Entanglement and quantum phase transition in the Heisenberg–Ising model

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We use the quantum renormalization-group (QRG) method to study the entanglement and quantum phase transition (QPT) in the one-dimensional spin-1/2 Heisenberg–Ising model [Lieb E, Schultz T and Mattis D 1961 Ann. Phys. (N.Y.) **16** 407]. We find the quantum phase boundary of this model by investigating the evolution of concurrence in terms of QRG iterations. We also investigate the scaling behavior of the system close to the quantum critical point, which shows that the minimum value of the first derivative of concurrence and the position of the minimum scale with an exponent of the system size. Also, the first derivative of concurrence between two blocks diverges at the quantum critical point, which is directly associated with the divergence of the correlation length.

Keywords: quantum renormalization-group, quantum phase transition, Heisenberg–Ising model

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1. Introduction

Quantum phase transition (QPT) occurs at absolute zero temperature.[1] It is caused by changing some coupling constants or external parameters, and driven by quantum fluctuations, which exist at $T = 0$ due to the Heisenberg uncertainty principle. As one tuning parameter changes the Hamiltonian, one may reach a critical point (CP) where the ground state of the system suffers an abrupt change mapped to a macroscopic change in system property. In general, QPT is characterized by detecting nonanalytic behaviors in some physical quantities of the system, such as magnetization, bipartite[2] and multipartite[3] entanglement, and quantum discord.[4] By investigating the extremal values of these quantities as well as the behavior of their first and second order derivatives, one can spotlight the CP of the system. The entanglement, which is the main difference between a quantum system and a classical system, plays an important role in QPT. Osterloh *et al*.[5] demonstrated for the first time that entanglement for a class of one-dimensional magnetic systems shows scaling behavior in the vicinity of the transition point. Since then, much effort has been devoted to studying the entanglement and QPT in spin systems.[6–9,11–15]

As is well known, renormalization group theory has been successfully applied to the studies of critical phenomena. Based on the idea of the renormalization, a lot of methods have been introduced, such as the quantum renormalization-group (QRG) method,[10] Monte Carlo RG (MCRG) method,[16] and the density-matrix RG (DMRG) method.[17] By contrast, MCRG and DMRG methods can usually obtain more accurate quantitative results. Though the QRG method usually presented poor quantitative results, it was used to investigate the quantum information properties of critical systems recently and found to be an efficient and powerful tool to study the QPT in various systems.[18–23]

In the present paper, we use the same method, i.e., QRG method, to study the entanglement and QPT in the one-dimensional spin-1/2 Heisenberg–Ising model. This model was initially discussed by Lieb *et al*.[24] and recently was extended to the case with anisotropic Heisenberg exchange by Yao *et al*.[25] and to the case with additional Dzyaloshinskii–Moriya interaction by Strecka *et al*.[26] The ground-state properties of the spin-1/2 Heiseberg–Ising chain and its various generalizations have been investigated, and relevant quantum phase transitions have been found.[24–26] In our work, we find that as the size of the system increases, the minimum value of the first derivative of concurrence tends to minus infinity and the position of the minimum approaches to the critical point. We also find a quantum phase boundary existing in the system and the scaling behavior appearing in the vicinity of the transition point.

The rest of this paper is organized as follows. In Section 2, we briefly introduce the QRG method and obtain a renormalized Heisenberg–Ising spin chain. In Section 3, we study block–block entanglement. In Section 4, we analyze the critical behavior of the system. We draw some conclusions from our work in Section 5.

2. Renormalization of the Heisenberg–Ising model

The main idea of the QRG method is to eliminate the degrees of freedom of the system by an iteration which reduces the number of variables step by step until reaching a fixed

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point. In order to do this, we divide the lattice into blocks by using Kadanoff's approach (see Fig. 1). We consider three sites as a block and each block can be treated independently to build the projection operator onto the lower energy subspace. In this way, we obtain an effective Hamiltonian, which has the same form as the original Hamiltonian. The original Hilbert space is also replaced by the renormalized subspace.[27,28]

The Hamiltonian of the Heisenberg–Ising model on a periodic chain with $2M$ sites can be written as

$$H=\sum_{i=1}^{M}(J\sigma_{2i-1}^{x}\sigma_{2i}^{x}+J\sigma_{2i-1}^{y}\sigma_{2i}^{y}+J_{z}\sigma_{2i-1}^{z}\sigma_{2i}^{z}+\lambda\sigma_{2i}^{z}\sigma_{2i+1}^{z}), \quad (1)$$

where J ($J>0$), J_z ($J_z>0$), and λ ($\lambda\geq 0$) are the coupling constants, and σ^{α} ($\alpha=x,y,z$) are Pauli matrices.

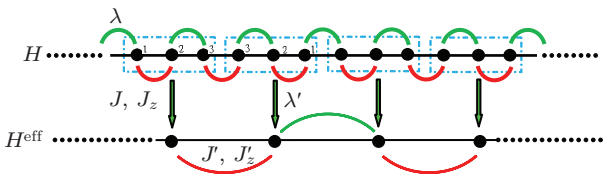


Fig. 1. (color online) Kadanoff's block renormalization-group method of the spin-1/2 Heisenberg–Ising chain where we consider three sites as a block.

By using Kadanoff's block approach, one can write Eq. (1) as

$$H=H^{\mathrm{B}}+H^{\mathrm{BB}}, \quad (2)$$

where H^{B} is the block Hamiltonian and H^{BB} is the inter-block Hamiltonian. The concrete forms of H^{B} and H^{BB} are

$$H^{\mathrm{B}}=\sum_{L=1}^{2M/3}h_{L}^{\mathrm{B}}, \quad (3)$$

$$H^{\mathrm{BB}}=\sum_{k=1}^{M/3}(J\sigma_{3,2k-1}^{x}\sigma_{3,2k}^{x}+J\sigma_{3,2k-1}^{y}\sigma_{3,2k}^{y}+J_{z}\sigma_{3,2k-1}^{z}\sigma_{3,2k}^{z}+\lambda\sigma_{1,2k}^{z}\sigma_{1,2k+1}^{z}), \quad (4)$$

where

$$h_{L}^{\mathrm{B}}=J\sigma_{1,L}^{x}\sigma_{2,L}^{x}+J\sigma_{1,L}^{y}\sigma_{2,L}^{y}+J_{z}\sigma_{1,L}^{z}\sigma_{2,L}^{z}+\lambda\sigma_{2,L}^{z}\sigma_{3,L}^{z}, \quad (5)$$

which is the L-th block Hamiltonian.

The three-site block Hamiltonian can be exactly diagonalized and solved. By calculation, we obtain two degenerate ground states, which will be used to construct the projection operator of the QRG. These two degenerate ground states are

$$|\psi_0\rangle=\frac{1}{\sqrt{a^2+1}}(a|\uparrow\downarrow\uparrow\rangle+|\downarrow\uparrow\uparrow\rangle), \quad (6)$$

$$|\psi_0'\rangle=\frac{1}{\sqrt{b^2+1}}(b|\uparrow\downarrow\downarrow\rangle+|\downarrow\uparrow\downarrow\rangle), \quad (7)$$

where

$$a=-\frac{\sqrt{\lambda^2+4J^2}+\lambda}{2J}, \quad (8)$$

$$b=\frac{-\sqrt{\lambda^2+4J^2}+\lambda}{2J}, \quad (9)$$

and $|\uparrow\rangle$, $|\downarrow\rangle$ are the eigenstates of σ^z. The corresponding ground state energy is

$$E_0=-J_z-\sqrt{\lambda^2+4J^2}. \quad (10)$$

In order to obtain the effective Hamiltonian, one must construct the projection operator at first. The projection operator P_0 can be constructed in a factorized form

$$P_0=\prod_{L=1}^{2M/3}P_0^{L}, \quad (11)$$

where P_0^L is the projection operator for the L-th block, which is defined as

$$P_0^{L}=|\Uparrow\rangle_L\langle\psi_0|+|\Downarrow\rangle_L\langle\psi_0'|. \quad (12)$$

The $|\Uparrow\rangle_L$ and $|\Downarrow\rangle_L$ in Eq. (12) are the renamed base sets in the renormalized subspace. The effective (renormalized) Hamiltonian is then

$$H^{\mathrm{eff}}=P_0HP_0^{\dagger}=P_0H^{\mathrm{B}}P_0^{\dagger}+P_0H^{\mathrm{BB}}P_0^{\dagger}. \quad (13)$$

The renormalizations of Pauli matrices are given by

$$P_0^{L}\sigma_{i,L}^{\alpha}P_0^{\dagger L}=\zeta_i^{\alpha}\sigma_L'^{\alpha} \quad (i=1,3;\ \alpha=x,y,z), \quad (14)$$

where

$$\zeta_3^{x}=\zeta_3^{y}=\frac{2J}{\sqrt{4J^2+\lambda^2}}, \quad \zeta_1^{z}=\frac{\lambda}{\sqrt{4J^2+\lambda^2}}, \quad \zeta_3^{z}=1, \quad (15)$$

with indexes 1 and 3 referring to sites labeled in a single block based on Fig. 1. Then the effective Hamiltonian can be obtained as

$$H^{\mathrm{eff}}=\sum_{k=1}^{M/3}(J'\sigma_{2k-1}^{x}\sigma_{2k}^{x}+J'\sigma_{2k-1}^{y}\sigma_{2k}^{y}+J_{z}'\sigma_{2k-1}^{z}\sigma_{2k}^{z}+\lambda'\sigma_{2k}^{z}\sigma_{2k+1}^{z}), \quad (16)$$

where J', J_z', and λ' are the renormalized coupling constants,

$$J'=\frac{4J^3}{4J^2+\lambda^2}, \quad J_z'=J_z, \quad \lambda'=\frac{\lambda^3}{4J^2+\lambda^2}. \quad (17)$$

Setting

$$g=\frac{\lambda}{J}, \quad (18)$$

we can derive an equation from Eq. (17),

$$g'=\frac{1}{4}g^3. \quad (19)$$

Thus, the large system with $N=3^{n+1}$ sites can be effectively described by a three-site block with the renormalized coupling constant after the n-th iteration of the QRG. By solving $g'\equiv g$, we can obtain two trivial fixed points $g=0,\infty$, and a nontrivial fixed point $g=2$ which specifies the slope of the critical line of this model.

3. Renormalization of the entanglement

In this section we investigate the ground-state entanglement of the spin-1/2 Heisenberg–Ising chain using the QRG method. We consider one of the degenerate ground states to define the density operator. The density operator is defined as

$$\rho = |\psi_0\rangle\langle\psi_0|, \tag{20}$$

where $|\psi_0\rangle$ has been introduced in Eq. (6). By tracing over the site 3 degrees of freedom, we can obtain the reduced density matrix for sites 1 and 2,

$$\rho_{12} = \frac{1}{a^2+1}\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & a^2 & a & 0 \\ 0 & a & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}. \tag{21}$$

We confine our interest to the nearest-neighbor entanglement between two sites, which is measured by concurrence.[29] C that presents the concurrence of sites 1 and 2, is defined as

$$C = \max\{\lambda_1 - \lambda_2 - \lambda_3 - \lambda_4, 0\}, \tag{22}$$

where λ_k ($k = 1, 2, 3, 4$) are the square roots of the eigenvalues in the descending order of the operator $R_{12} = \rho_{12}\tilde{\rho}_{12}$, with $\tilde{\rho}_{12} = (\sigma_y \otimes \sigma_y)\rho_{12}^*(\sigma_y \otimes \sigma_y)$,

$$\lambda_1 = \frac{2J}{\sqrt{4J^2+\lambda^2}}, \quad \lambda_2 = \lambda_3 = \lambda_4 = 0. \tag{23}$$

Thus, the concurrence is obtained

$$C = \frac{2J}{\sqrt{4J^2+\lambda^2}}. \tag{24}$$

Obviously, C is a function of J and λ. So, the renormalizations of J and λ determine the evolution of the concurrence as the size of the system becomes large. Figure 2 shows the plot of C versus J and λ in the thermodynamic limit. The concurrence ruptures at a line described by equation $\lambda = 2J$ which specifies the quantum phase boundary of this model.

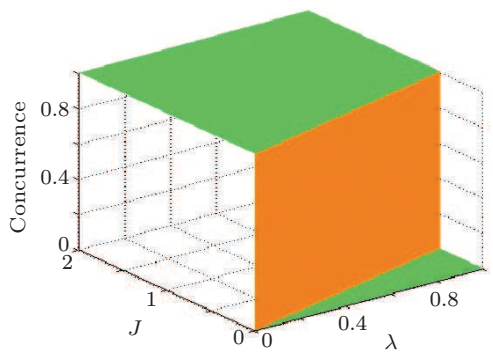


Fig. 2. (color online) Concurrence as a function of the coupling constants (J and λ) in the thermodynamic limit of Heisenberg–Ising spin-1/2 chain.

In order to clarify the discussion of the concurrence, we set C to be a function of g,

$$C = \frac{2}{\sqrt{4+g^2}}, \tag{25}$$

where g has been introduced in Eq. (18). Figure 3 shows the plots of C versus g for different QRG iterations. We can see that the plots of C for different QRG steps cross each other at the critical point $g_c = 2$.

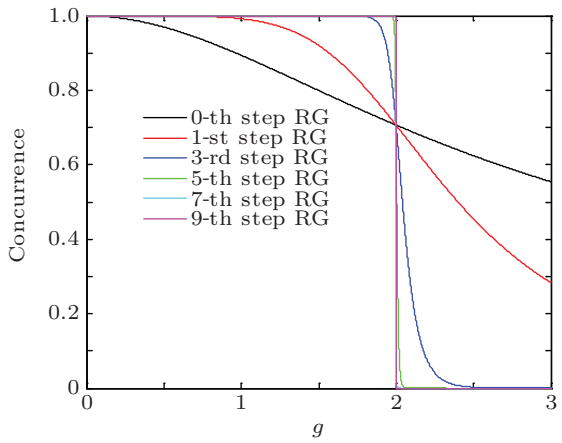


Fig. 3. (color online) Representation of the evolution of concurrence with g in terms of QRG iterations.

4. Non-analytic and scaling behavior

The non-analytic behavior of the entanglement is a feature of QPT. It is also accompanied by the scaling behavior in the vicinity of the critical point of the system because of the divergence of correlation length $\xi \sim (g - g_c)^{-\nu}$ at the critical point g_c. Specifically, a critical point of QPT is associated with a singularity in the derivative of the ground state energy.[2] Indeed, it was shown in Ref. [24] that the ground-state energy per site of the infinite Heisenberg–Ising model does exhibit non-analytic behavior at $g_c = \lambda = 2$ ($J = J_z = 1$). Moreover, in the anisotropic Heisenberg–Ising model, people found low-energy excitations with a gap when the Ising coupling

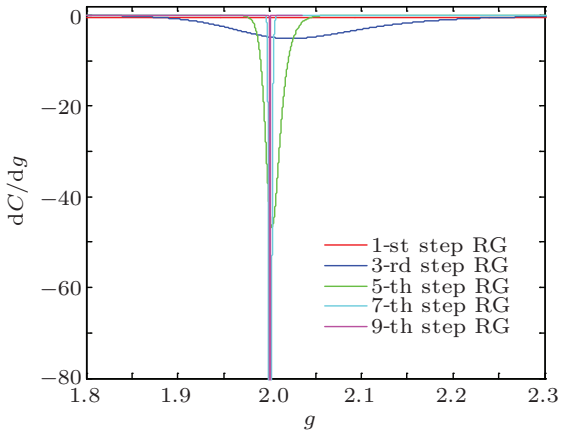


Fig. 4. (color online) First derivative of concurrence and its manifestation toward divergence as the number of QRG iterations increases (Fig. 3).

strength is not equal to 2, and this conclusion holds true for any kind of anisotropic Heisenberg exchange.[25] In Fig. 4 the first derivative of C ($\mathrm{d}C/\mathrm{d}g$) with respect to g is considered for the system of increasing size. On increasing the system size, the minimum of $\mathrm{d}C/\mathrm{d}g$ becomes more pronounced and the position of the minimum tends towards the critical point $g_c = 2$. When the size of the system reaches a thermodynamic limit, $\mathrm{d}C/\mathrm{d}g$ diverges at g_c (see Fig. 4).

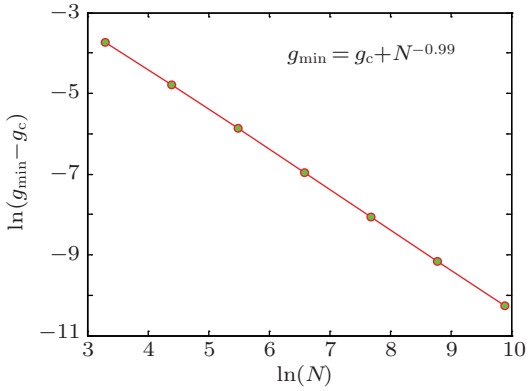


Fig. 5. (color online) Scaling behavior of $g_{\min}$ in terms of system size N, where $g_{\min}$ is the position of the minimum in Fig. 4.

A more detailed analysis shows that the position $g_{\min}$ of the minimum of $\mathrm{d}C/\mathrm{d}g$ scale as

$$g_{\min} = g_c + N^{-\theta}, \tag{26}$$

with $\theta = 0.99$, which is plotted in Fig. 5. The exponent θ is called the entanglement exponent. It should be emphasized that the exponent θ is directly related to the correlation length exponent υ close to the critical point. It is shown that $\upsilon = 1/\theta$.[18,19] The scaling behavior of $|\mathrm{d}C/\mathrm{d}g|_{g_{\min}}$ versus N is plotted in Fig. 6, which is fulfilled with

$$|\mathrm{d}C/\mathrm{d}g|_{g_{\min}} \sim N. \tag{27}$$

These results justify that the QRG implementation of entanglement truly captures the critical behavior of the infinite Heisenberg–Ising spin-1/2 chain in the vicinity of the critical point.

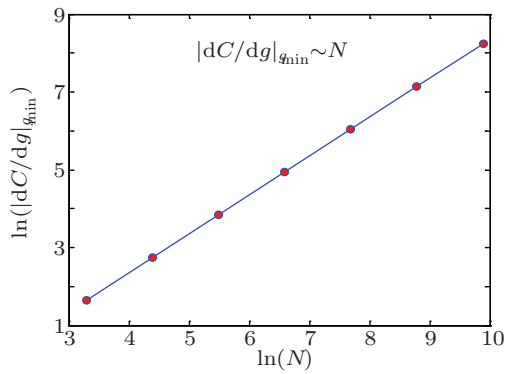


Fig. 6. (color online) Logarithm of absolute value of the minimum $\ln(|\mathrm{d}C/\mathrm{d}g|_{g_{\min}})$ versus the logarithm of chain size $\ln(N)$, which shows a scaling behavior. Each point corresponds to the minimum value of a single plot of Fig. 4.

5. Conclusion

In this paper, the entanglement and QPT in the spin-1/2 Heisenberg–Ising chain are investigated by using the QRG method. We use the concurrence as a measure of the quantum entanglement. In order to investigate the critical behavior of this system, the evolution of concurrence through the renormalization of the lattice is examined. As the size of the system becomes large, the concurrence develops to two different values on both sides of the critical point $g_c = 2$ which governs the quantum phase boundary ($\lambda = 2J$) of this model. In the thermodynamic limit, the first derivative of the concurrence shows a divergent behavior at the critical point, and it is also accompanied by a scaling behavior in the vicinity of the critical point since the correlation length diverges at the critical point. The scaling behavior characterizes how the critical point of the model is reached with the size of the system increasing. From this scaling behavior, we obtain the critical exponent $\upsilon = 1/0.99 \approx 1$, which is consistent with the universality class of the Ising model.

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