Entanglement entropy in an antiferromagnetic Heisenberg spin chain with boundary impurities

Jie Ren\textsuperscript{1}, Shiqun Zhu\textsuperscript{1,3} and Xiang Hao\textsuperscript{2}

\textsuperscript{1} School of Physical Science and Technology, Suzhou University, Suzhou, Jiangsu 215006, People’s Republic of China
\textsuperscript{2} Department of Physics, Suzhou University of Science and Technology, Suzhou, Jiangsu 215011, People’s Republic of China
E-mail: Jren01@163.com, szhu@suda.edu.cn

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Abstract
The effects of boundary impurities on the entanglement entropy in an antiferromagnetic Heisenberg opened spin-1/2 chain are investigated. The method of the density-matrix renormalization group is used to obtain the bipartite entanglement. The entropy increases when the length of the subsystem increases. It approaches a constant when the system length is very large. With the same impurity interaction, qutrit impurities of spin-1 can increase the entanglement entropy.

1. Introduction

Recently, entanglement has been recognized as an important resource of some quantum mechanical phenomena, such as quantum teleportation, quantum cryptography, quantum computation and violation of Bell’s inequality [1–3]. Many investigations show that an entanglement exists naturally in the spin chain when the temperature of the system is at zero. A useful many-body entanglement measure of a pure state is the von Neumann entanglement entropy [4], which can also quantify the quantum phase transition [5–11]. Bipartite entanglement in systems of atomic Bose–Einstein condensate has been studied [12, 13]. The entanglement entropy in the antiferromagnetic Heisenberg XX chain and the Ising model has been investigated [14]. In the isotropic antiferromagnetic Heisenberg model, the universal form of the entropy is predicted by [15]:

\[ S_L = \frac{c}{3} \log_2 L + k, \]  

where \( c \) is the central charge, and \( k \) is a non-universal constant. For a spin chain of an open boundary condition, the analogous formula \( c/3 \) should be replaced by \( c/6 \) for a part of the length \( L \) in an infinite one-dimension system [16, 17]. The analogous formula is dependent on the boundary conditions of the block and the rest of the chain. If the block has two boundaries with the rest of the chain then the factor is \( c/3 \), while if the block has just one boundary as in the case of a block consisting of the first adjacent spins of a semi-infinite chain, then the factor is \( c/6 \). Recently, it has been shown that a feeble central bound defect [18] or single impurity in the boundary [19] has a strong influence on the entropy, though the entropy measures the mutual coupling of the two parts of a system in wavefunction. A weak transverse boundary magnetic field impurity [20] and domain walls [21] generated by an antiparallel magnetic field have different effects on the entanglement entropy. Moreover, impurities show their strong influences on the spin correlation function [22, 23]. It would be interesting to investigate the effects of boundary impurities on the entanglement entropy in an open antiferromagnetic Heisenberg spin chain.

In this paper, the entanglement entropy of a spin-1/2 antiferromagnetic Heisenberg chain with boundary impurities located at two ends is investigated. In section 2, the Hamiltonian of an antiferromagnetic Heisenberg spin-1/2 chain is presented. By using the method of the density-matrix renormalization group (DMRG) [24, 25], the entropy of the ground state is calculated, and the effects of the impurities are analysed in section 3. A discussion concludes the paper.
2. Hamiltonian of a Heisenberg spin chain

The Hamiltonian of a spin-1/2 Heisenberg open chain with boundary impurities at two ends can be written as

\[ H = \sum_{i=2}^{N-2} J \mathbf{S}_i \mathbf{S}_{i+1} + \alpha (\mathbf{S}_1 \mathbf{S}_2 + \mathbf{S}_{N-1} \mathbf{S}_N), \]

where the coupling exchange \( J \) \( > 0 \) corresponds to the antiferromagnetic case, \( \mathbf{S}_i \) are spin operators, and \( N \) is the length of the spin chain. The coupling exchange \( \alpha \) is the impurity interaction. For simplicity, \( J = 1 \) is assumed in this paper.

The entropy is used as a measure of the bipartite entanglement. If \(|G_S\rangle\) is the ground state of a chain of \( N \) qubits, a reduced density matrix of \( L \) contiguous qubits can be written as

\[ \rho_L = \text{Tr}_{N-L}[|G_S\rangle \langle G_S|]. \]

The bipartite entanglement between the right-hand \( L \) contiguous qubits and the rest of the system can be measured by the entropy

\[ S_L = -\text{Tr}(\rho_L \log_2 \rho_L). \]

One of the properties of the entropy of a block of the system can be given by

\[ S_L = S_{N-L}, \]

since the spectrum of the reduced density matrix \( \rho_L \) is the same as that of \( \rho_{N-L} \).

3. Entanglement of entropy with impurities

In order to calculate the entropy accurately using the DMRG method, the length of the spin chain needs to be relatively long; it is chosen to be \( N = 256 \). The total number of the density-matrix eigenstates held in the system block is \( m = 128 \) in the basis truncation procedure.

To check the accuracy of the results from the DMRG method, an open boundary condition without impurities of \( \alpha = 1 \) is considered. The corresponding results of a finite spin chain, which is predicted by conformal field theory (CFT), can be considered as a benchmark. It can be written as

\[ S_L = \frac{c}{6} \log_2 \left[ \frac{N}{\pi} \sin \left( \frac{\pi}{N} L \right) \right] + A, \]

where \( c \) is the central charge, and \( A \) is a non-universal constant [26, 27]. There are large oscillations between the even and odd \( L \)-value entropy. To avoid these relatively large oscillations, the even-value entropy is chosen. The entropy \( S_L \) between contiguous \( L \) qubits and the remaining \( N - L \) qubits is plotted as a function of the subsystem \( L \) in figure 1 when \( N = 160, 200 \) and 256. For \( L < 8 \), the results of DMRG are slightly lower than those of CFT. For \( L > 8 \), an almost perfect agreement between the two results is obtained. For different values of \( N \) with large \( L \), \( S_L \) is small for small values of \( N \). For small \( L \), there is almost no difference between different values of \( N \). It seems that \( S_L \) approaching a constant for very large \( L \) is mainly due to the finite size effect. The entropy \( S_L \) is also plotted as a function of \( \log_2 \left[ \frac{N}{\pi} \sin \left( \frac{\pi}{N} L \right) \right] \) in the inset of figure 1. It is shown that the entropy appears as a straight line whose slope is very close to \( c/6 \).

The entanglement entropy \( S_L \) is plotted as a function of the subsystem length \( L \) for different values of the impurity interaction \( \alpha \) in figure 2(a). It is seen that the entropy \( S_L \) increases with the subsystem length \( L \) and then approaches a constant when \( L \) is very large for \( \alpha = 0.1, 2.0 \). When \( \alpha = 0.3, 0.5 \), the entropy \( S_L \) decreases slightly, then increases and approaches a constant for very large \( L \). The minimal value is 1.53 at \( L = 6 \) for \( \alpha = 0.3 \) and 1.16 at \( L = 4 \) for \( \alpha = 0.5 \). When \( \alpha = 0.1 \), \( S_L \) approaches a value of about 2.4 for very large \( L \). While for \( \alpha = 0.3, 0.5, 2.0 \), \( S_L \) approaches the value about 1.6 for very large \( L \). The influence of the impurity at two ends of the Heisenberg spin-1/2 chain depends on the value of the impurity interaction \( \alpha \). For \( \alpha = \alpha_0 = 0.235 \), the strength alternation of the even bond and the odd bond in the centre of the spin chain is minimized to close to zero [24]. For \( \alpha < \alpha_0 \), the even sublattice is favoured. This induces a larger value of \( S_L \). For \( \alpha > \alpha_0 \), the odd sublattice is favoured. This induces a smaller value of \( S_L \). If the value of \( \alpha \) is less than \( \alpha_0 = 0.235 \), the effect of the impurity on the entanglement entropy \( S_L \) is stronger. Therefore, the entanglement entropy, \( S_{L_{\alpha}} \), of \( \alpha = 0.1 \) is much larger than the \( S_L \) of \( \alpha = 0.3, 0.5 \) and 2.0 [18, 19, 24]. The entropy \( S_L \) is also plotted as a function of \( \log_2 \left[ \frac{N}{\pi} \sin \left( \frac{\pi}{N} L \right) \right] \) in the inset of figure 2(a). It is seen that \( S_L \) is almost a straight line as a function of \( \log_2 \left[ \frac{N}{\pi} \sin \left( \frac{\pi}{N} L \right) \right] \) for very large \( L \).

If \( S_{L_{\alpha}} \) is the entropy with impurities at two ends and \( S_{L_{\alpha 0}} \) is the entropy without impurities, the difference of the entropy \( \Delta S_L \) can be defined as

\[ \Delta S_L = S_{L_{\alpha}} - S_{L_{\alpha 0}}. \]
increases and then approaches a constant with an increase of the subsystem length $L$ when $\alpha = 2.0$. It seems that the effect of impurities decreases with the increase of the subsystem $L$ when $\alpha < \alpha_0 = 1.0$. However, the effect of the impurity increases when $\alpha > \alpha_0 = 1.0$. The entropy difference $\Delta S_L$ is also plotted as a function of $\log_2 \left( \frac{\pi}{N} \sin \left( \frac{\pi}{N} L \right) \right)$ in the inset of figure 2(b). It is seen that $\Delta S_L$ is almost a straight line as a function of $\log_2 \left( \frac{\pi}{N} \sin \left( \frac{\pi}{N} L \right) \right)$ for very large $L$. Similar to that shown in figure 2(a), the entropy difference $\Delta S_L$ of $\alpha = 0.1$ is much larger than $\Delta S_L$ of $\alpha = 0.3, 0.5$ and 2.0. This is mainly due to the fact that the small value of $\alpha < \alpha_0 = 0.235$ can induce a stronger effect on the impurities on $\Delta S_L$ since the even sublattice is favoured [18, 19, 24].

From figure 2, it is seen that both values of $S_L$ and $\Delta S_L$ decrease when $\alpha$ increases especially for a small value of $L$. There are large differences of $S_L$ and $\Delta S_L$ for different impurity interactions $\alpha$ when $L$ is small. If $L$ is quite large, $S_L$ and $\Delta S_L$ approach constants. If $\alpha = 0.3, 0.5$ and 2.0, $S_L$ approaches about 1.6 while $\Delta S_L$ approaches zero for quite large $L$. It seems that the effect of the impurity at two ends is very small for large $L$. If $\alpha = 0.1$, both $S_L$ and $\Delta S_L$ are quite large. It seems that the small value of the impurity interaction $\alpha < \alpha_0 = 0.235$ can induce a strong effect on $S_L$ and $\Delta S_L$.

The central charge $c$ in equation (6) plays an important role in the measurement of the entanglement entropy. The central charge $c$ can be calculated numerically by [17, 19]:

$$ c(L) = 6 \left[ \frac{S_{L+2} - S_{L-2}}{T(L+2) - T(L-2)} \right] .$$

where

$$ T(L) = \log_2 \left( \frac{N}{\pi} \sin \left( \frac{\pi}{N} L \right) \right) .$$

The central charge labelled by $c(L)$ is plotted in figure 3(a) as a function of the subsystem length $L$ for different values of the impurity interaction $\alpha$. When $\alpha = 0.1$, the central charge $c(L)$ increases to a peak and then decreases slowly with the increase of the subsystem length $L$. The central charge $c(L)$ decreases and then approaches a constant with the increase of the subsystem $L$ when $\alpha = 2.0$. When $\alpha = 0.3, 0.5$, the central charge $c(L)$ increases and almost approaches a constant with the increase of the subsystem length $L$. The central charges of $c(L = 6)$ and $c(L = 4)$ are negative when $\alpha = 0.3$ and 0.5, respectively. This corresponds to the minimum values of $S_L$ shown in figure 2(a). For $\alpha > 0.235$, the central charge $c(L)$ increases with increasing $\alpha$. For $\alpha = 0.1 < \alpha < 0.235$, $c(L)$ of $\alpha = 0.1$ is much larger than that of $\alpha = 0.3$; it decreases and finally approaches that of $\alpha = 0.3$ when $L$ is very large. The value of $c(L)$ of $\alpha = 0.1$ is larger than that of $\alpha = 0.5$ if $L < 20$. If $L > 20, c(L)$ of $\alpha = 0.1$ is smaller than that of $\alpha = 0.5$. This is mainly due to the stronger singlet bonds on the even-numbered links of the chain for $\alpha < 0.235$ [24]. Since the central charge may clarify the behaviour of the entropy for large values of the subsystem, the central charge $c(L = 80)$ is plotted as a function of the impurity interaction $\alpha$ in figure 2(b) when $1 \ll L (= 80) < N/2 (= 128)$. It is seen that the central charge $c$ reaches a minimum value when the impurity interaction $\alpha = 0.235$. When the impurity interaction $\alpha < 0.235$, the central charge $c$ decreases with the increase of the impurity interaction $\alpha$. The central charge $c$ increases with the increase of the impurity interaction $\alpha$ when $\alpha > 0.235$. It approaches 1.0 when the impurity interaction $\alpha$ is close to 2.0.

If the impurities are qutrits with spin-1 operators $\vec{S}$, the effects of qutrit impurities on the entropy can also be investigated. The entanglement entropy $S_L$ and the difference of the entropy $\Delta S_L$ are plotted in figures 4(a) and (b), respectively, as a function of the subsystem length $L$ for the impurity interaction $\alpha$ and different impurities. The entropy $S_L$ and the difference of the entropy $\Delta S_L$ are also plotted as a function of $\log_2 \left( \frac{5}{\pi} \sin \left( \frac{\pi}{N} L \right) \right)$ in the insets of figures 4(a) and (b). Similar to that shown in figure 2, both $S_L$ and $\Delta S_L$ of spin-1 decrease with the increase of $\alpha$. The entropy $S_L$ increases and then almost approaches a constant when the subsystem length $L$ increases. The entropy of impurities with spin-1 is much larger than those with spin-1/2. For the impurities of spin-1/2, the entropies of $\alpha = 0.5$ and $\alpha = 2.0$ are almost indistinguishable when the subsystem length $L$ is very large. While for the impurity of spin-1, the differences of the entropies of $\alpha = 0.5$ and $\alpha = 2.0$ are quite large and approach a constant when $L$ is very large. It is clear that the

![Figure 2](image-url)
effects of qutrit impurities on the entanglement entropy are much stronger than those of qubit impurities. It seems that it is easier to control the entropy of the system using qutrit impurities.

4. Discussion

It is clear that the impurity interaction and the impurity spin have a strong influence on the entanglement of two subsystems [19, 28, 29]. For pairwise entanglement between the impurity spin and the spin chain, the two boundary spins will have a strong tendency to form a singlet pair when the impurity interaction is large. This will reduce the entanglement between the boundary of the two spin subsystems and the rest of the system. The value of the entanglement entropy is mainly determined by the density-matrix spectra, extremely by the few largest eigenvalues of the reduced density matrix [18, 20, 25]. For qubit impurities, impurities can affect the entropy between two subsystems by changing the distribution of the reduced density-matrix spectra. If the impurities are qutrits with the same impurity interaction, not only is the distribution of the reduced density-matrix spectra changed, but also the degree of the freedom of density-matrix spectra of the subsystem is enlarged in the Hilbert space. This is similar to the result of entropy with increased subsystems [15, 20, 21].

The effects of boundary impurities on the bipartite entanglement in an antiferromagnetic Heisenberg open spin chain have been discussed. Using the method of the density-matrix renormalization group, the entanglement entropy is calculated for an even-number subsystem. The entanglement entropy decreases with the increase of the impurity interaction while it increases with the increase of the subsystem length. When the system length is very large, the entanglement entropy approaches a constant due to the finite size effect. The influences of boundary impurities with qutrits of spin-1 are much stronger than those of qubits of spin-1/2. With the same impurity interaction, qutrit impurities can increase the entanglement. All the results are dependent on the selection of an even subsystem. This shows that the entropy of a system with qutrit impurities can be more easily controlled.

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