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Impurity effects of transverse Ising model with multi-impurity

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ABSTRACT

We study the transverse Ising spin model with multi-impurity under the exact solution. The influence mechanisms of the concentration, configuration, impurity-inducing-interaction are investigated through the deformation energy, long-range order and the specific heat. It reveals a way that the impurities have crucial effects on the magnetic order of the system, which can be used to scale the order–disorder transition. In particular, the change of the exchange coupling interaction or magnetic field can lead to the deviation of the phase point. Moreover, the impurity excitation cannot be neglected in thermodynamic properties even though the concentration is only a few percent.

1. Introduction

The low-dimensional quantum magnets are intriguing model systems for studying correlated many-body quantum physics. This is because of the rich physics that they exhibit, and such systems are tractable from a computational and theoretical standpoint. The knowledge acquired by studying these relatively simple systems can be implemented in understanding physical phenomena in the more complex three-dimensional solids. In the low-dimensional systems, the order–disorder phenomena induced by impurity have attracted a lot of interest both from theoretical and experimental points of view [1–6]. For example, by studying the two-dimensional Ising model with random impurities, McCoy et al. [7] found that the impurity effect can explain the contradiction that the specific heat is singularity at the Curie temperature [8], which disagrees with the experimental result. The most striking feature of the model is that it displays “rounding” of the phase transition. Unfortunately, it is difficult to ascertain whether the rounding is specific to systems wherein the impurities exhibit long-range correlations or it is a general feature of disordered systems. The neutron diffraction experiment [9] illustrates that the Ising chain compound $Ca_3Co_{2-x}Mn_xO_6$ exhibits a long-range order for $0.75<x<1$, however, the long-range order is abruptly disappeared in the narrow vicinity of $x=1$. The long-range order exists only in the $Ca_3Co_{2-x}Mn_xO_6$ with reduced ionic order, this means that this order–disorder phenomenon is probably related to the disruption of the long-range magnetic interactions by the magnetic-site disorder. The nonmagnetic Ca substituted at the Sr sites of the Sr_2CuO_3 leads to a spin gap [10], which is independent to the interaction exchange coupling. This result suggests that the spin gap in an antiferromagnetic Heisenberg spin chain can also be induced by a local bound disorder of the intrachain exchange coupling. Though considerable efforts have been devoted to study the order–disorder phenomena, the understanding is incomplete for the order-disorder phenomena induced by impurities in the low-dimensional quantum magnetic systems.

The transverse Ising model (TIM) plays a particularly important role in the low-dimensional quantum magnetic systems, because it is the simplest model and surprisingly rich phase diagrams are found when competing interactions exist [11,12]. On the other hand, the TIMs are strongly affected by disorder in the case of low-dimension, which makes them particularly useful for combined theoretical and experimental studies of disorder in magnets [13–15]. In this paper, we investigate the order–disorder phenomena induced by impurities based on the TIM, and the main goal of this paper is to provide a good understanding of magnetic impurity effects. The related work has been considered [7,16–19], unfortunately, it is hard to study the problem precisely because of the difficulty in mathematics, which is crucial to study the quantum phase transition related impurity. Here we develop a general method to deal with the TIM with multi-impurity. The central point lies in the impurity information that can be expressed by host sites by introducing a displacement quantity related to impurity. So this method is universal, and can be used to a variety of impurity configurations such as $Ca_3Co_{2-x}Mn_xO_6$ [20], $LiHo_xY_{1-x}F_4$

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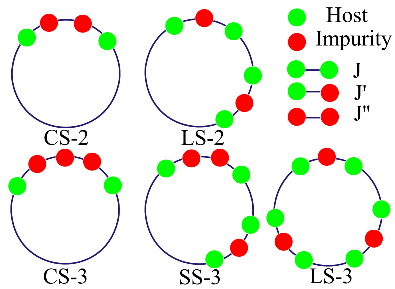

Fig. 1. (Color online) Schematic impurity configurations in periodic Ising spin chain. The CS refers to the impurities link together closely, the LS refers to the impurities divided by the host segment, and the SS refers to the combination of CS and LS.

[21], and $Ba_xSr_{1-x}TiO_3$ [22]. Here we report the solutions and the corresponding properties of the TIM with two impurities and three impurities without losing the generalization.

In order to investigate the impurity effect in detail, we classify the impurity configuration as five kinds for the spin chain with two impurities and three impurities, shown in Fig. 1. For the case of two impurities, the impurities can be closely linked together to form the compact structure (CS), or divided by host segment to form the loose structure (LS). For the case of three impurities, there exists another superposition structure (SS) which refers to the combination of CS and LS. Even in the simple Ising spin chains, we still find that the impurity configuration and the competition of impurities are crucial to the magnetic order, especially near the critical point. These results are important to understand the nature of impurity.

In Section 2 the exact solution of this model with multi-impurity is outlined. In Section 3, by calculating the deformation energy, long-range order of the system and the specific heat, we analyze the effects of impurity parameters on the magnetic order the system. In Section 4, we conclude with a summary and a possibility for application.

2. Exact solution of the models

On the basis of TIM, the Hamiltonian with multi-impurity can be written as $H = H_{\text{host}} + H_{\text{int}} + H_{\text{imp}}$

$$H_{\text{host}} = -J\sum_{\{r_j\}}\sigma_i^x\sigma_{i+1}^x - h\sum_{\{r_j\}}\sigma_i^z,$$
$$H_{\text{imp}} = -J''\sum_{\{l_j\}}S_i^xS_{i+1}^x - h'\sum_{\{l_j\}}S_i^z,$$
$$H_{\text{int}} = -J'\sum_{\{|j-i|=1\}}\sigma_i^xS_j^x, \tag{1}$$

where $\sigma^\alpha(\alpha = x,y,z)$ are Pauli matrices to represent the host spins, $S_i^\alpha(\alpha = x,y,z)$ refers a spin-1/2 magnetic impurity at the ith site, and N is the length of the chain. The periodic boundary condition is assumed. The first term and second term refer to the Ising spin chain segments of the host and impurity respectively, where J and h are Ising coupling strength and external magnetic field, the J'' and h' are impurity coupling strength and local magnetic field at the impurity, respectively. The third term is the interaction between host and impurity with the coupling strength J'.

We begin with the spin chain with two impurities. For the case of CS-2, there exists one host segment $\{x_1(1),\ldots,x_1(N-2)\}$ and two nearest-neighbor impurities in the spin chain. The Hamiltonian can be diagonalized by Jordan–Wigner transformation via expressing Pauli operators by Fermi operators. After performing a Bogoliubov transformation, we derived a compact Hamiltonian

$$H = \sum_k \Lambda(k)(\eta_k^\dagger\eta_k - 1/2), \tag{2}$$

where $\eta_k^\dagger, \eta_k$ are fermionic quasi-particle operators, and $\Lambda(k)$ is the energy spectrum. We choose the trial wave function as $\Phi(j) = A_k(e^{ikj} + e^{i\varphi}e^{-ikj})$ for the host, where A_k is the normalization constant, and the displacement quantity φ is introduced as the function of k to include the influence of impurity. The wave functions of impurity are $\tilde{\Phi}_1(1)$ and $\tilde{\Phi}_1(2)$. Define the parameters

$$a_1 = 4(h^2 + J^2), \quad a_2 = 4(h^2 + J'^2),$$
$$a_3 = 4(h'^2 + J'^2), \quad a_4 = 4(h'^2 + J''^2),$$
$$b_1 = 4hJ, \quad b_2 = 4hJ', \quad b_3 = 4h'J', \quad b_4 = 4h'J''. \tag{3}$$

Combining the wave function into the eigenvalue equation, we get the energy spectra and the wave functions of impurity

$$\Lambda_k^2 = a_1 + 2b_1 \cos k, \tag{4}$$

$$\tilde{\Phi}_1 = \frac{1}{b_2}[(\Lambda_k^2 - a_1)\Phi(N-2) - b_1\Phi(N-3)],$$
$$\tilde{\Phi}_2 = \frac{1}{b_3}[(\Lambda_k^2 - a_2)\Phi(1) - b_1\Phi(2)]. \tag{5}$$

The k is determined by the secular equation

$$(\xi_2\eta_3 + \xi_3\eta_2)\sin k = (\xi_1\eta_1 - \xi_3\eta_3)\sin(N-3)k + (\xi_1\eta_2 + \xi_2\eta_1)\sin(N-4)k + \xi_2\eta_2\sin(N-5)k, \tag{6}$$

where the parameters ξ and η are shown in the Supplementary material.

In the case of LS-2, the spin chain is divided into two host segments $\{x_1(1),\ldots,x_1(r)\}$ and $\{x_2(1),\ldots,x_2(N-r-2)\}$ by impurity, where r refers to the length of the first host segment. We suppose that the wave functions are $\Phi_1(j) = A_{k_1}(e^{ik_1j} + e^{i\varphi_1}e^{-ik_1j})$ and $\Phi_2(j) = A_{k_2}(e^{ik_2j} + e^{i\varphi_2}e^{-ik_2j})$ for the first and second segments, respectively. The wave functions of impurity are $\tilde{\Phi}_1(1)$ and $\tilde{\Phi}_2(1)$. Based on the eigenvalue equation, we can also get the energy spectra and the wave functions of impurity

$$\Lambda_{k_{1,2}}^2 = a_1 + 2b_1 \cos k_{1,2}, \tag{7}$$

$$\tilde{\Phi}_1 = \frac{1}{b_3}[(\Lambda_{k_1}^2 - a_2)\Phi_1(1) - b_1\Phi_1(2)],$$
$$\tilde{\Phi}_2 = \frac{1}{b_3}[(\Lambda_{k_2}^2 - a_2)\Phi_2(1) - b_1\Phi_2(2)]. \tag{8}$$

The k_1 and k_2 are determined by the secular equations

$$2\zeta_2\varsigma_2\sin(r-2)k_1 + 2\zeta_2\varsigma_1\sin(r-1)k_1 - 2\zeta_1\varsigma_2\sin k_1 + (\varsigma_1\nu_1 - \zeta_1\mu_1)e^{-ik_1} - \zeta_2\mu_1e^{-ik_1r} + \varsigma_2\nu_1e^{-2ik_1} = 0, \tag{9}$$

$$2\zeta_4\varsigma_4\sin(N-r-4)k_2 + \varsigma_4\nu_2e^{-2ik_2} + 2\zeta_4\varsigma_3\sin(N-r-3)k_2 - 2\zeta_3\varsigma_4\sin k_2 + (\varsigma_3\nu_2 - \zeta_3\mu_2)e^{-ik_2} - \zeta_4\mu_2e^{-ik_2(N-r-2)} = 0. \tag{10}$$

Note the two Eqs. (9) and (10) are dependent, as the parameters ς, ζ, μ, and ν are functions of k_1 and k_2 (see Supplementary material).

For the case of three and multiple impurities, the processes of calculation are similar with the case of two impurities. Obviously, Λ_k and k of CS-3 and LS-3 can be obtained on the base of CS-2 and LS-2, respectively, by adding one impurity parameter $\tilde{\Phi}_1(2)$. For the case of LS-3, the spin chain is divided into three host segments $\{x_i(j), i = 1,2,3\}$ by impurities. The corresponding wave function of impurities and host segments is $\{\tilde{\Phi}_i(1), i = 1,2,3\}$ and $\{\Phi_i(j) = A_{k_i}(e^{ik_ij} + e^{i\varphi_i}e^{-ik_ij}),\ i = 1,2,3\}$ respectively. We find that there exists a simple relation $3N_h + N_x = N_p$, where N_h, N_x, and N_p refer to the total number of host segment, impurity and introduced parameter, respectively. So one always can obtain the rigorous solution of the multi-impurity system for a finite size.