Spin gap in chains with hidden symmetries

M. N. Kiselev,[1] D. N. Aristov,[2,*] and K. Kikoin[3]
[1]*Physics Department, Arnold Sommerfeld Center for Theoretical Physics, and Center for NanoScience, Ludwig-Maximilians-Universität at München, 80333 München, Germany*
[2]*Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany*
[3]*Ben-Gurion University of the Negev, Beer-Sheva 84105, Israel*
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We investigate the formation of a spin gap in one-dimensional models characterized by groups with hidden dynamical symmetries. A family of two-parametric models of isotropic and anisotropic spin-rotator chains (SRC's) characterized by $SU(2)\times SU(2)$ and $SO(2)\times SO(2)\times Z_2\times Z_2$ symmetries is introduced to describe the transition from SU(2) to SO(4) antiferromagnetic Heisenberg chains. The excitation spectrum is studied with the use of the Jordan-Wigner transformation generalized for o_4 algebra and by means of the 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 the conventional Haldane problem.

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More than 20 years ago Haldane[1] 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 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 the Haldane conjecture has been proven a long time ago (see Refs. 2 and 3), the second part, although confirmed by many numerical[4] and experimental[5] studies and tested by some approximate analytical calculations,[6–10] remains a hypothesis. The problem of SU(2) Heisenberg chains has been attacked by modern tools such as, e.g., bosonization[6–8] (see also Ref. 11), various numerical methods,[4,12,13] and the recently proposed fermionization by means of the Jordan-Wigner transformation for higher spins.[14] However, the main focus of interest has been put either on $S=1$ chains characterized by SU(2) symmetry or on N-leg ladders described in terms of dynamic SO(N) groups.[16] There have also been made several conjectures concerning spontaneous discrete symmetry breaking in $S=1$ chain models associated with, e.g., existence of hidden Z_2 and $Z_2\times Z_2$ symmetries.[13,17] Nevertheless, the general question about the nature of the spin gap is still open.

In this paper we propose yet another approach to the spin gap problem. It is based on investigation of a family of two-parametric Hamiltonians described by dynamical groups.[18] This family includes the conventional two-leg ladder and several models intermediate between the ladder and the chain. Here we concentrate on the most instructive example of a "barbed-wire-like" chain with spins $1/2$ in each site coupled by the ferromagnetic exchange $J_\perp$ within a rung and the AF interaction $J_\parallel$ along the leg (Fig. 1). The model Hamiltonian is

$$H = J_\parallel \sum_i \vec{s}_{1,i}\vec{s}_{1,i+1} - J_\perp \sum_i \vec{s}_{1i}\vec{s}_{2i}. \quad (1)$$

This model is a natural extension of the $S=1$ chain 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[10,19]). Unlike earlier attempts to construct the representation of an $S=1$ state out of $s=1/2$ ingredients,[7,8] we respect in this case the SO(4) symmetry of the spin manifold on each rung.[20] As a result, *the singlet state cannot be projected out.* Moreover, it plays an integral part in the formation of the spin gap. We show that the hidden Z_2 symmetries in this model are an intrinsic property of the local SO(4) group of the 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 ($N\geqslant 2$)-leg ladder models and SU(2) chains. In particular we show also that the scaling dimension of a spin gap in a SRC differs from that in a two-leg ladder.

New variables on a rung are introduced to keep track of $S=1$ properties. We define $\vec{S}_i=\vec{s}_{1,i}+\vec{s}_{2,i}$, $\vec{R}_i=\vec{s}_{1,i}-\vec{s}_{2,i}$, where $\vec{S}_i$ stands for a triplet $S=1$ ground state and singlet $S=0$ excited state. The operator $\vec{R}$ describes dynamical triplet-singlet mixing.[18,20] Then

$$H = \frac{J_\parallel}{4}\sum_i [\vec{S}_i\vec{S}_{i+1} + \vec{S}_i\vec{R}_{i+1} + (\vec{S}\leftrightarrow\vec{R})] - \frac{J_\perp}{4}\sum_i (\vec{S}_i^2 - \vec{R}_i^2), \quad (2)$$

where the set of operators $\vec{S}_i$, $\vec{R}_i$ fully defines the o_4 algebra in accordance with the commutation relations

$$[S_i^\alpha, S_j^\beta] = i\delta_{ij}\varepsilon_{\alpha\beta\gamma}S_i^\gamma, \quad [R_i^\alpha, R_j^\beta] = i\delta_{ij}\varepsilon_{\alpha\beta\gamma}S_i^\gamma,$$

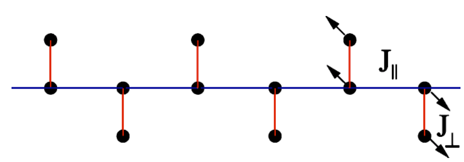

FIG. 1. Spin-rotator chain.

$$[R_i^\alpha, S_j^\beta] = i\,\delta_{ij}\varepsilon_{\alpha\beta\gamma}R_i^\gamma, \qquad (3)$$

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

$$(\vec{S}_i)^2 + (\vec{R}_i)^2 = 3, \quad (\vec{S}_i \cdot \vec{R}_i) = 0. \qquad (4)$$

In order to characterize low-lying excitations in the SRC we propose a fermionization procedure, which extends the Jordan-Wigner (JW) transformation to the SO(4) group, and a bosonization formalism based on this procedure. Our method incorporates the JW transformation for $S=1$ proposed by Batista and Ortiz (BO) in Ref. 14. The relationships between the SO(4) JW representation and the 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 ($S^\pm = S^x \pm iS^y$):

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

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

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

This representation satisfies commutation relations (3) for the SO(4) group and preserves the Casimir operators (4). The advantage of the 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

$$f_\uparrow = (a-b)/\sqrt{2}, \quad f_\downarrow^\dagger = (a+b)/\sqrt{2}. \qquad (5)$$

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

$$K_j = \exp\left(i\pi \sum_{k<j,\sigma} n_{\sigma k}\right) = \prod_{k<j}(1-2n_{\uparrow k})(1-2n_{\downarrow k}) \qquad (6)$$

($n_\sigma = f_\sigma^\dagger f_\sigma$). As a result of the JW transformation the SO(4) generators acquire the following form:

$$S_j^+ = \sqrt{2}[f_{\uparrow j}^\dagger(1-n_{\downarrow j})K_j + K_j^\dagger f_{\downarrow j}(1-n_{\uparrow j})],$$
$$S_j^- = (S_j^+)^\dagger, \quad S_j^z = n_{\uparrow j} - n_{\downarrow j}, \qquad (7)$$

$$R_j^+ = \sqrt{2}(f_{\uparrow j}^\dagger n_{\downarrow j}K_j + K_j^\dagger f_{\downarrow j}n_{\uparrow j}),$$
$$R_j^- = (R_j^+)^\dagger, \quad R_j^z = f_{\uparrow j}^\dagger f_{\downarrow j}^\dagger + f_{\downarrow j}f_{\uparrow j}. \qquad (8)$$

Part of the representation (7) describing $S=1$ coincides with the BO representation. Nevertheless, since $\vec{S}^2$ is no longer a conserved quantity, being defined by $\vec{S}_j^2 = 2[1-n_{\uparrow j}n_{\downarrow j}]$, the projection of the SO(4) group on the $S=1$ representation of the SU(2) group requires an additional Hubbard-like interaction responsible for the hidden constraint overlooked in the BO paper[14] (see also Ref. 15 where the unconstrained JW transformation is constructed for $S=3/2$). When the $S=1$ sector is fixed, three states $(n_\uparrow, n_\downarrow)$, namely, (1,0), (0,0), and (0,1), determine a threefold 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 a purely one-dimensional (1D) string operator K_j [Eq. (6)] in contrast to the meandering strings proposed for the theory of two-leg ladders (see Ref. 21 and references therein).

The Hamiltonian of the anisotropic *XXZ* SRC model is $H = H_\parallel + \Sigma_i H_{\perp,i}$, where

$$H_\parallel = \frac{J_\parallel^x}{8}\sum_i [S_i^+S_{i+1}^- + S_i^+R_{i+1}^- + (S \leftrightarrow R) + \text{H.c.}] + \frac{J_\parallel^z}{4}\sum_i [S_i^zS_{i+1}^z + S_i^zR_{i+1}^z + (S^z \leftrightarrow R^z)], \qquad (9)$$

$$H_{\perp,i} = \frac{J_\perp^x}{8}(R_i^+R_i^- + R_i^-R_i^+) + \frac{J_\perp^z}{4}(R_i^z)^2 - (\vec{R}_i \leftrightarrow \vec{S}_i).$$

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

$$S^+ \to R^+, \quad S^- \to R^-, \quad S^z \to S^z, \quad R^z \to R^z, \qquad (10)$$

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

After a JW transformation in the *a*-*b* basis (5)–(8) the Hamiltonian (9) is written as follows:

$$H_\parallel = J_\parallel^x \sum_i (a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i)\cos(\pi n_i^b) + J_\parallel^z \sum_i \left(n_i^a - \frac{1}{2}\right)\left(n_{i+1}^a - \frac{1}{2}\right) \qquad (11)$$

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

$$H_{\perp,i} = -\frac{J_\perp^x}{2}(a_i^\dagger b_i + b_i^\dagger a_i) - J_\perp^z\left(n_i^a - \frac{1}{2}\right)\left(n_i^b - \frac{1}{2}\right), \qquad (12)$$

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 the strongest deviations from the conventional Haldane gap regime[6,7] 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 the transformation $S^x \to -S^x$ and $S^y \to -S^y$ on the corresponding site. This situation is similar to the so-called Mattis disorder[22] where ran-

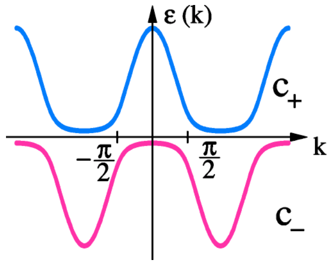

FIG. 2. Dispersion law for hybridized spin fermions $c_{\pm}$.

domness in an interaction is removed by proper redefinition of spin variables.

The kinematic factor $\sim\cos(\pi n_i^b)$ in $H_{\parallel}^x$ [Eq. (11)] can be eliminated by a unitary transformation $\tilde{H}=U^{\dagger}HU$ with $U=\exp(i\pi\Sigma_{l,j>l}n_j^a n_l^b)$. Then $H_{\perp}^z$ and $H_{\parallel}^z$ remain unchanged and the $J_{\perp}^x$ term acquires the string form

$$\tilde{H}_{\perp,i}^x = -\frac{1}{2}J_{\perp}^x\left[a_i^{\dagger}b_i \exp\left(-i\pi\sum_{j<i}[a_j^{\dagger}a_j + b_j^{\dagger}b_j]\right) + \text{H.c.}\right]. \tag{13}$$

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 the interacting case is also represented by two half-filled bands (see below). We note that the Hamiltonian $H_{\parallel}$ in Eq. (9) possesses U(1)×U(1) symmetry whereas only one local U(1) associated with b fermions exists in Eq. (11) due to the nonlocal character of the JW transformation.

Let us consider the $XY_{\parallel}$-$XY_{\perp}$ model ($J_{\parallel}^z=J_{\perp}^z=0$). We split the first term in Eq. (11) into the bare hopping and the kinematic term $\sim J_{\parallel}^x n_i^b(a_i^{\dagger}a_{i+1}+\text{H.c.})$ playing the part of the effective interaction H_{int}^{XY}. One gets after diagonalization of the hopping term

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

with $c_+=u_+a+u_-b$, $c_-=u_+b-u_-a$,

$$u_{\pm}^2(p) = \pm\varepsilon_{\pm}(p)/[\varepsilon_+(p)-\varepsilon_-(p)], \tag{15}$$

$$\varepsilon_{\pm}(p) = J_{\parallel}^x\cos p \pm [(J_{\parallel}^x\cos p)^2 + (J_{\perp}^x)^2]^{1/2}. \tag{16}$$

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

We represent H_{int}^{XY} in terms of new variables $c_{\pm}$ by expanding the Hamiltonian (11) in the vicinity of two Fermi points of the nonhybridized system:

$$H_{int}^{XY} = \frac{1}{2}\sum_{\{\mu,\nu,\alpha\}=\pm1,q} g_{\mu\mu'}^{\nu\nu'}(q)\rho_{\mu\mu',\alpha}(q)\Lambda_{\nu\nu',\alpha'}(-q) \tag{17}$$

where the operator $\rho_{\mu\mu'}$ is given by

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

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

$$\Lambda_{\nu\nu',\alpha}(q) = -\alpha\sum_k k\, c_{\alpha,\nu,k-q/2}^{\dagger}c_{\alpha,\nu',k+q/2}, \tag{19}$$

while its diagonal part is $\Lambda_{\nu\nu}=\text{div}\, j_{\nu\nu}=-\partial_t\rho_{\nu\nu}$.

In expressions (18) and (19) the index $\alpha=\pm$ stands for the "old" Fermi surface points $k_F^{\pm}=\pm\pi/2$ (we take unit lattice spacing), and k is measured from k_F. The indices $\mu,\mu',\nu,\nu'=\pm$ denote the branch of fermions $c_{\pm}$. We used the property of $u_{\pm,\alpha}(\pm\pi/2)\approx 1/\sqrt{2}$. The tensor $g_{\mu\mu'}^{\nu\nu'}$ for these scattering processes has the form

$$g_{\mu\mu'}^{\nu\nu'} = J_{\parallel}^x(\delta_{\mu\mu'}+\sigma_{\mu\mu'}^x)(\delta_{\nu\nu'}-\sigma_{\nu\nu'}^x). \tag{20}$$

We analyze Eq. (17) in terms of the g-ology approach[23] classifying various terms in $g_{\mu\mu'}^{\nu\nu'}(q)$ as forward and backward scattering and umklapp processes. We see, first, that if $|q|\ll\pi/2$ and $g\sim\pm J_{\parallel}^x$, both diagonal and off-diagonal matrix elements of $\Lambda_{\nu\nu'}$ vanish in accordance with Adler's principle.[24] Thus, the forward scattering processes leading to small renormalization of the coupling $\sim(J_{\perp}^x)^2/J_{\parallel}^x$ are irrelevant. The backward scattering processes $(\pm\pi/2\to\mp\pi/2)$ result in a reduction $J_{\parallel}\to J_{\parallel}^{1-\gamma}J_{\perp}^{\gamma}$ of the effective coupling $(0<\gamma<1$ is a constant). To get this estimate we cut off the logarithmic corrections to the coupling constant at $\Delta_{min}\sim(J_{\perp}^x)^2/J_{\parallel}$ where Δ_{min} determines the gap in the density of spin-fermion states $\varepsilon_{\pm}$. However, there is yet another energy scale $\Delta\sim J_{\perp}^x$ 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 the $S=0$ excited state on a rung from the triplet state. The crossover between the two energy scales will be discussed elsewhere. The Hamiltonian (17) allows also "interband" umklapp processes determined by the off-diagonal elements of $\rho_{\mu\mu'}$ and $\Lambda_{\nu\nu'}$ and responsible for the periodicity $Q=2\pi$. These processes, associated with the transfer of a pair of quasiparticles over the gap, do not change the leading term in Eq. (16).

The above arguments are complemented by bosonization calculations for the strongly asymmetric two-leg ladder with finite Fermi velocity u_b in the b subsystem, which may be set to zero at the end of the scaling procedure. The continuum representation for spin operators $\vec{s}_1,\vec{s}_2$ in Eq. (1) reads[11,25] $[i=a(1),b(2)]$

$$s_i^{\pm}(x) \sim e^{\pm i\theta_i}[\cos(\pi x)+\cos(2\phi_i)],$$

$$s_i^z(x) \sim \pi^{-1}\partial_x\phi_i + \cos(\pi x+2\phi_i) \tag{21}$$

with canonically conjugated variables ϕ_i and $\Pi_i=\partial_x\theta_i$. Keeping only the most relevant terms in the rung interaction $J_{\perp}^{\alpha}$, we arrive at the conventional equations of Abelian bosonization for the spin Hamiltonian (2),

$$H = \sum_{i=a,b} \int dx\left(\frac{\pi u_i K}{2}\Pi_i^2 + \frac{u_i}{2\pi K}(\partial_x \phi_i)^2 + J_\perp^x \cos(\theta_a - \theta_b) + J_\perp^z \cos 2\phi_a \cos 2\phi_b \right) \qquad (22)$$

with $K=1/2$ and $J_\perp \ll u_b \ll u_a = \pi J_\parallel/2$ for $J_\parallel = J_\parallel^x = J_\parallel^z$.

To find the scaling dimension of the gap we start with the case $J_\perp^x=0$, $J_\perp^z = J_\perp \neq 0$. Using the scaling procedure $(x\to\Lambda x, t\to\Lambda t)$, one has $\tilde{J}_\perp \to J_\perp \Lambda^{2-\beta}$ where $\beta/2 = K$ is the scaling dimension of $\cos 2\phi_i$. The renormalization of the b component stops when the renormalized $J_\perp$ becomes comparable with the lower scale of the energy u_b. The corresponding scale $\Lambda = \xi_b$ defines the first correlation length $\xi_b = (u_b/J_\perp)^{1/(2-\beta)}$ and the first energy gap $\Delta_b = u_b \xi_b^{-1} = u_b (J_\perp/u_b)^{1/(2-\beta)}$. At the second stage of the renormalization, with frozen $\langle \cos 2\phi_b\rangle \sim \xi_b^{-\beta/2}$, the factor $\cos 2\phi_a$ undergoes further enhancement. The procedure halts when the renormalized amplitude $\tilde{J}_\perp$ is comparable with u_a at $J_\perp \Lambda^{2-\beta/2}\xi_b^{-\beta/2} \sim u_a$, which defines a second correlation length $\xi_a = (\xi_b^{\beta/2} u_a/J_\perp)^{1/(2-\beta/2)}$ and a second gap $\Delta_a = u_a \xi_a^{-1}$. In our particular case $\beta=1$ these formulas simplify as follows:

$$\xi_b = (u_b/J_\perp), \quad \Delta_b = J_\perp,$$

$$\xi_a = \xi_b (u_a/u_b)^{2/3}, \quad \Delta_a = J_\perp (u_a/u_b)^{1/3}. \qquad (23)$$

One may decrease u_b in the regime of frozen ϕ_b down to $u_b \sim J_\perp$. Then $\Delta_a \sim J_\parallel (J_\perp/J_\parallel)^{2/3}$. Further decrease of u_b does not change the exponent $2/3$ of the spin gap fully determined by the scattering on the random potential $\cos 2\phi_a$.[26] 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 $\Delta \sim J_\perp$ (see, e.g., Ref. 27).

In the case $J_\perp^x \neq 0$, $J_\perp^{\ z}=0$ the scaling behavior of the spin gap $\Delta \sim J_\parallel (J_\perp^x/J_\parallel)^{2/3}$ 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, $J_\perp^x = J_\perp^z = J_\perp$, might be expected to yield the same estimate $\Delta \sim J_\parallel^{1/3}(J_\perp)^{2/3}$. A refined analysis (see, e.g., Ref. 28) including the less relevant terms in Eq. (17) may correct the gap values, but does not change this estimate.

To summarize, we introduced a 1D model intermediate between the spin $S=1$ chain and the two-leg ladder. Our SRC possesses special hidden Z_2 symmetries connected with discrete transformations in a 6D space of the SO(4) group characterizing the spin rotator. The SRC chain is mapped on the two-component unconstrained interacting fermions by means of an o_4 JW transformation. The two fermion fields are characterized by sharply different dynamics demanding a two-stage renormalization procedure. One of the two fields is frozen at $k\to \pm\pi/2$ and the scaling dimension β of the rung operator exchange $J_\perp$ is $\beta=1/2$ instead of $\beta=1$,[27,29] as in the conventional Haldane problem. As a result, the formation of massive excitations in the isotropic SRC model is characterized by a "two-thirds" scaling law.

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*On leave from Petersburg Nuclear Physics Institute, Gatchina 188300, Russia.

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