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# Effect of frustration on spin-wave excitation spectra and ground-state properties of the quasi-one-dimensional antiferromagnetic chain with asymmetrical sublattices

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ABSTRACT

We investigate the effect of frustration on spin-wave excitation spectra and the properties of the quasi-one-dimensional Heisenberg chain using a spin-wave–wave analysis, the exact diagonalization method and the density matrix renormalization group method. The results show that frustration can cause the softening of the acoustic excitation spectrum $\omega_3$, as well as the hardening of the optical excitation spectrum $\omega_1$. As a function of the frustration parameter $\alpha$, the phase diagram exhibits a ferromagnetic phase, a narrow canted phase and a singlet phase. The results obtained from numerical methods show that the spin gap obviously opens and the tetramer–dimer state dominates the properties of the ground state in the singlet phase.



## 1. Introduction

The study of quantum spin chains with frustration in quasi-one-dimensions has received considerable interest for decades. As a result of frustration, different quasi-one-dimensional (QOD) antiferromagnetic (AF) chains exhibit a variety of exotic quantum phases [1–4]. In recent years, the properties of many synthetic compounds can be described with some QOD AF chains. For example, in some parameter regions, the orthogonal-dimer spin chain is in the dimer phase and in others, it is in the plaquette phase [5]. The properties of the compound $SrCu_2(BO_3)_2$ can be described with this model [6]. Another example is the distorted-diamond model. The ground-state (GS) phase diagram of this model is composed of the ferromagnetic (F) phase, the dimer phase and the spin-liquid phase [7]. It can describe the property of the actual material $Cu_3Cl_6(H_2O)_2 \cdot 2H_8C_4SO_2$ [7]. Although the numbers of the two-sublattice's site spins are identical in many Heisenberg spin chains (using the Lieb and Mattis division method [8], if one site belongs to one sublattice, then another one connected with the site through the nearest interaction belongs to another sublattice), there exists some spin models with unequal site spins in two sublattices [7,9]. Sublattice symmetrical breaking causes obvious changes of the spin property in the GS of these systems. For instance, although the spin interaction of the AF distorted-diamond chain is AF, known from the Lieb–Mattis theorem, the breaking of the sublattice symmetry causes the GS of the model without frustration to possess the F long range order (LRO). When the frustration is relatively weak, the magnetic LRO is still possessed by that model, but it is destroyed in the case of strong frustration.

In this article, we study a QOD AF Heisenberg spin chain with frustration, as shown in Fig. 1. By periodically doping the spins (called side spin) adjacent to each spin site of the same sublattice in the one-dimensional Heisenberg spin chain, a QOD Heisenberg spin chain is

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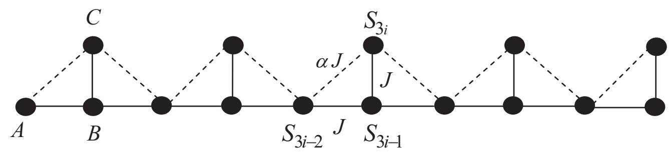


**Fig. 1.** The structure of the quasi-one Heisenberg spin chain.

constituted. The Hamiltonian is

$$H = J\sum_{i=1}^{N}(s_{3i-2}s_{3i-1} + s_{3i-1}s_{3i+1} + s_{3i-1}s_{3i}) + \alpha J\sum_{i=1}^{N}(s_{3i-2}s_{3i} + s_{3i}s_{3i+1}) \tag{1}$$

where $J(J>0)$ is the coupling constant along the chain and between the side spin and the nearest neighbor spin on the chain, and $\alpha J(\alpha \geq 0)$ is the coupling constant between the side spin and the next nearest neighbor spin on the chain. The model does not possess sublattice symmetry. It has been proved that the Lieb–Mattis FLRO exists in the GS [9] when $\alpha = 0$. Then the total spin of the GS is $S_g = \frac{1}{2}N$ according to the Lieb–Mattis theorem. In this paper, the aim is to study the effect of frustration on the properties of the model in the GS.

## 2. The magnetic phase

Although the Lieb–Mattis theorem does not work when $\alpha > 0$, it can be expected that the FLRO will survive up to some finite $\alpha$ due to the continuity principle. That means the total spin $S_g$ of the GS will still take the value $\frac{1}{2}N$ in the regime of small $\alpha$. In order to check this hypothesis, we use exact diagonalization (ED) (24 sites) to calculate the total spin of the GS $S_g$. From the result of ED, we find that $S_g$ always takes the value $\frac{1}{2} \times N = 4$ as $\alpha \leq 0.408$, which discloses that the FLRO with $S_g = \frac{1}{2}N = 4$ is always the GS of the model as $\alpha \leq 0.408$. At the transition point $\alpha_{c1} = 0.408$, $S_g$ changes from $\frac{1}{2}N = 4$ to 2. Another transition point is found at $\alpha_{c2} = 0.410$, where $S_g$ changes from $S_g = 2$ to a singlet GS with $S_g = 0$. So, a canted phase with $0 < S_g < \frac{1}{2}N$ exists in a very narrow parameter region, but that phase cannot be found in the systems with $N = 4$ and $N = 6$ due to finite-size effects.

Since the GS of the model possesses the FLRO, we firstly use spin-wave theory (SWT) to discuss the effect of frustration on this model in the regime of weak $\alpha$. For convenience, the model can be divided into three sublattices (denoted A, B and C) corresponding to the geometric position difference as shown in Fig. 1. After performing the standard Holstein–Primakoff and the Fourier transforms, Eq. (1) becomes

$$H = E_0 + Js\sum_k\left[2a_k^+a_k + 3b_k^+b_k + c_k^+c_k + 2\cos\frac{k}{2}(a_k^+b_k^+ + a_kb_k) + (b_k^+c_k^+ + b_kc_k)\right] + 2s\alpha J\sum_k\left[-c_k^+c_k - a_k^+a_k + \cos\frac{k}{2}(a_k^+c_k + a_kc_k^+)\right] \tag{2}$$

where $E_0 = -3JNs^2 + 2\alpha JNs^2$ is the energy of classical GS with Neel order and where the operators $a_k$, $b_k$ and $c_k$ obey bosonic commutation relations.

After defining the matrix retarded Green function [10] as

$$G(k,\omega) = \begin{pmatrix} \langle\langle a_k|a_k^+\rangle\rangle & \langle\langle a_k|b_k^+\rangle\rangle & \langle\langle a_k|c_k^+\rangle\rangle & \langle\langle a_k|a_k\rangle\rangle & \langle\langle a_k|b_k\rangle\rangle & \langle\langle a_k|c_k\rangle\rangle \\ \langle\langle b_k|a_k^+\rangle\rangle & \langle\langle b_k|b_k^+\rangle\rangle & \langle\langle b_k|c_k^+\rangle\rangle & \langle\langle b_k|a_k\rangle\rangle & \langle\langle b_k|b_k\rangle\rangle & \langle\langle b_k|c_k\rangle\rangle \\ \langle\langle c_k|a_k^+\rangle\rangle & \langle\langle c_k|b_k^+\rangle\rangle & \langle\langle c_k|c_k^+\rangle\rangle & \langle\langle c_k|a_k\rangle\rangle & \langle\langle c_k|b_k\rangle\rangle & \langle\langle c_k|c_k\rangle\rangle \\ \langle\langle a_k^+|a_k^+\rangle\rangle & \langle\langle a_k^+|b_k^+\rangle\rangle & \langle\langle a_k^+|c_k^+\rangle\rangle & \langle\langle a_k^+|a_k\rangle\rangle & \langle\langle a_k^+|b_k\rangle\rangle & \langle\langle a_k^+|c_k\rangle\rangle \\ \langle\langle b_k^+|a_k^+\rangle\rangle & \langle\langle b_k^+|b_k^+\rangle\rangle & \langle\langle b_k^+|c_k^+\rangle\rangle & \langle\langle b_k^+|a_k\rangle\rangle & \langle\langle b_k^+|b_k\rangle\rangle & \langle\langle b_k^+|c_k\rangle\rangle \\ \langle\langle c_k^+|a_k^+\rangle\rangle & \langle\langle c_k^+|b_k^+\rangle\rangle & \langle\langle c_k^+|c_k^+\rangle\rangle & \langle\langle c_k^+|a_k\rangle\rangle & \langle\langle c_k^+|b_k\rangle\rangle & \langle\langle c_k^+|c_k\rangle\rangle \end{pmatrix} \tag{3}$$

Then using the Green function theory, we can obtain the motion equation of the Green function as

$$DG = I \tag{4}$$

where

$$D = \begin{pmatrix} \omega - 2Js(1-\alpha) & 0 & -2s\alpha J\cos(k/2) & 0 & -2Js\cos(k/2) & 0 \\ 0 & \omega - 3Js & 0 & -2Js\cos(k/2) & 0 & -Js \\ -2s\alpha J\cos(k/2) & 0 & \omega - Js(1-2\alpha) & 0 & -Js & 0 \\ 0 & 2Js\cos(k/2) & 0 & \omega + 2Js(1-\alpha) & 0 & 2s\alpha J\cos(k/2) \\ 2Js\cos(k/2) & 0 & Js & 0 & \omega + 3Js & 0 \\ 0 & Js & 0 & 2s\alpha J\cos(k/2) & 0 & \omega + Js(1-2\alpha) \end{pmatrix}$$