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Transverse Ising model with multi-impurity

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ABSTRACT

We study the transverse Ising spin model with spin-1 impurities under the exact solution. We develop a universal method to deal with the multi-impurity problem by introducing a displacement quantity in the wave function and get a recursive formula to simplify the calculation of the partition function. This allows us to rigorously determine the impurity effects for a specific distribution of impurity in the thermodynamic limit. The low temperature behaviors are governed by the interplay between host and impurity excitations, and the quantum critical fluctuations around the critical point of the transverse Ising model are tuned by the transverse field and the concentration of impurity. However the impurity effects are limited, which depends on the host–impurity exchange interaction and the coupling strength of impurities.

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 experiment 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 singularity of specific heat at the Curie temperature [8]. 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]. So the TIM is often used to study order–disorder ferroelectrics with a tunnelling effect or the magnetic ordering in materials with singlet crystal field ground state [16].

In this paper, we investigate the order–disorder phenomena induced by impurities based on the TIM. Due to the difficulty in mathematics, it is hard to study the multi-impurity problem precisely. Here we develop a general method for dealing with the TIM with spin-1 impurities based on the hole decomposition [17,18]. By introducing a displacement quantity related to impurity in the wave function, the impurity sites information can be expressed by other sites. This method is not dependent on the configuration of the spin chain, which allows us to deal with any distribution of impurity. Here we consider the simplest case of the compact distribution of impurity in the free boundary condition. We analyze the relation between the impurity excitation and the quantum

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critical behavior in low temperature, the results indicate that the order–disorder transitions induced by impurities are strongly governed by the interplay hole and impurity fermion excitation.

In Section 2 the exact solution of this model with multi-impurity is outlined. In Section 3, by calculating the energy gap and the specific heat, we analyze the effects of impurity parameters on the order–disorder transition of the system. In Section 4, we conclude 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 $H = H_{\mathrm{TIM}} + H_{\mathrm{imp}}$

$$H_{\mathrm{TIM}} = -J\sum_{i,j}\sigma_i^z\sigma_j^z - \Gamma\sum_i\sigma_i^x,$$
$$H_{\mathrm{imp}} = -J'\sum_{i,j}\sigma_i^z S_j^z - J''\sum_{i,j}S_i^z S_j^z + D\sum_i (S_i^x)^2, \tag{1}$$

where $\sigma^\alpha(\alpha = x, y, z)$ are Pauli matrices to present the host spins, $S_i^\alpha(\alpha = x, y, z)$ refers a spin-1 magnetic impurity at the ith site. The summation runs over nearest neighbor sites. J' denotes the host–impurity exchange interaction, J'' is the coupling strength between impurities, and D is the single-ion anisotropy of the impurity. If the numbers of impurity are M, and the spin chain length is L, we define the concentration of impurity is $x=M/L$. We assume that the spin chain has a free boundary condition.

Based on the hole decomposition scheme, a quantum conserved quantity $\hat{N}_0 = M - \sum_i (S_i^z)^2$ can be induced in the system. The operator $\hat{N}_0$ commutes with H, which indicates that the hole states ($S_i^z = 0$) are decoupled from the spin polarized states ($S_i^z = \pm 1$). Therefore, the Hilbert space can be given by the sum of two subspaces: $\mathcal{H} = \mathcal{H}_0 \oplus \mathcal{H}_1$. The holes separate the system into many independent spin-1/2 Ising segments. The configurations of segments depend on the distribution of impurity. Here we consider a simple distribution that all impurity sites link compactly. In a system of p holes, there are at most $p + 1$ segments of spin-1/2. In the specific condition, the Hamiltonian equation (1) can be mapped to the following Hamiltonian:

$$H_{\mathrm{map}} = \sum_{n=1}^{p+1} h_n + \frac{1}{2}D(p + M), \tag{2}$$

where

$$h_n = -\sum_{i,j}J_{i,j}\sigma_i^z\sigma_j^z - \left(\Gamma - \frac{1}{2}D\right)\sum_i\sigma_i^x, \tag{3}$$

$J_{i,j} = J$, J' and J'' correspond to three different exchange interactions of host and impurity. Especially, for $J'' = J'$ the impurity only interacts with the nearest neighbor host, this means that the distribution of impurity can be extended to the normal alternate distribution (see Fig. 1). So for the single impurity segment, it is a special case of the compact distribution that the host and impurity

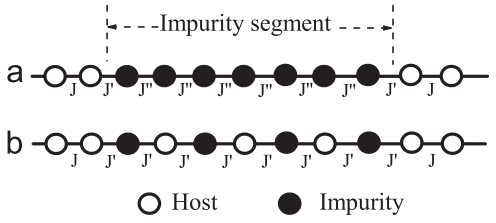

Fig. 1. The schematic impurity configuration in the free boundary condition, (a) and (b) refer to the compact and alternate configuration, respectively.

connect alternately. Obviously, the Hamiltonian equation (2) can be diagonalized, one needs only to diagonalize these segments h_n defined by Eq. (3). There are three kinds of probable segments h_n pure host or impurity segment and host–impurity segment. We can determine the properties of the pure host and impurity segment immediately from the normal TIM. For the host–impurity segment, we propose a trial method to diagonalize the Hamiltonian h_n ($J'' \neq J' \neq 0$). We suppose that the numbers of host site and impurity site are n and m respectively, the length of the segment is l_p.The Hamiltonian equation (3) can be diagonalized by Jordan–Wigner transformation [19] via expressing Pauli operators by Fermi operators. After performing a Bogoliubov transformation, we derived a compact Hamiltonian

$$h_n = \sum_k \Lambda(k)(\eta_k^\dagger\eta_k - 1/2), \tag{4}$$

where $\eta_k^\dagger$, η_k are fermionic quasi-particle operators, and $\Lambda(k)$ is the energy spectrum. We introduce the trial wave functions of host as $\Phi(j) = A_k(e^{ikj} + e^{i\varphi}e^{-ikj})$, $j = 1, \ldots, n$, where A_k is the normalization constant. The displacement quantity φ is the function of k to include the influence of impurity. The wave functions of impurity are $\{\Phi'(1), \Phi'(2), \ldots, \Phi'(m)\}$, which can be expressed by the wave functions of host by using the eigenvalue equation [20]. Define the parameters

$$a = 4\left[\left(\Gamma - \frac{1}{2}D\right)^2 + J^2\right],$$
$$b = 4J\left(\Gamma - \frac{1}{2}D\right), \tag{5}$$

combined the wave function into the eigenvalue equation, we can get the energy spectra

$$\Lambda_k^2 = a + 2b\cos k, \tag{6}$$

and the displacement quantity $e^{i\varphi} = -f(k)/f(-k)$, $f(k) = (\Lambda_k^2 - a)e^{ikn} - be^{ik(n-1)}$. The k is determined by the following secular equation:

$$\frac{\xi_1 e^{ik} + \xi_2 e^{2ik}}{\xi_1 e^{-ik} + \xi_2 e^{-2ik}} = \frac{\eta_1 e^{i(n-1)k} + \eta_2 e^{ink}}{\eta_1 e^{-i(n-1)k} + \eta_2 e^{-ink}}, \tag{7}$$

where $\xi_{1,2}$ and $\eta_{1,2}$ are function of k depending on the specific form of the segment.

We note that the process to resolve the unknown parameters $\{\Phi'(i), i = 1, 2, \ldots, m\}$, Λ_k, φ and k in subsystem h_n is not dependent on the details of the system. For the subsystem h_n, no matter how the impurity distributes, using the eigenvalue equations of h_n we can get all the unknown parameters including the wave functions of impurity. So it is straightforward to extend the results to the system with periodic boundary conditions and any distribution of impurity.

3. Results and discussion

To analyze the influence of the different impurity configuration on the properties of the system, we calculate the ground states, excitation energy and the thermodynamic properties. For simplification, the parameters are renormalized as $\lambda' = \lambda - \frac{1}{2}D/J$, $\lambda = \Gamma/J$, $\alpha = J''/J$, $\beta = J'/J$ and the energy units is $J=1$. In the following text, we set the length of the system is $L = 10^4$, at which the finite size effect can be ignored.