

Calculation of the singlet-triplet gap of the antiferromagnetic Heisenberg model on a ladder

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The ground-state energy and the singlet-triplet energy gap of the antiferromagnetic Heisenberg model on a ladder is investigated using a mean-field theory and the density-matrix renormalization group. Spin-wave theory shows that the corrections to the local magnetization are infinite. This indicates that no long-range order occurs in this system. A flux-phase state is used to calculate the energy gap as a function of the transverse coupling, J_{\perp} , in the ladder. It is found that the gap is linear in J_{\perp} for $J_{\perp} \gg 1$ and goes to zero for $J_{\perp} \rightarrow 0$. The mean-field theory agrees well with the numerical results.

I. INTRODUCTION

The antiferromagnetic (AF) Heisenberg ladders (two coupled spin chains) are relevant to the understanding of how the physics evolves from the purely one-dimensional (1D) to two-dimensional (2D) systems. Also, the $S = \frac{1}{2}$ Heisenberg model on the ladder can model the magnetic properties of systems such as the vanadyl pyrophosphate,¹ $(\text{VO})_2\text{P}_2\text{O}_7$. The calculation of the thermodynamic properties of this material will be addressed in a forthcoming work.² The relevance of the transverse coupling J_{\perp} for ground-state properties is examined in the present work.

From the theoretical point of view, two main reasons are behind the increasing interest in the Heisenberg ladder. The Haldane conjecture³ is that the energy gap of the elementary excitations of chains depends on whether the spin is an integer or a half integer. It is well known⁴ that the spin-one-half 1D Heisenberg model is gapless. However, it is not clear how the gap behaves when a transverse coupling J_{\perp} is turned on between the two chains of the Heisenberg ladder. In Ref. 5 the authors reported that a finite transverse coupling $J_{\perp c} \approx 0.4$ is required to get a finite gap. Later on, Barnes *et al.*⁶ concluded that the critical value vanishes at $J_{\perp c} = 0$. The second reason is the discovery of high-critical-temperature superconductors (HTCS's). The interest for these systems is due to the belief that the 2D Heisenberg model describes the AF interactions in the undoped copper-oxygen planes of HTCS's. The ladder problem can help us understand the crossover from 1D to 2D systems (this question is related to the stability of the Luttinger liquid).

Strong and Millis⁷ have also recently used this type of model to investigate the competition between magnetic ordering and the Kondo effect in heavy-fermion systems. Since the work of Doniach,⁸ it is widely believed that spin excitations of heavy fermions can be modeled by such a model. The major weakness is that the real Kondo effect is lost; only the spin compensation effect is shown.

The problem of a plane of coupled spin- $\frac{1}{2}$ chains was studied by Azzouz⁹ who found within a mean-field ap-

proximation that once J_{\perp} is nonzero, long-range AF order appears in the system. The gap remains zero because of the broken symmetry due to long-range order. For the ladder, no broken symmetry is expected to occur because of the 1D nature of the system. Indeed, the finite size in the transverse direction will bring different physics than the two-dimensional Heisenberg model. We believe that the gap starts to be nonzero for any finite J_{\perp} due to the finite size in the transverse direction.¹⁰ In the limit of large J_{\perp} the system is equivalent to weakly coupled singlets, and the gap is given in leading order by the singlet-triplet energy separation. The first term of the gap is linear in J_{\perp} . When J_{\perp} becomes of the same order as the parallel coupling the situation becomes more difficult to analyze.

In this paper, the ladder problem is investigated using a mean-field approach and exact diagonalization. The energy gap is found to be nonzero for any finite J_{\perp} . Comparison with the exact diagonalization, which is based on the density-matrix renormalization group¹¹ (DMRG) is reported. The agreement between these approaches is very good.

II. MEAN-FIELD TREATMENT

The Heisenberg model on the ladder is denoted as follows:

$$H = J_{\perp} \sum_{\langle i,j \rangle_{\perp}} \mathbf{S}_i \cdot \mathbf{S}_j + J \sum_{\langle i,j \rangle_{\parallel}} \mathbf{S}_i \cdot \mathbf{S}_j, \quad (1)$$

where the sums run over first-nearest neighbors $\langle i,j \rangle_{\parallel}$ along the chains and $\langle i,j \rangle_{\perp}$ perpendicular to the chains. J and J_{\perp} are AF coupling constants. In the following J is set equal to unity and periodic boundary conditions are imposed. Simple limits of this model can be analyzed. The first obvious one is realized for $J_{\perp} \gg 1$ as mentioned in the Introduction. In this case, one gets weakly coupled (by $J = 1$) singlets and the first excited state has an energy gap behaving as J_{\perp} in leading order. This excitation is obtained when the state of a single pair of spins changes from singlet to triplet. The second limit, less obvious, is $J_{\perp} = 0$. The two chains can be treated separately. It is

known from the exact results of des Cloiseaux⁴ that the 1D Heisenberg model has an energy spectrum of the form

$$\epsilon(k) = \frac{\pi}{2} |\sin k|, \quad (2)$$

which shows a zero gap. The intermediate regime ($J_{\perp} \sim 1$) is quite interesting and is the most complicated one. The dependence of the energy gap, hereafter denoted $E_g(J_{\perp})$, on the transverse coupling is investigated here using the same mean-field theory as in Ref. 7.

A. Review of the flux-phase and Néel-flux-phase states

The 2D generalization of Wigner-Jordan transformation of Ref. 7 can be easily implemented in the case of the ladder. One gets, following the notation of Fig. 1,

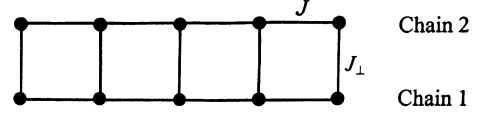


FIG. 1. The ladder system.

$$S_{i,1}^- = c_{i,1} \exp \left[i\pi \sum_{l=0}^{i-1} (n_{l,1} + n_{l,2}) \right] \quad (3)$$

for the chain 1 and

$$S_{i,2}^- = c_{i,2} \exp \left[i\pi \left[\sum_{l=0}^i n_{l,1} + \sum_{l=0}^{i-1} n_{l,2} \right] \right] \quad (4)$$

for the chain 2. The indices i run along the chains. The Hamiltonian is now written in this fermion representation. One finds the following spinless interacting fermion Hamiltonian:

$$H = \frac{-J}{2} \sum_{i,\delta} [c_{i,1} e^{-i\Phi_{i,i+\delta(1)}} c_{i+\delta,1}^\dagger + c_{i,2} e^{-i\Phi_{i,i+\delta(2)}} c_{i+\delta,2}^\dagger] + \frac{-J_{\perp}}{2} \sum_i c_{i,1} c_{i,2}^\dagger + J \sum_{i,j=1,2,\delta} (n_{i,j} - 1/2)(n_{i+\delta,j} - 1/2) + J_{\perp} \sum_i (n_{i,1} - 1/2)(n_{i,2} - 1/2). \quad (5)$$

The phases Φ are as follows:

$$\Phi_{i,i+1}(1) = \pi n_{i,2}, \quad \Phi_{i,i-1}(1) = -\pi n_{i-1,2}, \quad \Phi_{i,i+1}(2) = \pi n_{i+1,1}, \quad \Phi_{i,i-1}(2) = -\pi n_{i-1,1}, \quad (6)$$

and δ refers to the first-nearest neighbors of a given site. The mean-field solutions studied here are the flux phase,¹² with zero magnetization, and the Néel-flux phase with finite magnetization $m \equiv 2\langle n_{i,j} \rangle - 1$. The flux due to the XY term [the first and second terms in Eq. (5)] of the Hamiltonian is taken to be π per plaquette on average. For the Ising term [the last two terms of Eq. (5)], one chooses $\langle c_{i,j} c_{i+\delta,j}^\dagger \rangle = |\langle c_{i,j} c_{i+\delta,j}^\dagger \rangle| e^{-i\theta_{i,i+\delta(j)}}$ and $\langle c_{i,j} c_{i,j+\delta}^\dagger \rangle = |\langle c_{i,j} c_{i,j+\delta}^\dagger \rangle| e^{-i\theta'_{j,j+\delta(i)}}$ ($j=1,2$). In the following, we set $|\langle c_{i,j} c_{i+\delta,j}^\dagger \rangle| = Q$ and $|\langle c_{i,j} c_{i,j+\delta}^\dagger \rangle| = P$. The sum over θ 's around one plaquette is also taken to be π on average. The bipartite character and the different phases on each link of the system are summarized in Fig. 2. Despite the fact that a finite magnetization in a system like the ladder is not possible because of its smallness, we will discuss the Néel-flux phase and compare its physical meaning with the more physical flux-phase state.

B. Results and discussion

The mean-field Hamiltonian is written as follows:

$$H = \frac{J}{2} \sum_i (c_{i,1}^\dagger e^{-i\pi} c_{i+1,1} + c_{i,1}^\dagger c_{i-1,1} + c_{i,2}^\dagger c_{i+1,2} + c_{i,2}^\dagger e^{i\pi} c_{i-1,2}) + \frac{J_{\perp}}{2} \sum_i (c_{i,1}^\dagger c_{i,2} + c_{i,2}^\dagger c_{i,1}) + \frac{J}{2} \sum_{i,j=1,2,\delta} (m n_{i,j} - m n_{i+\delta,j} + m^2/2) + \frac{J_{\perp}}{2} \sum_i (m n_{i,1} - m n_{i,2} + m^2/2) + J \sum_{i,j=1,2} (Q c_{i,1}^\dagger e^{-i\pi} c_{i+1,1} + Q c_{i,1}^\dagger c_{i-1,1} + Q c_{i,2}^\dagger c_{i+1,2} + Q c_{i,2}^\dagger e^{i\pi} c_{i-1,2} + Q^2) + J_{\perp} \sum_i (P c_{i,1}^\dagger c_{i,2} + P c_{i,2}^\dagger c_{i,1} + P^2), \quad (7)$$

where a bipartite lattice due to AF correlations is used, Fig. 2 (the local magnetization is staggered: $m = m_A = -m_B$, where A and B are two adjacent sites). We get

$$H = \sum_{\mathbf{k}} E_{\pm}(\mathbf{k}) \alpha_{\mathbf{k},\pm}^\dagger \alpha_{\mathbf{k},\pm} \quad (8)$$

in k space, where the fermionic operator $\alpha_{\mathbf{k}}$ is obtained

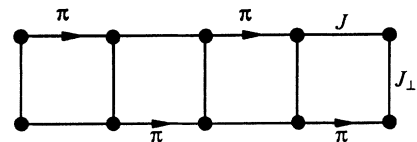


FIG. 2. The flux per plaquette is equal to π on average.

from $c_{\mathbf{k}}$ through the diagonalization of the Hamiltonian (7). The dispersion relation is given by

$$E_{\pm}(\mathbf{k}) = \pm [m^2(1+J_{\perp}/2)^2 + (1+2Q)^2 \sin^2 k_x + (1+2P)^2 (J_{\perp}/2)^2 \cos^2 k_y]^{1/2}, \quad (9)$$

where J_{\perp} is divided by a factor 2, since the periodic boundary conditions used in the transverse direction count J_{\perp} twice. The minimization of the free energy with respect to m , Q , and P gives a set of three self-consistent equations, which become

$$\begin{aligned} m &= \int (d^2k/2\pi) m (1+J_{\perp}/2) / E_{+}(\mathbf{k}), \\ Q &= \int (d^2k/2\pi) (1+2Q) \sin^2 k_x / E_{+}(\mathbf{k}), \\ P &= \int (d^2k/2\pi) (1+2P) (J_{\perp}/2) \cos^2 k_y / E_{+}(\mathbf{k}) \end{aligned} \quad (10)$$

at zero temperature. The integration is over the first Brillouin zone. By definition, we write $\int d^2k/2\pi \equiv \int (dk_x/2\pi)(1/2) \sum_{k_y}$, where k_y can take two values: 0 or π . One easily notes that $m=0$ is a solution. An interesting feature shown by such a solution is that when $J_{\perp}=0$ the k dependence of the dispersion relation yields

$$E_{\pm}(k) = \pm(1+2Q)|\sin k|. \quad (11)$$

The ground state corresponds to the situation, where the lower band is fully occupied and the upper band is empty. A fermion α created in the upper band produces the elementary excitation in the system and the corresponding energy excitation is given only by the dispersion relation of the upper band, namely,

$$\epsilon(k) = (1+2Q)|\sin k|. \quad (12)$$

One can calculate Q and finds $1+2Q \approx 1.63$. This result compares well with $\pi/2 \approx 1.57$ in the exact solution of Eq. (2). The interesting feature is that one recovers smoothly the 1D limit of the dispersion relation by taking $m=0$. The energy gap $E_g(J_{\perp}=0)$ is then equal to zero. When J_{\perp} is nonzero, the gap has the form

$$\begin{aligned} E_g(J_{\perp}) &= E_{+}[\mathbf{k}=(0, \pi)] \\ &= [m^2(1+J_{\perp}/2)^2 + (1+2P)^2 (J_{\perp}/2)^2]^{1/2}, \end{aligned} \quad (13)$$

which reduces to

$$E_g(J_{\perp}) = \frac{(1+2P)}{2} J_{\perp} \quad (14)$$

for $m=0$. Equation (13) is obtained by calculating the difference between the ground-state energy

$$E_{\text{GS}} = JQ^2 + J_{\perp}P^2 + (J+J_{\perp}) \frac{m^2}{4} - \frac{1}{2} \int \frac{d^2k}{2\pi} E_{+}(\mathbf{k}),$$

and the first excited state energy.

$$\begin{aligned} E_{\text{EX}} &= JQ^2 + J_{\perp}P^2 + (J+J_{\perp}) \frac{m^2}{4} \\ &\quad - \frac{1}{2} \int_{\mathbf{k} \neq (0, \pi)} \frac{d^2k}{2\pi} E_{+}(\mathbf{k}) + \frac{1}{2} E_{+}[\mathbf{k}=(0, \pi)]. \end{aligned}$$

For $m=0$ the results of the numerical calculation for the

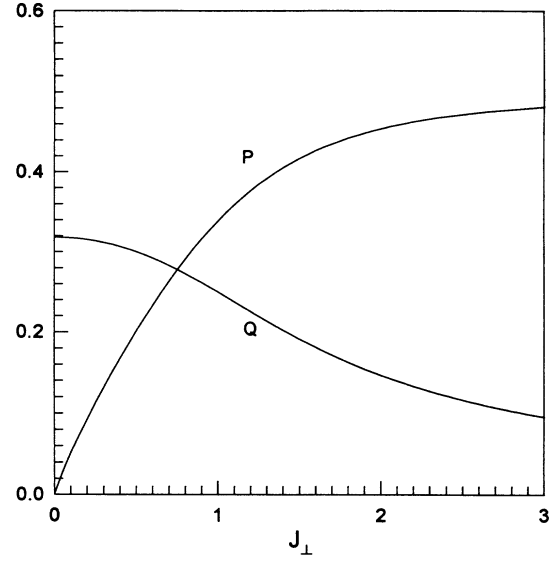


FIG. 3. The parameters Q and P as a function of J_{\perp} for $m=0$.

set of Eqs. (10) are displayed in Figs. 3 and 4. The parameters Q and P show no simple dependence on J_{\perp} . The energy gap, which is displayed in Fig. 4, has a linear behavior in $J_{\perp} \gg 1$. This is in good qualitative agreement with the simple limit $J_{\perp} = \infty$. It has a more complicated dependence for intermediate transverse coupling because of the J_{\perp} dependence of P (Fig. 3). For small J_{\perp} , $E_g(J_{\perp})$ has a simple power-law form

$$E_g(J_{\perp}) \approx c(J_{\perp})^g, \quad (15)$$

where the constant $c=0.76$ and the exponent $g=1.15$. This result compares qualitatively well with that of Strong and Millis⁷ who studied this problem in the case

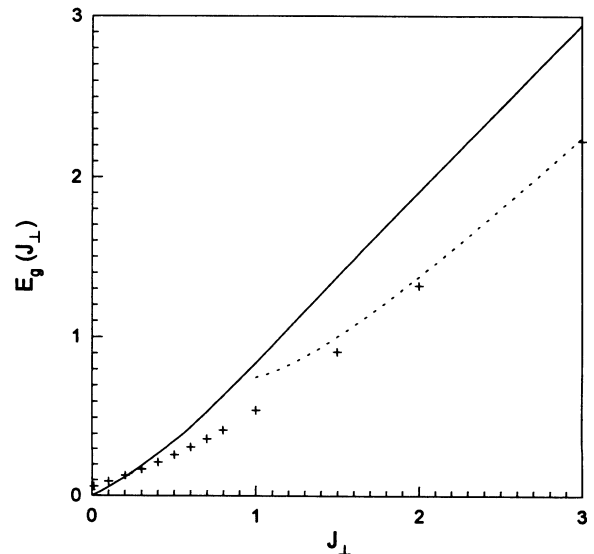


FIG. 4. The energy gap as a function of J_{\perp} . The full and dashed lines are, respectively, from our mean-field treatment ($m=0$) and the result of perturbation theory of Ref. 6. The '+' are the result of the DMRG calculation.

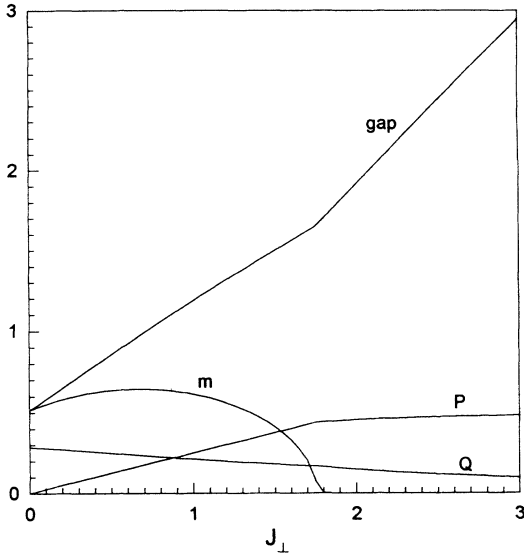


FIG. 5. The parameters of the nonzero magnetization solution of the mean-field approximation (plotted as a function of J_{\perp}).

of z anisotropy in the parallel Heisenberg coupling.

The Néel-flux-phase state has a nonzero m for $J_{\perp} < 1.76$. The different parameters of this state are displayed in Fig. 5. The gap is found to go to a finite limit when $J_{\perp} \rightarrow 0$. The finite magnetization in this state implies broken rotational symmetry. Gapless collective modes related to spin-wave excitation would then exist in the gap. The spin-wave theory goes beyond the mean-field approximation. For nonzero m , the quantum fluctuations due to spin wave excitations would have drastic repercussions on the value of m . As in 1D, these fluctuations destroy long-range order. Indeed, for the ladder,

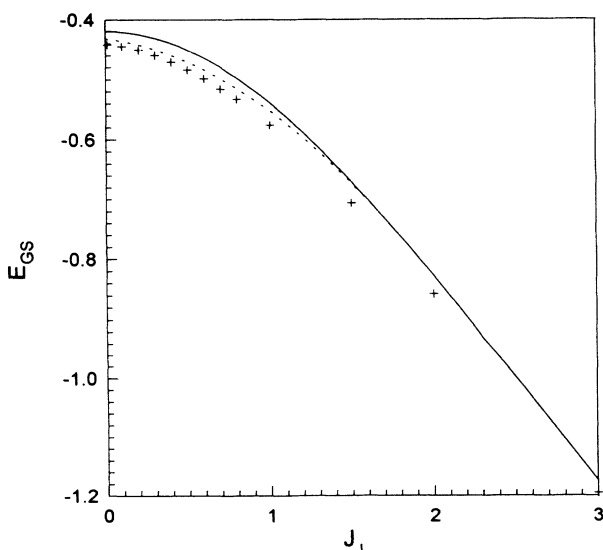


FIG. 6. The ground-state energy as a function of J_{\perp} . The full and dashed lines correspond, respectively, to zero and nonzero magnetization. The '+'s are the result of the DMRG calculation.

the corrections to the local magnetization in the standard spin-wave theory can be calculated and are found to be logarithmically singular

$$\Delta \langle S^z \rangle \sim \int \frac{dk}{k} \sim -\infty. \quad (16)$$

This implies that spin wave theory is not self-consistent, and no long-range order can occur at zero temperatures. So the flux-phase solution, $m=0$, is more adequate to describe the AF correlations even if its ground-state energy is slightly higher than that of the Néel-flux-phase state as shown in Fig. 6. All the physical information the nonzero solution contains is that the AF correlations are more important for $0 < J_{\perp} < 1.76$ as we see on Fig. 5 because the magnetization is zero for $J_{\perp} > 1.76$, but, to our opinion, these correlations are not strong enough to induce long range order (imagine that we can solve exactly this problem, then one would find a zero magnetization for any value of J_{\perp}). The Néel-flux-phase and flux-phase states give the same dispersion relation for $J_{\perp} > 1.76$.

III. NUMERICAL INVESTIGATION WITH THE DMRG

We have used the recently introduced density matrix renormalization group method¹¹ to find the ground-state energy of the Heisenberg ladder. Our Fortran codes are written with the version of the infinite lattice method with open boundary conditions. We first find the ground-state wave function of the finite 2×7 system and start the renormalization process by keeping 80 states in each block. Unlike the one-dimensional version suggested by White,¹¹ we insert only one pair of new sites in the middle of the two blocks to form the new superblock in each renormalization procedure so that the size of the Hilbert space is kept within our computer's capacity. We find this works reasonably well for the ground-state energy shown as crosses in Fig. 6. For the singlet-triplet energy gap, however, it works less well. Nevertheless, the gap we obtain numerically shows convincingly that it vanishes only as the J_{\perp} goes to zero, as should be apparent from the crosses of Fig. 4. The numerical results will be given in detail in a forthcoming work.¹³

IV. CONCLUSION

In conclusion, our mean-field theory (flux phase) describes accurately the low-lying excitations of the AF Heisenberg model on the ladder. The gap is found to increase smoothly with J_{\perp} . Its behavior as a function of J_{\perp} is shown in Fig. 4. The quantitative agreement between the analytical approach and the DMRG numerical solution is very good.

The accuracy of the flux phase in the case of the ladder is a precursor of high-dimensionality physics, since a finite flux can exit only in dimensions higher than 1. The

spin-energy excitations have a gap. Now, when charge degrees of freedom are introduced, the situation becomes more complicated. However, if we assume that a finite doping, δ_c , is required to bring the gap to zero, then one can conclude that the 1D Luttinger-liquid state is unstable for $\delta < \delta_c$ in the sense that the spin correlations decrease algebraically in 1D rather than exponentially for finite J_{\perp} . The system does not belong to the same universality class when $J_{\perp} > 0$ as that of the 1D system.

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