Field theoretical study of a spin-1/2 ladder with unequal chain exchanges

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We study the low-energy properties of a Heisenberg spin-1/2 zigzag ladder with different exchange constants on the two chains. Using a nonlinear σ-model field theory and abelian bosonization, we find that the excitations are gapless, with a finite spin wave velocity, if the values of the chain exchanges are small. If the chain exchanges are large, the system is gapped, and the energy spectra of the kink and antikink excitations are different from each other.

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I. INTRODUCTION

For the last several decades, one-dimensional and quasi-one-dimensional quantum spin systems have been studied extensively due to their unusual properties. Experimentally, many such systems are known to present a wide range of unusual properties, and a variety of analytical and numerical techniques exist for studying these systems theoretically. The three observations which make the low-dimensional spin systems particularly intersting are, (i) Haldane's conjecture for one-dimensional antiferromagnetic spin systems [1,2], (ii) the discovery of high-temperature superconductivity and its magnetic properties at low doping [3], and (iii) the discovery of ladder materials [4,5].

In spin ladders, two or more one-dimensional spin chains interact with each other. For ladders with the railroad geometry, it has been observed that spin-1/2 systems with an even number of legs are gapped, while systems with an odd number of chains have gapless excitations [6–8]. However, the frustrated zigzag ladder [9] shows gapless spin liquid state or the gapped dimer state, depending on the ratio of the exchanges of the rungs to the chains [10].

Another interesting kind of system is the spin-Peierls system such as $CuGeO_3$. The authors of Ref. [9] have explained the form of the ground state and the low-temperature thermodynamic properties of this sample by showing that there is spontaneous dimerization of the nearest neighbor interaction below a particular temperature. Their model includes a dimerization in the nearest neighbor exchange coupling.

Relatively less is known about a spin ladder with asymmetry in the chains. An extreme case of this situation, *i.e.*, when a chain is absent from the Fig. 1 (sawtooth chain), has been studied by two different groups [11,12].

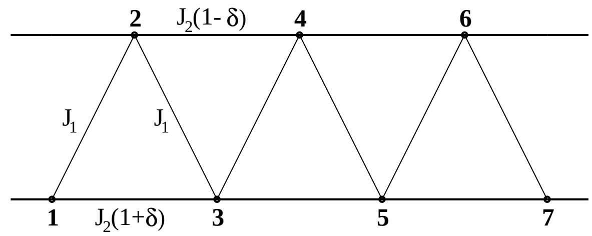

FIG. 1. Schematic diagram of a spin ladder with unequal chain exchanges.

The ground state is like that of the Majumdar-Ghosh model [13], except that the two kinds of low-energy excitations (kinks and antikinks) which interpolate between the two degenerate ground states have quite different excitation spectra.

In this paper, we study a two-chain ladder system with unequal exchange constants of the chains, rather than a dimerization in the rungs. Very recently, Voit *et al* [14] have studied this problem. We will discuss their results below. The plan of the paper is as follows. In Sec. II, we will analyze the problem using the nonlinear σ-model (NLSM) field theory. Sec. III will discuss the abelian bosonization approach.

II. NONLINEAR σ-MODEL STUDY

In this section we study the NLSM field theory of our model. The schematic plot is shown in Fig. 1. The system can be viewed either as a ladder with unequal exchanges on the two chains, or as a single chain with unequal next-nearest neighbor exchanges. The Hamiltonian is

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

where n is the site index, $J_1, J_2 \geq 0$, and $0 \leq \delta \leq 1$. If we view the system as two chains, then the lower (upper) chain contains the odd (even) numbered sites.

Using the NLSM field theory, one can describe the low-energy and long-wavelength excitations. In the Neel phase, this is given by an $O(3)$ NLSM with a topological term. Here we define two fields $\vec{\phi}_n$ and $\vec{l}_n$ as a linear combination of two spins as

$$\vec{\phi}_n = \frac{\vec{S}_{2n-1} - \vec{S}_{2n}}{2S} ,$$
$$\vec{l}_n = \frac{\vec{S}_{2n-1} + \vec{S}_{2n}}{2a} , \quad (2)$$

where a is the lattice spacing. It can be easily checked that

$$\vec{\phi}_n \cdot \vec{l}_n = 0 ,$$
$$\vec{\phi}_n^2 = 1 + \frac{1}{S} - \frac{a^2 \vec{l}_n^2}{S^2} . \quad (3)$$

Thus $\vec{\phi}_n$ becomes a unit vector in the large S limit. The unit cell of the classical ground state of the Neel phase is labeled by an integer n, and it contains the sites $2n-1$ and $2n$ respectively; the length of a unit cell is $2a$.

The fields $\vec{\phi}_n$ and $\vec{l}_n$ satisfy the commutation relations

$$[\vec{l}_{ma}, \vec{\phi}_{nb}] = \frac{i}{2a} \, \delta_{mn} \, \sum_c \, \epsilon_{abc} \, \vec{\phi}_{nc} \quad (4)$$

where m and n are the unit cell labels, a, b, c denote the x, y, z components of the field, and ϵ_{xyz} is the completely antisymmetric tensor with $\epsilon_{xyz} = 1$. This relation enables us to write $\vec{l}_n = \vec{\phi}_n \times \vec{\Pi}_n$, where the vector $\vec{\Pi}$ is canonically conjugate to $\vec{\phi}$ namely,

$$[\phi_{ma}, \Pi_{nb}] = \frac{i}{2a} \delta_{mn} \delta_{ab} . \quad (5)$$

To define the continuum limit of this theory, we introduce a spatial coordinate x which is equal to $2na$ at the location of the n^{th} unit cell. Summations are then replaced by integrals, *i.e.*, $\sum_n \to \int dx/(2a)$.

Since $\vec{\phi}_n$ is a unit vector, $\dot{\vec{\phi}}$ and $\vec{\phi}'$ are orthogonal to $\vec{\phi}$. In the low-energy and long-wavelength limit, the dominant terms in the Hamiltonian are those which have second order space-time derivatives of $\vec{\phi}$ and first order derivatives of $\vec{l}$ (since $\vec{l}$ contains the the first order derivatives of $\vec{\phi}$) [15,16]. To get the continuum Hamiltonian, we expand the fields $\vec{\phi}_{n+1} = \vec{\phi}(x+2a)$ and $\vec{l}_{n+1} = \vec{l}(x+2a)$, where $x = 2na$, as

$$\vec{\phi}(x+2a) = \vec{\phi}(x) + 2a\vec{\phi}'(x) + 2a^2 \vec{\phi}''(x) + \cdots ,$$
$$\vec{l}(x+2a) = \vec{l}(x) + 2a\vec{l}'(x) + \cdots . \quad (6)$$

Using Eqs. (2), (3), and (6), we obtain the Hamiltonian

$$H = \int dx \, [\, \frac{cg^2}{2} \, (\vec{l} + \frac{\theta}{4\pi} \vec{\phi}')^2 + \frac{c}{2g^2} \vec{\phi}'^2 \,] , \quad (7)$$

where

$$c = 2J_1 S a \sqrt{1 - 4J_2/J_1} ,$$
$$g^2 = \frac{2}{S\sqrt{1 - 4J_2/J_1}} ,$$
$$\theta = 2\pi S . \quad (8)$$

Note that the values of c, g^2 and θ turn out to be independent of δ in this approach. Further, this NLSM is valid only if $J_2/J_1 < 1/4$. For $J_2/J_1 > 1/4$, a different NLSM is required.

One can find the energy-momentum dispersion relation of the form $\omega = c|k|$, where c is the spin wave velocity, by considering small fluctuations around $\vec{\phi} = (0,0,1)$, and expanding the Hamiltonian in (7) to second order in those fluctuations. Similarly one can find the strength of the interaction between the spin waves, g^2, by expanding the Hamiltonian to fourth order in the fluctuations.

From Eq. (8), we see that the coefficient of the topological term $\theta = \pi$ for a spin-1/2 system. This implies that there is no gap in the low-energy excitation spectrum. This result is different from that of the zigzag ladder with a dimerization in the nearest neighbor interaction, *i.e.*, with a term like $J_1(-1)^n \vec{S}_n \cdot \vec{S}_{n+1}$. In that case $\theta = 2\pi S \, (1-\delta)$ is different from π for a spin-1/2 system [16,17], and the the low-energy excitations are gapped.

III. ABELIAN BOSONIZATION STUDY

In this section we study the low-energy excitations spectrum using abelian bosonization. We express our Hamiltonian as the following sum,

$$H = H_1 + H_2 + H_{2\delta} , \quad (9)$$

where

$$H_1 = J_1 \sum_n \vec{S}_n \cdot \vec{S}_{n+1} ,$$
$$H_2 = J_2 \sum_n \vec{S}_n \cdot \vec{S}_{n+2} ,$$
$$H_{2\delta} = -J_2 \, \delta \sum_n \, (-1)^n \, \vec{S}_n \cdot \vec{S}_{n+2} . \quad (10)$$

We can convert this Hamiltonian to a Hamiltonian of spinless fermions through the Jordan-Wigner transformation. The relations between the spin and the electron creation and annihilation operators are,

$$S_n^z = \psi_n^\dagger \psi_n - 1/2 ,$$
$$S_n^- = (-1)^n \psi_n \, \exp[i\pi \sum_{j=-\infty}^{n-1} n_j] ,$$
$$S_n^+ = (-1)^n \psi_n^\dagger \, \exp[-i\pi \sum_{j=-\infty}^{n-1} n_j] , \quad (11)$$

where $n_j = \psi_j^\dagger \psi_j$ is the fermion number at site j. The Hamiltonians in (10) then become

$$H_1 = -\frac{J_1}{2} \sum_n \, (\psi_{n+1}^\dagger \psi_n + \psi_n^\dagger \psi_{n+1})$$
$$+ J_1 \sum_n \, (\psi_n^\dagger \psi_n - 1/2)(\psi_{n+1}^\dagger \psi_{n+1} - 1/2) , \quad (12)$$

$$H_2 \ = J_2 \sum_n \ (\psi^\dagger_{n+2}\psi_n + \text{h.c.})(\psi^\dagger_{n+1}\psi_{n+1} - 1/2) + J_2 \sum_n \ (\psi^\dagger_n\psi_n - 1/2)(\psi^\dagger_{n+2}\psi_{n+2} - 1/2) \ , \quad (13)$$

$$H_{2\delta} = -J_2\delta\sum_n (-1)^n(\psi^\dagger_{n+2}\psi_n + \text{h.c.})(\psi^\dagger_{n+1}\psi_{n+1} - 1/2) - J_2\delta\sum_n (-1)^n(\psi^\dagger_n\psi_n - 1/2)(\psi^\dagger_{n+2}\psi_{n+2} - 1/2). \quad (14)$$

We will assume below that $J_1 >> J_2$. Since there is no applied magnetic field, the two Fermi points occur at $k_F = \pm\pi/2$. We can linearize the energy spectrum around these Fermi points, and express the lattice operators in terms of two continuum fields R and L which vary slowly on the scale of a lattice spacing,

$$\psi_n \ = \ \sqrt{a} \ [\ i^n R(n) \ + \ (-i)^n L(n) \ ] \ , \quad (15)$$

where R and L are describe the second-quantized fields of right- and left-moving fermions respectively. Now we bosonize our Hamiltonian following the standard procedure. The basic relations used to obtained the bosonized Hamiltonian are as follows [18].

$$S^z(x) \ = \ a \ [\ \rho(x) \ + \ (-1)^j \ M(x) \ ] \ , \quad (16)$$

where the fermion density $\rho(x) =: R^\dagger(x)R(x) : + : L^\dagger(x)L(x) :$, and the mass operator $M(x) =: R^\dagger(x)L(x) : + : L^\dagger(x)R(x) :$. (The double dots denote normal ordering). The bosonized expressions for ρ and M are given by

$$\rho(x) = \ - \ \frac{1}{\sqrt{\pi}} \ \partial_x\phi(x) \ , \qquad M(x) = \ \frac{1}{\pi a} \ \cos(2\sqrt{\pi}\phi(x)) \ . \quad (17)$$

The bosonized version of H_1 is known to be

$$H_1 = \int dx \ [\ \frac{v_1 K}{2} \ \Pi^2 \ + \ \frac{v_1}{2K} \ (\partial_x\phi)^2 + \frac{v_1}{(\pi a)^2} : \cos(4\sqrt{\pi}\phi) : \ ] \ , \quad (18)$$

where $v_1 = \pi J_1 a/2$ is the spin wave velocity, and $K = 1/2$ is the bosonization interaction parameter for the isotropic spin-1/2 antiferromagnet. The last term in (18) is marginal, and is known to have no effect at long distances in the sense of the renormalization group (RG) [18]. Using Eqs. (13), (15), and (16), we get the following expression for H_2, where we have ignored terms of the order of a^4 and higher,

$$H_2 = J_2 a^2 \ \sum_n \ [- \ (\rho_{n+1} - (-1)^n M_{n+1}) \times (\rho_n + \rho_{n+2} + (-1)^n M_n + (-1)^n M_{n+2}) + (\rho_n + (-1)^n M_n)(\rho_{n+2} + \ (-1)^n M_{n+2})]. \quad (19)$$

To derive this expression, we have used Taylor expressions such as

$$R(n+2) \ = \ R(n) \ + \ 2aR'(n) \ + \ 2a^2R''(n) \ + \ \cdots \quad (20)$$

to write

$$R^\dagger(n+2)R(n) \ + \ R^\dagger(n)R(n+2) = \ R^\dagger(n+2)R(n+2) \ + \ R^\dagger(n)R(n) \ + \ O(a^2) \ . \quad (21)$$

On keeping only the terms which do not oscillate as $(-1)^n$ (which would give zero in the continuum limit) and then expressing the operators ρ and M in the bosonic language, the above expression becomes

$$H_2 \ = v_2 \ \int dx \ [-\frac{1}{\pi}(\partial_x\phi)^2 + \frac{3}{2(\pi a)^2}\cos(4\sqrt{\pi}\phi)], \quad (22)$$

where $v_2 = J_2 a$. Both the terms in (22) have scaling dimension 2, and they are marginal. It is known that they have no effect in the RG sense as long as $J_2/J_1 < 0.241$ [19]. Finally, one can find the bosonized expression for $H_{2\delta}$. To begin with, the nonoscillatory part of the Hamiltonian is given by

$$H_{2\delta} = -J_2\delta a^2 \sum_n \ [\rho_n M_{n+2} + M_n\rho_{n+2} - \rho_{n+1}(M_n + M_{n+2}) + M_{n+1}(\rho_n + \rho_{n+2})]. \quad (23)$$

Now we perform an operator product expansion of the above Hamiltonian. In the limit $z \to w$, we can use the following expansion [20,21],

$$\partial_z\phi(z) : e^{i\beta\phi(w)} : \ = -\frac{i\beta}{z-w} : e^{i\beta\phi(w)} : + : \partial_z\phi(z)e^{i\beta\phi(z)} : \quad (24)$$

for $K = 1/2$. The second term in (24) is a total derivative, and its contribution will therefore vanish in the Hamiltonian where it appears inside an integral over all x. From the first term in Eq. (24), we see that the various terms in Eq. (23) cancel each other in pairs which have $z - w = \pm a$ or $\pm 2a$. If this cancellation had not occurred, the bosonized version of $H_{2\delta}$ would have been proportional to the operator $\cos(2\sqrt{\pi}\phi)$, which has scaling dimension 1 and would therefore have been relevant. However, due to the cancellation, $H_{2\delta}$ contains no relevant operators with scaling dimension less than 2. Thus the system continues to remain gapless (and lies in the same spin-liquid phase as the model described by the nearest neighbor Hamiltonian H_1) even if $\delta \neq 0$, provided that $J_2 << J_1$. This is in contrast to a dimerization in J_1; in that case abelian bosonization correctly produces a relevant term which leads to a gapped phase.

Recently Voit *et al* [14] have studied the same model as ours using abelian bosonization followed by a perturbative renormalization group analysis. They claim that the perturbation due to the unequal chain exchanges ($J_2\delta$ terms) is relevant but that it does not lead to a gapped phase; instead, they argue that it leads to a different fixed point where the system is gapless and has a vanishing spin velocity. In our study, we have shown that due to some cancellations, the $J_2\delta$ terms do *not* lead to any relevant terms in the continuum theory, and therefore that the system remains gapless if J_2 is small.

Finally, let us discuss the low-energy excitations of this model when J_2 becomes larger. In particular, we find that these are given by kinks and antikinks when $J_2 = J_1/2$, for all values of δ lying in the range $[0,1]$. (The Majumdar-Ghosh model is a special case of this where $\delta = 0$). Then the Hamiltonian in (1) can be written, up to a constant, as the sum

$$H = \frac{J_1}{4} \sum_n [(1+\delta)(\vec{S}_{2n-1} + \vec{S}_{2n} + \vec{S}_{2n+1})^2 + (1-\delta)(\vec{S}_{2n} + \vec{S}_{2n+1} + \vec{S}_{2n+2})^2] \; . \quad (25)$$

Hence the ground state is given by a configuration in which the total spin of each triangle is $1/2$. Since this can be done either by forming a singlet with the pair of spins $(2n-1, 2n)$ for all values of n, or by forming a singlet with the pair of spins $(2n, 2n+1)$ for all values of n, we see that the ground state is doubly degenerate. Let us denote these two ground states by A and B respectively. The lowest-energy excitations (kink and antikink) are formed by interpolating between these two ground states. The kink has the ground state A on the left and the ground state B on the right, while the antikink has the ground state B on the left and the ground state A on the right. For general values of δ, we find that the kink and antikink dispersion are nondegenerate in contrast with the Majumdar-Ghosh model [11,12]. A simple variational calculations gives the kink and antikink dispersions to be $J_1(1-\delta)(5+4\cos k)/8$ and $J_1(1+\delta)(5+4\cos k)/8$ respectively. Hence the minimum gap for the kink and antikink excitations are $J_1(1-\delta)/8$ and $J_1(1+\delta)/8$ respectively, occurring at $k = \pi$. This result has been also obtained by the Voit *et al* [14].

To summarize, we have studied the low-lying excitations of a zigzag ladder with unequal chain exchanges. Both the NLSM and abelian bosonization show that the system remains gapless if $J_2 << J_1$. We have also shown that the system is gapped (with two degenerate ground states) for $J_2 = J_1/2$. It would be interesting to use numerical techniques like the density-matrix renormalization group [22], to study the complete phase diagram of the ground state as a function of the two parameters J_2/J_1 and δ.

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