Quantum corrections of the biquadratic interaction in the 1D spin-1/2 frustrated ferromagnetic systems

Javad Vahedi1, Saeed Mahdavifar2
1 Department of Physics, Science and Research Branch, Islamic Azad University, Tehran, Iran
2 Department of Physics, University of Guilan,41335-1914, Rasht, Iran

(Dated: May 10, 2014)

Quantum corrections of the biquadratic interaction in the 1D spin-1/2 frustrated ferromagnetic Heisenberg model are studied. The biquadratic interaction for spin-1/2 chains is eliminated and transformed to the quadratic interaction. Doing a numerical experiment, new insight as to how the classical phases get modified on the inclusion of quantum fluctuations is provided. Observed results suggest the existence of an intermediate region in the ground state phase diagram of the frustrated ferromagnetic spin-1/2 chains with combination of dimer and chiral orders. In addition, from the quantum entanglement viewpoint, differences between quantum phases are also obtained. The nearest neighbor spins never be entangled in the frustrated ferromagnetic chains but are entangled up to the Majumdar-Ghosh point in the frustrated antiferromagnetic chains. On the other hand, the next nearest neighbor spins in the mentioned intermediate region are entangled.

PACS numbers: 75.10.Jm; 75.10.Pq

I. INTRODUCTION

The explore of novel order in frustrated models in low dimensional quantum systems have been studied extensively from theoretical and experimental point of view. An example which shows a variety of intriguing phenomena is frustrated ferromagnetic spin-1/2 chain with added nearest-neighbor biquadratic interaction:

\[ H = \sum_{n=1}^{N} \left[ J_1 \vec{S}_n \cdot \vec{S}_{n+1} + J_2 \vec{S}_n \cdot \vec{S}_{n+2} - A(\vec{S}_n \cdot \vec{S}_{n+1})^2 \right], \tag{1} \]

where \( J_1 < 0, J_2 > 0 \) are the nearest-neighbor (NN) and next-nearest-neighbor (NNN) exchange couplings. \( \vec{S}_n \) represents the spin-1/2 operator at the \( n \)-th site, and \( A \) denotes the biquadratic exchange. We introduce parameters \( \alpha = \frac{J_2}{J_1} \) and \( a = \frac{A}{J_1} \) for convenience.

The pure frustrated ferromagnetic model (\( a = 0 \)) is well studied\textsuperscript{2,3,4,5}. Beside a general interest in understanding frustrations and phase transitions, it helps people to understand intriguing magnetic properties of a novel class of edge-sharing copper oxides, described by the frustrated ferromagnetic model\textsuperscript{6,7,8}. Several compounds with edge-sharing chains are known, such as \( \text{Li}_2\text{CuO}_2 \), \( \text{La}_2\text{CuO}_4 \), and \( \text{Cu}_2\text{Y}_2\text{Cu}_2\text{O}_8 \). Though the pure frustrated ferromagnetic model has been a subject of many studies\textsuperscript{9,10,11,12} the complete picture of the quantum phases of this model has remained unclear up to now. It is known that the ground state is ferromagnetic for \( \alpha = \frac{J_2}{J_1} < \frac{1}{2} \). At \( \alpha_c = 1/4 \) the ferromagnetic state is degenerate with a singlet state. The wave function of this singlet state is exactly known\textsuperscript{13,14}. For \( \alpha > \frac{1}{4} \), however, the ground state is an incommensurate singlet. It has been long believed that at \( \alpha > \frac{1}{4} \) the model is gapless\textsuperscript{15,16} but the one-loop renormalization group analysis indicates\textsuperscript{17,18} that the gap is open due to a Lorentz symmetry breaking perturbation. However, existence of the energy gap has not been yet verified numerically\textsuperscript{19}. Using field theory considerations it has been proposed\textsuperscript{20} that a very tiny but finite gap exists which can be hardly observed by numerical techniques.

In a very recent work\textsuperscript{21}, T. Kaplan presents the classical ground state phase diagram of the frustrated model with added biquadratic exchange interaction (\( a \neq 0 \)). By considering spins as vector and using a kind of cluster method which is based on a block of three spins, he found the classical ground state phase diagram as Fig.\textsuperscript{22}. The classical phase diagram exhibits the ferromagnetic, the spiral, the canted-ferro, and up-up-down-down spin structures. In the non frustrated Heisenberg case (\( \alpha = 0 \)), the spiral phase is caused by the contest between the Heisenberg and the biquadratic interactions. There are two known sources of these terms: Firstly, purely electronic: higher order terms in the hopping amplitudes or orbital overlap (leading order yields the Heisenberg interactions)\textsuperscript{23,24} and Secondly, lattice induced: spin-lattice interaction\textsuperscript{25}.

The presence of chiral phase in quasi-one dimensional frustrated magnets has been intensively studied during the last decade.\textsuperscript{26,27,28,29,30,31,32,33,34} This interest was triggered by the prediction of a ground state with non-zero vector spin chirality, \( \langle \vec{S}_i \times \vec{S}_m \rangle \neq 0 \). As it is pointed in ref.\textsuperscript{30}, classical states with spontaneously broken chirality only exist together with helical long range order. The helical order breaks the continuous symmetry of global spin rotations along the \( z \)-axis. Consequently, the existence of long range helical order is in most cases precluded by zero point fluctuations of 1D quantum systems\textsuperscript{35,36} (Mermin-Wagner theorem\textsuperscript{37}). On the other hand, chiral orderings are allowed because they only break discrete symmetries. For this reason, chiral orders in quantum spin systems can be thought as remnants of the helical order in classical systems. This is one of the main motivations for finding chiral orders in quantum spin Hamiltonian whose ground state exhibits helical order in the \( S \rightarrow \infty \) limit\textsuperscript{38}.
The structure of the paper is as follows: In Sec. II we check the validity of classical phase diagram capture exhaustively with the accurate lanczos scheme from quantum point of view. In Sec. III we will use the entanglement of formation (EoF) to check the presence of quantum point of view. In Sec. IV we will present our results.

II. QUANTUM PHASE DIAGRAM

By considering operator \(2(S_n \cdot S_{n+1}) + 1/2\) as the permutation operator, the 1D frustrated ferromagnetic Hamiltonian is transformed to the following model

\[
H^\text{F} = \sum_{n=1}^{N} \left[-(1 + \frac{\alpha}{2})S_n \cdot S_{n+1} + \alpha S_n \cdot S_{n+2}\right] + \text{constant}.
\]  

This is nothing but the isotropic spin-1/2 Heisenberg model with NN exchange \((1 + \frac{\alpha}{2})\) and NNN exchange \(\alpha\). From quantum point of view, one encounter with four different cases by changing the strength of the biquadratic and the frustration exchanges

(I) \(\alpha < 0, \ a < -2\), nonfrustrated AF – F model  
(II) \(\alpha < 0, \ a > -2\), nonfrustrated F – F model  
(III) \(\alpha > 0, \ a < -2\), frustrated AF – AF model  
(IV) \(\alpha > 0, \ a > -2\), frustrated F – AF model.

It is known that the ground state of the 1D spin-1/2 non-frustrated F-F model has the ferromagnetic long-range order. On the other hand the spectrum of the non-frustrated AF-F model is gapless. The 1D frustrated AF-AF is well known. In the classical limit the system develops spiral order for \(\frac{\alpha}{1+\alpha/2} > \frac{1}{4}\) whereas a quantum phase transition into a dimerized phase occurs at \(\alpha_c \approx 0.2411\ | 1 + a/2 \). This dimerized phase is characterized by a singlet ground state with twofold degeneracy and an excitation gap to the first excited state. At the Majumdar-Ghosh point \(35\), i.e. \(\alpha = 0.5 \ | 1 + a/2 \) the ground state is exactly solvable. In addition, the ground state of the frustrated F-F model is ferromagnetic for \(\frac{\alpha}{1+\alpha/2} < \frac{1}{4}\). At \(\alpha_c = \frac{1}{4}(1 + a/2)\) the ferromagnetic state is degenerate with a singlet state. For \(\alpha > \alpha_c\), the existence of a tiny gapped region suggested. Recently, the possible relevance of this model to the several quasi-1D edge-sharing cuprates \(36,37,38,39,40\) is raised very serious. \(41,42,43,44\) These compounds can exhibit multiferroic behavior in low-temperature chiral spin ordered phases. Theoretically, the study of the anisotropy effect clearly has shown that the chiral phase appears and extends up to the vicinity of the SU(2) point for moderate values of frustration \(42,44\) in well agreement with the experimental results.

In the following, to find the ground state quantum phase diagram and providing proper insight as how the classical phases can modify by the inclusion of quantum fluctuations, we did a numerical experiment by using the Lanczos method. To explore the nature of the spectrum and the quantum phase transitions, we diagonalized numerically chains with length up to \(N = 24\) for different values of the biquadratic exchanges. The energies of the few lowest eigenstates were obtained for chains with periodic boundary conditions.

We start our study with magnetization where defined as

\[
M^\gamma = \frac{1}{N} \sum_{j=1}^{N} \langle GS | S_j^\gamma | GS \rangle \tag{3}
\]

where \(\gamma = x, y, z\) and the notation \(\langle GS | ... | GS \rangle\) represents the ground state expectation value. One of the most intriguing properties of quasi-one dimensional frustrated systems is the dependence of the magnetization on the applied magnetic field at \(T = 0\). The magnetization is characterized by a swift increase (or even discontinuity) in the magnetization when the external field exceeds a critical value. It is expected that the magnetization exhibits a true jump (the metamagnetic transition) when the frustration \(\alpha\) is a little larger than \(\alpha_c = 0.25\). \(41,44\) In Fig. 2(a) and Fig. 2(b), for chain size \(N = 24\), we have plotted \(M^x\) as a function of frustration and biquadratic parameters respectively in order to sweep all parts of the ground state phase diagram. As it can be seen from Fig. 2(a), the magnetization is saturated, \(M^x = 0.5\), in the ground state of the nonfrustrated F-F model and for some values of the frustration, \(\alpha < \alpha_c = \frac{1}{4}(1 + a/2)\) in the frustrated F-AF model. At the critical point \(\alpha_c = \frac{1}{4}(1 + a/2)\), a sudden jump is happened which is known as the metamagnetic phase transition. \(5\) Numerical results presented in Fig. 2(b) show that quantum fluctuations destroy the suggested classical long range order.
canted ferromagnetic order in the nonfrustrated AF-F model. By changing the biquadratic exchange a metamagnetic phase transition between nonfrustrated AF-F and F-F models happens at the exact critical biquadratic exchange $a = -2.0$. In the insets of Fig. 2, we have plotted the magnetization for a fixed value of the biquadratic interaction Fig. 2(a) and frustration parameter Fig. 2(b) for different chain sizes $N = 12, 16, 20, 24$. It is completely clear that there is not any size effect on the numerical results of the magnetization that confirms the presence of critical lines in the thermodynamic limit. In conclusion the quantum critical line which separates the ferromagnetic phase from the spiral phase is consistent with the classical line, but our calculations show that the vertical critical line which separates the ferromagnetic phase from up-up-down-down phase no longer exists in the quantum level and quantum correlations expand the ferromagnetic phase to live even in the region $\alpha \geq 0.5$ and $\alpha \geq 2.0$.

To display the quantum ground state magnetic phase diagram of the model and check the nature of the classical suggested up-up-down-down phase we have calculated the quantum dimer order parameter which is defined as

$$d = \frac{1}{N} \sum_{j} \langle GS|\vec{S}_{j} \cdot \vec{S}_{j+1} - \vec{S}_{j} \cdot \vec{S}_{j+2}|GS\rangle. \quad (4)$$

In Fig. 2(a), we have plotted the dimer order parameter $d$ as a function of the frustration parameter $\alpha$ with different fixed values of the biquadratic parameter $a = 1.0, 1.2, \ldots, 3.0$ for chain size $N = 24$. It is clear from Fig. 2(a) that in the frustrated F-F model, for values of the frustration $\alpha < \alpha_{c1} = \frac{1}{4}(1 + a/2)$ the dimer order parameter is equal to zero in well agreement with fully polarized ferromagnetic phase. By further increasing the frustration and for $\alpha > \alpha_{c1}$, the dimer order parameter starts to increase and reaches its saturation value ($\approx 0.5$) at $\alpha = \alpha_{c2}(a)$. At the first critical point, $\alpha = \alpha_{c1}$, quantum fluctuations suppress the ferromagnetic ordering and the system undergoes a quantum phase transition from the ferromagnetic phase into a phase with dimer ordering. The positive value of the dimer order parameter in the region $\alpha > \alpha_{c1}$, shows the dimerization between nearest neighbors which is named “Dimer-I”. The oscillations (quasi-plateaus) at finite $N$ in the region $\alpha_{c1} < \alpha < \alpha_{c2}$, are the result of level crossing between the ground state and excited states of the model. At the second quantum critical point, $\alpha = \alpha_{c2}$, the ground state of the system goes into a phase with almost fully polarized dimer state between nearest neighbors. We have also checked the size effects on the dimerization and numerical results are shown in the inset of Fig. 2(a) with fixed biquadratic exchange $a = 2.0$ for different chain lengths $N = 12, 16, 20, 24$.

In Fig. 2(b), the dimer order parameter is plotted vs the frustrated parameter for a chain size $N = 24$ and different values of the biquadratic parameter $a < -2.0$. Indeed, in order to check the nature of the classical suggested canted ferromagnetic phase, we have plotted the dimer order parameter as a function of the frustrated parameter for fixed values of biquadratic exchanges in this region. As it can be seen from Fig. 2(b), in the region $\alpha < 0$, namely nonfrustrated AF-F model, the ground state of the system has the long-range dimerization between nearest neighbors, so called the Dimer-I phase. In the case of the frustrated AF-AF model, as soon as the frustration increases from $\alpha_{c}$, the dimerization order parameter starts to increase and becomes zero at almost Majumdar-Ghosh point $\alpha = 0.5 \mid 1 + a/2 \mid$. The value of the the critical frustration, $\alpha_{c}$, depends on

FIG. 2: (Color online.) Magnetization ($M^x$) curve versus (a) frustration parameter $\alpha$ with different fixed biquadratic parameters $a = 1.0, 1.2, \ldots, 3.0$ for chain with length $N = 24$. (b) biquadratic parameter $a$ with different fixed frustration $\alpha = -0.1, -0.2, -0.3$ for chain with length $N = 24$. In both plots the inset shows scaling behavior for chain with lengths $N = 12, 16, 20, 24$. 
rapidly and reaches to the saturation value ($d \to 1$). By more increasing the frustration, a

dimer ordering between next nearest spins $N = 24$. In both plots the inset shows scaling behavior for
chain with lengths $N = 12, 16, 20, 24$. The vector chiral phase is characterized by long-range order of the vector chiral correlation defined as

$$C_I = \sum_{l=1}^{N} \langle GS | \chi_j \chi_{j+l} | GS \rangle.$$  

To find a deeper insight into the nature of the quantum phases we have calculated numerically the vector chiral correlation for chains with periodic boundary conditions and lengths $N = 12, 16, 20, 24$. In Fig. 4 we have presented Lanczos results on the vector chiral correlation, $C_I$, as a function of the frustration parameter $\alpha$ for different chain lengths $N = 12, 16, 20, 24$. As is clearly seen, in the region $\alpha < \alpha_{c1} = 1/2, (1 + b)/2$ there is no long-range chiral order along the $x$ axis in well agreement with the ferromagnetic phase. By increasing the frustration, in an intermediate region, $\alpha_{c1} < \alpha < \alpha_{c2}$, the ground state shows a profound chiral order. It is important to note that the growth of the results in the intermediate region by increasing size of the system, shows the diverging in the thermodynamic limit $N \to \infty$ the characteristic of the true long-range order of the chirality. As soon as the frustration increases from $\alpha_{c2}$, the chirality drops rapidly. The constant value of the vector chiral correlation in the region $\alpha > \alpha_{c2}$ shows that the $C_I / N$ takes zero value in the thermodynamic limit $N \to \infty$. Also, we did our numerical experiment for other values of the biquadratic exchange in the region $\alpha > -2.0$ and found the same qualitative picture. Therefore, in the intermediate region $\alpha_{c1} < \alpha < \alpha_{c2}$ and for values of the biquadratic exchange, $a > -2$ corresponding to the frustrated F-AF model, the dimer ordering between next nearest spins coexists with the chirality.

Another way of the quantum mechanical mimic of the classical pitch angle is the possibility to study at which
wave vector $q$ the static spin structure factor
\[
S^\alpha(q) = \sum_{j} e^{iqj} \langle GS \mid \sigma_j^\alpha \sigma_j^\alpha \mid GS \rangle.
\] (7)

is peaked. In Fig. (4b), we have plotted the structure factor versus $0 \leq q \leq 2\pi$ with fixed parameters $a = 2.0$ and $\alpha = 0.68$. As it can be seen, the structure factor shows two peaks around the $q \sim 1.0$ and $q \sim 5.0$ in the predicted chiral phase.

III. GROUND STATE ENTANGLEMENT

In recent years interest of the quantum information community to study in condensed matter has stimulated an exciting cross fertilization between the two areas. It has been found that entanglement plays a crucial role in the low-temperature physics of many of these systems, particularly in their ground states. The pioneering study of quantum information in the condensed matter area was the observation that two body entanglement in the ground state of a cooperative system, exhibits peculiar scaling features approaching a quantum critical point. These seminal studies showed that at quantum phase transitions the dramatic change in the ground state is associated to a change in the way entanglement is distributed among the elementary constituents. We here focus on one of the most frequently used entanglement measure: concurrence. A knowledge of two-site reduced density matrix enables one to calculate concurrence, a measure of entanglement between two spin at site $i$ and $j$. The reduced density matrix defined as
\[
\rho_{ij} = \frac{1}{4} \left( 1 + \sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y + \sigma_i^z \sigma_j^z \right)
\] (8)

where $\sigma_i^x$ is the Pauli matrix and the concurrence $C$ is given by $C = \text{max} \{e_1 - e_2 - e_3 - e_4, 0\}$, where $e_i$'s are square roots of the eigenvalues of the operator $\rho_{ij} = \rho_{ij}(\sigma_i^x \otimes \sigma_j^x)\rho_{ij}(\sigma_i^x \otimes \sigma_j^x)$ in descending order. $C = 0$ implies an unentangled state whereas $C = 1$ corresponds to maximum entanglement.

The numerical Lanczos results describing the concurrence are shown in Fig. 5. In this figure the concurrence between two NN spins is plotted as a function of the frustration $\alpha$. It can be seen that NN spins do not show any entanglement for the biquadratic exchange $a = 2.0$. Increasing the frustration and reaches its nearly saturated value at $\alpha = \alpha_{c1}$. As soon as the frustration increases from $\alpha_{c1}$, a jump happens which is the characteristic of the metamagnetic phase transition. In the intermediate region, $\alpha_{c1} < \alpha < \alpha_{c2}$, the concurrence between NNN spins increases by increasing the frustration and reaches its nearly saturated value at $\alpha = \alpha_{c2}$. In the region $\alpha > \alpha_{c2}$, the concurrence between NNN spins remains almost constant. Indeed the quantum correlations between two NNN spins in the intermediate region, increases with increasing the frustration and takes the almost maximum value at $\alpha_{c2}$. In the inset of Fig. 5(a), we have plotted the concurrence between NN spins as a function of the frustration for the biquadratic exchange $a = 2.0$. It can be seen that the NN spins do not show any entanglement.
in the frustrated F-AF model. To complete our study of the entanglement phenomena we have calculated the concurrence between NN and NNN spins in different sectors of the ground state phase diagram. For example, we have presented our numerical results for the biquadratic exchange $a = -3$ in Fig. 5(b). As it can be seen, in the region of frustration, $\alpha < 0$, corresponding to the non-frustrated AF-F model, the NNN spins are not entangled but NN spins are entangled (inset of Fig. 5(b)). On the other hand, in the frustrated AF-AF model, the NN spins remain entangled up to the Majumdar-Ghosh point and then after the Majumdar-Ghosh by increasing the frustration parameter only the NNN spins will be entangled.

IV. SUMMARY AND DISCUSSION

We have considered the frustrated ferromagnetic chains spin-$\frac{1}{2}$ with added nearest-neighbor biquadratic interaction. In a very recent work, the classical ground state phase diagram of the model was studied. The existence of ferromagnetic, spiral, canted-ferro and up-up-down-down spin structures was shown. To find the quantum corrections, first, using a permutation operator we eliminated the biquadratic interaction and transformed it to the quadratic interaction. By changing the biquadratic parameter, it is shown that the transformed Hamiltonian covers all types of NN and NNN interaction models. Then, we did a numerical experiment to observed quantum corrections.

Our numerical experiment showed that the quantum fluctuations are strong to change the classical ground state phase diagram. As it can be seen from Fig. 6 depending on the values of the frustration and the biquadratic exchange parameters, the ground state of the system can be found in the ferromagnetic, the Dimer-I, the Dimer-II and the chiral magnetic orders.

In very recent works, it was shown that the chiral phase appears in anisotropic frustrated ferromagnetic chains and extends up to the vicinity of the SU(2) point for moderate values of frustration in well agreement with the experimental results. The complete picture of the quantum phases of this model has remained unclear up to now. Also, several authors have discussed deeply in this area. The existence of a tiny but finite gap in the region of the frustration $\alpha > 0.24$ is one of the

FIG. 6: (Color online) Modified quantum phase diagram.
interesting and still puzzling effects in frustrated ferromagnetic chains.

It is also worth mentioning, using the coupled cluster method for infinite chain and exact diagonalization for finite chain, author in ref.[52], have studied the effect of a third-neighbor exchange $J_3$ on the ground state of the spin half Heisenberg chain with ferromagnetic nearest-neighbor interaction $J_1$ and frustrating antiferromagnetic next-nearest-neighbor interaction $J_2$. By setting $J_1 = -1$, they have proposed that the quantum phase diagram consist of spiral and ferromagnetic phases in the $J_2 - J_3$ plane. Across the $J_3 = 0$ line, in the proposed diagram the second-order transition will take place from FM to spiral phase. Our study shows, there should be the mentioned region and It is surprising that this region have the two ordering phases: Dimer-II and chiral. However more research is needed in this respect.

From quantum entanglement point of view, difference between quantum phases is also studied. We showed that the concurrence function is a very useful tool to recognize the different quantum phases specially in different sectors of the ground state phase diagram.

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V. ACKNOWLEDGEMENT

It is our pleasure to thank T. Vekua and T. Nishino, for very useful comments.

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