Exact solutions of an Ising spin chain with a spin-1 impurity*

Xuchu Huang(黄旭初)†

Department of Physics, Changji University, Changji 831100, *China*

(Received 3 August 2016; revised manuscript received 26 November 2016; published online 13 February 2017)

An exact solution of a single impurity model is hard to derive since it breaks translation invariance symmetry. We present the exact solution of the spin-1/2 transverse Ising chain imbedded by a spin-1 impurity. Using the hole decomposition scheme, we exactly solve the spin-1 impurity in two subspaces which are generated by a conserved hole operator. The impurity enlarges the energy deformation of the ground state above a pure transverse Ising system without impurity. The specific heat coefficient shows a small anomaly at low temperature for finite size. This indicates that the impurity can tune the ground state from a magnetic impurity space to a non-magnetic impurity space, which only exists for spin-1 impurity comparing with spin-1/2 impurity and a pure transverse Ising chain without impurity. These behaviors essentially come from adding impurity freedom, which induces a competition between hole and fermion excitation depending on the coupling strength with its neighbor and the single-ion anisotropy.

Keywords: exact solution, spin chain, impurity

PACS: 75.10.Pq, 02.30.Ik, 75.10.Dg **DOI:** 10.1088/1674-1056/26/3/037501

1. Introduction

The low dimension spin system had revealed many interesting spin orders at low temperature, such as spin-liquids without long range order, spin excitations with energy gap, ferromagnetic order or antiferromagnetic order, and spin glasses.[1–6] These spin orders may demonstrate significant change when a magnetic or non-magnetic impurity is imbedded in the spin chain.[7–11] An antiferromagnetic Heisenberg spin $S = 1/2$ chain with one impurity is a typical model under frequent theoretical and experimental investigations. Some experimental implementation of these impurity models had been found in the spin-Peierls chain $CuGeO_3$ and spin-ladder $SrCu_2O_3$ in which the magnetic atoms Cu are substituted by a few percent of non-magnetic Zn or Mg.[12–14] These non-magnetic impurities result in a collective magnetic order freezing phase at low temperature.[15,16] When a few magnetic Cu atoms in $SrCuO_2$ are substituted by Ni atoms as impurity, the low-energy spin excitation spectrum would be depleted and a spin-pseudogap is open. This character is captured by the one-dimensional Heisenberg model with site defects.[17] Theoretical researches suggests that impurity has a strong influence on electron transportation. Kane and Fisher showed that even a small impurity atom could reflect electrons in a one-channel Luttinger liquid and make the one dimensional link completely insulating.[18]

An exact solution of quantum spin models provides the most accurate predictions of physical phenomena.[19] In some special cases, the exact solution of a Heisenberg chain with an impurity problem was studied by Andrei and Johannesson using Bethe's Ansatz.[20] They modeled a spin-$1/2$ Heisenberg chain embedded by impurity atoms with spin $S > 1/2$. Later on, Lee and Schlottmann generalized this model to impurity with arbitrary spins, and exactly diagonalized the model Hamiltonian to reach its thermodynamics behavior.[21] In the Heisenberg model, all the three components of spin are involved in physics. To simplify the impurity problem in the quantum spin model, a simpler quantum spin model, the quantum transverse Ising model (TIM), also attracted broad interest.[22] To some extent, TIM could be viewed as a special case of the Heisenberg model. The quantum spin Ising model could be exactly solved by a hole decomposition scheme (HDS) method.[23–25] We also used the hole decomposition to derive the exact solution of the spin-1 quantum Ising model.[26,27] The impurity system mentioned above includes many impurity atoms, while the single impurity model is more complicated since it breaks translation symmetry.[28,29] An exact solution of the single impurity model may have potential applications in quantum information for manipulating qubits.

We consider spin-1 impurity embedded in the spin-$1/2$ Ising spin chain, and use the HDS method and Jordan–Wigner transformation to map the model into the usual spin-$1/2$ transverse Ising model.[23] The exact solution we obtained reveals many fine structures of quantum critical behavior induced by impurity. This method also can be used to deal with two or three dimensional spin chain with spin-1 impurity.

2. Exact solution of the transverse Ising model with an impurity

We consider N spin-1/2 particles coupled to a spin-1 impurity. The neighboring spin-1/2 particles couple to each other by Ising model coupling rule $\sigma_i^z\sigma_j^z$. A transverse magnetic field is applied for the x-component of spin. The spin-1 par-

*Project supported by the Xinjiang Natural Science Foundation of China (Grant No. 2016D01C003).

†Corresponding author. E-mail: hxuchu@163.com

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ticle couples to the first spin-1/2 particle and the last spin-1/2 particle. Thus the N spin-1/2 particles and spin-1 particle form a ring under the period boundary condition. If the spin-1 particle has a stronger electric dipole moment than the spin-1/2 particle, it may induce an anisotropic electric field in the system, which usually occurs in the molecule magnetic system. Thus we introduce a spin dependent anisotropic interaction of spin-1 impurity. The Hamiltonian for this anisotropic impurity system reads

$$\begin{aligned} H = & -\sum_{i=1}^{N-1} J\sigma_i^z\sigma_{i+1}^z - \sum_{i=1}^{N} h_x\sigma_i^x - J_{\rm L}\sigma_N^z S_0^z \\ & - J_{\rm R} S_0^z\sigma_1^z - 2D_x(S_0^x)^2 - D_z(S_0^z)^2, \end{aligned} \tag{1}$$

where σ_i^α ($\alpha = x,y,z$) is Pauli operators for the spin 1/2 particle. J and h_x are the Ising coupling strength and transverse magnetic field, respectively. The spin-1 impurity is represented by S_0^α with $S = 1$, which is located at the zeroth site. The system is the same if the impurity is at a different site. The impurity particle is a special channel that connects the head and tail of the long chain of spin-1/2 particles. In a realistic impurity system, the distance between the impurity particle and its left-hand neighbor usually is not exactly the same as that between impurity and its righthanded neighbor. For the most general case, the coupling strength between the spin-1 impurity and its lefthanded neighbor, the Nth $S = 1/2$, is $J_{\rm L}$, while $J_{\rm R}$ labels the coupling of impurity with its right-hand neighbor, the 1st $S = 1/2$ particle. The strength of single-ion anisotropy for the spin-1 impurity is denoted by $D_{x,y,z}$. Usually $D_{x,y,z}$ represents the crystal field due to distortion of the lattice structure of the environment.

The eigenstates of this model could be expressed in the Hilbert space of S_0^z, $S_0^z \mid \psi\rangle = m \mid \psi\rangle$ ($m = \pm 1, 0$). However, S_0^z is not conserved quantity for this model. Based on HDS, for the $S = 1$ impurity quantum Ising model, the hole number operator $N_0 = 1 - (S_0^z)^2$ is a conserved quantum operator. This quantum number commutes with Hamiltonian $[H, N_0] = 0$.[23,30] The eigenvalue of this hole number operator $p = 0, 1$, i.e., $N_0 \mid \psi_N\rangle = p \mid \psi_N\rangle$. This hole operator behaves like a fermion and its eigenvalue is either one or zero. Obviously, from the commute relation of the Hamiltonian, it is clear that the hole state $p = 1$ does not couple with the polarized spin state $p = 0$. The eigenstates of the quantum impurity model could be classified into two subspaces by the eigenvalue of N_0. The total Hilbert space is the sum of two subspaces: $\mathcal{H} = \mathcal{H}_0 \oplus \mathcal{H}_1$. The Hamiltonian Eq. (1) has a reduced formulation in each subspace

$$\begin{aligned} H_{(p=0)} &= -\sum_{i=0}^{N} J_i\sigma_i^z\sigma_{i+1}^z - \sum_{i=1}^{N} h_x\sigma_i^x - D_x\sigma_0^x - D_z, \\ H_{(p=1)} &= -\sum_{i=1}^{N-1} J_i\sigma_i^z\sigma_{i+1}^z - \sum_{i=1}^{N} h_x\sigma_i^x - D_x, \end{aligned} \tag{2}$$

where we required $J_0 = J_{\rm R}$, $J_N = J_{\rm L}$, and $J_i = J$ for $i \neq 0, N$. Then this spin-1 impurity model reduced to an $S = 1/2$ transverse Ising model. For $p = 0$, the impurity is a magnetic impurity since the z-component of spin-1 is ± 1. For $p = 1$, the impurity is a non-magnetic impurity, as the quantum number of the magnetic moment operator is zero. We would exactly solve this quantum impurity model in the two subspace separately.

For the magnetic impurity space $p = 0$, the transverse Ising model can be reduced to a quadratic fermion model by Jordan–Wigner transformation[31] $H_{(p=0)} = \sum_{i=0}^{N} c_i^\dagger M_{ij} c_j +$ constant. Here $c_i^\dagger$ and c_i are fermionic operators, the matrix M_{ij} contains off-diagonal elements (see Appendix). We make a Bogoliubov transformation to map the conventional fermion operator $(c_i^\dagger, c_i)$ into a fermionic operator of quasiparticle $(\eta_k^\dagger, \eta_k)$. The Hamiltonian could be diagonalized in the form of quasiparticle operators

$$H_{(p=0)} = \sum_k \Lambda(k)(\eta_k^\dagger\eta_k - 1/2), \tag{3}$$

where fermionic quasi-particle operators $\eta_k^\dagger$ and η_k carry quasi-momentum k and $\Lambda(k)$ is the eigen-energy of quasiparticles. In order to find the explicit form of $\Lambda(k)$, we apply a trial wave function $\Phi(j) = A_k \mathrm{e}^{\mathrm{i}kj} + A_k \mathrm{e}^{\mathrm{i}\varphi}\mathrm{e}^{-\mathrm{i}kj}$ so that it obeys the eigen-equation

$$M\Phi = \Lambda_k^2\Phi. \tag{4}$$

The deflection factor φ in the trial wave function is a function of k which carries the scattering wave of the impurity.[32] Combining the trial wave function into Eq. (4) gives us the energy spectrum

$$\Lambda(k) = \sqrt{4h_x^2 + 4J^2 + 8h_xJ\cos k}. \tag{5}$$

The wave vector k is computed self-consistently from the secular equation

$$\begin{aligned} & 8h_xJB_k\sin k - 4h_xJ(C_k + D_k)\sin(N-2)k \\ = \; & 16h_x^2J^2\sin(N-3)k + (C_kD_k - B_k^2)\sin(N-1)k. \end{aligned} \tag{6}$$

The momentum dependent coefficients are listed in the Appendix.

In non-magnetic impurity space, the Hamiltonian Eq. (2) becomes simpler since the impurity at the zeroth site is no longer coupled to its neighbor spins. The Hamiltonian $H_{(p=1)}$ can also be diagonalized by choosing almost the same trial wave function. The energy spectrum has almost the same form

$$\tilde{\Lambda}_k = \sqrt{4h_x^2 + 4J^2 + 8h_xJ\cos\tilde{k}}, \tag{7}$$

where the redefined wave vector $\tilde{k}$ is determined by a simple equation

$$[\sin N\tilde{k}/\sin(N+1)\tilde{k}] = -h_x/J \equiv -\lambda. \tag{8}$$

This equation can also be obtained from the secular equation Eq. (6) by choosing the couplings $J_{\rm L}$ and $J_{\rm R}$ as zero.

3. The impurity excitation and ground state

3.1. The impurity excitation

The lowest energy level represents the ground state. We compare the lowest energy level in both $p=0$ and $p=1$ space

$$E_0(p=0,x) = -\sum_k \Lambda(k)/2 - D_z, \tag{9}$$

$$E_0(p=1,x) = -\sum_{\tilde{k}} \Lambda(\tilde{k})/2 - D_x, \tag{10}$$

to find out which one is the ground state at different coupling strength. The momentum vectors k and $\tilde{k}$ must obey the secular equations (6) and (8). $x = J_{\rm imp}/J$ refers to the strength of impurity. We consider the special situation $J_{\rm R} = J_{\rm L} \equiv J_{\rm imp}$, and set $J = \hbar = k_{\rm B} \equiv 1$ without losing the generality.

The quantum critical behaviors of the system are related to the impurity excitation, which have two ways: the hole excitation gap Δ_h and the impurity fermion excitation gap Δ_x. The excitation gap is determined by the minimal energy for creating a hole or an impurity fermion from the ground states to the excited states. The impurity excitation gap $\Delta_{\rm imp} = \min\{\Delta_h, \Delta_x\}$ depends on the exchange coupling and single-ion anisotropic of impurity, and the competition of Δ_x and Δ_h can induce a switch of the ground state between the two subsystems $p=0$ and $p=1$. For a positive anisotropic interaction $D_z > 0$, the magnetic impurity subsystem $p=0$ has the lowest energy, so the ground state is confined in the magnetic impurity subspace. If the anisotropic interaction is zero $D_z = 0$, the system trends to a one-hole subsystem if and only if $J_{\rm imp} = 0$. For a negative anisotropic interaction $D_z < 0$, the non-magnetic impurity subsystem $p=1$ bears the lowest energy. Figure C1 in the Appendix C shows the exact dependence of ground state energy on the coupling strength between the impurity and its neighboring particles $x = J_{\rm imp}/J = J_{\rm L}/J = J_{\rm R}/J$. A rough approximation of this dependence is a negative parabola $E_{\rm Ground} \approx -(J_{\rm imp}/J)^2$. Thus a non-zero impurity coupling strength lowers the ground state energy.

Since the transverse Ising model has an exact solution of ground state energy, we can also exactly find the ground state energy of an impurity imbedded transverse Ising model. Here we are interested in how much energy arises for the ground state when an impurity is introduced into the Ising spin chain. We compute the impurity-induced deformation of the ground state $\Delta E(p,x)$ between a pure transverse Ising model and an impurity imbedded transverse Ising model

$$\Delta E(p,x) = E_{[0,\rm TIM]} - E_0(p,x). \tag{11}$$

Figure 1 shows the exact dependence of deformation on the impurity coupling strength and effective magnetic field. Figure 1(a) suggests that the ground state deformation is approximately a positive parabolic function of the impurity coupling. No matter whether the impurity coupling interaction is positive or negative, the deformation grows larger with the increase of the coupling. The minimal value appears when the impurity coupling becomes zero. Figure 1(b) shows that the deformation increases in an approximate linear way in the case of a weak magnetic field.

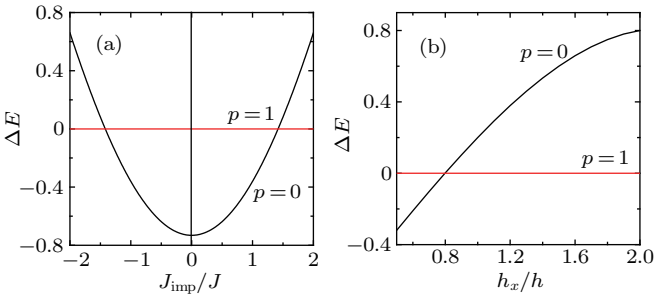


Fig. 1. (color online) (a) The dependence of impurity induced energy deformation $\Delta E(p,x)$ on the impurity coupling strength $J_{\rm imp}/J$. Here we choose $\lambda = h_x/J = 2$. (b) The dependence of impurity induced energy deformation on the effective magnetic field h_x/J. Here $x = J_{\rm imp}/J = 1$.

3.2. The impurity effects on the ground state

For the pure transverse Ising model without impurity, the quantum fluctuation due to a small effective magnetic field h_x tend to drive the spin chain away from an ordinary magnetic order, while the doping of an impurity into the spin chain enhances the disordered scattering. As shown by the impurity-induced deformation in Fig. 1, both the impurity coupling strength and effective magnetic field would enlarge the deformation. However, the impurity coupling strength demonstrates a faster promotion of the deformation than the effective magnetic field. When both of these factors have small values, the magnetic field plays a dominant role. Thus there is a competition between the impurity coupling strength and the effective magnetic field. The critical point lies at the balanced point of the two powers.

We exactly plotted the competitive relation of the impurity coupling strength and the effective magnetic field at the ground state in Fig. 2. The ground state of this impurity system is divided into three regions for the different impurity coupling strength $x(=J_{\rm imp}/J)$ and the effective magnetic field $\lambda(=h_x/J)$. Region I denotes a non-magnetic impurity space and there is a hole in this space for $p=1$. A trivial point joints the upper and lower critical lines together in the limit of $\lambda = 0$. Region II is a magnetic impurity space and the hole is diminished for $p=0$. The boundary between regions I and II is a jointed three-sectional curve with an apparent turning point. The transition between regions I and II is induced by the impurity. The ground state switches from non-magnetic impurity space $p=1$ to a magnetic impurity space $p=0$. The hole annihilates during this transition. Region III refers to magnetic-disordered due to the strong transverse magnetic field. The boundary between regions II and III is exactly at $|h_x| = J$, i.e., $\lambda = \pm 1$. A Z_2 symmetry breaking occurs here

when the ordered–disordered phase transition happens. In region III, the width is decided by crystal field D_x and the maximal and minimal points will join together when $D_x = D_z$.

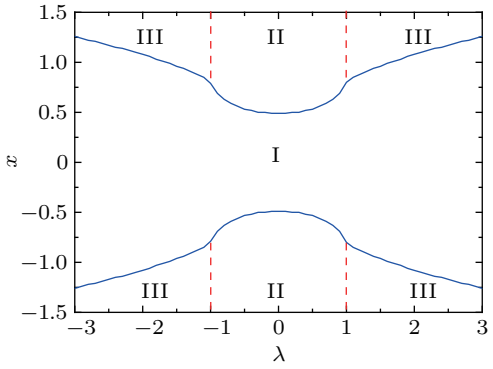


Fig. 2. (color online) The dependence of the ground state for x and λ, where $x = J_{\rm imp}/J$ denotes the impurity strength and $\lambda = h_x/J$ describes the competition mechanism between the Ising coupling and the transverse magnetic field.

4. Thermodynamic anomalous behavior induced by impurity

Specific heat as a thermodynamic quantity can demonstrate the quantum critical point.[33] For example, the specific heat of superfluid ^{4}He has a sharp peak at the temperature $T = 2.17$ K which marks the quantum phase transition from normal fluid to superfluid. We can exactly compute the specific heat of this impurity model based on HDS. The total partition function of this model is the sum of that of the two sectors, $Z = Z(p = 0) + Z(p = 1)$. As long as we have the partition function, the free energy, entropy, and specific heat can be computed exactly.

Figure 3 presents how specific heat evolves at finite temperature for different magnetic field strength $\lambda = h_x/J = 0.5, 1$, and 1.5. We note that there is no expected singularity, and only the λ-like peak has a small shift with the change of magnetic field strength. The specific heat decays faster for a larger magnetic field. At high temperature after the maximal point, the specific heat for a smaller magnetic field is always above the larger magnetic field. A strong magnetic field tends to bend spins into an order phase. In this case, the thermal fluctuation becomes relatively weaker, so its specific heat becomes smaller. However, the specific heat still exhibits the singular behavior in a multi-impurity spin system, since the configuration and concentration of impurity also can induce the phase transition when the parameters are larger than a critical value.[27]

We also calculate the specific heat coefficient at low temperatures for finite size, which is identical to the scaled free energy. From the specific heat coefficient we can observe the thermodynamic anomalous behavior in detail, which should be capable of yielding important information on the nature of the impurity.[34,35] In Fig. 4(a), we calculate the specific heat coefficient C/T at the quantum critical point $\lambda = h_x/J = 1$ within $x = J_{\rm imp}/J \in [0, 3]$. The specific heat coefficient converges to $\pi/12$ when temperature goes to zero $T \to 0$. This universal number $\pi/12$ is exactly the same as a pure $S = 1/2$ transverse Ising model. This suggests that the impurity system and the pure $S = 1/2$ transverse Ising model belong to the same universality class.

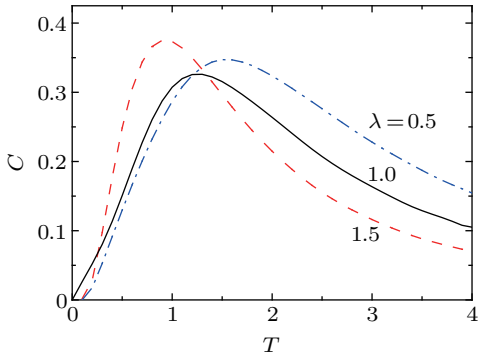


Fig. 3. (color online) The curve of specific heat C vs temperature T for different effective magnetic field $\lambda = h_x/J = 0, 5, 1.0$, and 1.5. In the computation, we chose $x = J_{\rm imp}/J = 1$, $D_z = -0.4J$, $D_x = 1.0J$, and $N = 2000$.

In Fig. 4(b), we show the temperature dependent specific heat coefficient for different impurity coupling strength x. For a large impurity coupling strength x, the specific heat coefficient is a monotonically growing curve. As x reduces, a small anomaly (or peak) began to appear. When $x = 0.9$, a sharp peak comes into being. This peak only occurs at very low temperature $T \in (0, 0.2J)$. This sharp peak suggests a thermal fluctuation. A strong impurity coupling strength freezes the system into a stable phase. Suppose that the impurity effect is strong enough to affect the block properties, e.g., adding the concentration of impurity, the quantum scattering that blocks particle transportation may also become weaker when the impurity coupling becomes weaker, then it is possible to transform an insulating state into a conducting state.

Notice that the impurity above is a spin-1 particle. One may ask if the spin-1 impurity is replaced by a special spin-1/2 particle, whether it would induce a similar anomaly or not. So we calculated $S = 1/2$ impurity in the same model as the $S = 1$ impurity. The light blue dash line in Fig. 4(c) corresponds to the specific heat coefficient of spin-1/2 impurity. It almost overlaps with the dark blue dash line which denotes the specific heat coefficient of a pure transverse Ising model. But the specific heat coefficient of spin-1 impurity is completely different from these two curves, above which a small plateau shows up at the low temperature region. So the spin-1 impurity is completely different from spin-1/2 impurity. Only $S = 1$ impurity could induce a singular peak at low temperature. The $S = 1$ impurity coupling strength could grow strong enough to suppress the singular peak, then it slides into a similar behavior like a pure transverse Ising model. Certainly, if the chain

length is increased, the small anomaly will be suppressed and even vanish as $N \to \infty$.

A closer observation on Fig. 4(b) tells us that the value of the exact temperature where the small peak locates is proportional to the hole gap Δ_h. For instance, the hole gap at different impurity coupling strength obeys the inequality $\Delta_h(x=0.9) < \Delta_h(x=0.6) < \Delta_h(x=1.0)$, while the critical temperature of the peak also obeys $T_c(x=0.9) < T_c(x=0.6) < T_c(x=1.0)$. This hints that the thermal fluctuations are induced by the hole excitation of impurity, in other words, it is the origin that the ground state switches from the magnetic impurity space to non-magnetic impurity space. For $x = 1.5$, the hole gap is about $0.9740J$ which is large enough, so this transition is not due to thermodynamical fluctuations. It is intrinsically related to the spin-1 quantum operator, and the eigenvalue of the spin-1 operator could be $[+1, 0, -1]$.

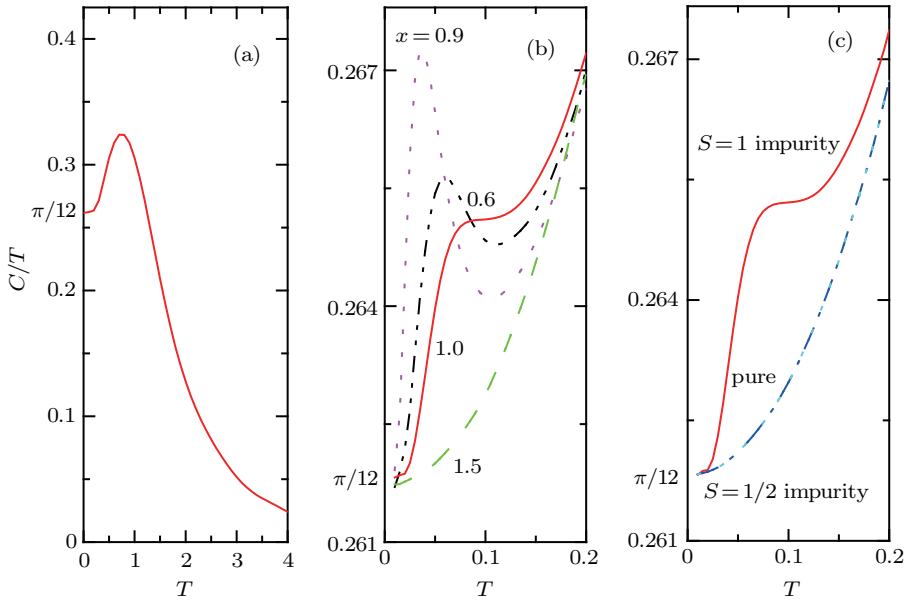


Fig. 4. (color online) The specific heat coefficients C/T vs temperature T for $\lambda = h_x/J = 1$, $D_z = -0.4J$, $D_x = 1.0J$, and $N = 2000$, (a) within the temperature window $T \in [0,4]$; (b) for the impurity strength $x = J_{\rm imp}/J = 0.6, 0.9, 1.0$, and 1.5 within the low temperature range of $[0, 0.2]$; (c) for the systems with $S = 1/2$ impurity (the light blue dashed line) and $S = 1$ impurity (the solid red line), and for the pure $S = 1/2$ Ising system (the dark blue dashed line), where $x = 1$.

5. Conclusion

Impurity models are only exactly solvable in some special cases. As the impurity breaks the translational invariant symmetry, it is hard to derive an exact result for a quantum impurity model. We exactly solved the transverse Ising model imbedded with an $S = 1$ quantum impurity. The Hilbert space of this model is divided into two spaces due to a conserved quantum operator, the hole operator. With this exact spectrum of ground state and excited states, we found that the impurity could enlarge the energy deformation of the ground state above a pure transverse Ising model. The deformation grows approximately linearly with respect to an effective magnetic field. We computed the dependence of the ground state on impurity parameters. There exists a tuned behavior of the ground state, which depends on the effective magnetic field and the impurity coupling strength. We computed the specific heat coefficient to explore the anomalous behavior at low temperature for finite size. The specific heat coefficient shows a sharp peak when the impurity coupling strength becomes weak enough. While this peak is the special transition point induced by spin-1 impurity, there is no such sharp transition point for a pure transverse Ising model and spin-1/2 impurity model. This transition point indicates the switch of the ground state from a magnetic impurity space to a non-magnetic impurity space. Since the magnetic impurity space to a non-magnetic impurity space is determined by the eigenvalue of the conserved quantum operator of spin-1, it is essentially a competition of hole excitation and fermion excitation. As the spin-1 impurity could induce some special thermodynamics, it maybe also has some exotic effect on the quantum entanglement at low temperature. In the future, we shall study the quantum entanglement, geometric phase, and potential topological phases.

Appendix A: $p = 0$ sector

Considering the effect of impurities, we choose the wave function for $p = 0$ sector

$$\Phi(j) = \begin{cases} A_k \mathrm{e}^{\mathrm{i}kj} + A_k \mathrm{e}^{\mathrm{i}\varphi} \mathrm{e}^{-\mathrm{i}kj}, & j = 1, 2, \cdots, N, \\ \Phi(0), & j = 0, \end{cases} \tag{A1}$$

where the displacement quantity φ is the function of k, and indicates that the particles of spin $1/2$ are effected by impurity. Defining

$$a = 4h^2 + 4J^2, \quad a_0 = 4h_0^2 + 4J_{\rm L}^2, \quad a_1 = 4h^2 + 4J_{\rm R}^2,$$
$$b = 4hJ, \quad b_0 = 4h_0 J_{\rm R}, \quad b_1 = 4hJ_{\rm L},$$

we have

$$M\Phi = \Lambda_k^2 \Phi, \tag{A2}$$

where M is an $(N+1)\times(N+1)$ symmetric matrix, $M_{01} = a_0$, $M_{02} = b_0$, $M_{0N} = b_1$, $M_{11} = a_1$, and for the other case $M_{ii} = a$, $M_{i,i+1} = b$.

If we define

$$A_1 = \frac{b_0 b_1}{\Lambda^2(k) - a_0}, \quad B_1 = \frac{b_0^2}{\Lambda^2(k) - a_0} + a_1 - \Lambda^2(k),$$
$$A_2 = \frac{b_1^2}{\Lambda^2(k) - a_0} + a - \Lambda^2(k), B_2 = A_1,$$

we could get the secular equation

$$b(A_1 + B_2)\sin k - b(B_1 + A_2)\sin(N-2)k$$
$$= b^2 \sin(N-3)k + (B_1 A_2 - A_1 B_2)\sin(N-1)k.$$

The trial wave function for the impurity is $\Phi(0)$, and we have

$$\begin{pmatrix} \Phi(0) = \Phi(0) \\ \Phi(1) = A_k \mathrm{e}^{\frac{\mathrm{i}\varphi}{2}}(\mathrm{e}^{\mathrm{i}k - \frac{\mathrm{i}\varphi}{2}} + \mathrm{e}^{-\mathrm{i}k + \frac{\mathrm{i}\varphi}{2}}) \\ \Phi(2) = A_k \mathrm{e}^{\frac{\mathrm{i}\varphi}{2}}(\mathrm{e}^{2\mathrm{i}(k - \frac{\varphi}{4})} + \mathrm{e}^{-\mathrm{i}2(k - \frac{\varphi}{4})}) \\ \vdots \\ \Phi(N) = A_k \mathrm{e}^{\frac{\mathrm{i}\varphi}{2}}(\mathrm{e}^{\mathrm{i}(k - \frac{\varphi}{2N})N} + \mathrm{e}^{-\mathrm{i}(k - \frac{\varphi}{2N})N}) \end{pmatrix}. \tag{A3}$$

The secular equation can be obtained from Eq. (4), which reads

$$8h_x J B_k \sin k - 4h_x J(C_k + D_k)\sin(N-2)k$$
$$= 16h_x^2 J^2 \sin(N-3)k + (C_k D_k - B_k^2)\sin(N-1)k, \tag{A4}$$

where

$$B_k = \frac{16h_x D_x J_\mathrm{R} J_\mathrm{L}}{\Lambda^2(k) - 4D_x^2 - 4J_\mathrm{L}^2},$$
$$C_k = \frac{16D_x^2 J_\mathrm{R}^2}{\Lambda^2(k) - 4D_x^2 - 4J_\mathrm{L}^2} + 4h_x^2 + 4J_\mathrm{R}^2 - \Lambda^2(k),$$
$$D_k = \frac{16h_x^2 J_\mathrm{L}^2}{\Lambda^2(k) - 4D_x^2 - 4J_\mathrm{L}^2} + 4h_x^2 + 4J^2 - \Lambda^2(k).$$

The deflection factor φ is determined by $\mathrm{e}^{\mathrm{i}\varphi} = -\frac{f(k)}{f(-k)}$, where

$$f(k) = C_k \mathrm{e}^{\mathrm{i}k} + B_k \mathrm{e}^{\mathrm{i}kN} + 4h_x J \mathrm{e}^{2\mathrm{i}k}. \tag{A5}$$

Appendix B: $p = 1$ sector

For there is only one impurity, in the $N_0 = 1$ sector the Hamiltonian is the transverse Ising chain with a hole and the open boundary, and the displacement $\delta = 0$. The wave function is $\Phi(k) = A_k \sin(kj), j = 1, \ldots, N$. The M matrix is

$$M = \begin{pmatrix} a_2 & b & 0 & \ldots & 0 & 0 \\ b & a & b & \ldots & 0 & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & \ldots & b & a & b \\ 0 & 0 & \ldots & 0 & b & a \end{pmatrix}, \tag{B1}$$

where $a_2 = 4h^2$. Thus, the secular equation in the $p = 1$ sector is

$$\frac{\sin Nk}{\sin(N+1)k} = -h_x/J \equiv -\lambda. \tag{B2}$$

Appendix C: the ground state energy

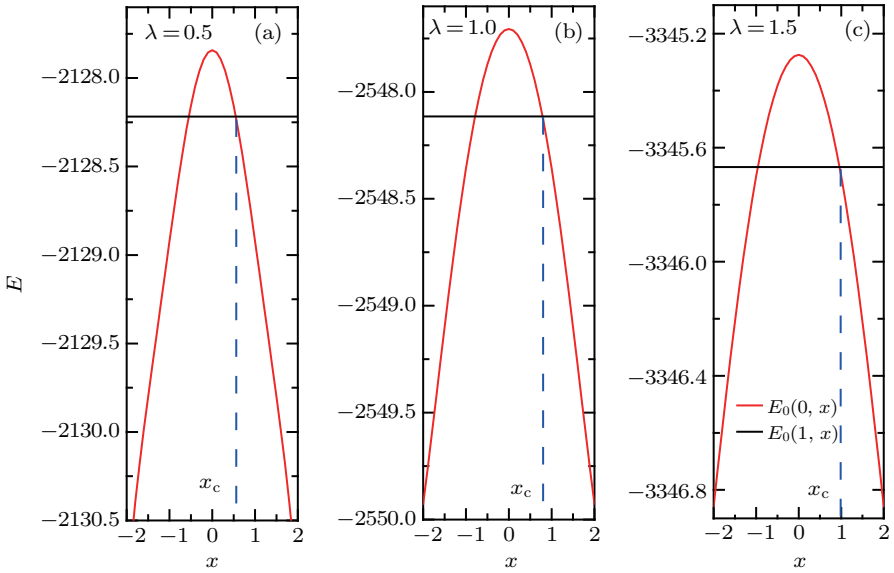


Fig. C1. (color online) The lowest energy in $p = 0$, 1 subsystems dependent on the impurity strength x at $D_z = -0.4J$ and $D_x = 1.0J$.

Acknowledgment

The author thanks Prof. Zhihua Yang(Xinjiang Technical Institute of Physics & Chemistry, CAS) and Dr. Tieyan Si(Harbin Institute of Technology) for their valuable suggestion.

References

[1] Balents L 2010 *Nature* **464** 199
[2] Gopalan S, Rice T M and Sigrist M 1994 *Phys. Rev. B* **49** 8901
[3] Binder K and Young A P 1986 *Rev. Mod. Phys.* **58** 801
[4] Fisher D S and Huse D A 1986 *Phys. Rev. Lett.* **56** 1601
[5] Dioguardi A P, Crocker J, Shockley A C, Lin C H, Shirer K R, Nisson D M, Lawson M M, apRoberts-Warren N, Canfield P C, Bud'ko S L, Ran S and Curro N J 2013 *Phys. Rev. Lett.* **111** 207201
[6] Yuan Z G and Zhang P 2015 *Chin. Phys. Lett.* **32** 60301
[7] Pasupathy A N, Bialczak R C, Martinek J, Grose J E, Donev L A K, McEuen P L and Ralph D C 2004 *Science* **306** 86
[8] Nishida Y 2013 *Phys. Rev. Lett.* **111** 135301
[9] Zhang Y H, Kahle S, Herden T, Stroh C, Mayor M, Schlickum U, Ternes M, Wahl P and Kern K 2013 *Nat. Commun.* **4** 2110
[10] Chen J J, Duan J Z, Zhang X Z, Jiang X and Duan W S 2015 *Acta Phys. Sin.* **64** 0238101 (in Chinese)
[11] Liao K S, Li Z F, Li L, Wang C, Zhou X H, Dai N and Li N 2015 *Acta Phys. Sin.* **64** 227302 (in Chinese)
[12] Hase M, Terasaki I and Uchinokura K 1993 *Phys. Rev. Lett.* **70** 3651
[13] Uchiyama Y, Sasago Y, Tsukada I, Uchinokura K, Zheludev A, Hayashi T, Miura N and Böni P 1999 *Phys. Rev. Lett.* **83** 632
[14] Fujiwara N, Yasuoka H, Fujishiro Y, Azuma M and Takano M 1998 *Phys. Rev. Lett.* **80** 604
[15] Shender E F and Kivelson S A 1991 *Phys. Rev. Lett.* **66** 2384
[16] Bobroff J, Laflorencie N, Alexander L K, Mahajan A V, Koteswararao B and Mendels P 2009 *Phys. Rev. Lett.* **103** 047201
[17] Simutis G, Gvasaliya S, Mansson M, Chernyshev A L, Mohan A, Singh S, Hess C, Savici A T, Kolesnikov A I, Piovano A, Perring T, Zaliznyak I, Buchner B and Zheludev A 2013 *Phys. Rev. Lett.* **111** 067204
[18] Kane C L and Fisher M P A 1992 *Phys. Rev. B* **46** 15233
[19] Yang L J, Cao J P and Yang W L 2015 *Chin. Phys. B* **24** 107502
[20] Andrei N and Johannesson H 1984 *Phys. Lett. A* **100** 108
[21] Lee K J B and Schlottmann P 1988 *Phys. Rev. B* **37** 379
[22] Qiao J and Zhou B 2015 *Chin. Phys. B* **24** 110306
[23] Oitmaa J and von Brasch A M A 2003 *Phys. Rev. B* **67** 172402
[24] Oitmaa J and Zheng W 2003 *Physica A* **328** 185
[25] Yang Z H, Yang L P, Dai J H and Xiang T 2008 *Phys. Rev. Lett.* **100** 067203
[26] Huang X C and Yang Z H 2015 *J. Magn. Magn. Mater.* **381** 372
[27] Huang X C and Yang Z H 2015 *Solid State Commun.* **204** 28
[28] Eggert S and Affleck I 1992 *Phys. Rev. B* **46** 10866
[29] Schlottmann P 2000 *Nucl. Phys. B* **565** 535
[30] Yang Z H, Yang L P, Wu H N, Dai J H and Xiang T 2009 *Phys. Rev. B* **79** 214427
[31] Jordan P and Wigner E 1928 *Z. Phys.* **47** 631
[32] Zvyagin A A 1997 *Phys. Rev. Lett.* **79** 4641
[33] Yuan Z G and Zhang P 2015 *Chin. Phys. Lett.* **32** 060301
[34] Ando Y, Miyamoto N, Segawa K, Kawata T and Terasaki I 1999 *Phys. Rev. B* **60** 10580
[35] Custers J, Gegenwart P, Wilhelm H, Neumaier K, Tokiwa Y, Trovarelli O, Geibel C, Steglich F, Pépin C and Coleman P 2003 *Nature* **424** 524