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Critical behaviors of mutual information in the one-dimensional spin-1 bilinear biquadratic model

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Abstract

The critical behaviors of the mutual information in the one-dimensional spin-1 bilinear biquadratic model are studied. It is found that all the quantum phase transition points including the order–disorder ones and the infinite-order ones in the system can be quantified from the singularity analysis of the mutual information of two sites with the longest distance, because the mutual information captures the correlation properties about the critical fluctuations. More interestingly, the special structure of the wavefunction and the special symmetric property of the system can be indicated by the entropy correlation behaviors. The finite size scaling laws of the mutual information and its derivative are also studied.

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1. Introduction

Many interesting phenomena in many-body systems are caused by correlations. The ground state of a system may favor different quantum states with the changing of model parameters. These quantum states compete with each other and the phase transition happens at the critical point. The order parameter is used to characterize the quantum phase transition. The quantum phase transition is a very important issue in modern condensed matter physics [1]. Due to the correlations, the subsystems are entangled. The quantum entanglement is a very interesting topic in the quantum information and quantum computation sciences [2]. Several measurements of entanglement are proposed to quantify the correlations such as von Neumann entropy, concurrence [3, 4], entanglement of formation [3, 4], negativity [5–7], tangle [8, 9] and block entanglement [10, 11]. Recently, it has been found that the quantum phase transition point can be detected by the singularity of measurement of entanglement

[12–22]. This fact can be understood as follows. The order parameter is heavily dependent on the correlation functions, which may show some singular behaviors at the critical point because the wavefunction of the system is singular at the phase transition point. Some necessary information about the critical fluctuations in the correlation functions is kept in the local reduced density matrix because the elements of the reduced density matrix are determined by the correlation functions. As a result, the measurement of entanglement calculated from the reduced density matrix may show some singular behaviors at the critical point. Therefore, the singular point of the measurement of entanglement or its derivative can give some information about the phase transition point. If the minimum, maximum or discontinuous point of the measurement of entanglement or its derivative is the singular point, it may correspond to a phase transition point. While if the minimum, maximum or discontinuous point is not the singular point, it does not correspond to a phase transition point. According to Landau's phase transition theory, if the measurement of entanglement itself has a singularity, the singular point corresponds to a critical point of the first-order phase transition. If the first-order derivative of the measurement of entanglement has a singularity, the singular point corresponds to a second-order phase transition point. The fidelity susceptibility is also an interesting quantity [23, 24]. It comes from the overlap between the original state and final state after some evolutions. It is found that the fidelity susceptibility can be used to determine the quantum phase transition point [25–29].

The strongly correlated systems with a high intrinsic degree of freedom have many applications. Many new quantum states and novel phenomena appear in the high-spin systems. The phase diagrams of this kind of systems are rather rich because every site can contain more information. The study of entanglement quantifying in the high-spin systems is quite complicated. One reason is that some definitions of measurements of entanglement are valid only for the 2×2 that is two qubits systems such as the concurrence. Moreover, some local measurements are failed to quantify the phase transition for this includes the long range or global correlations.

Based on the above considerations, we study the long range correlation behaviors from the view of entropy in the one-dimensional spin-1 bilinear biquadratic model. This system is very interesting for it has both the order–disorder phase transitions and the infinite order ones. We calculate the mutual information of two sites with the longest distance in the system. We find that all the quantum phase transition points can be quantified accurately by the mutual information with the longest distances from the numerical exact diagonalization and the finite size scaling analysis. More interesting, we also find that the mutual information can give the information about the SU(3) integrable point and the valence bond solid (VBS) state. Our results agree with the previous results [30–35]. This method is simple and can be applied to other models.

The paper is organized as follows. In section 2, we introduce the one-dimensional spin-1 bilinear biquadratic model and its phase diagram. We derive the analytic expression for the correlation entropy in section 3 and study it by the numerical exact diagonalization method in section 4. Section 5 is the summary.

2. The model

The Hamiltonian of the one-dimensional spin-1 bilinear biquadratic model reads

$$H = \sum_{j=1}^N [\cos \theta \mathbf{S}_j \cdot \mathbf{S}_{j+1} + \sin \theta (\mathbf{S}_j \cdot \mathbf{S}_{j+1})^2], \quad (1)$$

where \mathbf{S}_j is the spin-1 operator at the site j , N is the total number of the sites and θ is the coupling parameter. In the following, we use the periodic boundary condition. It is well known that the ground-state phase diagram of the system (1) can be divided into four regions.

- (i) If $-0.25\pi < \theta < 0.25\pi$, the system favors the Haldane phase. In this region, the system has a unique disordered ground state, the correlation functions exponentially decay, and the elementary excitation has a gap. The eigenstate of the system is the VBS state at the point of $\theta_{VBS} = 0.1024\pi$ [36, 37]. The system has a continuous transition from the Haldane gapped phase to the gapless trimerized phase at the Lai–Sutherland critical point $\theta_{c1} = 0.25\pi$. This is a infinite order phase transition, which belongs to the Kosterlitz–Thouless-type transition [38, 39]. At the critical point θ_{c1} , the system has the SU(3) symmetry and can be solved exactly by the Bethe ansatz method [40–42].
- (ii) If $0.25\pi < \theta < 0.5\pi$, the system favors the trimerized phase. In this region, the elementary excitation is gapless. At the critical point $\theta_{c2} = 0.5\pi$, the ground state of the system has a transition from the trimerized phase to the ferromagnetic phase. It is a first-order phase transition.
- (iii) If $0.5\pi < \theta < 1.25\pi$, the ground state of the system is an ordered ferromagnetic state and the elementary excitation is gapless.
- (iv) If $1.25\pi < \theta < 1.75\pi$, the system is in the dimerized phase region. The ground state is a singlet state with two-fold degeneracy due to the Z_2 symmetry. The order parameter is the dimer–dimer correlation function. At the critical point of $\theta_{c3} = 1.25\pi$, the system has a transition from the gapless ferromagnetic state to the gapped dimerized state, which is a first-order phase transition. In the region of θ slightly larger than 1.25π , some authors predict that the system has a nondimerized nematic phase [43], while other authors argue that the nematic phase does not exist [34]. At the point of $\theta_{bk} = 1.5\pi$, the system can be solved exactly by the Bethe ansatz method [44, 45]. At the critical point $\theta_{c4} = 1.75\pi$, the system has a transition from the dimerized phase to the Haldane phase. It is a second-order phase transition. The system (1) is also integrable at the critical point θ_{c4} [46, 47].

3. Correlation entropy

The correlation function is a fundamental tool to quantify the correlation effects. It has many applications in condensed matter physics. The correlation function has a counterpart quantity in the quantum information theory. That is the mutual information or the correlation entropy, which measures the correlation effects from the view of entropy. The definition of the correlation entropy is [48–51]

$$S(A : B) = S(A) + S(B) - S(AB), \quad (2)$$

where A and B are two interacting subsystems in the real physical system, $S(p) = -\text{tr}(\rho_p \log_2 \rho_p)$ is the partial entropy of the subsystem $p = A, B$ and AB , the $\rho_p = \text{tr}_{\bar{p}} \rho$ is the reduced density matrix of subsystem p , $\text{tr}_{\bar{p}}$ stands for tracing over all except the selected subsystem p and ρ is the density matrix of the system. The correlation entropy measures the total correlation between two subsystems A and B . At the critical point, the entropy correlation length tends to infinity and the correlation entropy is an exponential decay. Far away from the critical point, the entropy correlation length is finite and the correlation entropy decays as a power-law. The correlation entropy captures the key feature of the correlation information

about critical fluctuations and can be used to quantify the critical phenomena in both the quantum and the classical systems.

The previous studies show that some measurements of entanglement such as von Neumann entropy of two sites with nearest neighbor, entanglement of formation and concurrence cannot give all the phase transition points of the system. In this paper, we consider the global correlation effects and study the correlation entropy between two sites with the longest distance. From the analysis of symmetry of the system (1), we obtain the reduced density matrix of two sites l and j as [52]

$$\rho_{lj} = \alpha_0 + \alpha_1 \mathbf{S}_l \cdot \mathbf{S}_j + \alpha_2 (\mathbf{S}_l \cdot \mathbf{S}_j)^2, \quad (3)$$

where the coefficients are determined by the correlation functions as

$$\begin{aligned} \alpha_0 &= 1 - 2\langle (S_l^z S_j^z)^2 \rangle, \\ \alpha_1 &= \frac{1}{4}\langle (S_l^z S_j^z)^2 \rangle + \frac{1}{4}\langle S_l^z S_j^z \rangle - \frac{2}{3}, \\ \alpha_2 &= \frac{3}{2}\langle S_l^z S_j^z \rangle - \frac{2}{3}. \end{aligned} \quad (4)$$

The system (1) is an isotropic model and has the rotational invariant, thus the correlation functions along the x , y and z directions are equal, $\langle S_l^x S_j^x \rangle = \langle S_l^y S_j^y \rangle = \langle S_l^z S_j^z \rangle$. The correlation functions between different directions are zero. The reduced density matrix (3) can be diagonalized analytically. From this, we obtain the partial entropy of two sites l and j as $S(l:j) = -\sum_{n=1}^9 \lambda_n \log_2 \lambda_n$, where λ_n are the eigenvalues of the reduced density matrix (3). Taking the partial trace of the density matrix (3), we obtain the single-site reduced density matrix. From this, we obtain the von Neumann entropy of a single site as $\log_2 3$. Then the correlation entropy between two sites l and j reads

$$S(l:j) = 2 \log_2 3 + \sum_{n=1}^9 \lambda_n \log_2 \lambda_n, \quad (5)$$

where

$$\begin{aligned} \lambda_1 &= \lambda_2 = \lambda_3 = \lambda_4 = \alpha_0 + \alpha_1 + \alpha_2, & \lambda_5 &= \lambda_6 = \alpha_0 - \alpha_1 + \alpha_2, \\ \lambda_7 &= \sqrt[3]{\delta_1} + \sqrt[3]{\delta_2} - \frac{b}{3}, & \lambda_8 &= \omega \sqrt[3]{\delta_1} + \omega^2 \sqrt[3]{\delta_2} - \frac{b}{3}, \\ \lambda_9 &= \omega^2 \sqrt[3]{\delta_1} + \omega \sqrt[3]{\delta_2} - \frac{b}{3}, & \omega &= \frac{1}{2}(-1 + i\sqrt{3}), \\ \delta_1 &= -\frac{q}{2} + \sqrt{\frac{q^2}{4} + \frac{p^3}{27}}, & \delta_2 &= -\frac{q}{2} - \sqrt{\frac{q^2}{4} + \frac{p^3}{27}}, \\ p &= -\frac{b^2}{3} + c, & q &= \frac{2b^3}{27} - \frac{bc}{3} + d, & b &= -3\alpha_0 + 2\alpha_1 - 6\alpha_2, \\ c &= 3\alpha_0^2 - \alpha_1^2 + 9\alpha_2^2 + 12\alpha_0\alpha_2 - 4\alpha_0\alpha_1 - 4\alpha_1\alpha_2, \\ d &= (\alpha_0 - \alpha_1 + \alpha_2)(2\alpha_1^2 - \alpha_0^2 - 4\alpha_2^2 - 5\alpha_0\alpha_2 + \alpha_0\alpha_1 - 2\alpha_1\alpha_2). \end{aligned} \quad (6)$$

Equation (5) gives a relation between the correlation entropy and the correlation functions.

According to the coupled angular momentum theory, the reduced density matrix (3) can also be written as [52]

$$\rho_{lj} = G|0, 0\rangle\langle 0, 0| + \frac{F}{3} \sum_{S_l^z = -1}^1 |1, S_l^z\rangle\langle 1, S_l^z| + \frac{1-G-F}{5} \sum_{S_l^z = -2}^2 |2, S_l^z\rangle\langle 2, S_l^z|, \quad (7)$$

where S_l^z is the total spin along the z direction of the two spins, and the coefficients G and F are defined by

$$G = \frac{1}{3}[\langle(\mathbf{S}_l \cdot \mathbf{S}_j)^2\rangle - 1], \quad F = 1 - \frac{1}{2}[\langle\mathbf{S}_l \cdot \mathbf{S}_j\rangle + \langle(\mathbf{S}_l \cdot \mathbf{S}_j)^2\rangle]. \quad (8)$$

Under the coupled basis, the reduced density matrix (7) is diagonalized naturally. The results obtained from equations (3) and (7) are the same.

Compared with the correlation functions, the correlation entropy has many advantages. From equation (5), we see that the correlation entropy is a reasonable combination of the correlation functions. Meanwhile, both the correlation function and its square have contributions to the correlation entropy. Then the correlation entropy includes some information related to the critical fluctuations. Generally speaking, if we consider an anisotropic system, the correlation functions along the x , y and z directions are not equal. In this case, the correlation functions along one direction cannot supply all the necessary critical information and the correlation functions along other directions should be considered. The order parameter may be difficult to construct because it is hard to integrate these correlation effects. More detailed calculations show that the correlation entropy includes all kinds of correlation functions, i.e. that along the same directions and that between two different directions. The correlation effects are combined naturally in the correlation entropy.

The correlation entropy shows different behaviors from that of the correlation functions. The correlation entropy has its own finite size scaling law and critical exponents. The correlation entropy enters the scaling regions before the correlation functions [9]. That is to say for some small system sizes, the correlation entropy has the finite size scaling behaviors while the correlation functions do not.

When treating the phase transition by using the correlation entropy method, we do not need a pre-assumed order parameter for the correlation entropy characterizes the total correlation effects. Let us focus on the system (1) and give an example. The order parameter quantifying the phase transition at the critical point θ_{c1} is [53]

$$g(l) \equiv \left\langle S_0^z \left(\prod_{j=1}^{l-1} e^{i\pi S_j^z} \right) S_l^z \right\rangle. \quad (9)$$

From equation (9), we see that the order parameter is non-local and we must calculate the correlation functions with different distances to obtain the global information of the critical phenomena. The order parameter of the trimer phase in the system (1) is $o \equiv \langle S_{j-1}^z S_j^z S_{j+1}^z \rangle$. Then we should calculate the three-body correlation functions to determine the order parameter and the critical point. Thus quantifying the phase transition points by the correlation functions is not much effective. If we use the correlation entropy method, we do not need the explicit form of the order parameter and the phase transition point can be determined directly. Please see the next section for this point.

The correlation entropy method is valid for both the quantum and the finite-temperature phase transitions. It is also valid for the order–disorder phase transitions and the infinite order ones.

4. The results

System (1) does not have the exact solutions except for several special values of the model parameter θ . We use the numerical exact diagonalization method to calculate the correlation entropy of the system. The numerical results of the system with finite system size should be

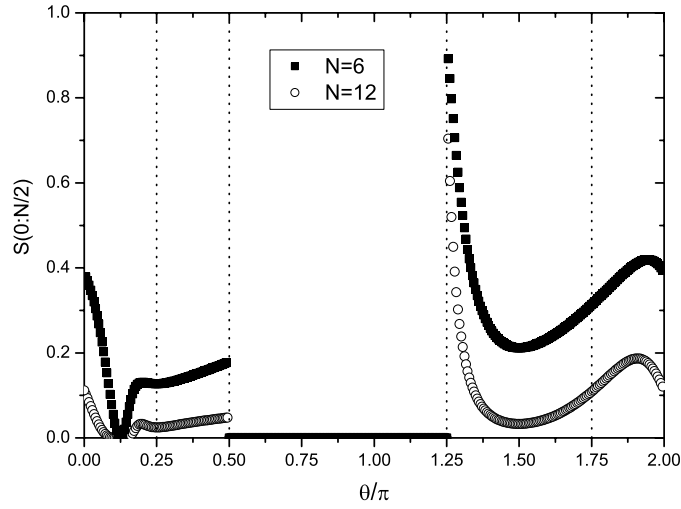


Figure 1. The curves of the correlation entropy $S(0 : N/2)$ versus the coupling parameter θ with the system size $N = 6, 12$. We see that the curve has five singular points, $\theta_{VBS} = 0.1024\pi$, $\theta_{c1} = 0.25\pi$, $\theta_{c2} = 0.5\pi$, $\theta_{c3} = 1.25\pi$ and $\theta_{c4} = 1.75\pi$. The θ_{VBS} corresponds to the valence bond solid state, and θ_{c1} , θ_{c2} , θ_{c3} and θ_{c4} correspond to the phase transition points. At the VBS point, the correlation entropy is zero. The correlation entropy arrives at the minimum exactly at the critical point θ_{c1} for any system size. The correlation entropy is discontinuous at the critical points θ_{c2} and θ_{c3} , which means that they are two first-order phase transition points. The first-order derivative of the correlation entropy is divergent at the critical point θ_{c4} , which corresponds to a second-order phase transition point. The valley near 1.5π and the peak near 1.9π are the results that the derivative of correlation entropy has a singularity at the critical point 1.75π .

generalized to that with infinite system size because the quantum phase transition happens in a infinity system at the zero temperature. Therefore, the finite size scaling analysis is necessary.

In order to see the entropy correlation behaviors more clearly, we consider the correlation entropy between two sites with the longest distance. That is to say if the system size is N , we calculate the correlation entropy between two sites with the distance $N/2$. Because every site has three spin states, $|+\rangle$, $|0\rangle$ and $|-\rangle$, the Hilbert space of the system (1) is 3^N . The ground-state properties can be obtained by diagonalizing Hamiltonian (1) in some invariance subspaces so that the system size could be larger. After some algebra, we obtain the curve of the correlation entropy $S(0 : N/2)$ versus the coupling parameter θ , which is shown in figure 1. Figure 1 only gives the results for the system sizes $N = 6$ and 12 . For other system sizes, we exactly diagonalize Hamiltonian (1) in different invariance subspaces for different coupling regions. For example, in the region of $0 \leq \theta \leq 0.5\pi$, we calculate the correlation entropy with the system size $N = 6, 9, 12$, while in the region of $1.25\pi \leq \theta \leq 2\pi$, we calculate the correlation entropy with the system size $N = 4, 6, 8, 10, 12, 14$.

The correlation functions and their square terms versus the coupling parameter θ are shown in figure 2. From it, we see that the correlation functions are discontinuous at the critical points $\theta_{c2} = 0.5\pi$ and $\theta_{c3} = 1.25\pi$, which means that they are two first-order phase transition points. The correlation functions do not show any singular behaviors at the critical points $\theta_{c1} = 0.25\pi$ and $\theta_{c4} = 1.75\pi$.

We explain the inflexions of the correlation entropy $S(0 : N/2)$ one by one. From figure 1, we see that the first inflexion of the curve appears near the point 0.12π . By carefully checking

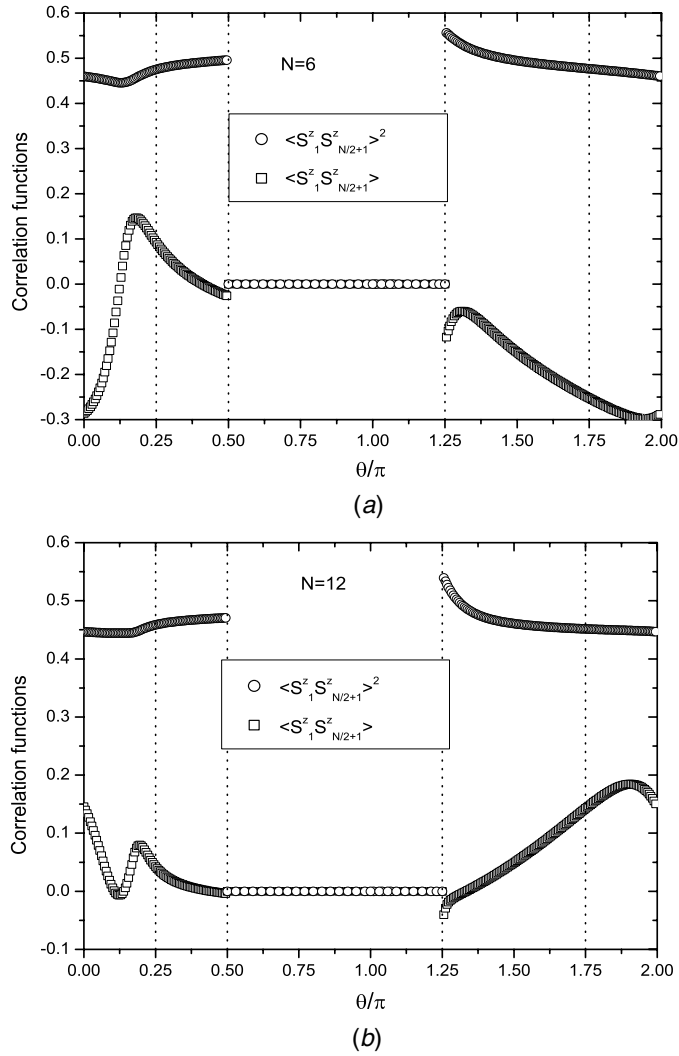


Figure 2. The curves of the correlation functions and their square terms versus the coupling parameter θ with the system size (a) $N = 6$ and (b) $N = 12$. The correlation functions do not show any singular behavior at the critical points $\theta_{c1} = 0.25\pi$ and $\theta_{c4} = 1.75\pi$.

the numerical data, we find that the value of correlation entropy $S(0 : N/2)$ at this inflexion is zero, which means the subsystems with the longest distance are separable, $\rho_{0N/2} = \rho_0 \otimes \rho_{N/2}$. This point indicates the valence bond solid state of the system. Furthermore, for any values of the system size N , we can always find a coupling θ_{VBSm} at which the correlation entropy between two sites with longest distance is zero. The coupling θ_{VBSm} depends on the system sizes. For different system sizes, the coupling θ_{VBSm} are different. Then we should consider the finite size scaling behaviors of the coupling θ_{VBSm} . The curve of the coupling θ_{VBSm} versus the system size scale N^{-3} is plotted in figure 3, where the system size $N = 6, 8, 10, 12, 14$. We see that the data for the θ_{VBSm} with different system sizes fall on a straight line. The fitting gives $\theta_{VBSm}/\pi = 0.10443 + 4.43926N^{-3}$. If the system size tends to infinity, the coupling

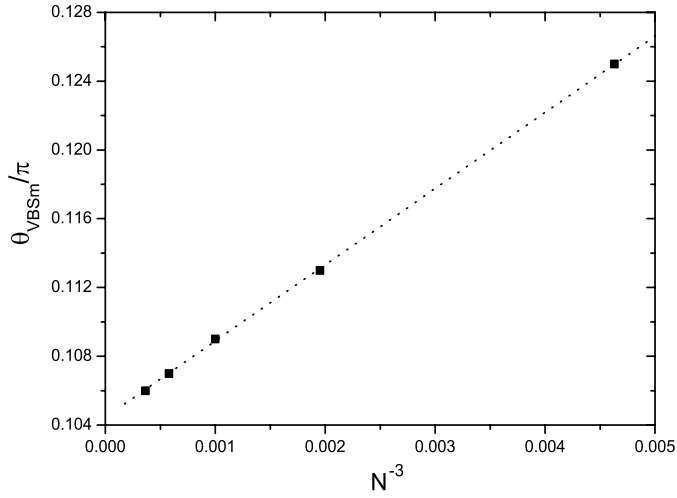


Figure 3. The finite size scaling behaviors of the coupling θ_{VBSm} with the system size scale N^{-3} . The data are fitted with a straight line as $\theta_{VBSm}/\pi = A + BN^{-3}$, where $A = 0.10443 \pm 0.00007$ and $B = 4.43926 \pm 0.02850$. When the system size tends to infinity, the coupling θ_{VBSm} takes the value of $0.10443\pi \pm 0.00007\pi$, which is close to the actual value 0.1024π .

θ_{VBSm} tends to $0.10443\pi \pm 0.00007\pi$, which is very close to the actual value 0.1024π . Then we arrive at a very interesting issue that the correlation entropy can be utilized not only to determine the critical point but also to find the special structure of the wavefunction of the system.

From figure 1, we find that the correlation entropy $S(0 : N/2)$ takes the minimum exactly at the point of $\theta_{c1} = 0.25\pi$ for the system size $N = 6, 12$. It is also true for the case of $N = 9$. Therefore, the critical point θ_{c1} does not depend on the system size. Further study shows that the system (1) has the SU(3) symmetry at this point. Then Hamiltonian (1) is equivalent to a SU(3) permutation operator plus a constant. Therefore, the correlation entropy can also indicate the special symmetry point of the system.

From figure 1, the curve of correlation entropy is discontinuous at the points of $\theta_{c2} = 0.5\pi$ and $\theta_{c3} = 1.25\pi$. These critical points correspond to the first-order phase transitions in the system (1).

We focus the region of $1.25\pi < \theta < 2\pi$ in figure 1. The correlation entropy $S(0 : N/2)$ is a concave function near the coupling 1.6π , while it is a convex function near the coupling 1.8π . Then the derivative of correlation entropy $S'_\theta(0 : N/2)$ must have a maximum at certain θ_m , which gives us a hint to determine the second-order phase transition point. Please note that the correlation entropy $S(0 : N/2)$ must have one minimum and one maximum to show the concave and convex behaviors, thus the valley near the coupling 1.5π and the peak near the coupling 1.9π are trivial and do not mean anything. We find that the maximum of the derivative of the correlation entropy $S'_{\theta_m}(0 : N/2)$ and θ_m are oscillated with the increasing system size N , please see figure 4. This is because the correlation function with the longest distance $N/2$ has a factor $(-1)^{N/2}$. Then the correlation entropy and its derivative calculated from the correlation functions are also oscillated with the increasing system size. The oscillation effects can be erased by considering the cases of odd $N/2$ and even $N/2$ respectively and the results must be the same. Without losing generality, we consider the case that $N/2$ is odd. The θ_m versus the system size $N = 6, 10, 14$ is shown in figure 5. The linear fitting gives

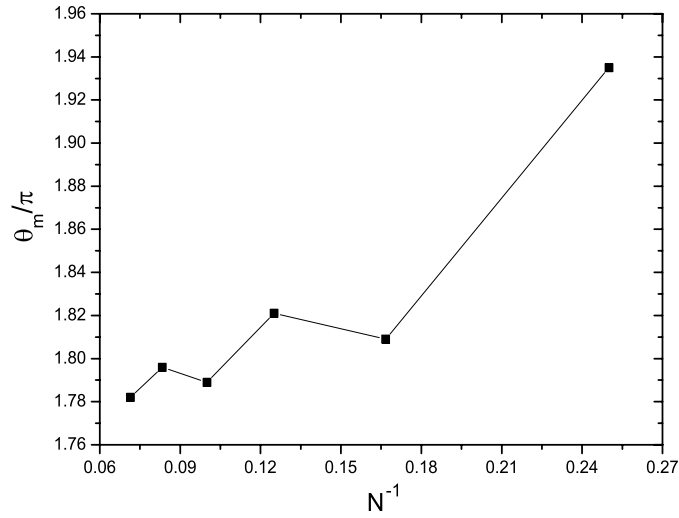


Figure 4. The finite size scaling behaviors of the coupling θ_m , at which the derivative of the correlation entropy $S'_{\theta_m}(0 : N/2)$ arrives at its maximum. The coupling θ_m are oscillated with the increasing system size N . This is because the correlation functions with the longest distance have a factor $(-1)^{N/2}$, then the correlation entropy and its inflexions calculated from the correlation functions have an oscillation. The oscillation effects can be erased by treating the odd $N/2$ and even $N/2$ respectively and the results are the same.

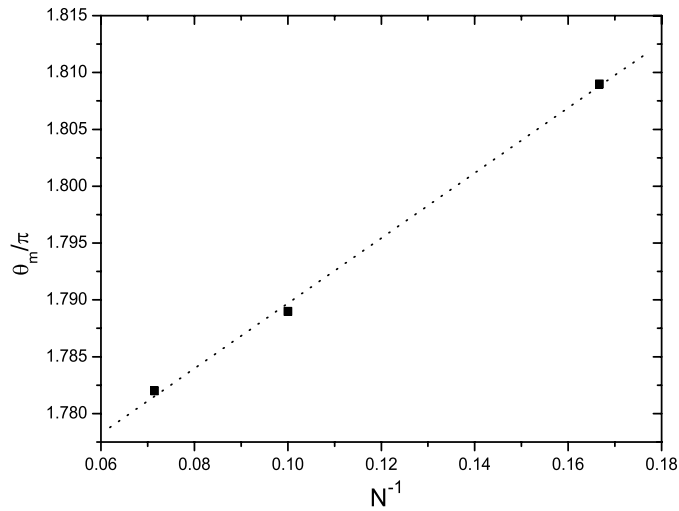


Figure 5. The finite size scaling behaviors of the coupling θ_m with the system size $N = 6, 10, 14$. The linear fitting gives $\theta_m/\pi = A + BN^{-1}$, where $A = 1.76105 \pm 0.00151$ and $B = 0.28643 \pm 0.01266$. When the system size tends to infinity, θ_m takes the value of $0.176\pi \pm 0.00151\pi$, which is reasonably close to the actual value 0.175π .

$\theta_m/\pi = 1.76105 + 0.28643N^{-1}$. When the system size tends to infinity, the θ_m takes the value of $0.176\pi \pm 0.00151\pi$, which is reasonably close to the actual critical value $\theta_{c4} = 0.175\pi$. The curve of the maximum of the derivative of correlation entropy $S'_{\theta_m}(0 : N/2)$ versus system

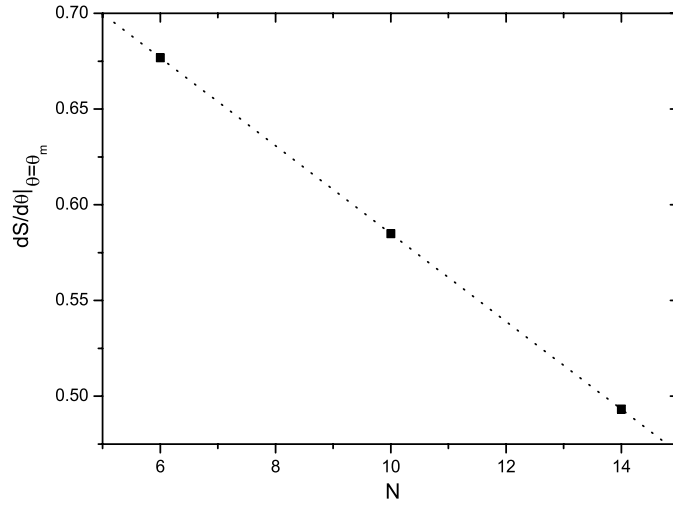


Figure 6. The curve of the maximum of the derivative of correlation entropy $S'_{\theta_m}(0 : N/2)$ versus the system size $N = 6, 10, 14$. The linear fitting gives $S'_{\theta_m}(0 : N/2) = A - BN$, where $A = 0.81452 \pm 0.00026$ and $B = 0.02295 \pm 0.00025$, which means the maximum of the derivative of correlation entropy is divergent when the system size N tends to infinity.

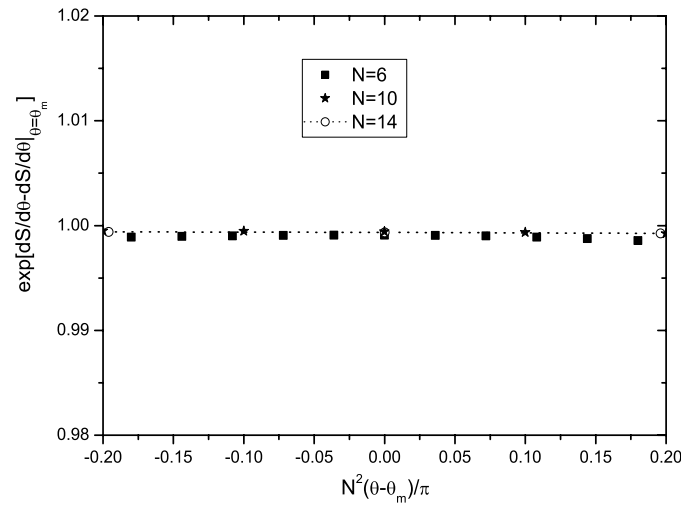


Figure 7. The finite size scaling behaviors of the maximum of the derivative of correlation entropy $S'_{\theta_m}(0 : N/2)$.

size N is shown in figure 6. The linear fitting gives $S'_{\theta_m}(0 : N/2) = 0.81452 - 0.02295N$. Thus the maximum of the derivative of correlation entropy is divergent when the system size tends to infinity. The finite size scaling behaviors of the maximum of the derivative of correlation entropy are shown in figure 7. We see that all the data for $N = 6, 10, 14$ fall on a single line. The phase transition at the coupling $\theta_{c4} = 1.75\pi$ is the second-order one because the above analysis is based on the first-order derivative of correlation entropy.

5. Conclusion

In conclusion, we study the long-range entropy correlation effects and quantum phase transitions in the one-dimensional spin-1 bilinear biquadratic model. From the singular analysis and finite size scaling behaviors of the correlation entropy or its derivative, we find that all the critical points in the system (1) can be determined by the correlation entropy. We also find that the correlation entropy can indicate the valence-bond solid state and the integrable SU(3) symmetric property of the system.

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