Quantum phase transition induced by local defects in Heisenberg spin chains

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We propose a model of one-dimensional Heisenberg spin chain with a single local defect attached to one end of the spin chain which exhibits nontrivial quantum phase transition in the parameter space characterizing the local defect. By calculating the ground state energy, entanglement entropy, and total spin of the system using density matrix renormalization group, we found that a quantum phase transition, which is robust enough to survive in the thermodynamic limit, always exists when the defect is symmetric with respect to the spin chain. On the other hand, in the absence of this symmetry, the quantum phase transition only remains in systems with even number of spin sites. The quantum phase transition is characterized by crossover of two energy functions along with discontinuous total spin (in systems with even number of spin sites) and entanglement entropy at the critical point in the parameter space.

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I. INTRODUCTION

The one-dimensional (1D) spin-1/2 quantum Heisenberg model1–4 can be solved analytically by the Bethe ansatz method for regular lattice with periodic boundary conditions. In realistic situations, magnetic defects widely exist and can affect the properties of the otherwise perfectly ordered systems. In particularly shown in Fig. 1, consists of a finite 1D spin chain with a triangle defect formed by two extra spin sites (labeled as \(a\) and \(b\)) connecting to spin site \(N\), we call the system a 1D spin chain with a triangle defect. The total Hamiltonian \(H\) of the system can be expressed as the sum of a regular part,

\[
H_t = J \sum_{i=1}^{N-1} S_i \cdot S_{i+1},
\]

a part of the defect,

\[
H_d(g) = g S_a \cdot S_b,
\]

and an interaction part,

\[
H_i = \alpha S_N \cdot S_a + \beta S_N \cdot S_b.
\]

To be specific, we only consider antiferromagnetic spin-1/2 systems with \(J > 0\) and set \(J = 1\). The components of the spin vector \(S\) are \(S_\alpha = \sigma_\alpha/2\) (\(\alpha = x, y, z\)), \(\sigma_\alpha\) being the Pauli matrices acting on the relevant subspace (corresponding to the spin site) of the \(2^{(N+2)}\)-dimensional Hilbert space. The parameter \(g\), introduced to characterize the defect, can be adjusted by varying the distance between \(a\) and \(b\). Generally, when their distance is larger (smaller) than the lattice constant of the regular chain, \(g\) will be smaller (larger) than 1. The parameters \(\alpha\) and \(\beta\), which characterize the interaction between the regular part and the defect part, can be either the same (symmetric defect with \(\mathbb{Z}_2\) symmetry) or different (asymmetric defect).

II. MODEL OF SPIN CHAIN WITH LOCAL DEFECT

The physical system studied in this paper, as schematically shown in Fig. 1, consists of a finite 1D spin chain (with the spin sites being labeled from 1 to \(N\)) and two extra spin sites (labeled as \(a\) and \(b\)) connecting to spin site \(N\). Since \(N\), \(a\), and \(b\) form a triangle, we call the system a 1D spin chain with a triangle defect. The total Hamiltonian \(H\) of the system can be expressed as the...
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FIG. 2. (Color online) Eigenenergies as a function of $g$ for the $N=1$ (a) and $N=2$ (b) spin chains with symmetric triangle defect. Solid and dashed lines correspond to the lowest two energy functions and the open circles denote the crossover points of them, which are $g_c = 1$ and $g_c = 0.5$ for $N = 1$ and $N = 2$, respectively.

We first consider the case of symmetric defect, $\alpha = \beta$. To be specific, we set $\alpha = \beta = 1$. In this case $H_d$ commutes with the total Hamiltonian. Therefore, the ground state of the total system comes from eigenstates of $H_d$, which are linear functions of $g$, as demonstrated explicitly below.

We begin with the simplest case where $N = 1$. The total Hamiltonian can be rewritten as

$$H = \frac{1}{2} \left( (S_a + S_b + S_1)^2 - (S_a + S_b + S_1)^2 - S_2^2 \right) + \frac{g}{2} \left( (S_a + S_b)^2 - S_a^2 - S_b^2 \right). \quad (4)$$

The eigenstates of $H$ are degenerate and can be classified by the total spins corresponding to the operators $(S_1 + S_a + S_b)^2$ and $(S_a + S_b)^2$, which can take the following values: $(1, 0)$, $(\frac{3}{2}, 1)$, and $(\frac{1}{2}, 1)$. The eigenenergies as a function of $g$ corresponding to these sets of eigenvalues are $E(g) = -\frac{2}{3}g + \frac{1}{2}g$, and $-\frac{1}{2} + \frac{1}{2}g$. There is a crossover of the lowest two energy functions, occurring at $g_c = 1$, as shown in Fig. 2(a).

Analytical results for the case of $N = 2$ can be obtained similarly. The total Hamiltonian can be written as

$$H = \frac{1}{2} \left( (S_a + S_b + S_1 + S_2)^2 - (S_a + S_b + S_1 + S_2)^2 - S_2^2 \right) + \frac{g}{2} \left( (S_a + S_b)^2 - S_a^2 - S_b^2 \right).$$

(5)

The eigenstates of $H$ can be classified by the total spins corresponding to the operators $(S_1 + S_2 + S_a + S_b)^2$, $(S_1 + S_2 + S_a + S_b)^2$, and $(S_a + S_b + S_2)^2$, which can take the following values: $(2, \frac{3}{2}, 1), (\frac{3}{2}, 1, 1), (\frac{1}{2}, 1), (0, \frac{3}{2}, 1), (1, \frac{1}{2}, 0)$, and $(0, 0, 0)$. The corresponding energy functions are $E(g) = \frac{3}{4} + \frac{1}{2}g$, $\frac{3}{8} + \frac{1}{2}g$, $\frac{1}{2} + \frac{1}{2}g$, $-\frac{1}{2} + \frac{1}{2}g$, $\frac{1}{4} + \frac{1}{2}g$, and $-\frac{1}{4} - \frac{1}{2}g$. There is a crossover of the lowest two energy functions occurring at $g_c = 1/2$, as shown in Fig. 2(b).

Due to the crossover of the energy functions with varying $g$, the wave function of the ground state changes abruptly from $g < g_c$ to $g > g_c$. This suggests that $g_c$ is the critical point of a quantum phase transition at zero temperature. To further explore the nature of the quantum phase transition with varying $g$, we use the DMRG method to numerically calculate the ground state energy, the bipartite entanglement entropy (in terms of the Von Neumann entropy of the reduced density matrix with an appropriate bipartition of the system), and the total spin of systems with larger $N$.

To be specific, we first consider the cases with $N = 42$ and $N = 41$. The results are shown in Fig. 3. The ground state energy in each case jumps from one type of eigenstate to another at the critical point, which is found to be about $g_c = 0.66$ and $g_c = 0.72$ for $N = 42$ and $N = 41$, respectively. Associated with the crossover of the energy functions, there is an abrupt upward (downward) jump of the bipartite entanglement entropy in the $N = 42$ ($N = 41$) system, regardless of the way of bipartition. More interestingly, the total spin of the $N = 42$ system changes from 0 to 1 as $g$ approaches $g_c$ from above, which means that there is a quantum phase transition from the conventional antiferromagnetic phase to another new phase. On the other hand, the $N = 41$ system exhibits a constant total spin of 1/2 for all $g$ values, presumably due to the lack of full pairing in a system with an odd number of spin sites. In both sides of $g_c$, the ground state energy is linear with respect to $g$, while the entropy and total spin keep constant, due to the commutative property $[H_d, H] = 0$. Therefore, the ground state in each side defines a phase with definite properties (except for the energy) which are invariant with varying $g$. 
The quantum phase transition exists in systems with arbitrary \( N \). The eigenvalue of \( H_4 \) is \( E_4(g) = \frac{4}{3} g \) when \( g \to -\infty \) and \( E_4(g) = -\frac{4}{3} g \) when \( g \to +\infty \). Since \([H_4, H] = 0\), the ground state energy \( E_{gs}(g) \) of the whole system has the same \( g \)-dependence as \( E_4(g) \) in each limit, which results in an unavoidable turning point of \( E_{gs}(g) \) in the \( g \)-space. This turning point is exactly the critical point \( g_c \). Our numerical results, as presented in Fig. 4(a), show that \( g_c \) lies in the interval of \([0.5, 1.0]\) and increases (decreases) monotonically for even (odd) \( N \). The values of \( g_c \) for even and odd \( N \) may or may not converge to the same value in the thermodynamic limit of \( N \to \infty \). The difference of the entanglement entropy between the phase with \( g > g_c \) and the phase with \( g < g_c \), \( \Delta S = S(g > g_c) - S(g < g_c) \), also shows a trend of convergence to a finite value with increasing \( N \) for both even and odd \( N \), as can be seen from Fig. 4(b). Therefore, the quantum phase transition in the \( g \)-space caused by the single local defect is robust enough to survive in the thermodynamic limit.

**IV. QUANTUM PHASE TRANSITION IN SPIN CHAINS WITH ASYMMETRIC DEFECT**

We next consider the case of asymmetric defect, \( \alpha \neq \beta \), in which case \( H_4 \) and \( H \) do not commute. To be specific, we consider the case in which \( \alpha < 1 \) and \( \beta = 1 \). We use DMRG to calculate the ground state energy, bipartite entanglement entropy, and total spin for different values of \( \alpha \): 0.5, 0.6, 0.7, 0.8, 0.9, and 1, the last being the symmetric case.

The results for systems with \( N = 42 \) and \( N = 41 \) are presented in Fig. 5. The energy functions for all the \( \alpha \) values in the \( N = 42 \) system still develop a relatively sharp turning point \( g_c \) in the \( g \)-space, although they are not strictly straight around \( g = g_c \). This suggests that quantum phase transition in the \( g \)-space may still be possible. More convincing evidence comes from the behaviors of entanglement entropy and total spin, both of which change abruptly at the same critical points. In accordance with the bending of the energy function, the entropy is not invariant but converges to a constant with increasing \( g \) in the phase with \( g > g_c \), different from the symmetric case with \( \alpha = \beta \). The total spin, on the other hand, still keeps a constant value of 1 in the phase with \( g < g_c \) and 0 in the phase with \( g > g_c \). We have checked that the quantum phase transition survives in the thermodynamic limit.

Different from the case of systems with even \( N \), systems with odd \( N \) do not develop a quantum phase transition in the \( g \)-space when \( \alpha \neq \beta \), as evidenced by the smooth energy functions and continuous entropy functions shown in Figs. 4(d-e). The total spins, as in the case of \( \alpha = \beta \), are always 1/2 due to an extra unpaired spin in odd-\( N \) systems.

To better understand the different behaviors in systems with even and odd \( N \), we perform perturbative analysis in the limit of \( |x| = |\alpha - 1| << 1 \) (\( \beta \) is fixed to 1). The unperturbed system with \( \alpha = \beta = 1 \) can be approximated by a two-level system with states \(|1\rangle \) and \(|2\rangle \) and energies \( E_1(g) \) and \( E_2(g) \) close to the critical point \( g = g_c \). The effective Hamiltonian with the addition of the perturbation reads

\[
H_{\text{eff}} = \left( \begin{array}{cc} E_1(g) + xV_{11} & xV_{12} \\ xV_{21} & E_2(g) + xV_{22} \end{array} \right)
\]

where \( V_{ij} \equiv \langle i|S_N \cdot S_i|j\rangle \) \((i,j = 1,2)\). The eigenvalues of the effective Hamiltonian can be solved analytically,

\[
E_{\pm} = \frac{E_1(g) + xV_{11} + E_2(g) + xV_{22} \pm \sqrt{\Delta}}{2},
\]

where \( \Delta = [(E_1(g) + xV_{11}) - (E_2(g) + xV_{22})]^2 + 4x^2|V_{12}|^2 \). An energy gap would open up if \( \Delta \neq 0 \) for all \( g \) and unavoidable crossover of energy functions only remains when \( V_{12} = 0 \). Although a rigorous proof is yet to be found, we have confirmed numerically that \( V_{12} = 0 \) \((V_{12} \neq 0)\) for even (odd) \( N \). Therefore, the quantum phase transition in the \( g \)-space remains in even-\( N \) systems due to the unavoidable crossover of the energy functions but disappears in odd-\( N \) systems due to the energy gap opened up by the uncompensated interaction between the spin sites \( N \) and \( a \) when \( \alpha \neq \beta \) \((x \neq 0)\).

**V. CONCLUSIONS**

In summary, we have proposed a model of one-dimensional Heisenberg spin chain with a single local defect attached to one end of the chain and studied its ground state properties, including ground state energy, entanglement entropy, and total spin, by density matrix renormalization group calculations. The local defect is characterized by an interaction strength \( g \). When the local defect has a \( Z_2 \) symmetry with respect to the spin chain, the is always a quantum phase transition in the \( g \)-space, which is caused by an unavoidable crossover of the lowest two energy functions which have distinct properties. The total spin (only in systems with even number
of spin sites) and entanglement entropy are discontinuous at the critical point but keep constant away from it. This quantum phase transition is robust and survives in the thermodynamic limit. When the $Z_2$ symmetry is broken, the quantum phase transition remains for systems with even number of spin sites, but vanishes for systems with odd number of spin sites.

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