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Analytical approach to dimerized and frustrated Heisenberg chains

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Abstract

We present a self-consistent quantum-theoretical analysis of the ground-state energy and low-energy excitation spectrum of a dimerized and frustrated Heisenberg chain by the bosonization representation in the continuum-limit approach. The frustration effects on the ground-state energy and energy gap are investigated for $\alpha > \alpha_c$ where α is the frustration parameter and α_c is its critical value, above which a frustration-induced energy gap is opened. It is shown that as α increases, the ground-state energy decreases and the energy gap increases. We find that the dimerization dependence of the ground-state energy and energy gap for small dimerization obeys the Cross–Fisher power law only at $\alpha = \alpha_c$, but departs significantly from it when $\alpha > \alpha_c$. The present results are in good agreement with numerical analyses from the density–matrix renormalization-group and exact diagonalization methods. The relevance of our calculated results to recent experiments on the spin-Peierls compounds $CuGeO_3$ is also discussed.

1. Introduction

The discovery of the spin-Peierls (SP) transition in the inorganic material $CuGeO_3$ [1] has led to intense investigations of one-dimensional (1D) spin systems. The SP transition was observed experimentally in $CuGeO_3$ at a temperature $T_{SP} \approx 14$ K. The basic structure of $CuGeO_3$ consists of edge-sharing CuO_6 octahedra forming CuO_4 chains along the crystallographic c axis. The dimerization of $S = 1/2$ Cu ions has been determined below 14 K by neutron diffraction measurements [2]. The magnetic properties of the SP compound $CuGeO_3$ may be described by an $S = 1/2$ antiferromagnetic Heisenberg chain with both dimerization and

frustration, i.e., an alternation δ of the nearest-neighbour (NN) exchanges and a next-nearest-neighbour (NNN) exchange αJ. The model Hamiltonian is given by

$$H = J \sum_i \{[1 + \delta(-1)^i] S_i S_{i+1} + \alpha S_i S_{i+2}\} \tag{1}$$

where S_i is the $S = 1/2$ spin operator on site i and the summation over i is taken over all the sites in the Heisenberg chain, $J > 0$ is the NN exchange coupling, and α the frustration parameter from the NNN coupling. It has been shown that the magnetic susceptibility of $CuGeO_3$ in a uniform phase ($\delta = 0$) can be accurately reproduced by a frustrated Heisenberg chain model [3]; from this fit the frustration was estimated to be $\alpha \approx 0.35$. The ground state of the uniform model can be exactly solved for $\alpha = 0.5$ [4]. The ground state is doubly degenerate for the ring and the two states are representable as the two Kekule structures of the valence–bond theory. Analytical and numerical studies [5–7] of the model on the $\delta = 0$ line show a transition from a gapless phase for $\alpha < \alpha_c$ to a gapped phase for $\alpha > \alpha_c$. The value of α_c has been accurately computed to be 0.2411 [7]. The $\alpha = 0$ and $\delta > 0$ line corresponds to a dimerized spin chain, in which the excitation spectrum is always gapped. In addition, the frustrated SP model can also describe the two-leg spin-ladder system with frustration.

Recently, much theoretical attention has been attracted to the frustrated SP model. Chitra *et al* [8] studied the ground-state phase diagram and low-energy properties by using a density–matrix renormalization group (DMRG) technique. Zang *et al* [9] used a renormalization group method and the bond-operator mean-field approximation to calculate the ground-state phase diagram and excitation spectrum. By the exact diagonalization method, numerical studies of the low-energy excitation spectrum have been given by Bouzerar *et al* [10]. On the other hand, in recent years the field-theoretical continuum-limit approach has been successfully used to study the SP compounds and spin-ladder systems [5, 11–13]. It is well known that the SP systems can be mapped, via the Jordan–Wigner transformation and bosonization under the continuum-limit approximation [5], onto a 1D single-frequency sine-Gordon (SG) model with a boson-field operator $\cos(\beta\phi/2)$. Therefore, it is interesting to discuss the frustration effects on these systems in the frame of the SG model. In the presence of frustration, by adding another boson-field operator $\cos\beta\phi$ in the phase Hamiltonian of the SP chain, the frustrated SP chain can be mapped onto a 1D double-frequency SG model [14]. In contrast to the single-frequency SG model, which can be solved exactly at special values of β and whose excitation spectrum is well understood [15], we know less about the excitation spectrum of the double-frequency SG model. Since there are different scaling dimensions of the relevant operators in the double-frequency SG model, $\dim[\cos\beta\phi] = 4\dim[\cos(\beta\phi/2)]$, the conventional way of treating the double-frequency SG model is to keep only the more relevant term $\cos(\beta\phi/2)$ then reduce to a single-frequency SG model. Recent studies on the frustrated spin-Peierls model have shown that the interplay between the two relevant operators is important [10] and the conventional treatment of the double-frequency SG model is no longer valid in determining the excitation spectrum of the system. As a result, it is highly desirable to develop an effective approach in studying the frustration effects on the elementary excitation spectrum of a frustrated SP chain in the frame of the 1D double-frequency SG model.

Due to the problem of infrared divergence, the traditional perturbation approach becomes invalid in determining the low-energy behaviour of the single-frequency SG model. Although the renormalization group theory can give the scaling flow of the model, other useful information such as the single-particle excitation spectrum and many-particle bound states cannot be easily obtained. Recently, a self-consistent quantum theory [16] has been developed for the low-energy properties of the single-frequency SG model. Based on this method, the infrared divergence is effectively removed and the excitation spectrum can be obtained self-consistently. In the present paper, we extend this method to the double-frequency SG model

and perform an analytical study on the low-energy properties of the frustrated SP chain.

This paper is organized as follows. In section 2 we map the frustrated SP system, in the adiabatic limit, onto the 1D double-frequency SG model via the Jordan–Wigner transformation and bosonization representation in the continuum limit. Using the self-consistent quantum theory, the ground-state energy and the energy gap as functions of dimerization and frustration parameters are derived analytically with the help of a self-consistent equation of a renormalization parameter. In section 3 we focus our attention on the frustration effects on the ground-state energy and energy gap of a general α–δ model for $\alpha > \alpha_c$. The theoretical results are compared with recent experimental data of $CuGeO_3$ as well as with existing numerical results. We also discuss contributions of both dimerization and frustration to the energy gap which is opened by the two mechanisms above. A brief summary of the results is given in section 4.

2. Theoretical approach

First, using the Jordon–Wigner transformation: $S_i^+ = c_i^+ \exp[\mathrm{i}\pi \sum_{j<i} c_j^+ c_j]$, $S_i^- = \exp[-\mathrm{i}\pi \sum_{j<i} c_j^+ c_j] c_i$, and $S_i^z = c_i^+ c_i - 1/2$, we transform Hamiltonian (1) into the spinless fermion Hamiltonian

$$H = J \sum_i [1 + \delta(-1)^i] \left[(c_i^+ c_{i+1} + c_{i+1}^+ c_i)/2 + (n_i - 1/2)\,(n_{i+1} - 1/2) \right] + \alpha \{ [c_i^+ (n_{i+1} - 1/2) c_{i+2} + h.c.] + (n_i - 1/2)(n_{i+2} - 1/2) \}. \tag{2}$$

In the continuum limit, Hamiltonian (2) can be bosonized to obtain a tractable bosonic theory in 1+1 dimensions [14]. The resulting continuum Hamiltonian is given by

$$H = \int \mathrm{d}x [A(\partial_x \varphi)^2 + C p^2 - B \sin\varphi - D \cos 2\varphi] \tag{3}$$

with

$$[\varphi(x),\, p(x')] = i\delta(x - x'). \tag{4}$$

The constants in equation (3) are $A = (Ja/8\pi)[1 + (3 + 7\alpha)/\pi]$, $B = J\delta/a$, $C = 2\pi a J[1 - (1+\alpha)/\pi]$, and $D = (J/2a)(1 - 3\alpha)$, where a is the lattice constant. The frustration parameter α appears in A, C,and D, but B is independent of α because it comes only from the NN interaction. By making the transformation $\varphi \to \varphi + \pi/2$ and rescaling the boson field operator $\varphi(x)$ and its canonical momentum operator $p(x)$ as $\phi(x) = (A/C)^{1/4} \varphi(x)$, $P(x) = (C/A)^{1/4} p(x)$, Hamiltonian (3) can be further transformed into the following double-frequency SG model

$$H = v \int \mathrm{d}x \left[\frac{1}{2} (\partial_x \phi)^2 + \frac{1}{2} P^2 - \frac{\alpha_1}{\beta^2} \cos\beta\phi - \frac{\alpha_2}{\beta^2} \cos\frac{\beta}{2}\phi \right] \tag{5}$$

where $v = 2\sqrt{AC}$ is the spin wave velocity, and

$$\alpha_1 = -\frac{2D}{A} = -8\pi^2 \frac{1 - 3\alpha}{\pi + 3 + 7\alpha} \tag{6}$$

$$\alpha_2 = \frac{2B}{A} = 16\pi^2 \frac{\delta}{\pi + 3 + 7\alpha} \tag{7}$$

$$\beta^2 = 4\sqrt{\frac{C}{A}} = 16\pi \sqrt{\frac{\pi - 1 - \alpha}{\pi + 3 + 7\alpha}}. \tag{8}$$

Next, we attempt to apply the self-consistent quantum theory [16] to the 1D double-frequency SG model. Since the integrand in equation (5) is a minimum at $\phi = 0$ for positive

α_1 and α_2, we can make a perturbation expansion in the vicinity of $\phi = 0$ for two cosine terms in equation (5) and omit the higher order terms. On the other hand, since frustration and dimerization provide two principally different mechanisms for the energy-gap formation, we adjust parameters α_1 and β according to [10] as follows:

$$\alpha_1 = 8\pi^2 \frac{\alpha - \alpha_c}{\pi + 3 + 7\alpha} \tag{9}$$

$$\beta^2 = 8\pi \sqrt{\frac{1 - (\alpha - \alpha_c)}{1 + (\alpha - \alpha_c)}} \tag{10}$$

where $\alpha_c = 0.2411$. In this paper we consider only the case of $\alpha \geqslant \alpha_c$. Here we briefly outline the procedure of the self-consistent theory. In momentum space the Bose field operator $\phi(x)$ and its canonical momentum operator $P(x)$ are defined as

$$\phi(x) = \sum_k (2 \mid k \mid)^{-1/2} \exp(\mathrm{i}kx)(b_k + b_{-k}^+) \tag{11}$$

$$P(x) = -i \sum_k (\mid k \mid /2)^{1/2} \exp(\mathrm{i}kx)(b_k - b_{-k}^+). \tag{12}$$

where the summation over k is performed in the range $0 \leqslant \mid k \mid \leqslant \pi/a$. Then we consider the following Bogoliubov transformation in order to deal with the infrared divergence:

$$U = \exp\left[\sum_k (\gamma_k/2)(b_k^+ b_{-k}^+ - b_k b_{-k})\right] \tag{13}$$

where b_k and b_k^+ satisfy the standard boson commutator, and γ_k will be determined below. The transformed Hamiltonian $\widetilde{H} = UHU^{-1}$ is given by

$$\begin{aligned}\widetilde{H} = \sum_k v \mid k \mid \left[b_k^+ b_k \cosh(2\gamma_k) - (b_k^+ b_{-k}^+ + b_k b_{-k})\frac{1}{2}\sinh(2\gamma_k) + \frac{1}{2}\cosh(2\gamma_k)\right] \\ - \frac{v\alpha_1}{\beta^2}\int \mathrm{d}x \cos\left[\sum_k \beta(2 \mid k \mid)^{-1/2} \mathrm{e}^{-\gamma_k} \exp(\mathrm{i}kx)(b_k + b_{-k}^+)\right] \\ - \frac{v\alpha_2}{\beta^2}\int \mathrm{d}x \cos\left[\sum_k \frac{\beta}{2}(2 \mid k \mid)^{-1/2} \mathrm{e}^{-\gamma_k} \exp(\mathrm{i}kx)(b_k + b_{-k}^+)\right].\end{aligned} \tag{14}$$

We normally order the cosine terms in equation (14) and expand them to second order in the bosonic operators. The resulting Hamiltonian is given by

$$\widetilde{H} = \widetilde{H_0} + \widetilde{H_1} + \widetilde{H_2} \tag{15}$$

where

$$\widetilde{H_0} = v \sum_k \left[\frac{1}{2} \mid k \mid \cosh(2\gamma_k) - \frac{\alpha_1 \xi^4}{a^2\beta^2} - \frac{\alpha_2 \xi}{a^2\beta^2}\right] \tag{16}$$

$$\widetilde{H_1} = v \sum_k \left[\mid k \mid \cosh(2\gamma_k) + \frac{\alpha_1 \xi^4 \exp(-2\gamma_k)}{2a^2 \mid k \mid} + \frac{\alpha_2 \xi \exp(-2\gamma_k)}{8a^2 \mid k \mid}\right] b_k^+ b_k \tag{17}$$

$$\widetilde{H_2} = -\frac{v}{2} \sum_k \left[\mid k \mid \sinh(2\gamma_k) - \frac{\alpha_1 \xi^4 \exp(-2\gamma_k)}{2a^2 \mid k \mid} - \frac{\alpha_2 \xi \exp(-2\gamma_k)}{8a^2 \mid k \mid}\right] (b_k^+ b_{-k}^+ + b_k b_{-k)} \tag{18}$$

with

$$\xi = \exp\left(-\frac{\beta^2}{16} \sum_k \frac{\mathrm{e}^{-2\gamma_k}}{\mid k \mid}\right). \tag{19}$$

In equation (15) unimportant constant terms have been neglected. The $\widetilde{H}_2$ term in equation (18) contains nondiagonal terms of the boson operators, which can be removed by selecting appropriate γ_k:

$$\gamma_k = \frac{1}{4}\ln\left(1 + \frac{\alpha_1\xi^4}{a^2k^2} + \frac{\alpha_2\xi}{4a^2k^2}\right). \tag{20}$$

Combining equations (19) and (20), we obtain a self-consistent equation for ξ

$$\xi = \left(\frac{\alpha_1\xi^4 + \frac{1}{4}\alpha_2\xi}{\left[1 + \sqrt{1 + \alpha_1\xi^4 + \frac{1}{4}\alpha_2\xi}\right]^2}\right)^{\beta^2/32\pi} \tag{21}$$

where an upper cutoff of the integral, $1/a$, has been used. Substituting equation (20) into equations (16) and (17), we find the ground-state energy per site to be

$$E_0 = v\left(\frac{1}{4\pi a^2}\sqrt{1 + \alpha_1\xi^4 + \frac{1}{4}\alpha_2\xi} - \frac{\alpha_1\xi^4}{a^2\beta^2} - \frac{\alpha_2\xi}{a^2\beta^2}\right) \tag{22}$$

and the single-particle excitation spectrum

$$\omega_k = \sqrt{v^2k^2 + \Delta^2} \tag{23}$$

with the energy gap given by

$$\Delta = \sqrt{\Delta_1^2 + \Delta_2^2} \tag{24}$$

where $\Delta_1 = v\sqrt{\alpha_1\xi^4}/a$ and $\Delta_2 = v\sqrt{\alpha_2\xi}/2a$ stand for the contributions of frustration and dimerization to the energy gap, respectively. We will take $a = 1$ below.

3. Results and discussions

Equations (21)–(24) constitute one of the main results of this paper, suitable for the $S = 1/2$ Heisenberg chain with both dimerization and frustration. They can reproduce previous theoretical results in several special cases.

(1) In the frustrated case without dimerization ($\delta = 0$ and so $\alpha_2 = 0$), behaviour of the model is governed by the term $\alpha_1\cos\beta\phi$ which describes the frustration effects. It is found [16] that for $\beta^2 > 8\pi$, there is no nonzero solution of ξ in equation (21), indicating gapless behaviour; on the other hand for $\beta^2 < 8\pi$, there is a nonzero solution of ξ and so the gap appears. The critical value is $\beta^2 = 8\pi$, corresponding to $\alpha = \alpha_c$. As a result, with increasing frustration, the system undergoes a transition at α_c from the gapless phase to the gapped phase. This is a second-order Kosterlitz–Thouless-type phase transition [17].

(2) In the case of $\alpha = \alpha_c$ and small δ, it follows from equations (9) and (10) that $\alpha_1 = 0$ and $\beta^2 = 8\pi$ so that equation (5) reduces to a standard single-frequency SG model with the term $\alpha_2\cos(\beta\phi/2)$. The self-consistent equation (21) for ξ is simplified to

$$\xi^{3/2}\left(\sqrt{\xi + \frac{4}{\alpha_2}} + \sqrt{\frac{4}{\alpha_2}}\right) = 1. \tag{25}$$

There is always a nonzero solution of ξ in equation (25) for any δ, indicating that a finite gap always exists in this case. Let us calculate analytically the asymptotic behaviour of the ground-state energy and the energy gap as functions of the dimerization parameter in the limit of $\delta \ll 1$. To investigate behaviour near the uniform limit, it is appropriate to

calculate the difference between the ground-state energies for a small dimerization and in the uniform limit:

$$\epsilon_0(\delta) = \frac{1}{J}[E_0(0,\alpha) - E_0(\delta,\alpha)]. \tag{26}$$

Since $1/\alpha_2 \gg 1$ and $\xi \ll 1$ in the limit $\delta \to 0$, it follows from equations (7) and (25) that $\alpha_2 \propto \delta$ and $\xi \propto \delta^{1/3}$. Taking into consideration that $\alpha_2\xi \propto \delta^{4/3}$, from equations (24) and (26), we obtain $\Delta(\delta) \propto \delta^{2/3}$ and $\epsilon_0 \propto \delta^{4/3}$. The results obtained for small δ are in excellent agreement with the Cross and Fisher theory [18], which has also been obtained from the DMRG studies [8] and from the exact diagonalization results [10].

(3) Along the line $2\alpha + \delta = 1$, the ground state of the model is known to be exactly solvable. In the α–δ plane, this line is a boundary between two distinct regimes: for $2\alpha + \delta \leqslant 1$, the dominant peak in the static magnetic structure factor is always at $q^* = \pi$; whereas for $2\alpha + \delta > 1$, with increasing α and δ, q^* continuously decreases from π to $\pi/2$ [8], exhibiting incommensurate behaviour. Our calculation shows that along the line $2\alpha + \delta = 1$, the variation of $E_0(\delta)$ in units of J varies linearly with δ, as shown in figure 1. The slope of the straight line is -0.46, which is somewhat different from a variational result of $-3/8$ [8]. Figure 2 shows the variation of the gap with δ along this line, which is in better agreement with the DMRG result (circular points) [8].

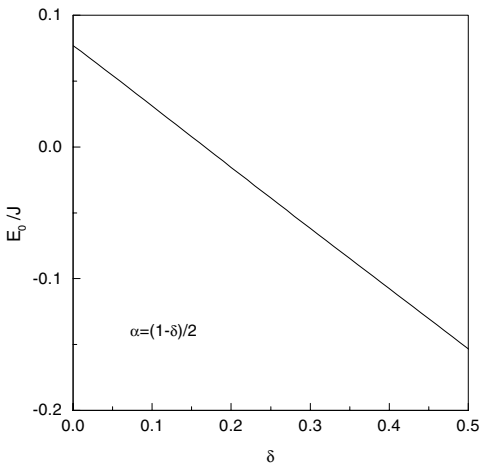


Figure 1. Ground-state energy per site as a function of δ along the line $2\alpha + \delta = 1$.

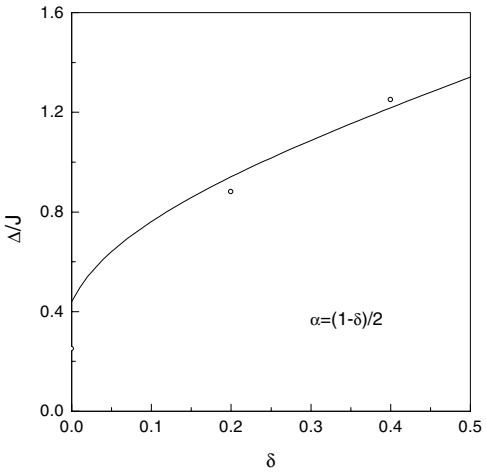


Figure 2. Energy gap as a function of δ along the line $2\alpha + \delta = 1$. Circular points stand for the DMRG data [8].

From equations (21)–(24), one can study variations of ϵ_0 and Δ with δ and α in a more general case. It is found that for fixed δ, with increasing α, ϵ_0 increases or the ground-state energy $E_0(\delta,\alpha)$ decreases, as shown in figure 3. At the same time, the increase in the gap with α is shown in figure 4. On the other hand, with increasing δ for fixed α, the ground-state energy decreases and the gap increases.

We now compare the calculated results with recent experimental data of $CuGeO_3$ [1]. Many authors have made an attempt at evaluating α and J from experimental data of the magnetic susceptibility [1]. Riera and Dobry [19] obtained $\alpha = 0.36$ and $J = 160$ K by fitting the maximal point of magnetic susceptibility. Using Faraday rotation, Nojiri *et al* [20] estimated $J \simeq 183$ K. The magnetic susceptibility of $CuGeO_3$ in the uniform phase can be accurately reproduced by a frustrated Heisenberg chain model with $\alpha \approx 0.35$ [3], very close

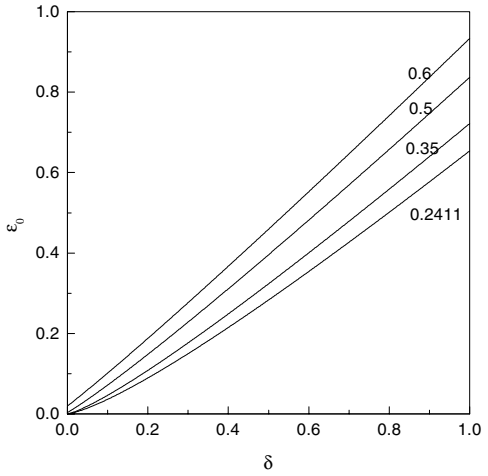


Figure 3. Change in the ground-state energy per site as a function of δ for different α.

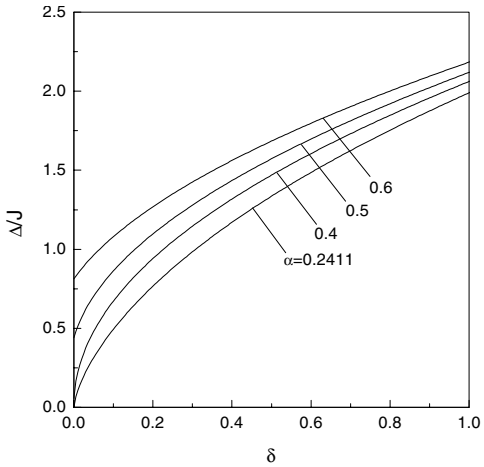
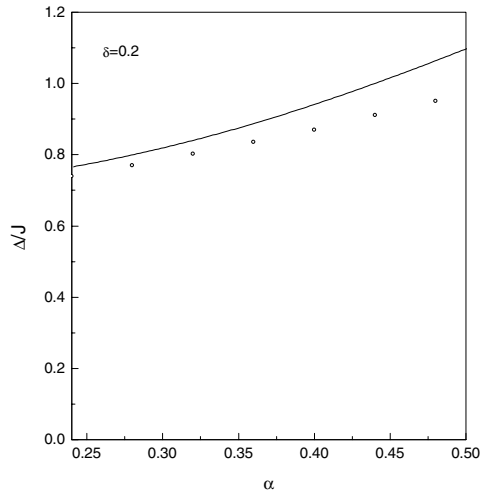


Figure 4. Energy gap as a function of δ for different α.

to the previous estimate [19]. From $J \approx 160$ K and $\alpha = 0.35$ and by taking dimerization $\delta = 0.012$, the frustrated Heisenberg chain model [21] can reproduce $\Delta \approx 2.15$ meV which was experimentally determined by inelastic neutron scattering [22]. With $J = 160$ K and $\alpha = 0.35$, we get $\delta = 0.0096$, which is in good agreement with the estimate by exact diagonalization [23] but slightly smaller than $\delta = 0.012$ [21].

We wish to make a comparison between the present analytical results and numerical data. Figure 5(a) shows the calculated gap (solid line) as a function of α for a fixed value of $\delta = 0.2$, in which circular points stand for the extrapolated values of Δ using exact diagonalization techniques with periodic boundary conditions for chains with up to $L = 26$ sites [10]. On the



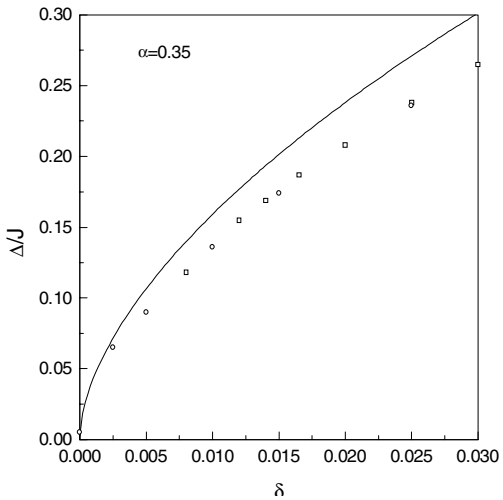


Figure 5. (a) Energy gap as a function of α for $\delta = 0.2$. Cricular points stand for the exact diagonalization data [10]. (b) Energy gap as a function of δ for $\alpha = 0.35$.
Square and cricular points stand for the exact diagonalization data from [21] and [23], respectively.

other hand, figure 5(b) shows the calculated gap as a function of δ for selected $\alpha = 0.35$, in which square and circular points stand for the numerical data from the Lanczos diagonalization techniques [21, 23]. It is found that our analytical results are somewhat greater than numerical data with a relative difference of less than about 12%. This difference may stem from the fact that we have neglected the renormalization of the parameters in transforming the lattice model equation (1) into the continuum model equation (3) [24]. The renormalized values of the parameters in the continuum models can be found by solving the appropriate renormalization ground equations [25] but a detailed discussion of this problem is beyond the scale of the present paper. On the other hand, the higher-order terms are omitted when we expand the exponential functions in equation (14) to obtain equations (15)–(18). The comparison with numerical results indicates that the present theory gives an appropriate description for the case of weak dimerization.

In order to see the asymptotic behaviour of the ground-state energy ϵ_0 and the gap Δ as a function of δ for various frustrations, figures 6 and 7 show the log–log plots of ϵ_0 and Δ versus δ, respectively. It is found that the Cross–Fisher power law [18] holds only at $\alpha = \alpha_c = 0.2411$, but is no longer valid for $\alpha > \alpha_c$. When α increases, the deviation from linear behaviour becomes large, which can be clearly seen in figures 6 and 7. Similar behaviour has also been found by Yokoyama and Saiga [23]. Finally, we discuss the contributions of the two cosine terms in equation (5) to the energy gap. For $\alpha > \alpha_c$, frustration and dimerization provide two independent mechanisms for energy–gap formation. Figure 8 shows the ratio $r = \Delta_1/\Delta_2$ as a function of δ for different α. It is found that r is small for α close to α_c; when α increases, r rapidly increases, especially for $\delta < 0.2$. This result is consistent with that of [10].

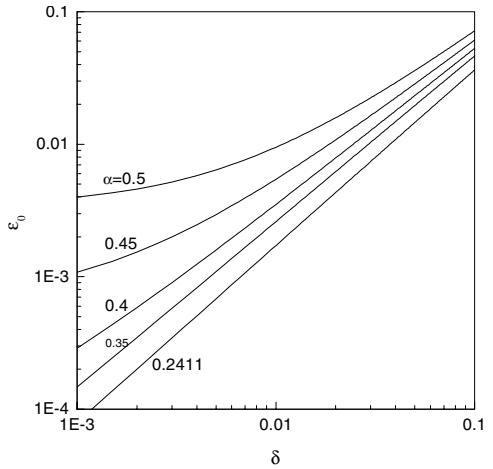


Figure 6. Log–Log plot of ϵ_0 versus δ for different α.

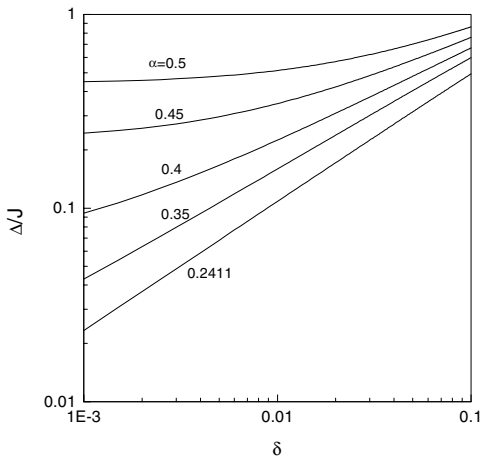


Figure 7. Log–Log plot of Δ/J versus δ for different α.

4. Summary

We have analytically studied the ground-state energy and elementary excitations of a dimerized and frustrated Heisenberg chain by the bosonization technique in the continuum-limit approach combined with the self-consistent quantum theory. It has been shown that as the frustration parameter α increases from $\alpha_c = 0.2411$, the ground-state energy decreases and the energy gap increases. For small δ and at $\alpha = \alpha_c$, the energy gap scales as δ to the power $2/3$, while the change in the ground-state energy scales with the power $4/3$. The Cross–Fisher power law

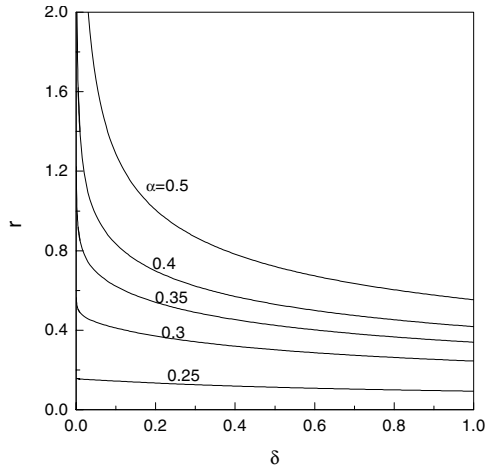


Figure 8. Ratio Δ_1/Δ_2 as a function of δ for different α

holds only at $\alpha = \alpha_c$, but becomes invalid with increasing α. Our analytical results are in good agreement with other numerical results from the DMRG and from exact diagonalization. The calculated results are of relevance for the magnetic excitations in the SP compound $CuGeO_3$. Starting from the 1D quantum double-frequency SG model, we have discussed contributions of the dimerization and frustration to the energy gap. These are two independent mechanisms that give rise to the energy gap. The frustration-induced energy gap increases gradually as α is increased from α_c.

Acknowledgments

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