IOP Publishing Physica Scripta
Phys. Scr. 95 (2020) 055806 (7pp) https://doi.org/10.1088/1402-4896/ab73d7

Quantum phases of the 1D anisotropic spin-1/2 frustrated ferromagnetic model: view point of quantum correlations

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Received 26 November 2019, revised 26 January 2020
Accepted for publication 5 February 2020
Published 3 March 2020

Abstract

We have studied the ground state phases of the one-dimensional (1D) spin-$1/2$ anisotropic frustrated ferromagnetic model, using the numerical Lanczos method. We have focused on the quantum correlations as the concurrence and the quantum discord (QD) between the nearest neighbor (NN) and the next-nearest neighbor (NNN) spins. Numerical results show that the Tomonaga-Luttinger liquid (TLL), the even-parity dimer, and the vector chiral phases can be distinguished from each other using the long-distance quantum correlations. Specially, the critical points are explicitly detected in the first derivative of the concurrence between the nearest neighbor spins with respect to the frustration parameter.

Keywords: spin-$1/2$ frustrated chains, entanglement, quantum discord, quantum phases

(Some figures may appear in colour only in the online journal)

1. Introduction

Frustration refers to a condition where different competing interactions affect spins simultaneously. The spins conflict and as a result, they do not get an orientation satisfying all underlying interactions, that causes spins to fluctuate [1]. The topology of the lattice or interaction between farther-neighbor spins can drive a spin system into a frustrated state. Pauling [2] and Wannier [3] began the study of frustration more than 65 years ago. Wannier studied frustration in a triangular lattice with antiferromagnetic interactions, the simplest geometrical spin frustration. In this lattice, all three spins cannot be antiparallel and have to compromise.

1D strongly correlated frustrated spin systems have recently generated great interests for both experimental and theoretical researches in condensed matter physics [4–8]. These systems have been noticed specially because they have various phases in the ground state, high ground state degeneracy, and also gapful or gapless as well as magnetic or non-magnetic phases. Besides, some materials based on copper oxides can be described by frustrated chains such as $Rb_2Cu_2Mo_3O_{12}$ [9, 10], $LiCuVO_4$ [11–14], Li_2ZrCuO_4 [15], $La_6Ca_8Cu_{24}O_{41}$ [16], $LiCuSbO_4$ [17], and $PbCuSO_4$ [18]. Recently, there have been experimental efforts to generate frustrated configurations, in which, a system of four frustrated spins as a tetramer plaquette and a two-dimensional triangular optical lattice have been successfully simulated [19, 20].

In this paper, we consider a 1D spin-$1/2$ model with ferromagnetic exchange interaction ($J_1 < 0$) between the nearest-neighbors (NN) and antiferromagnetic ($J_2 > 0$) exchange interaction between the next-nearest-neighbors (NNN) that induces the frustration (see figure 1). The Hamiltonian of the system is defined as

$$\mathcal{H} = J_1\sum_{n=1}^{N}(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + \Delta S_n^z S_{n+1}^z) + J_2\sum_{n=1}^{N}(S_n^x S_{n+2}^x + S_n^y S_{n+2}^y + \Delta S_n^z S_{n+2}^z), \quad (1)$$

where S_n is the spin-$1/2$ operator of the n-th site and Δ is the anisotropy parameter. We have considered Δ in the easy-plane

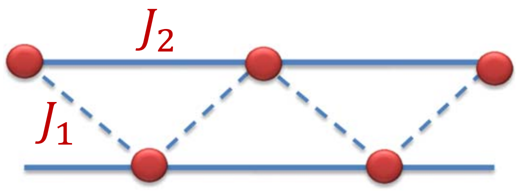

Figure 1. A sketch of the one-dimensional frustrated spin chain with J_1 exchange interaction between the nearest-neighbors and J_2 exchange interaction between the next-nearest-neighbors.

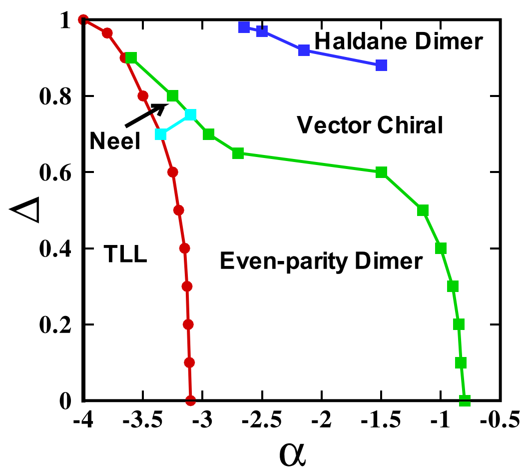

Figure 2. Ground state phase diagram of the 1D anisotropic spin-$1/2$ frustrated ferromagnetic Heisenberg model obtained in [33].

case, $0 \leqslant \Delta \leqslant 1$. From the theoretical point of view, this model has been the subject of many studies [21–48]. For $\Delta = 1$ ($SU(2)$-symmetric case) and the region with $\alpha = \frac{J_1}{J_2} < -4$, the ground state is in the saturated ferromagnetic phase and placed in the subspace $S_{tot} = \frac{N}{2}$ with the degeneracy $N + 1$ and becomes an incommensurate singlet state ($S_{tot} = 0$) for $\Delta = 1$ and $\alpha > -4$. Moreover, the lattice translational symmetry is thought to be broken [21–23]. At the critical point, $\alpha_c = -4$, two distinct configurations with the energy $\frac{E}{N} = -\frac{3}{16}J_1$ construct the degenerate ground state [22, 28]. It is suggested that in the incommensurate singlet state, the energy gap is strongly suppressed [29].

Furukawa *et al* [31–33] studied the ground state phase diagram of the model for $0 \leqslant \Delta < 1$ by means of the infinite time evolving block decimation algorithm and the bosonization approach. It was suggested that there is a variety of phases, including the Haldane dimer, the TLL, the Neel, the even-parity dimer, and the vector chiral phases (see figure 2). In the region with $\alpha \lesssim -4$, the anisotropic system is in the TLL phase. By increasing the frustration parameter α, depending on the anisotropy parameter, a quantum phase transition into the Neel phase or the even-parity dimer occurs [30, 31]. It is also pointed out that by further increasing α, the model converts to the vector chiral ordered phase. Furthermore, the existence of a narrow intermediate phase where the vector chiral and dimer orders coexist in $0.61 \lesssim \Delta \lesssim 0.63$ and $\alpha = -2$ is recognized by entanglement entropy [33].

Here, we use the Lanczos numerical method as a powerful tool for diagonalizing the Hamiltonian of finite size chains (up to $N = 28$ spins). We show how the competition between different couplings in a frustrated chain is reflected in quantum correlations such as the concurrence and the QD. It has been realized that quantum correlations can influence the low-temperature behavior of the bulk properties such as magnetic orders in a system. In addition, it can be used to pinpoint quantum phase transitions. These facts raised the interest in probing the relationship between quantum correlations and quantum phase transitions in this model. We also show that quantum correlations as the concurrence and the QD can help us to determine the critical regions in such a very complicated model. Our numerical results show that quantum correlations are able to separate three different phases: the TLL, the even-parity dimer, and the vector chiral phases.

The rest of the paper goes in the following sequence. In section 2, the concurrence as a measure of entanglement and the QD have been defined. In section 3, using the Lancsoz method, the Hamiltonian has been diagonalized and numerical results are presented. The results have been summarized in section 4.

2. The concurrence and the quantum discord

Due to the long-range correlations among the constituents of the system near the quantum critical points, the ground state of the 1D spin-$1/2$ frustrated ferromagnetic model must be nontrivial. It is suggested that in these complicated situations, quantum correlations could be also useful for studying quantum phase transitions [49]. Furthermore, it is widely argued that distinguishing quantum phase transitions in frustrated spin systems is feasible by analysis of the quantum correlation measures as the concurrence [50] and the QD [51]. It should be noted that in the mentioned works the frustrated antiferromagnetic model is considered.

One of the most important predictions of modern quantum physics is the entanglement [52, 53]. The entanglement is a unique property of any superposition state in quantum systems that consist of two or more elements. It is known that at the quantum critical point where the quantum phase transition happens, fluctuations of the order parameter extend throughout the system and the length of correlation diverges. Consequently, quantum correlations can mark quantum phase transitions at the critical points [54, 55]. The entanglement between two spins can be measured by the concurrence. The concurrence between two spins at sites n and $n + m$ is determined by the corresponding reduced density matrix [56]

$$\rho_{n,n+m} = \begin{pmatrix} X^{+}_{n,n+m} & 0 & 0 & 0 \\ 0 & Y^{+}_{n,n+m} & Z^{*}_{n,n+m} & 0 \\ 0 & Z_{n,n+m} & Y^{-}_{n,n+m} & 0 \\ 0 & 0 & 0 & X^{-}_{n,n+m} \end{pmatrix}, \qquad (2)$$

where

$$\begin{aligned} X^{+}_{n,n+m} &= \langle P^{\uparrow}_{n} P^{\uparrow}_{n+m}\rangle, \\ Y^{+}_{n,n+m} &= \langle P^{\uparrow}_{n} P^{\downarrow}_{n+m}\rangle, \\ Y^{-}_{n,n+m} &= \langle P^{\downarrow}_{n} P^{\uparrow}_{n+m}\rangle, \\ Z_{n,n+m} &= \langle S^{+}_{n} S^{-}_{n+m}\rangle, \\ X^{-}_{n,n+m} &= \langle P^{\downarrow}_{n} P^{\downarrow}_{n+m}\rangle, \end{aligned} \tag{3}$$

and $P^{\uparrow} = \frac{1}{2} + S^{z}$, $P^{\downarrow} = \frac{1}{2} - S^{z}$, $S^{\pm} = S^{x} \pm iS^{y}$. One should note that the brackets symbolize expectation values on the ground state of the system. Finally, the concurrence is obtained as

$$C_m = \max\{0, 2(|Z_{n,n+m}| - \sqrt{X^{+}_{n,n+m}X^{-}_{n,n+m}})\}. \tag{4}$$

It is known that there exist quantum correlations that are not spotlighted by the entanglement measures. These unilluminated correlations are thoroughly included in the formulation of so-called the QD as a measure for representing all quantum correlations [57, 58]. The QD coincides with the entanglement for pure quantum states, but for mixed quantum states, these two measures differ from each other. QD has motivated a search for a complete description of all quantum correlations specially where no entanglement exists [59, 60]. Here, we follow Sarandy's prescription [61] to study the QD in the frustrated model. The QD between a pair of spins at sites n and $n + m$ is defined as

$$QD_m = \mathcal{I}(\rho_{n,n+m}) - \mathcal{C}(\rho_{n,n+m}), \tag{5}$$

where $\mathcal{I}$ denotes the mutual information and $\mathcal{C}$ stands for the classical correlations. Mutual information is given by

$$\mathcal{I}(\rho_{n,n+m}) = S(\rho_n) + S(\rho_{n+m}) + \sum_{\alpha=0}^{3} \lambda_\alpha \log(\lambda_\alpha), \tag{6}$$

where λ_α are eigenvalues of $\rho_{n,n+m}$ and can be read as

$$\begin{aligned} \lambda_0 &= 0.25(1 + c_2 + |c_3|), \\ \lambda_1 &= 0.25(1 + c_2 - |c_3|), \\ \lambda_2 &= 0.25(1 - c_2 + |c_1|), \\ \lambda_3 &= 0.25(1 - c_2 - |c_1|). \end{aligned} \tag{7}$$

In addition, the entropy is determined as

$$S(\rho_n) = S(\rho_{n+m}) = -\left[\left(\frac{1+c_3}{2}\right)\log\left(\frac{1+c_3}{2}\right) + \left(\frac{1-c_3}{2}\right)\log\left(\frac{1-c_3}{2}\right)\right], \tag{8}$$

where we define new variables as

$$\begin{aligned} c_1 &= 2Z_{n,n+m}, \\ c_2 &= X^{+}_{n,n+m} + X^{-}_{n,n+m} - Y^{+}_{n,n+m} - Y^{-}_{n,n+m}, \\ c_3 &= X^{+}_{n,n+m} - X^{-}_{n,n+m}. \end{aligned} \tag{9}$$

The classical correlations, $\mathcal{C}(\rho_{n,n+m})$, are given by

$$\begin{aligned} &\mathcal{C}(\rho_{n,n+m}) \\ &= \max_{\{\Pi^{B}_{n}\}}\left(S(\rho_n) - \frac{S(\rho_0) + S(\rho_1)}{2}\right. \\ &\quad \left. - c_3\cos(\theta)\frac{S(\rho_0) - S(\rho_1)}{2}\right), \end{aligned} \tag{10}$$

where

$$\begin{aligned} S(\rho_k) = &-\left(\frac{1+\theta_k}{2}\right)\log\left(\frac{1+\theta_k}{2}\right) \\ &+ \left(\frac{1-\theta_k}{2}\right)\log\left(\frac{1-\theta_k}{2}\right), \end{aligned} \tag{11}$$

and $\theta_k = \sqrt{\sum_{d=1}^{3} q_{kd}^2}$. In this equation q_k is defined as

$$\begin{aligned} q_{k1} &= (-1)^k c_1\left[\frac{\sin(\theta)\cos(\phi)}{1 + (-1)^k c_3 \cos(\theta)}\right], \\ q_{k2} &= \tan(\phi) q_{k1}, \\ q_{k3} &= (-1)^k\left[\frac{c_2\cos(\theta) + (-1)^k c_3}{1 + (-1)^k c_3\cos(\theta)}\right], \end{aligned} \tag{12}$$

where $0 \leqslant \theta \leqslant \pi$ and $0 \leqslant \phi \leqslant 2\pi$. Therefore, the QD between a pair of spins located at sites n and $n + m$ can be calculated.

In recent years, the entanglement and the QD have been analyzed as a function of the distance between a pair of spins in the transverse magnetic field for spin-1/2 chains [54, 55, 62–70]. In the next section, the concurrence and the QD between spin pairs with different distances in the 1D ferromagnetic frustrated anisotropic spin-1/2 model will be studied and different ground state phases are recognized from the viewpoint of the quantum correlations.

3. Numerical experiment

The theoretical investigation of physical problems requires appropriate handling of very high-rank matrices. Although the matrix is sparse in a lot of applications, it is not possible to solve the problem by direct diagonalization of a very large matrix using the standard methods. The Lanczos numerical method with appropriate implementations has emerged as one of the most applicable computational procedures, mainly when the ground state is desired [71]. In fact, it is a method for tridiagonalizing Hermitian matrices. In following, we briefly summarize some basic features of the Lanczos method in its standard formulation. To explain this method briefly, let us consider Hamiltonian of the system as $\mathcal{H}$, with unknown eigenvalues and eigenstates. First, an initial normalized state, $|f_0\rangle$, is chosen arbitrary as the seed state of the procedure. Applying the operator of Hamiltonian $\mathcal{H}$ on the initial normalized state, a new state orthogonal to $|f_0\rangle$ is obtained as

$$|F_0\rangle = \mathcal{H}|f_0\rangle - \gamma_0|f_0\rangle, \tag{13}$$

where $\gamma_0 = \langle f_0|H|f_0\rangle$. The normalization of the new state, $|F_1\rangle$, is indicated by $\beta_1 = |\langle F_1|F_1\rangle|$, $|f_1\rangle = \frac{1}{\beta_1}|F_1\rangle$. By iterating l

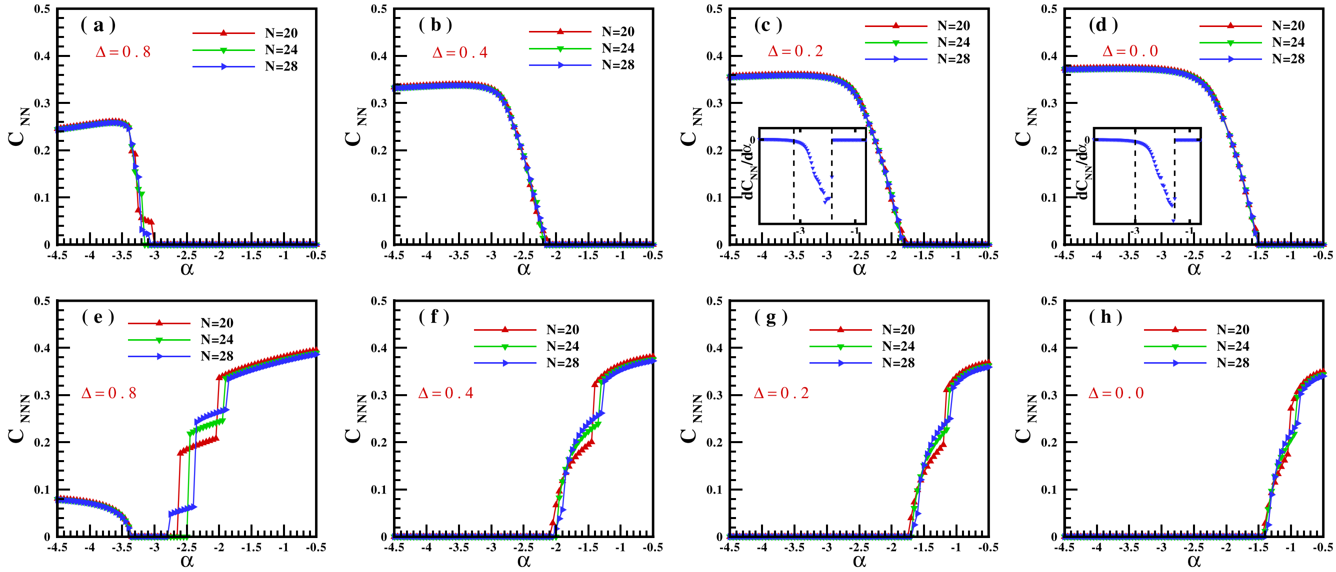

Figure 3. Concurrence between the NN spin pairs as a function of frustration parameter for (a) $\Delta = 0.8$, (b) $\Delta = 0.4$, (c) $\Delta = 0.2$, (d) $\Delta = 0.0$ and concurrence between the NNN spin pairs for (e) $\Delta = 0.8$, (f) $\Delta = 0.4$, (g) $\Delta = 0.2$, (h) $\Delta = 0.0$, using Lanczos method for chain sizes $N = 20, 24, 28$. The insets of (c) and (d) parts show the first derivative of the concurrence with respect to the frustration parameter for $\Delta = 0.2$ and $\Delta = 0.0$, respectively, for chain size $N = 28$.

times the procedure, a general form is obtained as

$$|F_{l+1}\rangle = \mathcal{H}|f_l\rangle - \gamma_l|f_l\rangle - \beta_l|f_{l-1}\rangle. \tag{14}$$

Finally, in the basis set $\{|f_l\rangle\}$, the Hamiltonian is presented by a tridiagonal matrix as

$$\mathcal{H} = \begin{pmatrix} \gamma_0 & \beta_1 & 0 & 0 & \dots & & \\ \beta_1 & \gamma_1 & \beta_2 & 0 & 0 & \dots & \\ 0 & \beta_2 & \gamma_2 & \beta_3 & 0 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}. \tag{15}$$

It should be noted that the number of steps to be carried out in the Lanczos procedure, can be reasonably small. The diagonalization of tridiagonal matrix form of the Hamiltonian gives low energy states of the system.

Here, we used the Lanczos numerical method and diagonalized the Hamiltonian of the system for different values of the frustration α and anisotropy parameter Δ. Periodic boundary conditions are considered for chains with lengths $N = 12,\ 16,\ \dots\ 28$, but only results of three largest sizes ($N = 20, 24, 28$) are reported. The ground state of the system, $|GS\rangle$, is calculated by applying the Lanczos algorithm and subsequently, quantum correlations are obtained.

Numerical results of the concurrence between the NN and the NNN spin pairs for different chain lengths, $N = 20$, 24, 28, and different values of the anisotropy parameter, $\Delta = 0.8, 0.4, 0.2, 0.0$, are presented in figure 3. Figure 3(a) shows that the NN spin pairs are entangled in the TLL phase. This is in complete agreement with previous studies that the NN spin pairs are entangled in the TLL phase of 1D spin-1/2 systems [54, 56, 66, 72]. By increasing the frustration parameter, α, the concurrence between the NN spin pairs grows very slowly and will be maximized at the first critical frustration point, α_{c_1}. As soon as the frustration parameter crosses the first critical point, the concurrence between the NN spin pairs decreases rapidly and vanishes at the second critical frustration point, α_{c_2}. In the region $\alpha > \alpha_{c_2}$, the NN spin pairs are not entangled. For the same anisotropy parameter value, $\Delta = 0.8$, the behavior of the concurrence between NNN spin pairs is shown in figure 3(e). It should be noted that only in the middle region, $\alpha_{c_1} < \alpha < \alpha_{c_2}$, the NNN spin pairs are not entangled. Unlike the NN spin pairs, when $\alpha > \alpha_{c_2}$, the NNN spin pairs are entangled and the value of the concurrence increases by α.

Moreover, the same behavior is observed for other values of the anisotropy parameter, $\Delta = 0.4, 0.2, 0.0$, in figure 3. For $\alpha < \alpha_{c_1}$, the NN spin pairs are entangled and concurrence value remains almost constant by increasing α. As soon as the frustration increases from α_{c_1}, the concurrence between the NN spin pairs starts to decrease and vanishes at the second critical frustration point α_{c_2}. Finally, in the vector chiral phase, the NN spin pairs are not entangled. In contrast, figures 3(f)–(h) show that the NNN spin pairs are only entangled for $\alpha > \alpha_{c_2}$.

In insets of figures 3(c) and (d), the first derivative of the concurrence between NN spin pairs is plotted versus the frustration parameter. As it is clearly seen, the concurrence derivative is explicitly able to separate the even-parity dimer region (located between two dashed lines in the mentioned figure) from two other phases. In the even-parity dimer phase, we observe non-zero value of the concurrence between NN spin pairs. This fact accord with the picture that the ground state is approximated by the product state of $(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$ that are maximally entangled. By increasing α in this phase, the states with less entanglement create. Ultimately, new states which can be expressed as a separable state become dominant and the system undergoes a phase transition to an unentangled phase.

In addition to the concurrence, we have calculated the QD between the NN and NNN spin pairs. The Lanczos results are presented in figure 4. As a general behavior, the QD

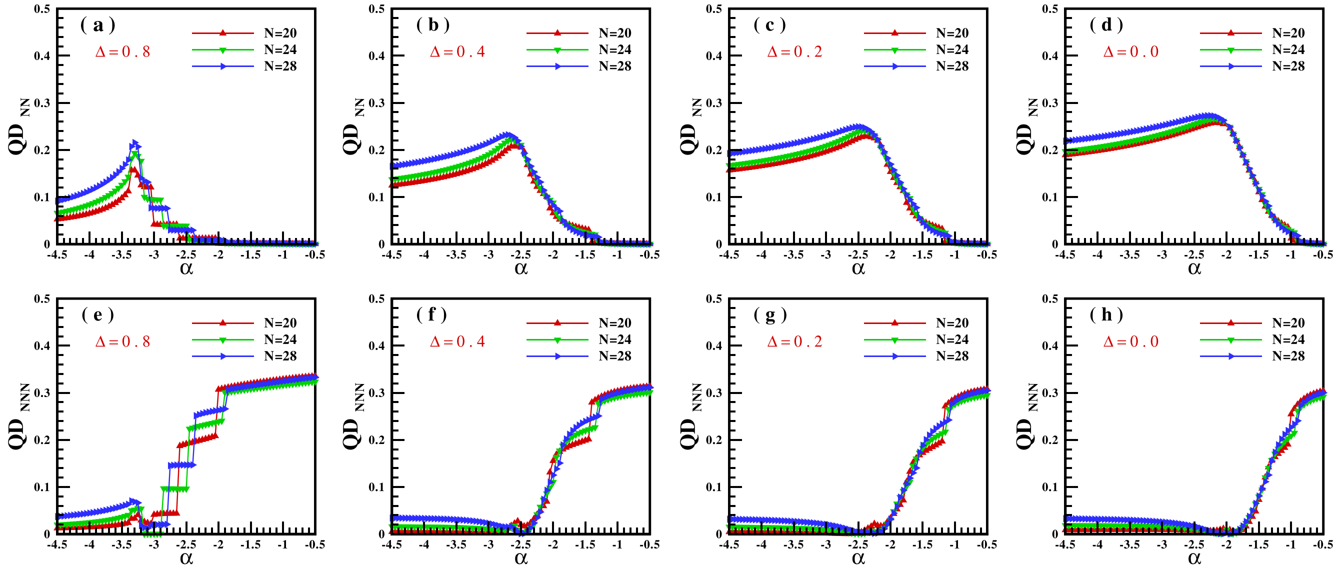

Figure 4. QD between the NN spin pairs as a function of frustration parameter for (a) $\Delta = 0.8$, (b) $\Delta = 0.4$, (c) $\Delta = 0.2$, (d) $\Delta = 0.0$ and QD between the NNN spin pairs for (e) $\Delta = 0.8$, (f) $\Delta = 0.4$, (g) $\Delta = 0.2$, (h) $\Delta = 0.0$, using Lanczos method for chain sizes $N = 20$, 24, 28.

between the NN spin pairs grows by increasing the frustration (figures 4(a)–(d)). It will be maximized exactly at the first critical frustration point $\alpha_{c_1}(\Delta)$. As soon as the frustration crosses the first critical point, the QD between the NN spin pairs starts to decrease and shows a monotonic behavior in the region $\alpha_{c_1} < \alpha < \alpha_{c_2}$ (It is clearly seen in figure 4(d) without finite size level crossing). Finally, for $\alpha > \alpha_{c_2}$, it shows a plateau with a value of approximately zero. As it is seen in figures 4(e)–(h), QD between the NNN spin pairs also shows very interesting behavior. In the TLL phase, a quasi-plateau is observed. Close to the first critical frustration parameter, α_{c_1}, it starts to increase and exactly at the first critical point a maximum is seen as a cusp for $\Delta = 0.8$. Finally, in the region $\alpha > \alpha_{c_2}$, the QD between the NN spin pairs shows an increasing behavior.

To have a complete knowledge of the concurrence behavior in different phases, we added a density plot of the concurrence in figure 5. The concurrence between the NN and NNN spin pairs in the $(\Delta - \alpha)$ plane for a chain size $N = 20$ are sketched in figures 5(a) and (b), respectively. As it is displayed in panel (a) of the figure 5, in the TLL phase, the NN spin pairs are entangled and by increasing frustration, the concurrence almost remains constant. Moreover, in vector chiral phase, concurrence between the NN spin pairs is disappeared. Between these two phases, we observed the even-parity dimer region with decreasing concurrence values.

The concurrence for the NNN spin pairs is displayed in the panel (b) of figure 5. In contrast with the nearest neighbor spin pairs, in the both TLL and even-parity dimer phases, the concurrence for NNN spin pairs has zero values, except in a small area in the TLL phase near $\Delta = 1$. Therefore, the boundary line between TLL and even-parity dimer phases is not recognizable in this diagram. Furthermore, in the vector chiral phase by increasing frustration parameter, the NNN spins start to be entangled and the concurrence value increases by increasing frustration. It is worthy noting that

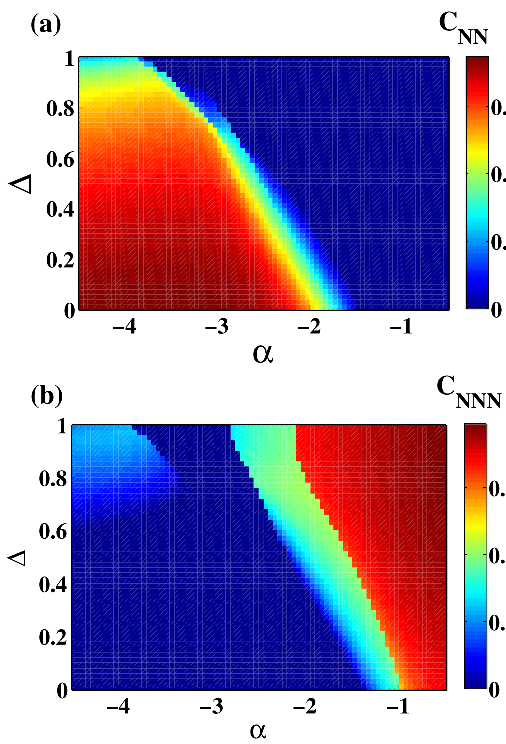

Figure 5. Density plot of the concurrence between (a) the NN (b) the NNN spin pairs in (Δ-α) plane, for $N = 20$ using the Lanczos method results.

$(\Delta,\ \alpha) = (1, -4)$ transition point is clearly signaled by concurrence between NN and NNN spins.

4. Summary

In this work, we considered a 1D spin-$\frac{1}{2}$ anisotropic Heisenberg model with ferromagnetic interaction between the

NN spins which is frustrated by antiferromagnetic interaction between the NNN spins. Using the Lanczos numerical method we did a numerical experiment on the ground state phases by focusing on the quantum correlations. We calculated the ground state of the finite chains with lengths $N = 20$, 24, and 28. Different values of the anisotropy and frustration parameters are considered. The results of our numerical experiment showed that quantum critical points can be extracted from the behavior of quantum correlations. In fact, entanglement between the NN spin pairs is almost constant in the TLL phase region, $\alpha < \alpha_{c_1}(\Delta)$. In the middle region, $\alpha_{c_1}(\Delta) < \alpha < \alpha_{c_2}(\Delta)$, it shows a monotonic decreasing behavior. Finally, in the vector chiral phase, $\alpha > \alpha_{c_2}(\Delta)$, the NN spin pairs are not entangled. On the contrary, the NNN spin pairs are only entangled in the vector chiral region.

In addition to the entanglement, we studied the QD between the NN and the NNN spin pairs. From the numerical results, we found that the QD between NN spin pairs will be maximum at the first critical point, $\alpha_{c_1}(\Delta)$. At the second critical point $\alpha_{c_2}(\Delta)$, it will almost become zero. Moreover, the QD between the NNN spin pairs exists in the region $\alpha > \alpha_{c_2}(\Delta)$ and increases by increasing frustration.

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