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Phase transition of spin–orbital models with a four-spin ring exchange

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ABSTRACT

We extend the bond-operator mean-field theory to study the rung singlet phase and its phase boundary, the triplet excitation, and the spin gap of the spin–orbital models with four-spin exchanges. The theory gives a well description of the rung singlet phase and phase boundaries in two-dimensional (2D) and three-dimensional (3D) cases are predicted. It is shown that consideration of the ring exchange suppresses the excitation spectrum and decreases the spin gap. For 2D and 3D spin–orbital models, positive ring and leg coupling tend to collaborate with each other to break the rung singlet phase. On the boundary line $J_{leg} = J_{ring} < J_{rung}/4$, the rung singlet density is one and a second-order phase transition occurs.

1. Introduction

The multiple-spin exchange interactions have drawn steady research interest from both theoretical and experimental points of view over the years [1–4]. These four-spin exchange terms, such as $(S_i \cdot S_j)(S_k \cdot S_l)$, are usually derived from fourth-order perturbation in the strong coupling limit (small t/U) of the Hubbard model and can induce many exotic ground states [4]. The most important mechanism is the so-called ring exchange [1–3], which is introduced first to describe the magnetic properties of solid ^{3}He. Recently it was suggested that inclusion of a small ring exchange can induce obvious effect on some strongly correlated systems like spin ladders and the high-T_c cuprates [1,5,6]. Among low-dimensional spin systems, two-leg antiferromagnetic spin-ladder systems provide an important playground for studying the effect of ring exchange terms. The motivation to study the effect of ring exchange is that the magnon dispersion at the zone boundary obtained by inelastic neutron scattering experiments cannot be described within a nearest-neighbor Heisenberg model. It is also found that the inclusion of a cyclic spin exchange term of about 20% can reproduce the dispersion [5].

The Hamiltonian of the spin–orbital chain (also called spin ladder) with extended four-spin exchange interactions (as Fig. 1(a)) is usually defined as

$$H = J_{rung}\sum_i S_{1,i}S_{2,i} + J_{leg}\sum_i (S_{1,i}S_{1,i+1} + S_{2,i}S_{2,i+1}) + \frac{J_{ring}}{2}\sum_{\langle ijkl\rangle}(P_{ijkl} + P_{ijkl}^{-1}), \quad (1)$$

where J_{rung} and J_{leg} denote the rung and leg coupling constants, the index i refers to the rungs, and 1, 2 label the two legs. The cyclic permutation operator P_{ijkl} for four spins on a plaquette is given by

$$P_{ijkl} + P_{ijkl}^{-1} = 4(S_iS_j)(S_kS_l) + 4(S_iS_l)(S_jS_k) - 4(S_iS_k)(S_jS_l) + S_iS_j + S_kS_l + S_iS_l + S_jS_k + S_iS_k + S_jS_l. \quad (2)$$

In Fig. 1(b), (c), the extended coupled spin-ladder models are also illustrated in two-dimensional (2D) and three-dimensional (3D) cases. Consideration of the four-spin ring exchange has been widely studied [5–15] in recent years, which can induce the gapped staggered dimer phase, scalar chiral phase, rung singlet phase and other exotic phases. Especially the scalar chiral phase can be realized by ring exchange [2,7], which is considered to be difficult to realize in SU(2)-symmetric systems in the past. In most cases we understand the ground state of model (1) with the help of numerical techniques, such as the density–matrix renormalization group (DMRG) [7,8,12], numerical exact diagonalization of small clusters [11,14]. Analytical investigations of the influence of this exchange have employed perturbative approaches [9], spin-wave analysis [13], exact diagonalization in combination with conformal field theory [5].

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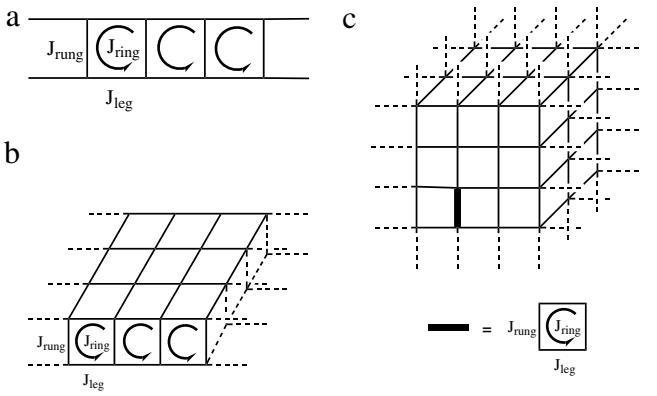

Fig. 1. Schematic structure of spin–orbital models with additional ring exchange of (a) one dimension, (b) two dimension, and (c) three dimension.

The bond-operator mean-field approach [16,17] is an important method to discuss the disordered and frustrated spin systems and superior than SU(2) mean-field approximation in many cases, which is proposed firstly by Sachdev [16]. Its basic idea is to introduce a set of bond operators to create and annihilate singlet and triplet bonds between a pair of spins. The effect of the local hardcore constraint is handled by Brueckner approximation as introduced by Kotov et al. [18]. Until now, this method has been applied widely and successfully to many spin systems, such as spin-ladder system [17,19], the bilayer model [18,20], $J_1 - J_2$ model [21], and so on. For the spin-ladder system, bond-operator approach reproduces the dispersion and the spin gap in the rung singlet phase [17], which ensures us to extend the discussion with taking the ring exchange into account.

In the present paper, we use the bond-operator formalism to study the spin–orbital model with a four-spin ring exchange. The starting point is the dimer limit of uncoupled rungs. In Section 2 we give the theoretical framework and the self-consistent equations for the present model. In Section 3 we study the effect of the four-spin ring exchange on the elementary excitations, the energy gap and other physical quantities. The limitation of the present mean-field approach is discussed. We also present the exactly soluble condition for generalized spin-ladder system with rung singlet ground state, while a similar result is also proposed by variational ansatz. Finally, Section 4 gives the summary.

2. Theoretical framework

For a pair of spins, four operators $s^\dagger$, $t_x^\dagger$, $t_y^\dagger$, $t_z^\dagger$ are introduced to create the four states in Hilbert space. A representation of the spins between two ladders in terms of these singlet and triplet operators is given by $S_1^\alpha = \frac{1}{2}(s^\dagger t_\alpha + t_\alpha^\dagger s - i\epsilon_{\alpha\beta\gamma} t_\beta^\dagger t_\gamma)$, $S_2^\alpha = \frac{1}{2}(-s^\dagger t_\alpha - t_\alpha^\dagger s - i\epsilon_{\alpha\beta\gamma} t_\beta^\dagger t_\gamma)$, where α, β, and γ represent components along the x, y, and z axes, respectively, and ϵ is the antisymmetric Levi-Civita tensor. The s and t_α operators satisfy the bosonic commutation relations with a local constraint $s^\dagger s + t_\alpha^\dagger t_\alpha = 1$. Substituting the operator representation into the original Hamiltonian (1), we get

$$
\begin{aligned}
H &= H_0 + H_1 + H_2,\\
H_0 &= \sum_i \left[\frac{J_{rung}}{4} + \frac{3}{8}J_{ring} - (J_{rung} + 2J_{ring}) s_i^\dagger s_i\right]\\
&\quad - \sum_i \mu_i (s_i^\dagger s_i + t_{i,\alpha}^\dagger t_{i,\alpha} - 1),\\
H_1 &= \frac{J_{leg} + J_{ring}}{2} \sum_{i,\alpha} \left(s_i^\dagger s_{i+1} t_{i,\alpha} t_{i+1,\alpha}^\dagger + h.c.\right)\\
&\quad + \frac{J_{leg} - J_{ring}}{2} \sum_{i,\alpha} \left(s_i^\dagger s_{i+1}^\dagger t_{i,\alpha} t_{i+1,\alpha} + h.c.\right),\\
H_2 &= \frac{J_{leg} + J_{ring}}{4} \sum_{i,\alpha,\beta} (1 - \delta_{\alpha,\beta})\\
&\quad \times \left(t_{i,\alpha}^\dagger t_{i+1,\beta}^\dagger t_{i+1,\alpha} t_{i,\beta} - t_{i,\alpha}^\dagger t_{i+1,\alpha}^\dagger t_{i+1,\beta} t_{i,\beta} + h.c.\right)\\
&\quad + 2J_{ring} \sum_i s_i^\dagger s_i s_{i+1}^\dagger s_{i+1},
\end{aligned}
\tag{3}
$$

where a site-dependent chemical potential μ_i has been introduced to impose the local constraint. For a relatively large J_{rung}, we take $\langle s_i \rangle = \bar{s}$, which means that s bosons are condensed. It can be seen that the consideration of J_{ring} renormalizes the coupling parameters of the individual terms in the original Heisenberg Hamiltonian. We also define two mean fields P and Q as $P = \langle t_{i,\alpha}^\dagger t_{i+1,\alpha} \rangle$, $Q = \langle t_{i,\alpha}^\dagger t_{i+1,\alpha}^\dagger \rangle$ to decouple the Hamiltonian. Then the Hamiltonian can be solved by a mean-field approach.

Defining a generalized Nambu spinor $\Psi_k^\dagger = (t_{k,1}^\dagger, t_{k,2}^\dagger, t_{k,3}^\dagger, t_{-k,1}, t_{-k,2}, t_{k,3})$ and after Fourier transformation, the decoupled Hamiltonian can be written in a compact form:

$$
\begin{aligned}
H &= \frac{1}{2}\sum_k \Psi_k^\dagger H_{\alpha\alpha} \Psi_k + N[-(J_{rung} + 2J_{ring})\bar{s}^2 + 2J_{ring}\bar{s}^4\\
&\quad + \left(\frac{5}{2} - \bar{s}^2\right)\mu - 3(J_{leg} + J_{ring})(P^2 - Q^2)],
\end{aligned}
\tag{4}
$$

where $H_{\alpha\alpha} = \Lambda_k \Omega_1 + \Delta_k \Omega_2$ with $\Omega_1 = \sigma_x \otimes \sigma_0$, $\Omega_2 = \sigma_0' \otimes \sigma_0$, σ_x is the Pauli matrix, σ_0' is the 2×2 unit matrix and σ_0 is the 3×3 unit matrix, $\Lambda_k = -\mu + (J_{leg} + J_{ring})(\bar{s}^2 + 2P)\cos k$, $\Delta_k = (J_{leg} - J_{ring})\bar{s}^2 \cos k - 2(J_{leg} + J_{ring})Q \cos k$. Here $\Omega_{1(2)}$ are expressed in the form of direct product of $\sigma_{x(0')}$ and σ_0. The corresponding Matsubara Green's function (GF) is thus deduced to $G^{-1}(k, i\omega_n) = i\omega_n \sigma_z \otimes I - H_{mf}(k)$, where ω_n is the bosonic Matsubara frequency. The poles of the GF matrix give rise to the quasiparticle spectra: $\epsilon(k) = \sqrt{\Lambda_k^2 - \Delta_k^2}$. From the free energy of the system, the saddle-point equations at $T = 0$ K are derived as

$$
\begin{aligned}
&\frac{3}{2}\int_{-\pi}^{\pi} \frac{dk}{2\pi} \frac{1}{\sqrt{1 - \Gamma_k^2}} = \frac{5}{2} - \bar{s}^2,\\
&\frac{1}{2}\int_{-\pi}^{\pi} \frac{dk}{2\pi} \frac{\cos k}{\sqrt{1 - \Gamma_k^2}} = P,\\
&\frac{1}{2}\int_{-\pi}^{\pi} \frac{dk}{2\pi} \frac{-\Gamma_k \cos k}{\sqrt{1 - \Gamma_k^2}} = Q,\\
&3J_{leg}(P + Q) + 3J_{ring}(P - Q) = \mu + J_{rung} + 2J_{ring}(1 - 2\bar{s}^2),
\end{aligned}
\tag{5}
$$

where $\Gamma_k = \Delta_k / \Lambda_k$. For the $2D$ and $3D$ cases, one can obtain the self-consistent equations directly by replacing $\cos k$ with $(\cos k_x + \cos k_y)/2$ and $(\cos k_x + \cos k_y + \cos k_z)/3$ in the dispersion relation in Eq. (5). For a given value of J_{leg}/J_{rung} and J_{ring}/J_{rung}, we have a set of solutions for μ, $\bar{s}^2$, P and Q. It has be shown in numerous former studies that most rungs occupy the singlet state for a relatively large J_{rung} and so the effect of P and Q are small [17,19].

The bond-operator mean-field theory has been applied successfully to the spin-ladder system without taking the ring exchange into account [19]. In 2D case, the model reduces to the well-known bilayer spin model for $J_{ring} = 0$. It is shown that the zero-temperature quantum phase transition occurs at a critical ratio of $J_{leg}/J_{rung} \approx 0.86$. Without taken the four-spin exchange terms into account, the 2D model considered here is also called net spin model, where a set of exactly soluble net spin models for any spin S have been presented [22]. In the following discussion, J_{rung} is taken as the energy unit. For small J_{leg} and J_{ring}, the spectrum is real and positive everywhere in the Brillouin zone. From the expression of