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Ferrimagnetic states in $S = 1/2$ frustrated Heisenberg chains with period 3 exchange modulation

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Abstract

The ground state properties of the $S = 1/2$ frustrated Heisenberg chain with period 3 exchange modulation are investigated using the numerical diagonalization and density matrix renormalization group (DMRG) method. It is known that this model has a magnetization plateau at one third of the saturation magnetization M_s. On the other hand, the ground state is ferrimagnetic even in the absence of frustration if one of the nearest neighbour bond is ferromagnetic and the others are antiferromagnetic. In the present work, we show that this ferrimagnetic state continues to the region in which all bonds are antiferromagnetic if the frustration is strong. This state further continues to the above-mentioned $1/3$ plateau state. In between, we also find the noncollinear ferrimagnetic phase in which the spontaneous magnetization is finite but less than $M_s/3$. The intuitive interpretation for the phase diagram is given and the physical properties of these phases are discussed.

1. Introduction

Frustrated quantum spin chains have been the subject of extensive studies for decades. One of the most remarkable phenomena driven by frustration is the transition to a spontaneously dimerized ground state as demonstrated by the exact solution of Majumdar and Ghosh [1]. In the magnetic field, another type of translational symmetry breakdown has recently been found by Okunishi and Tonegawa [2, 3] and Tonegawa *et al* [4] resulting in a nontrivial magnetization plateau at one third of the saturation magnetization M_s. The present author and Affleck [5] have investigated the effect of period 3 exchange modulation on this plateau state. It turned out that the transition between the classical plateau state and the quantum plateau state takes place within the $1/3$ plateau state.

Another remarkable effect of frustration is the stabilization of the ferrimagnetic ground state. Yoshikawa and Miyshita [6] proposed a model of a frustrated quantum chain which shows a ferrimagnetic ground state. Remarkably, this model not only has a Lieb–Mattis type ground state in which magnetization is fixed to a value determined by the difference of number of sites of two sublattices but also has a noncollinear ferrimagnetic ground state where magnetization is not a simple fraction of full magnetization. In this state, the local magnetization profile has an incommensurate structure.

In the present paper, we show that the $S = 1/2$ frustrated Heisenberg chain with period 3 exchange modulation also shows Lieb–Mattis type and noncollinear type ferrimagnetism in an appropriate parameter range. The former continues to the $1/3$ plateau state investigated in [5].

This paper is organized as follows. In section 2, we present the model Hamiltonian. The ground state phase diagram obtained by numerical diagonalization is presented in section 3. The property of each phase is also discussed based on the density matrix renormalization group (DMRG) calculation. In the section 4 we summarize our results.

2. Hamiltonian

The Hamiltonian of the $S = 1/2$ frustrated Heisenberg chain with period 3 exchange modulation is given by

$$\mathcal{H} = J\sum_{l=1}^{N/3}[(1-\alpha)\,(\boldsymbol{S}_{3l-1}\boldsymbol{S}_{3l} + \boldsymbol{S}_{3l}\boldsymbol{S}_{3l+1}) + (1+\alpha)\boldsymbol{S}_{3l+1}\boldsymbol{S}_{3l+2}] + J\delta\sum_{i=1}^{N}\boldsymbol{S}_i\boldsymbol{S}_{i+2} \tag{1}$$

where $\boldsymbol{S}_i$ is the spin $1/2$ operator and N is the number of sites. This model has a magnetization plateau at one third of the saturation magnetization M_{s} as investigated in [5]. On the other hand, it is obvious that the ground state is ferrimagnetic for $\alpha < -1$ even in the absence of frustration. In this paper, we concentrate on the ground state properties of this model in the region $-1 < \alpha < 0$ and $\delta > 0$.

3. Ground state properties

The ground state phase diagram is obtained for $\alpha \leqslant 0$ and $0 \leqslant \delta \leqslant 0.8$ as shown in figure 1 by the numerical diagonalization of a finite size system with $N = 12$, 18 and 24. For $\delta > 0.8$, the strong finite size effect prevents the precise determination of phase boundary.

For small $|\alpha|$, the ground state is the gapless Tomonaga–Luttinger liquid for small δ and the Majumdar–Ghosh type spontaneously dimerized phase for larger δ. The transition between these two phases is the Brezinskii–Kosterilitz–Thouless type transition and the phase boundary can be determined by the level spectroscopic method [7] using the numerical diagonalization data for $N = 12$, 18 and 24.

Typical magnetization curves calculated by the DMRG method in these two nonmagnetic phases are shown in figure 2(a) for $(\alpha, \delta) = (-0.2, 0.2)$ and (b) for $(\alpha, \delta) = (-0.8, 0.8)$ and $N = 96$ with the open boundary condition. It is evident that the spin gap is absent in the former case while it is present in the latter case. The magnetization plateau at $M = M_{\mathrm{s}}/3$ is always present, reflecting the period 3 exchange modulation.

For large negative α and large δ, the ground state is ferrimagnetic with magnetization $M = M_{\mathrm{s}}/3$. Even though the present model is not strictly bipartite due to next nearest neighbour exchange interaction, this phase can be regarded as the Lieb–Mattis type ferrimagnetic phase because it is directly connected to the Lieb–Mattis ferrimagnetic state with $M = M_{\mathrm{s}}/3$ at $\alpha < -1$ and $\delta = 0$. For small δ and $\alpha \simeq -1$, the three spins connected by the $(1-\alpha)$-bonds form an effective spin $1/2$ doublet.

$$|\Uparrow\rangle = \frac{1}{\sqrt{6}}\left(|\uparrow\uparrow\downarrow\rangle - 2\,|\uparrow\downarrow\uparrow\rangle + |\downarrow\uparrow\uparrow\rangle\right) \tag{2}$$

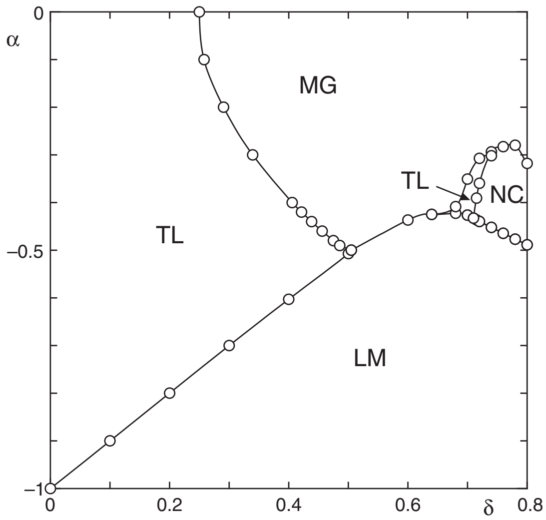

Figure 1. Ground state phase diagram for $-1 \leqslant \alpha \leqslant 0$ for $0 \leqslant \delta \leqslant 0.8$. TL, MG, NC and LM stand for Tomonaga–Luttinger liquid phase, Majumdar–Ghosh type dimer phase, noncollinear and Lieb–Mattis ferrimagnetic phases, respectively.

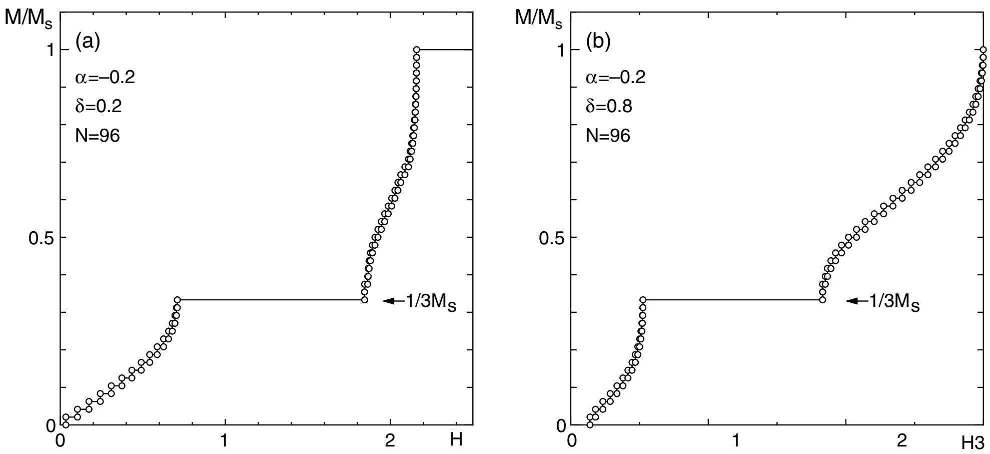

Figure 2. Magnetization curve in (a) Tomonaga–Luttinger liquid phase with $(\delta, \alpha) = (0.2, -0.2)$ and (b) Majumdar–Ghosh type dimer phase with $(\delta, \alpha) = (0.8, -0.2)$ for $N = 96$ calculated by the DMRG method.

$$|{\Downarrow}\rangle = \frac{1}{\sqrt{6}} \left(|{\downarrow\downarrow\uparrow}\rangle - 2\,|{\downarrow\uparrow\downarrow}\rangle + |{\uparrow\downarrow\downarrow}\rangle\right). \tag{3}$$

By elementary manipulation, the effective exchange interaction between these effective spins turns out to be $2J(1 + \alpha - \delta)/9$. Therefore the ground state in this region is a Lieb–Mattis type ferrimagnetic state for $1 + \alpha < \delta$ and the Tomonaga–Luttinger liquid state otherwise. A typical magnetization curve calculated by the DMRG method in this phase is shown in figure 3(a) for $(\alpha, \delta) = (-0.8, 0.8)$ and $N = 96$ with open boundary conditions. Comparing this magnetization curve with figure 2, it is clear that this ferrimagnetic state continues to the *classical* plateau state in the nonmagnetic phases. It should be noted that the *quantum*

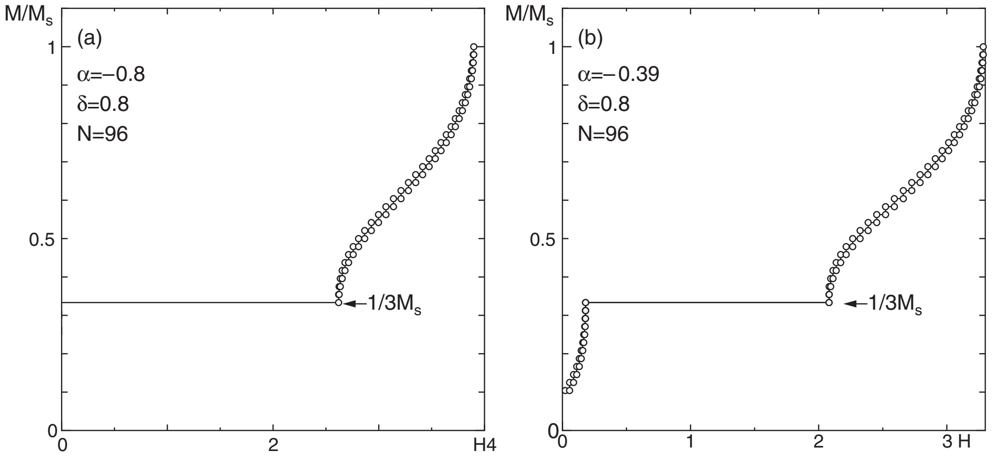

Figure 3. Magnetization curves in (a) the Lieb–Mattis type ferrimagnetic phase with $(\delta, \alpha) = (0.8, -0.8)$ and (b) the noncollinear ferrimagnetic phase with $(\delta, \alpha) = (0.8, -0.39)$ for $N = 96$ calculated by the DMRG method.

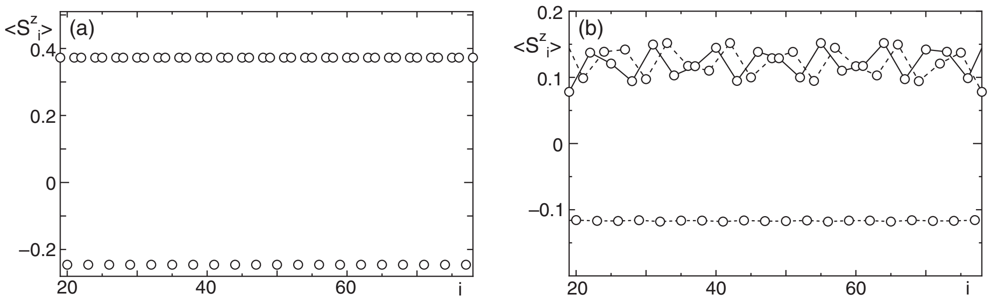

Figure 4. Local magnetization profile (a) in the Lieb–Mattis type ferrimagnetic phase with $\delta = 0.7$ and $\alpha = -0.7$ and (b) in the noncollinear ferrimagnetic phase with $\delta = 0.8$ and $\alpha = -0.39$ for $N = 96$ calculated by the DMRG method. In order to exclude the boundary effects, only the sites in the middle of the system $19 \leqslant i \leqslant 78$ are shown. The lines are guides for the eye drawn to make clear the incommensurate modulation of the magnetization profile.

plateau state is realized only for $\alpha > 0$ [5]. The local magnetization profile $\langle S_i^z \rangle$ calculated by the DMRG method clearly shows a three-sublattice structure as shown in figure 4(a) for $(\alpha, \delta) = (-0.7, 0.7)$ and $N = 96$ with open boundary conditions. It should also be noted that spins are not fully polarized even in the Lieb–Mattis type phase although the total magnetization is exactly quantized to $M_s/3$.

With the decrease in $|\alpha|$, the ferrimagnetic state with magnetization less than $M_s/3$ appears for $\alpha \gtrsim 0.72$. This phase has similarity with the noncollinear ferrimagnetism studied by Yoshikawa and Miyashita [6]. As a representative, the magnetization curve in this state calculated by the DMRG method is presented in figure 3(b) for $(\alpha, \delta) = (-0.39, 0.8)$ and $N = 96$ with open boundary conditions. It is clear that the magnetization starts from a nonzero value less than $M_s/3$ at $H = 0$. The magnetization profile in this state calculated by the DMRG method is shown in figure 4(b) for the same set of parameters. As in the case of Yoshikawa and Miyashita [6], the magnetization profile has incommensurate modulation.

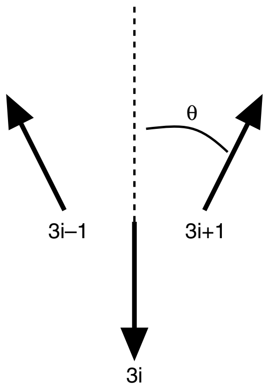

Figure 5. Classical noncollinear spin configuration.

The presence of the noncollinear ferrimagnetic state can be also understood within the classical picture. If we assume the noncollinear spin configuration depicted in figure 5 and minimize the classical energy calculated using the Hamiltonian (1) with respect to the angle θ, we find the nonzero solution of θ for $\delta > -1 - 3\alpha$ corresponding to the noncollinear ferrimagnetic phase. For $\delta < -1 - 3\alpha$, we find $\theta = 0$ corresponding to the Lieb–Mattis type ferrimagnetism. However, the observed incommensurate ferrimagnetic spin profile cannot be understood within this classical picture. We expect that this phenomenon is essentially due to the combined effect of quantum fluctuation and frustration.

Finally, in the narrow region between the ferrimagnetic phase and the spontaneously dimerized phase, another Tomonaga–Luttinger liquid phase is found. Considering the difference in the spin structures of the spontaneously dimerized phase and the noncollinear ferrimagnetic phase, it is reasonable to expect an intermediate critical phase between these two phases. However, it still possible that this phase does not survive in the thermodynamic limit because of the limitation of the system size and ambiguity in the extrapolation procedure.

4. Summary

The phase diagram of the $S = 1/2$ frustrated Heisenberg chains with period 3 exchange modulation is determined by analysing the exact numerical diagonalization data. In addition to the Tomonaga–Luttinger liquid phase, a dimer phase, a Lieb–Mattis type ferrimagnetic phase and a noncollinear ferrimagnetic phase are found. A physical interpretation of the phase diagram based on the perturbational argument and classical picture is given. A typical magnetization curve in each phase is presented. It is shown that the magnetization profile has incommensurate modulation in the noncollinear ferrimagnetic phase. This feature has a similarity to the model investigated by Yoshikawa and Miyashita [6] which also has frustration and noncollinear ferrimagnetism. Therefore we may regard the incommensurate spin profile as a characteristic of the noncollinear quantum ferrimagnetism induced by frustration.

Another Tomonaga–Luttinger liquid phase is found in the narrow region between the dimer phase and the noncollinear ferrimagnetic phase. Further investigation of the nature of this phase is left for future studies.

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