1/(2-\beta/2)} \) and the second gap \( \Delta_a = u_a \xi_a^{-1} \).

In our particular case \( \beta = 1 \) these formulas simplify as follows:

\[
\begin{align*}
\xi_b & = (u_b/J_{1i}), \quad \Delta_b = J_{1i} \\
\xi_a & = \xi_b (u_a/u_b)^{2/3}, \quad \Delta_a = J_{1i} (u_a/u_b)^{1/3}.
\end{align*}
\] (23)

One may decrease \( u_a \) in the regime of frozen \( \phi_a \) down to \( u_a \sim J_{1i} \). Then \( \Delta \sim J_{1i} (J_{1i}/u_a)^{2/3} \). Further decrease of \( u_a \) does not change the exponent \( 2/3 \) of the spin gap fully determined by the scattering on the random potential \( \cos 2\phi_a \). The two-stage renormalization procedure is essential for understanding the SRC model in the limit \( u_a \sim u_b \), Eq. (23) leads to standard scaling of the spin gap \( \Delta \sim J_{1i} \) (see e.g. 24).

In the case \( J_{1i}^z \neq 0, J_{1i}^z = 0 \) the scaling behavior of the spin gap \( \Delta \sim J_{1i} (J_{1i}/J_{1i})^{2/3} \) is determined by the backward scattering processes of the field \( a \) on the random potential associated with fluctuations of \( \cos \theta_a \).

The fully isotropic case, \( J_{1i}^z = J_{1i} = J_{1i} \), might be expected to yield the same estimate \( \Delta \sim J_{1i}^{1/(3)} (J_{1i}^{2/3}) \). A refined analysis (see e.g. 27) including the less relevant terms in (17) may correct the gap values, but does not change this estimate.

To summarize, we introduced a new 1D model intermediate between the spin \( S=1 \) chain and the 2-leg ladder. Our SRC possesses special hidden \( Z_2 \) symmetries connected with discrete transformations in a 6D space of SO(4) group characterizing the spin rotator. The SRC chain is mapped on the two-component unconstrained interacting fermions by means of \( \phi_0 \) JW transformation. Two fermion fields are characterized by sharply different dynamics. One of two fields is frozen at \( k \rightarrow \pm \pi/2 \) and the scaling dimension \( \beta \) of the rung operator exchange \( J_{1i} \) is \( \beta = 1/2 \) instead of \( \beta = 1 \) in a conventional Haldane problem. As a result, new scaling "two third" law for the spin gap arises.

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