Physica B 462 (2015) 25–29

Contents lists available at ScienceDirect

Physica B

journal homepage: www.elsevier.com/locate/physb

Quantum entanglement investigation on impurity effects in the transverse Ising chain

Xuchu Huang [a,b], Tieyan Si [c], Zhihua Yang [a,*]

[a] Key Laboratory of Functional Materials and Devices for Special Environments of CAS, Xinjiang Technical Institute of Physics & Chemistry of CAS, 40-1 South Beijing Road, Urumqi 830011, China
[b] University of Chinese Academy of Sciences, Beijing 100049, China
[c] Harbin Institution of Technology, 92 West Dazhi Street, Nan Gang District, Harbin 150001, China

ARTICLE INFO

Article history:
Received 4 August 2014
Received in revised form
9 December 2014
Accepted 12 January 2015
Available online 13 January 2015

Keywords:
Impurity effect
Quantum entanglement
Correlation function
Concurrence

ABSTRACT

The impurity effects of the transverse Ising spin model with a magnetic impurity are investigated via the correlation function and entanglement on the basis of an exact solution. The non-analytical transition point from an ordered phase to a disorder phase is significantly shifted by the impurity coupling with local host spins. The maximal entanglement point which usually appears around the critical point shows strong dependence on the impurity coupling strength with local host spin and the independent transverse field upon the impurity itself. Quantum entanglement in disordered spin phase is much stronger than that in ordered spin phase. The exact concurrence of impurity spin with local host spin suddenly increases to a large value from zero at a threshold value. The maximal entanglement point between impurity and local host spin increases as the impurity coupling strength increases. So the impurity coupling strength and local transverse field on the impurity can control position of critical point and maximal entanglement point.

1. Introduction

Non-thermal physical parameters can control the quantum phase transition induced by quantum fluctuation at zero temperature [1,2]. The most frequently investigated non-thermal parameter is quantum entanglement of many body system. As revealed by many recent researches on quantum models of spin-1/2 chains [3–5], entanglement act as a critical ingredient for the occurrence of quantum phase transition. Quantum entanglement in condensed matter system also provides a promising physical implementation of quantum information theory [6–8]. Quantum entanglement in quantum many body system with impurity demonstrates many interesting phenomena since a few impurities can induce a significant transformation of magnetic order in different quantum phases [9–12]. Even if the impurity is a non-magnetic particle which does not break spin-rotational symmetry, such as a random bond, an interstitial spin or a vacancy, the highly degenerated states of the pristine system are still locally distinguishable [13].

Recently there is an increasing numerical research interest on quantum entanglement of impurity system [14–18]. Osenda et al. numerically studied an anisotropy XY model with an impurity in periodic boundary condition, it shows that the entanglement strongly depends on the anisotropy parameter and the impurity parameter [19]. Wang investigated an XY model with an impurity in open boundary condition by numerical method, and found that the entanglement between the impurity and the nearest neighbor host admits a threshold value which depends on the impurity strength [20]. LeHur studied the impurity entanglement in spin-boson model using bosonic numerical renormalization group method, it exhibits a second-order quantum phase transition [21]. Quantum Monte Carlo method and the density matrix renormalization group method also made progress in studying quantum entanglement of impurity system [22,23].

Despite the rapid development of numerical research on entanglement of impurity system, the theoretical research based on exact solution of quantum impurity system is rare due to the high difficulty of finding an exact solution of quantum impurity system. The latest progress on the exact solution of quantum impurity problem is made in 1984 by Andrei and Johannesson, they found the integrable model of the Heisenberg chain with impurities in periodic boundary condition [24]. An impurity of spin $S > 1/2$ is embedded in a spin-1/2 Heisenberg chain. The exact solution was derived by Bethe Ansatz [24]. However this method for exact solution based on Bethe Ansatz is not suitable for two or three dimensional Heisenberg model. It only works for one dimensional

* Corresponding author.
E-mail address: zhyang@ms.xjb.ac.cn (Z. Yang).

http://dx.doi.org/10.1016/j.physb.2015.01.007
0921-4526/

chain.

In this paper, we propose an exact method for solving spin models with impurity. By introducing a proper wave function the information of impurity site can be expressed by other sites, so this method not only works for one dimensional spin chain, but also can be generalized and applied to two or three dimensional transverse Ising model. The general procedure is first to transform the Pauli spin operators to Fermi operators, then express the wave function of impurity by a displacement quantity. Based on the exact solution of transverse Ising model, we computed the spin–spin correlation both in short and long-range order, and the entanglement of the ground state. The impurity spin produces a small disturbance to the short and long-range order near the critical point, but it does not change the short and long-range order transition in the transverse Ising model. The entanglement between the impurity and the analysis of neighbor host shows singular behaviors at a threshold value of impurity parameter. This threshold value can be reduced by the impurity strength. While the magnitude of the small entanglement peak can be reduced by the local transverse field of impurity.

The structure of this paper is as follows. In Section 2 the exact solution of this model is outlined. The short and long-range correlation functions are considered in Section 3. The nearest-neighbor entanglement is calculated in Section 4. In Section 5 we discussed the effect of impurity on short and long range order and some outlooks for the future.

2. The quantum impurity model

An impurity spin is introduced into the transverse Ising model with periodic boundary condition:

$$H = -\sum_{j=1}^{N-1} J\sigma_j^x\sigma_{j+1}^x - h\sum_{j=1}^{N}\sigma_j^z - J_L\sigma_1^x S_0^x - J_R\sigma_N^x S_0^x - h_0 S_0^z. \quad (1)$$

Here the index of the spin operators i and j could be two dimensional spatial index and three dimensional index, here we use a single letter for brevity. σ_j^α $(\alpha = x, y, z)$ is the Pauli matrix which indicates the host sites for $j = 1, \ldots, N$, and S_0^α $(\alpha = x, y, z)$ indicates a spin-1/2 magnetic impurity at the zeroth site, h_0 refers to the local transverse field of impurity. The interaction strength parameters are renormalized by spin coupling coefficient J. In the following text, $\lambda = h/J$ indicates the competition between the Ising coupling and the transverse field. Without losing the generality, we set $J_L = J_R = J_{imp}$ and $\gamma = J_{imp}/J$ to express the impurity strength. The Hamiltonian equation (1) is diagonalized by Jordan–Wigner transformation [25] to express Pauli operators by Fermi operators [26,27]. On the basis of Jordan–Wigner transformation, we introduce the Bogoliubov transformation as follows:

$$\eta_k = \sum_j (g_{kj}c_j + h_{kj}c_j^\dagger), \quad \eta_k^\dagger = \sum_j (g_{kj}^* c_j + h_{kj}^* c_j^\dagger), \quad (2)$$

where $\eta_k^\dagger, \eta_k$ are fermionic quasi-particle operators with quasi-momentum k, c_j, $c_j^\dagger$ are Fermi operators in Jordan–Wigner transformation, and g_{kj}, h_{kj} should be complex in general. Then we can derive a compact Hamiltonian:

$$H = \sum_k \Lambda(k)(\eta_k^\dagger\eta_k - 1/2), \quad (3)$$

$\Lambda(k)$ is the energy spectrum. We chose the trial wave functions as

$$\Phi_k(j) = \begin{cases} A_k(e^{ikj} + e^{i\varphi}e^{-ikj}), & j = 1, \ldots, N \\ \Phi_k(0), & j = 0, \end{cases} \quad (4)$$

where A_k is the normalization constant, j denotes the location of spin site. The displacement quantity φ is introduced as the function of k to include the influence of impurity. So the element $\Phi_k(0)$ of the wave function as an unknown parameter can be expressed by other elements. If we define $\Phi_k(j) = g_{kj} + h_{kj}$, $\Psi_k(j) = g_{kj} - h_{kj}$, and combine the trial wave function equation (4) into the eigenvalue equation (3), we get the energy spectra and the zeroth order wave function $\Phi_k(0)$:

$$\Lambda(k) = 2\sqrt{h^2 + J^2 + 2hJ\cos k}, \quad (5)$$

$$\Phi_k(0) = \frac{hJ_L\Phi_k(N) + h_0J_R\Phi_k(1)}{h^2 - h_0^2 + J^2 - J_L^2 + 2hJ\cos k}. \quad (6)$$

Here the wave vector k is determined by the secular equation

$$8ah_xJ\sin k - 4h_xJ(b+c)\sin(N-2)k = 16h_x^2J^2\sin(N-3)k + (bc - a^2)\sin(N-1)k. \quad (7)$$

The three parameters in the secular equations are

$$a = \frac{16hh_0J_RJ_L}{\Lambda^2(k) - 4h_0^2 - 4J_L^2},$$

$$b = \frac{16h_0^2J_R^2}{\Lambda^2(k) - 4h_0^2 - 4J_L^2} + 4h^2 + 4J_R^2 - \Lambda^2(k),$$

$$c = \frac{16h^2J_L^2}{\Lambda^2(k) - 4h_0^2 - 4J_L^2} + 4h^2 + 4J^2 - \Lambda^2(k).$$

The displacement quantity $e^{i\varphi} = -F(k)/F(-k)$ also depends on these three parameters above as well as the Ising coupling strength, $F(k) = be^{ik} + ae^{ikN} + 4hJe^{2ik}$. The ground state energy directly reads $E_0 = -\frac{1}{2}\sum_k \Lambda(k)$. The excited state above ground state can be interpreted as fermion excitation [28].

3. Effects of impurity on short range and long range order

We first study how the short range and long range order parameter behaves at different impurity coupling strength. The spin–spin correlation function between two spins separated by arbitrary distance is calculated [26,29], $\rho_{i,j}^{\alpha\beta} = \langle\sigma_i^\alpha\sigma_j^\beta\rangle(\alpha, \beta = x, y, z)$, $\rho_i^z = \langle\sigma_i^z\rangle$. The spin–spin correlation functions are given by [26]

$$\langle\sigma_i^x\sigma_j^x\rangle = \begin{bmatrix} G_{i,i+1} & G_{i,i+2} & \cdots & G_{ij} \\ \vdots & & & \vdots \\ G_{j-1,i+1} & \cdots & & G_{j-1,j} \end{bmatrix},$$

$$\langle\sigma_i^y\sigma_j^y\rangle = \begin{bmatrix} G_{i+1,i} & G_{i+1,i+1} & \cdots & G_{i+1,j-1} \\ \vdots & & & \vdots \\ G_{ij} & \cdots & & G_{j,j-1} \end{bmatrix},$$

$$\langle\sigma_i^z\sigma_j^z\rangle = (G_{ii}G_{jj} - G_{ji}G_{ij}), \quad \langle\sigma_i^z\rangle = G_{ii}. \quad (8)$$

From the inverse transformation of η_k, $\eta_k^\dagger$

$$c_j^\dagger = \sum_k \frac{\Phi_k(j) + \Psi_k(j)}{2}\eta_k^\dagger + \frac{\Phi_k^*(j) - \Psi_k^*(j)}{2}\eta_k,$$

$$c_j = \sum_k \frac{\Phi_k^*(j) + \Psi_k^*(j)}{2}\eta_k + \frac{\Phi_k(j) - \Psi_k(j)}{2}\eta_k^\dagger, \quad (9)$$