Classical Investigation of Frustrated and Dimerized Heisenberg Chains

J. Vahedi\textsuperscript{1}, S. Mahdavifar\textsuperscript{2}, M. R. Soltani\textsuperscript{3}, M. Elahi\textsuperscript{1}

\textsuperscript{1}Department of Physics, Science and Research Branch, Islamic Azad University, Tehran, Iran
\textsuperscript{2}Department of Physics, University of Guilan, 41335-1914, Rasht, Iran
\textsuperscript{3}Department of Physics, Shahr-Ray branch, Islamic Azad University, Tehran, Iran.

(Dated: May 10, 2014)

PACS numbers: 75.10.Pq, 75.10.Hk

I. INTRODUCTION

During the last decades several classical techniques such as the well-known Luttinger-Tisza method\textsuperscript{1}, vertex model\textsuperscript{2} and so on have been introduced to solve classical Hamiltonian exactly. The Luttinger-Tisza method is more effective in systems with bilinear interactions and vertex model usually applied for treating frustrated model\textsuperscript{3,4}.

In a very recent work\textsuperscript{5}, T. Kaplan have used a kind of cluster method, hereafter simply LK method, which is based on a block of three spins to solve frustrated classical Heisenberg model in one dimension with added nearest neighbor biquadratic exchange interactions. He asserted that the LK method is not limited to one dimension or to translationally invariant spin Hamiltonian\textsuperscript{6} and expanded his approach to determine the phase diagram of frustrated classical Heisenberg and XY models with added nearest neighbor biquadratic exchange interactions in $d = 2$ dimension. In order to check the validity of Kaplan’s phase diagram conjecture, we have investigated his model\textsuperscript{5} with an accurate algorithm (Lanczos method), and our results, which will be presented elsewhere\textsuperscript{6}, showed that LK method, albeit is a classical approach but has the capability to work for aspects of a quantum treatment.

Actually, these are our stimulating reasons to take a quite well known frustrated and dimerized Heisenberg model and determine its classical ground state phase diagram exactly with strong, but not well known LK method which is able to solve problems rigorously\textsuperscript{7}. Let us start with definition of the dimerized and frustrated Heisenberg model as follow

$$H = J_1 \sum_n \left[ 1 + (-1)^n \delta \right] \vec{S}_n \cdot \vec{S}_{n+1} + J_2 \sum_n \vec{S}_n \cdot \vec{S}_{n+2}, \quad (1)$$

where $\vec{S}_n$ is the $n$th classical vector of the length $S$. A spin system is frustrated when the global order because of the competition of different kinds of interaction is incompatible with the local order, so chain with both antiferromagnetic-antiferromagnetic exchanges ($J_1 > 0, J_2 > 0$) and ferromagnetic-antiferromagnetic exchanges ($J_1 < 0, J_2 > 0$), hereafter simply AF-AF and F-AF respectively, are frustrated.

Quantum study of this model is well done for the spin-1/2 and spin-1 chains\textsuperscript{9,10,11,12,13,14,15,16}. It is found that the quantum fluctuations play a prominent role at zero temperature in the ground state phase diagram of the models. This model shows a dimerization transition at $\delta = \delta_c$. For $S = 1/2$, the transition point is always $\delta_c = 0$, since the Lieb-Schultz-Mattis theorem implies either gapless excitations or two-fold degeneracy of the ground states at $\delta = 0$. In fact, on the undimerized line $\delta = 0$, for AF-AF case, there exists a critical frustration parameter $\alpha_c = 0.2411\textsuperscript{17,18}$. For $\alpha < \alpha_c$, the system is a gapless Tomonaga-Luttinger Liquid (TLL); that is, the dimerization transition at $\delta = \delta_0 = 0$ is of second order. On the other hand, for $\alpha > \alpha_c$, the ground state is doubly degenerate, exhibiting a spontaneous dimerization. This implies a first-order dimerization transition at $\delta = \delta_c = 0$. For $S = 1$, $\delta = 0$ (for a small $\alpha$) belongs to Haldane phase and does not exhibit a transition line. Instead, dimerization transition between the Haldane phase and the dimerized phase occurs\textsuperscript{19,20} at a finite $\delta_c$, which depends on the frustration $\alpha$. Albeit the shape of the phase diagram is thus different, topology of the phase diagram is a bit similar to that for $S = 1/2$. In fact, also for $S = 1$, there is a critical frustration $\alpha_c$; the transition is second order with the critical point described by a TLL for $\alpha < \alpha_c$, and first order for $\alpha > \alpha_c$.

But there is not a classical clear picture of different ground state phases of the mentioned model. Having a classical picture, from one hand help us to know that quantum fluctuations destroy which one of the classical orderings. On the other hand for arbitrary large spin model, the classical picture is the same with the quan-
The schematic picture of the ground state phase diagram. In this work we focus on the 1D frustrated and dimerized systems with arbitrary spin $S$ (see FIG. 1). To find the exact classical ground state phase diagram of the model, the LK cluster method is used. In the absence of the dimerization, by increasing the frustration a classical phase transition occurs at $\alpha_c = +0.25$ ($-0.25$) from the antiferromagnetic (ferromagnetic) phase into the spiral magnetic phase. Our results show that the dimerization parameter induces new magnetic phases including stripe-antiferromagnetic phase (or uud and duu phases). Existing of these magnetic phases is independent of length of spins.

The outline of the paper is as follows. In forthcoming sections we will extensively explain the LK method with implementing it to our model and in the section III we will summarize our results.

## II. THE LK CLUSTER METHOD

In order to implement LK method we follow exactly the procedure in Ref. [2]. Without losing the generality and setting periodic boundary conditions, Eq. (1) can be rewritten as:

$$H_c = \sum_i h_c(S_{i-1}, S_i, S_{i+1}),$$  

(2)

where the "cluster energy" involve three neighboring spins is

$$h_c(S_1, S_2, S_3) = \frac{J_1}{2}\left((1 - \delta)S_1 \cdot S_2 + (1 + \delta)S_2 \cdot S_3\right) + \frac{J_2}{2}(S_1 \cdot S_3).$$  

(3)

It is clear that

$$H_c \geq \sum J \min h_c(\vec{S}_{j-1}, \vec{S}_j, \vec{S}_{j+1}).$$  

(4)

To minimize $h_c$ respect spins directions, we first consider coplanar spins, and label the angles $\theta, \theta'$ made by the end spins with the central spin (see FIG. 2) which in coplanar case we set $\phi = 0, \phi' = 0$. The cluster energy is given by

$$h_c(\theta, \theta') = S^2\left\{\frac{1 - \delta}{2}\cos \theta + \frac{1 + \delta}{2}\cos \theta' + \alpha \cos(\theta - \theta')\right\},$$  

(5)

where $\alpha = J_2/J_1$. Minimizing $h_c$ respect $\theta, \theta'$ gives the following equation:

$$\frac{\partial h_c}{\partial \theta} = -S^2\left[(1 - \delta)\sin \theta + 2\alpha \sin(\theta - \theta')\right]$$

$$\frac{\partial h_c}{\partial \theta'} = -S^2\left[(1 + \delta)\sin \theta' - 2\alpha \sin(\theta - \theta')\right].$$  

(6)

Let’s first deal with a case without dimerization, by setting $\delta = 0$ in Eq. (6) we have

$$\frac{\partial h_c}{\partial \theta} = -S^2\left[\sin \theta + 2\alpha \sin(\theta - \theta')\right]$$

$$\frac{\partial h_c}{\partial \theta'} = -S^2\left[\sin \theta' - 2\alpha \sin(\theta - \theta')\right].$$  

(7)

its solutions are

$$(\theta, \theta') = (0, 0), (\pi, \pi), (\pi, 0), (0, \pi),$$

$$(\theta, \theta') = (\theta_0, -\theta_0), \text{ (Spiral- type), where}$$

$$\cos \theta_0 = -\frac{1}{4\alpha} \rightarrow |\alpha| \geq \frac{1}{4}.\hspace{2cm}(8)$$

The solutions $(\pi, \pi), (0, 0)$ are related to collinear antiferromagnetic and ferromagnetic states respectively. The antiferromagnetic (ferromagnetic) state will minimize the energy in the case of $J_1 > 0$ ($J_1 < 0$). Solutions $(\pi, 0) \rightarrow (\downarrow, \uparrow, \uparrow)$ and $(0, \pi) \rightarrow (\uparrow, \downarrow, \downarrow)$ are degenerate states and show spins propagate in the down-up-up and up-up-down respectively. Spiral state $(\theta_0, -\theta_0)$ with uniform rotation is also degenerate state. In following we present results of the antiferromagnetic case $J > 0$.

By setting minimization conditions into the Eq. (5) we have the following energies:

$$h_{\text{antiferro}} = h_c(\pi, \pi) = S^2(-1 + \alpha),$$

$$h_{\text{uudd}} = h_c(0, \pi) = S^2(-\alpha),$$

$$h_{\text{spiral}} = h_c(\theta_0, -\theta_0) = S^2(-\frac{1}{8\alpha} - \alpha).\hspace{2cm}(9)$$

By equating these energies in pairs we have found only one critical point, $\alpha_c = 0.25$. Because of the continuity
the derivative $\frac{\partial h}{\partial \alpha}$, a second-order phase transition occurs when passing through $\alpha = 0.25$. The ground state is in the antiferromagnetic phase in the region of the frustration $\alpha < 0.25$ and in the spiral phase in region $\alpha > 0.25$. In general, the antiferromagnetic phase is recognized by the nonzero value of the Neel order parameter defined as

$$M^z_{st} = \frac{1}{N} \sum_n (-1)^n S^z_n,$$  \hspace{1cm} (10)

and the spiral phase in the ground state phase diagram of the spin systems is characterized by the nonzero value of the spiral order parameter

$$\chi = \frac{1}{N} \sum_n |S_n \times S_{n+1}|.$$  \hspace{1cm} (11)

Using Eq. (8) we have found the spiral order parameter as

$$\chi = 0 \quad , \quad \alpha < \alpha_c,$$

$$\chi = S^2 \sqrt{1 - \frac{\alpha^2}{\alpha^2}} \quad , \quad \alpha > \alpha_c.$$ \hspace{1cm} (12)

In Fig. 3 we have plotted the spiral order parameter as a function of the frustration parameter $\alpha$ for the nondimerized model ($\delta = 0$). As is clearly seen from this figure, there is no long-range spiral order in the region of frustration $\alpha < \alpha_c = 0.25$. However, in the region $\alpha > \alpha_c = 0.25$ the spins of the system show a profound spiral order which grows by increasing the frustration parameter $\alpha$.

It has been discovered that continuous phase transitions have many interesting properties. The phenomena associated with continuous phase transitions are called critical phenomena, due to their association with critical points. It turns out that continuous phase transitions can be characterized by parameters known as critical exponents. Critical exponents describe the behavior of physical quantities near continuous phase transitions. It is believed, that they are universal, i.e. they do not depend on the details of the physical system. Our analytical results show that the spiral order parameter $\chi$ approaches zero in a singular fashion as $\alpha$ approaches $\alpha_c$, vanishing asymptotically as

$$\chi \propto (1 - \frac{\alpha_c}{\alpha})^{1/2};$$  \hspace{1cm} (13)

which shows that the critical exponent for spiral order parameter is a simple fraction $\varepsilon = 1/2$.

Now, we back to our original problem $\delta \neq 0$, finding the exact ground state phase diagram of the classical frustrated and dimerized Heisenberg chains. One can immediately see the possibility of having two spirals, one on the even sites, the other on the odd sites, both with the same wave length, but with a phase difference as described in the following:

$$\theta, \theta' = (0, 0), (\pi, \pi), (\pi, 0), (0, \pi), \quad \text{Spiral- type},$$

$$\cos \theta_0 = -\frac{16\delta \alpha^2 - (1 - \delta)^2}{4\alpha(1 - \delta)^2(1 + \delta)},$$

$$\sin \theta_0 = 0 \rightarrow \theta_0 = n\pi \rightarrow \varepsilon = 0.$$ \hspace{1cm} (14)
By substituting them into the Eq. (5), the ground state energy of cluster in different sectors becomes

\[ h_{\text{antiferro}} = h_c(\pi, \pi) = S^2(-1 + \alpha), \]
\[ h_{\text{uud}} = h_c(0, \pi) = S^2(-\delta - \alpha), \]
\[ h_{\text{duu}} = h_c(\pi, 0) = S^2(\delta - \alpha), \]
\[ h_{\text{spiral}} = h_c(\theta_0, -\theta_0 + \epsilon) = S^2\left(\frac{\delta - 1}{2}\right) + (1 + \cos \theta_0)\left\{ (1 - \delta) + \sqrt{(1 - \delta)^2 \cos^2 \theta_0 + 4\delta}\right\}. \]

As it can be seen from the above equations, in respect to the case of \( \delta = 0 \), dimerization exchange removed the degeneracy between \((\downarrow, \uparrow, \uparrow)\) and \((\uparrow, \downarrow, \downarrow)\) states. The \((\downarrow, \uparrow, \uparrow)\) state, defines as a phase with opposite magnetization on odd \((J_{\uparrow\uparrow})\) bonds, but \((\uparrow, \downarrow, \downarrow)\) state denotes by opposite magnetization on even \((J_{1\uparrow\downarrow})\) bonds. Using the conditions in Eq. (13) allow us to find the stability of different phases. Doing some calculations, one can find two critical lines as

\[ \alpha_c = \frac{1 - \delta^2}{4\delta}, \]
\[ \alpha_c = \frac{\delta^2 - 1}{4\delta}. \] (15)

These critical lines separate spiral phase from the \(\text{uud}\) and the \(\text{duu}\) phases. There is a discontinuity in the derivative \(\frac{\partial h}{\partial \alpha}\), and therefore a first-order phase transition through the mentioned critical lines. In addition, one should note that the ordering of the \(\text{uud}\) and \(\text{duu}\) phases, in principle is a type of the stripe-antiferromagnetic phase. Therefore, the order parameter for distinguishing these phases is defined as

\[ M_{sp}^z = \frac{2}{N} \sum_{n=1}^{N} (-1)^{n+1}(S_{2n-1}^z + S_{2n}^z), \text{ for } \text{uud} \]
\[ = \frac{2}{N} \sum_{n=1}^{N} (-1)^{n+1}(S_{2n}^z + S_{2n+1}^z), \text{ for } \text{duu}. \] (16)

We have also found antiferromagnetic phase that is stable for

\[ \alpha < \frac{1 - \delta^2}{4} \text{ for } \delta > 0, \]
\[ \alpha > \frac{\delta^2 - 1}{4} \text{ for } \delta < 0. \] (17)

The zero value of \(M_{sp}^z\) in the region \(\alpha < \alpha_c\) is in complete agreement with the fully polarized antiferromagnetic and spiral phases in this region. By more increasing the dimerization and for \(\alpha > \alpha_c\), clearly be seen that the ground state of the system is in the \(\text{uud}\). Also one predicts that the tripe antiferromagnetic as a function of the \(\alpha\) displays a jump for certain parameters which is one of the most important indications of the first-order phase transition. We emphasize that a first-order phase transition occurs between the spiral and the \(\text{duu}\) phases, for negative values of the dimerization.

The FIG. 4 (a) shows the exact classical ground state phase diagram of the model in \(\delta - \alpha\) plane. It should be mentioned that the same phase diagram can be also found in the ferromagnetic side which we do not depict. In the absence of dimerization, \(\delta = 0\), there are antiferromagnetic(ferromagnetic) and spiral phases which is separated by two critical point at \(\alpha_c = \pm 0.25\) which the neg-
The antiferromagnetic is separated from spiral by critical line. The antiferromagnetic phase remains stable up to the critical line $\alpha = 0$. The spiral phase is separated from antiferromagnetic and ferromagnetic states respectively. We have also the solutions $(\pi, \pi), (0, 0)$ that are related to the antiferromagnetic and ferromagnetic states respectively. We have also the solutions $(\pi, 0) \rightarrow (\downarrow, \uparrow)$ and $(0, \pi) \rightarrow (\uparrow, \downarrow, \downarrow)$ that are related to the $uud$ and $duu$ states respectively. Spiral phase also exists same as the coplanar case. The stability of different phases in the non-coplanar case is also checked and behaves same as the coplanar case.

III. CONCLUSION

To summarize, we have studied the classical ground state magnetic phase diagram of the dimerized and frustrated Heisenberg chain using LK cluster method. In coplanar case and in the absence of dimerization effect this approach could detect antiferromagnetic(ferromagnetic) and spiral phases. We have shown that turning the dimerization yields to remove the degeneracy between two $uud$ and $duu$ phases. We have argued that in the ground state phase diagram of the system there are first order transition lines. These lines separate spiral and $uud$ or $duu$ phases. On the other hand two second order phase transition points also exist, which separate antiferromagnetic(ferromagnetic) and spiral phases. By helping this approach we have calculated the spiral exact critical exponent $\varepsilon = 1/2$.

We check the possible configurations which can minimize the above equations. By taking arbitrary $(\phi, \phi')$, we have the solutions $(\pi, \pi), (0, 0)$ that are related to the antiferromagnetic and ferromagnetic states respectively. We have the solutions $(\pi, 0) \rightarrow (\downarrow, \uparrow)$ and $(0, \pi) \rightarrow (\uparrow, \downarrow, \downarrow)$ that are related to the $uud$ and $duu$ states respectively. Spiral phase also exists same as the coplanar case. The stability of different phases in the non-coplanar case is also checked and behaves same as the coplanar case.
[1] J. M. Luttinger and L. Tisza Phys. Rev. 70, 954 (1946); J. M. Luttinger and Laszo Tisza Phys. Rev. 72, 257 (1947).
[2] R.J. Baxter, *Exactly solved models in statistical mechanics*, London, Academic Press, (1982).
[3] E. H. Lieb, Physical Review 162, 162-172 (1967).
[4] B. Sutherland, J. Math. Phys. 11, 3183 (1970).
[5] T. Kaplan, Phys. Rev. B 80, 012407 (2009); T. Kaplan, Phys. Rev. B 80, 229906 (2009).
[6] D. H. Lyons and T. A. Kaplan, J. Phys. Chem. Solids, 25, 645 (1964).
[7] L. X. Hayden, T. A. Kaplan and S. D. Mahanti, Phys. Rev. Lett. 105, 047203 (2010).
[8] J. Vahedi and S. Mahdavifar, in preparation.
[9] S. Pati, R. Chitra, D. Sen, H. R. Krishnamurthy, and S. Ramasesha, Phys. Rev. B 52, 6581 (1995).
[10] S. Pati, R. Chitra, D. Sen, H. R. Krishnamurthy and S. Ramasesha, Europhys. Lett., 33, 707 (1996).
[11] S. Mahdavifar, Eur. phys. J. B 77, 77 (2010).