Excitation spectrum of Heisenberg spin ladders

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(Received 3 August 1992)

Heisenberg antiferromagnetic spin "ladders" (two coupled spin chains) are low-dimensional magnetic systems which for $S=\frac{1}{2}$ interpolate between half-integer-spin chains, when the chains are decoupled, and effective integer-spin one-dimensional chains in the strong-coupling limit. The spin-$\frac{1}{2}$ ladder may be realized in nature by vanadyl pyrophosphate, $(VO)_2P_2O_7$. In this paper we apply strong-coupling perturbation theory, spin-wave theory, Lanczos techniques, and a Monte Carlo method to determine the ground-state energy and the low-lying excitation spectrum of the ladder. We find evidence of a nonzero spin gap for *all* interchain couplings $J_\perp > 0$. A band of spin-triplet excitations above the gap is also analyzed. These excitations are unusual for an antiferromagnet, since their long-wavelength dispersion relation behaves as $(k-k_0)^2$ (in the strong-coupling limit $J_\perp \gg J$, where J is the in-chain antiferromagnetic coupling). Their band is folded, with a minimum energy at $k_0=\pi$, and a maximum between $k_1=\pi/2$ (for $J_\perp=0$) and 0 (for $J_\perp=\infty$). We also give numerical results for the dynamical structure factor $S(q,\omega)$, which can be determined in neutron scattering experiments. Finally, possible experimental techniques for studying the excitation spectrum are discussed.

I. INTRODUCTION

The subject of quantum antiferromagnetism in low-dimensional systems has been a very active field in recent years. One specific area of research is one-dimensional spin chains, in particular the excitation spectrum as a function of spin. Much of the recent interest in this field was stimulated by Haldane's conjecture[1] that integer-spin chains have a spin-excitation energy gap, whereas half-integer-spin chains are gapless. Although this has now been convincingly demonstrated numerically for $S=1$ (Ref. 2) and $S=\frac{3}{2}$ (Ref. 3), a detailed understanding of this result is lacking, and studies of related generalizations of the Heisenberg chain might be expected to lead to additional insights.

Recently, the closely related field of two-dimensional spin systems has been the subject of intense study, due to speculations that the $S=\frac{1}{2}$ square-lattice antiferromagnetic copper-oxygen planes might be a vital component of the mechanism of high-temperature superconductivity.[4] As a result of considerable analytical and numerical work the two-dimensional Heisenberg antiferromagnet is now relatively well understood.[5-7] If the antiferromagnetic interaction in insulators such as La_2CuO_4 is indeed responsible for high-temperature superconductivity, perhaps due to magnetic hole-pairing forces which remain effective even after doping leads to a metallic state, one might expect other antiferromagnets to superconduct under hole doping as well.

The related low-dimensional system investigated in this paper is the Heisenberg antiferromagnetic "ladder." This system is the standard spin-$\frac{1}{2}$ Heisenberg model on a ladder of two coupled spin chains. The ladder Hamiltonian has a strength-J interaction along the long (chain) axis of the ladder, and a $J_\perp$ interaction across the rungs,

$$H = J \sum_{\leftrightarrow} \mathbf{S}_i \cdot \mathbf{S}_j + J_\perp \sum_{\updownarrow} \mathbf{S}_i \cdot \mathbf{S}_j \tag{1}$$

in a self-explanatory notation. $\mathbf{S}_i$ is a spin-$\frac{1}{2}$ operator at site i of the ladder. Johnston *et al.*[8] suggested that this Hamiltonian might describe the magnetic properties of vanadyl pyrophosphate, $(VO)_2P_2O_7$, in their experimental study of the magnetic susceptibility of this material. Unfortunately, at that time there were no theoretical results available for the susceptibility of the Heisenberg ladder, so Ref. 8 instead used the dimerized Heisenberg chain susceptibility to fit their data. This model gave a good fit for chain parameters $J_1=65.7$ K and $J_2/J_1=0.7$. (J_1 and J_2 are the alternating spin-spin interaction strengths in the dimer chain model. $J_1 \neq J_2$ implies an energy gap for spin excitations.[9]) The accuracy of the fit implies that either the ladder and dimerized chain give very similar results for $\chi(T)$, or perhaps the magnetic interaction actually follows a dimerized chain, as in $Cu(NO_3)_2 \cdot \frac{5}{2}H_2O$.[8,10]

More recently, Dagotto, Riera, and Scalapino[11] studied the Heisenberg ladder numerically on finite clusters of up to 2×12 sites using a Lanczos algorithm, and found that the spin gap as a function of $J_\perp$ showed some evidence for

a $J_\perp(\text{crit}) \approx 0.4J$, below which the system appeared gapless. Unfortunately, the bulk-limit properties were not clear in this finite-cluster study, and those authors were unable to establish the existence of a nonzero critical $J_\perp$ with certainty. They also noted that vanadyl pyrophosphate was interesting because it might become a superconductor under hole doping. Dagotto *et al.*[11] note that ladder models are interesting as intermediates between one- and two-dimensional systems, both of which have shown interesting and unusual magnetic and superconducting properties. It is plausible that experimental and theoretical studies of ladders may lead to other interesting physical phenomena.

In this paper we attempt to establish the excitation spectrum of the undoped Heisenberg ladder by applying several analytical and numerical techniques, which are described in Secs. II and III. The most useful analytical approach appears to be a strong coupling expansion about the local "rung Hamiltonian" obtained by setting $J=0$ (discussed in Sec. II A). Even at $O(J^2/J_\perp)$ this approximation gives predictions for the singlet-triplet energy gap and the dispersion relation of the spin-triplet band that are in reasonable agreement with our numerical results for $J_\perp/J \gtrsim 2$. We have also derived spin-wave results for the ladder (in Sec. II B), but these are suspect in light of the erroneous spin-wave prediction of a gapless spectrum for integer-spin chains. Indeed, we find that spin-wave theory fails to reproduce basic qualitative features of the spin-triplet dispersion relation, although the spin-wave ground-state energy per spin is fairly accurate for $J_\perp/J \lesssim 1$.

We have also carried out extensive numerical studies of the Heisenberg spin ladder. We calculated Lanczos energies for the spin-singlet ground state and the spin-triplet excited state on 2×4 to 2×12 clusters, the spin-triplet dispersion relation on a 2×12 cluster, and generated Monte Carlo results for the ground-state energy per spin and singlet-triplet gap on lattices up to 2×32 in extent. The ground-state energy and gap are discussed in Sec. III A, and the spin-triplet dispersion relation is treated in Sec. III B. Our principal conclusion is that a careful analysis of these results supports the presence of a singlet-triplet gap for *all* $J_\perp>0$, which argues against the possibility of a nonzero critical $J_\perp$. The interpolation between the $S=\frac{1}{2}$ chain dispersion relation obtained at $J_\perp=0$ and the strong-coupling limit ($J_\perp\to\infty$) is clearly evident in our results, and involves a folded band of spin excitations. We also present results for the dynamical structure factor $S(k,\omega)$ (in Sec. III C), which is accessible in neutron-scattering experiments. Finally, we conclude in Sec. IV by summarizing these results and by discussing experimental techniques which might be useful in the study of the spin excitations of this system.

II. ANALYTICAL RESULTS

A. Strong-coupling expansion

A straightforward study of the Heisenberg ladder is possible using a strong-coupling expansion. In this technique the two-spin rungs are treated as the unperturbed system

$$H_0 = J_\perp \sum_{\updownarrow} \mathbf{S}_i \cdot \mathbf{S}_j \ , \tag{2}$$

and the interactions along the chains form the perturbing Hamiltonian,

$$H_I = J \sum_{\leftrightarrow} \mathbf{S}_i \cdot \mathbf{S}_j \ . \tag{3}$$

Each two-site rung has a spin-zero ground state with $E_0^{\text{rung}} = -3J_\perp/4$ and a spin-one excited state with $E_1^{\text{rung}} = +J_\perp/4$. Thus in this strong-coupling expansion the ladder is treated as a generalized integer-spin chain in which the rung "sites" have both spin-0 and spin-1 degrees of freedom. The unperturbed strong-coupling ground state is a direct product of spin-0 rung states,

$$|\psi_0(0)\rangle = |[0][0]\cdots[0]\rangle \ , \tag{4}$$

with a zeroth-order energy for a $2\times L$ ladder of $E_0(0) = -\frac{3}{4}J_\perp L$. H_I applied to $|\psi_0(0)\rangle$ of Eq. (4) excites two nearest-neighbor rungs to spin-1 states, with their magnetic quantum numbers correlated to maintain total spin 0. This $O(J/J_\perp)$ correction to $|\psi_0(0)\rangle$ gives to $O(J^2/J_\perp)$ a ground-state energy per spin of

$$\frac{E_0}{2L} = -\frac{3}{8}J_\perp - \frac{3}{16}\frac{J^2}{J_\perp} \ . \tag{5}$$

In contrast, the excited states constitute a degenerate perturbation problem. The unperturbed first excited state in the strong-coupling limit has a single rung promoted to spin 1, and is $3L$-fold degenerate. One such state (with $S_{\text{tot}}=1$ and $S^z_{\text{tot}}=+1$) is

$$|\psi_1(0)\rangle = |[1,+][0]\cdots[0]\rangle \ . \tag{6}$$

H_I has the effect of moving the rung excitation to nearest-neighbor rungs, as well as giving a diagonal contribution. Since the nearest-neighbor excited-rung basis states are degenerate under H_0, the resulting H eigenstates are translational superpositions which are momentum eigenstates. At lowest order in strong coupling these are

$$|\psi_1(k)\rangle = \frac{1}{\sqrt{L}} \sum_{l=1}^{L} e^{ikx_l} |[0][0]\cdots[1,+]\cdots[0]\rangle \ , \tag{7}$$

where the excitation $[1,+]$ is on the lth rung, and the $O(J^2/J_\perp)$ energy we find for this band of spin-triplet excitations is

$$E_1(k) = -\frac{3}{4}J_\perp L + J_\perp + J\cos(k) - \frac{3}{8}\frac{J^2}{J_\perp}(L-2) \ . \tag{8}$$

Subtracting E_0 at this order, we find for the $O(J^2/J_\perp)$ spin-triplet dispersion relation

$$\omega(k) = J_\perp + J\cos(k) + \frac{3}{4}\frac{J^2}{J_\perp} \ . \tag{9}$$

This energy is minimized by $k=\pi$, and thus the gap at $O(J^2/J_\perp)$ is

$$E_{\text{gap}} = \omega(\pi) = J_\perp - J + \frac{3}{4}\frac{J^2}{J_\perp} \ . \tag{10}$$

Note that (at least for $J_\perp \gg J$) the gap is primarily a measure of the rung interaction $J_\perp$, whereas the spin-triplet bandwidth $W=2J$ is determined by the coupling J along the chains. This conclusion remains qualitatively correct even in the $J_\perp=0$ "chain limit"; in that limit the bandwidth monotonically decreases from $2J$ to $(\pi/2)J$, whereas the gap goes to zero with $J_\perp$.

The predicted k dependence of the spin-triplet dispersion relation $\omega(k)=c_0+c_1\cos(k)$ is unusual for an isotropic antiferromagnet, as their antiferromagnetic spin excitations typically have linear-k energies at long wavelengths. However, we shall see that the k^2 behavior only dominates for $J_\perp \gg J$; for $J_\perp$ comparable to J the linear-k coefficient is reduced by the rung interaction, but is not eliminated.

B. Spin-wave theory

The predictions of linear spin-wave theory for the Heisenberg ladder are especially interesting in view of the failure of spin-wave theory (SWT) to predict a gap for integer-spin Heisenberg chains. Applying the standard Holstein-Primakoff transformation to a spin-S ladder with two sublattices leads to the linearized Hamiltonian

$$H^{\mathrm{SWT}}=\sum_k \omega^{\mathrm{SWT}}(k)(\alpha_k^\dagger\alpha_k+\beta_k^\dagger\beta_k)+E_0^{\mathrm{SWT}} , \tag{11}$$

where the ground-state energy per spin is

$$\frac{E_0^{\mathrm{SWT}}}{2L}=(J+J_\perp/2)\left[-S(S+1)+\frac{S}{L}\sum_k \sqrt{1-\Gamma(k)^2}\right] \tag{12}$$

and the dispersion relation is

$$\omega^{\mathrm{SWT}}(k)=(J+J_\perp/2)2S\sqrt{1-\Gamma(k)^2} . \tag{13}$$

The function $\Gamma(k)$ is

$$\Gamma(k)=\frac{J\cos(k_x)+(J_\perp/2)\cos(k_y)}{J+J_\perp/2} , \tag{14}$$

and the sum over k is over the reduced antiferromagnetic Brillouin zone. The full Brillouin zone spans the range $-\pi<k_x\le\pi$ (L values of k_x) and $k_y=0$ and π, and for the reduced zone one may fix $k_y=0$ and sum over the full range of k_x.

The bulk-limit spin-wave result for the ground-state energy per spin involves an integral over k_x,

$$\lim_{L\to\infty}\frac{E_0^{\mathrm{SWT}}}{2L}=-(J+J_\perp/2)\left\{S(S+1)-\frac{S}{\pi}\int_0^\pi \sqrt{1-\Gamma(k_x,0)^2}\,dk_x\right\} . \tag{15}$$

For $S=\frac{1}{2}$ and $J_\perp=0$ we recover the usual spin-wave energy per spin for the chain of $\approx -0.4317J$, rather close to the exact result $-(\ln 2-\frac{1}{4})J\approx -0.4431J$. In the strong-coupling limit $J_\perp \gg J$ the spin-wave result approaches the correct energy $-\frac{3}{8}J_\perp$. However, for moderately large $J_\perp/J$ the spin-wave result departs considerably from the correct energy. For example, at the equal-strength point $J_\perp=J$, spin-wave theory predicts a bulk-limit energy of $E_0^{\mathrm{SWT}}/(2L)=-0.553J$, close to our numerical result (to be discussed) of $E_0/(2L)\approx -0.578J$. However, at the larger value $J_\perp/J=2$ we find $E_0^{\mathrm{SWT}}/(2L)=-0.769J$, far from the correct value of $E_0/(2L)\approx -0.859J$. This behavior is evident in Fig. 1.

The result $\omega(k)^{\mathrm{SWT}}$ in Eq. (13) for the dispersion relation is clearly unphysical; in the limit $J_\perp \gg J$ we must recover a gap of order $J_\perp$, and in contrast spin-wave theory predicts a gapless system for all J and $J_\perp$ [$\omega^{\mathrm{SWT}}(k)$ approaches zero as $k_x\to 0$ for $k_y=0$]. This unphysical result may be visualized more simply by applying spin-wave theory to a single rung. Generalizing to an anisotropic interaction, the single-rung Hamiltonian is

$$H=J_\perp\left[S_1^zS_2^z+\frac{g}{2}(S_1^+S_2^-+S_1^-S_2^+)\right] . \tag{16}$$

Here spin-wave theory predicts a gap for S_z excitations equal to $J_\perp S\sqrt{1-g^2}$ (i.e., zero at the isotropic point), whereas the actual energy gap for S_z excitations (for $S=\frac{1}{2}$) is $(J_\perp/2)(1+g)$, equal to $J_\perp$ at the isotropic point.

It is not surprising that spin-wave theory is more accurate for the ground-state energy than the gap, since it gives a better result for the single rung as well. There we find $E_0^{\mathrm{SWT}}/J_\perp=S\sqrt{1-g^2}-S(S+1)$, which equals the correct $S=\frac{1}{2}$ result at both the Ising and isotropic points. Of course, the spin-wave prediction for the approach to the bulk limit will be an incorrect power law in $1/L$, since it is based on a gapless dispersion relation. We instead anticipate an exponential approach to the bulk-limit ground-state energy, as we find evidence that the system has a gap for all $J_\perp>0$.

III. NUMERICAL RESULTS

A. Ground-state energy and the spin gap

The ground-state energy per spin is interesting as a test of approximate analytic methods, and also because the approach to the bulk limit can be used as evidence of a spin-excitation energy gap. We used a Lanczos technique to determine the ground-state energy per spin as well as the singlet-triplet energy gap on $2\times L$ lattices for $L=4$, 6, 8, 10, and 12. Since the intermediate- and weak-coupling region $0\le J_\perp/J\le 1$ is of greatest interest, we generated results for representative values in this range, specifically $J_\perp/J=0$, 0.2, 0.4, 0.6, 0.8, and 1. We also studied several large $J_\perp/J$ values to test strong-coupling perturbation theory. Our Lanczos results for the ground-state energy and the gap are presented in Tables I and II.

TABLE I. Lanczos (Ref. 18) and Monte Carlo results for the ground-state energy per spin ($E_0/2LJ$) of the $2\times L$ Heisenberg ladder.

L \ $J_\perp/J$	0.0	0.2	0.4	0.6	0.8	1.0
4	−0.500 000	−0.503 782	−0.515 856	−0.536 654	−0.565 808	−0.602 511
6	−0.467 133	−0.472 005	−0.487 058	−0.511 605	−0.544 412	−0.584 437
8	−0.456 387	−0.462 023	−0.478 718	−0.504 825	−0.538 967	−0.580 203
	−0.456 3(1)	−0.462 3(2)	−0.479 0(1)	−0.504 7(1)	−0.539 0(1)	−0.580 0(2)
10	−0.451 545	−0.457 740	−0.475 373	−0.502 232	−0.537 031	−0.578 860
12	−0.448 949	−0.455 583	−0.473 761	−0.501 045	−0.536 229	−0.578 375
24	−0.444 584					
	−0.444 7(2)	−0.452 6(2)	−0.471 9(2)	−0.499 5(2)	−0.535 4(2)	−0.578 1(2)
32			−0.472 6(4)	−0.500 1(2)	−0.535 7(1)	−0.578 4(2)
∞	−0.443 147					
	−0.443	−0.453	−0.472	−0.500	−0.535	−0.578

As the bulk-limit behavior of the gap for $J_\perp/J \leq 0.5$ is not clear from these results, we also used a Monte Carlo technique to generate energies for larger clusters. We applied the guided-random-walk (GRW) algorithm (see Ref. 12, and references cited in Ref. 7) to the Heisenberg ladder on the 2×24 cluster at the $J_\perp/J$ values given above, as well as checking for consistency on smaller clusters and confirming stability with a few tests on the 2×32 lattice. For importance sampling we used a simple $\exp(-\xi V_{\text{Ising}})$ guiding wave function, with the optimum ξ determined numerically to be $\xi \approx 0.89 - 0.26 J_\perp/J$ over this range. A Euclidean-time resolution of $h_\tau = 0.05/L$ was used, and the measurements of E_0 or E_1 tabulated here usually represent averages over 2^{18} walks. (The exceptions were $L=8$, 8×10^4 walks, and $L=32$, 3.2×10^5 walks.) The initial state was taken to be a Néel state, with a single flipped spin for the spin-triplet states. To test convergence of our results we extracted energies for a range of measurement times τ_1 (with $\tau_2 = \tau_1 + 1$), and found convergence to near the quoted statistical accuracy by $\tau_1 = 6$ except for the case $J_\perp/J = 0.2$ on the $L=24$ lattice, which had the smallest gap. (The definitions of these algorithm parameters are given in Refs. 7 and 12.) Our Monte Carlo energies with statistical errors are presented in Tables I and II.

To extrapolate these energies to the bulk limit we require an ansatz for the asymptotic finite-size dependence. We used the form

$$f(L) = f(\infty) + c_0 \frac{e^{-L/L_0}}{L^p} , \tag{17}$$

which incorporates a power law in L times an exponential, to allow for the presence of a gap. We fitted our Lanczos data sets in the tables to this function, with a power $p=1$ for E_{gap} and $p=2$ for $E_0/2LJ$ (motivated by $S=\frac{1}{2}$ chain results). This proved to give a useful description of our numerical results, even for the smallest (2×4) lattice. The fitted bulk limit values are given in Tables I and II, and are shown in Figs. 1 and 2 as well. The two parameters in (17) were found to be $c_0 \approx 3.8$ and $L_0 \approx 4J/J_\perp$.

The ground-state energy per spin, shown in Table I and Fig. 1, shows quadratic dependence $\propto J_\perp^2/J$ for small $J_\perp/J$. The first-order correction to the energy of the chains ($\propto J_\perp$) is zero because the transverse matrix elements vanish trivially, and from isotropy the Ising terms must vanish as well. In principle the coefficient of $J_\perp^2/J$ could be calculated in second-order perturbation theory in the "rung Hamiltonian" Eq. (2), but this would be a difficult problem involving a sum over matrix elements to excited chain states with arbitrarily high spin. Although

TABLE II. Lanczos (Ref. 18) and Monte Carlo results for the singlet-triplet energy gap $[E_1(k_x=\pi) - E_0]/J$ on the $2\times L$ Heisenberg ladder.

L \ $J_\perp/J$	0	0.2	0.4	0.6	0.8	1.0
4	1.000 000	0.884 574	0.809 103	0.775 491	0.780 783	0.820 089
6	0.684 790	0.568 341	0.515 473	0.515 531	0.555 218	0.626 570
8	0.522 680	0.411 971	0.382 605	0.406 755	0.467 232	0.557 398
	0.526(3)	0.417(3)	0.385(3)	0.402(2)	0.467(3)	0.555(4)
10	0.423 238	0.320 667	0.310 876	0.351 259	0.425 567	0.528 106
12	0.355 848	0.262 569	0.267 717	0.319 647	0.404 006	0.514 999
24	0.182 721					
	0.19(1)	0.17(2)	0.21(1)	0.29(1)	0.39(1)	0.51(1)
32			0.20(3)	0.28(2)	0.37(1)	0.51(2)
∞	0.000 000					
	0.03(3)	0.07(3)	0.18(2)	0.28(2)	0.38(1)	0.50(1)

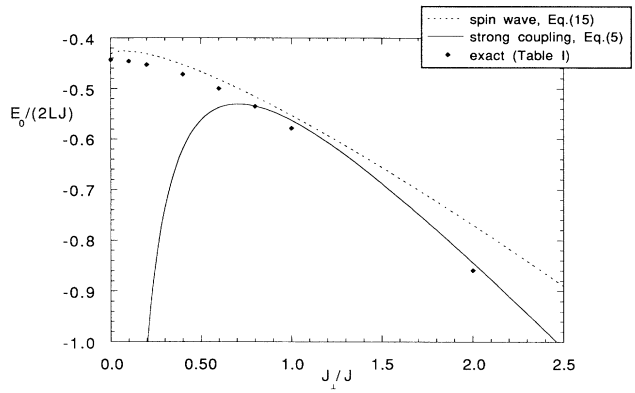

FIG. 1. The ground-state energy per spin from spin-wave theory [Eq. (15)], strong-coupling expansion [Eq. (5)], and numerical results (Table I).

spin-wave theory follows the true ground-state energy qualitatively for $J_\perp/J<1$ (see Fig. 1), there are discrepancies in detail. For example, spin-wave theory predicts a linear term in $J_\perp/J$, which is incorrect. At larger $J_\perp/J$ the strong-coupling formula Eq. (5) evidently approaches the numerical result, and is more accurate than spin-wave theory for $J_\perp/J \gtrsim 0.7$. It would be useful to evaluate higher-order terms in the strong-coupling expansion for comparison with the numerical predictions.

Our results for the singlet-triplet gap are shown in Table II and Fig. 2. The bulk-limit extrapolated values follow from Eq. (17) using the Lanczos data, and the errors are subjective estimates based on a comparison with the chain limit and the Monte Carlo results. There is no indication of a critical value $J_\perp(\text{crit})>0$. The existence of a gap for any nonzero ladder interaction is reminiscent of the dimerized spin-$\frac{1}{2}$ chain, which develops a gap in response to any amount of alternation.[9] Several other models are known to have similar qualitative behavior.

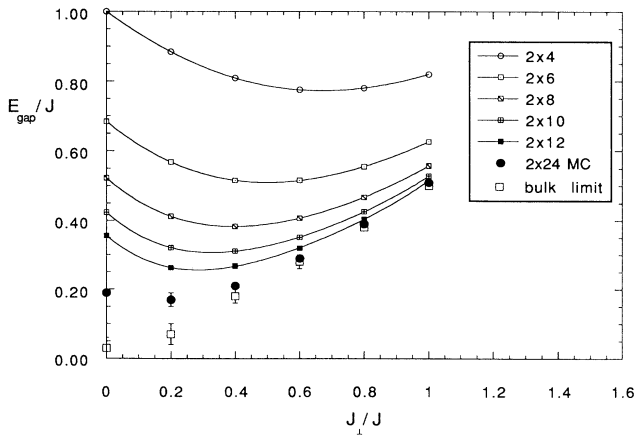

FIG. 2. Numerical results (Table II) for the singlet-triplet energy gap versus $J_\perp$. We show Lanczos results for 2×4 to 2×12 lattices, Monte Carlo results for 2×24, and an extrapolation to the bulk limit. The curves are quartic fits to the Lanczos data.

Examples include the half-filled Kondo lattice in one dimension,[13] which has a gap for all values of the antiferromagnetic coupling; the repulsive Hubbard model in two dimensions at half filling, which has an antiferromagnetic gap for any Hubbard coupling $U/t>0$; and the attractive Hubbard model in two dimensions at half filling, which has a superconductive gap for any attractive coupling. In these Kondo and Hubbard examples the gap depends on the coupling strength through an essential singularity, and is therefore inaccessible to perturbative expansions about the gapless system.

In our numerical results we similarly see evidence that the perturbative (in $J_\perp/J$) singlet-triplet gap has a zero radius of convergence in the bulk limit. If the Lanczos data shown in Fig. 2 are fitted with a polynomial in $J_\perp$, the linear coefficient c_1 in $E_{\text{gap}}\approx c_1 J_\perp + c_2 J_\perp^2/J$ apparently has a finite (negative) bulk limit, but the quadratic coefficient c_2 diverges linearly with L. This singular behavior explains how (E_{gap}/J) as a function of $(J_\perp/J)$ can have a finite negative slope at $J_\perp=0$ for all L (see Fig. 2) and still remain positive for all $J_\perp>0$ in the bulk limit. Unfortunately, our bulk-limit numerical results are not sufficiently accurate to allow us to determine the functional dependence of the gap on $J_\perp$ for small $J_\perp/J$.

In contrast to the ground-state energy, the theoretical techniques we have employed do not give useful results for the gap in the limit of small $J_\perp/J$; the strong-coupling result Eq. (10) is only useful for $J_\perp/J \gtrsim 1$, and spin-wave theory incorrectly predicts a gapless system for all $J_\perp$.

B. Spin-triplet dispersion relation

In our discussion of the strong-coupling limit $J_\perp/J \gg 1$ we found that there is a band of spin-triplet excitations, with an asymptotic bandwidth of $2J$ and a dispersion relation [Eq. (9)] that, surprisingly for an isotropic antiferromagnet, is quadratic in wave number for long wavelengths. This strong-coupling dispersion relation, $\omega(k)=J_\perp + J\cos(k) + \frac{3}{4}J^2/J_\perp$, differs considerably from the exact result for the chain limit $J_\perp=0$,[14]

$$\omega(k)=\frac{\pi}{2}J\sin(k)\ . \tag{18}$$

Despite the different k dependences it is notable that the bandwidth changes only from $(\pi/2)J$ to $2J$ as the rung coupling $J_\perp$ increases from zero to infinity; evidently this bandwidth, if experimentally accessible, could serve as a measure of the in-chain coupling J. For fixed J the spin-wave velocity falls as $J_\perp$ increases, from the chain value of $(\pi/2)J$ at $J_\perp=0$ to zero as $J_\perp\to\infty$.

The form of this triplet band of spin excitations at intermediate $J_\perp/J$ may be seen qualitatively in Fig. 3, which shows Lanczos data from the 2×12 lattice together with the two theoretical bulk limits. The Lanczos data suggests that any $J_\perp>0$ lifts the chain degeneracy of $k_x=0$ and $k_x=\pi$ states, with $k_x=\pi$ becoming the band minimum. This is accompanied by a shift of the wave number k_1 of the highest energy level, from $k_1=\pi/2$ for $J_\perp=0$ to $k_1=0$ in the limit $J_\perp/J\to\infty$. The shape of the spin-triplet band, as opposed to the total bandwidth, is a

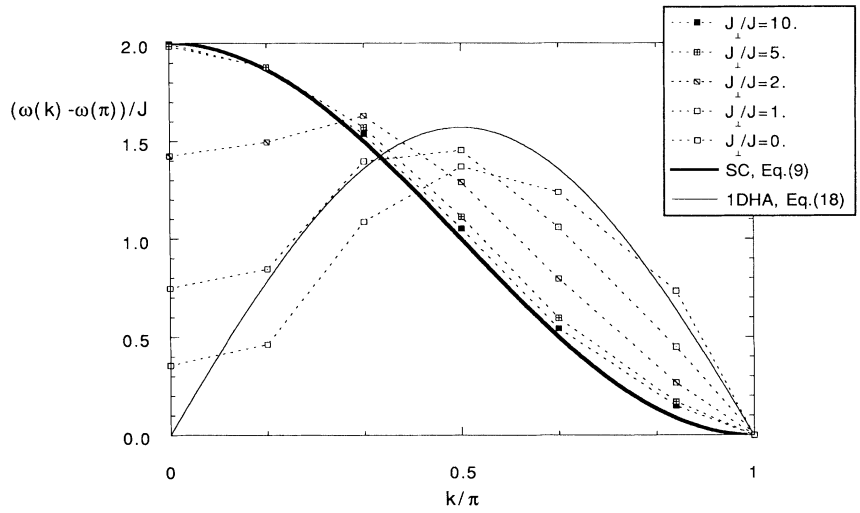

FIG. 3. Energies of spin-triplet excited states relative to the band minimum. We show 2×12 Lanczos results together with the theoretical bulk limit for the one-dimensional chain [Eq. (18)] and the strong-coupling limit [Eq. (9)].

sensitive test of the relative coupling $J_\perp/J$. From Fig. 3 it is clear that strong-coupling theory gives reasonably accurate results for the dispersion relation for $J_\perp/J \gtrsim 5$, but it would be useful to extend these calculations to higher order to clarify the approach to the small-$(J_\perp/J)$ form.

C. Structure factor $S(k,\omega)$

Measurements of the dynamical structure factor $S(k,\omega)$ in neutron scattering experiments have proven to be very useful in the study of Haldane gaps in $S=1$ chains.[15] A similar approach should also be useful in the study of excitations of candidate Heisenberg ladder systems such as $(VO)_2P_2O_7$. The dynamical structure factor is defined by

$$S(k,\omega)=\sum_n |\langle n|S_k^\dagger|0\rangle|^2\delta(\omega-(E_n-E_0)) , \qquad (19)$$

where $|0\rangle$ is the ground state, E_0 the ground-state energy, and $\{|n\rangle\}$ is the set of spin-1 excited states which can be created from the ground state by the Fourier-transformed spin operator $S_k^\dagger$.

Using recently developed Lanczos techniques for the study of dynamical properties of spin and electronic models,[6] we have calculated $S(k,\omega)$ for a 2×8 cluster at several values of $J_\perp/J$. Although this cluster is rather small, our numerical results suggest that the residual finite size effects for $J_\perp/J \geq 2$ are not large, and for smaller $J_\perp$ they at least provide a qualitative picture of the behavior of $S(k,\omega)$ as the interchain coupling $J_\perp$ is decreased. Our results are shown for $k=(\pi,\pi)$ in Fig. 4; this momentum allows excitation of the lowest-lying spin-triplet state, and would be chosen experimentally to determine the singlet-triplet gap. The full band structure can be explored by following the location of the first peak in ω as a function of k.

Notice that the Hamiltonian is symmetric under a reflection with respect to the plane which bisects the rungs. For large $J_\perp$ the ground state obeys this symmetry since each rung comprises a spin singlet which changes sign under the reflection and in our numerical studies we have considered an even number of rungs. The spin triplet contains one triplet which does not change sign under reflection and thus the spin-triplet state is odd. As a result one must employ an operator which is odd in order to excite a spin-triplet state. This may be achieved by staggering $S_k^\dagger$ in the transverse direction and is the reason we choose $k=(\pi,\pi)$.

It is easiest to interpret our results by beginning with the largest value of $J_\perp$. In Fig. 4(f) we show results far into the strong-coupling regime, with $J_\perp=10J$. Here an asymptotic regime has been reached in which the first excitation at $\omega\approx9J$ corresponds to a good approximation to the excitation of one isolated rung from a spin-singlet to a triplet state. The remaining Figs. (4e)–4(a) show results as $J_\perp$ decreases to $5.0J$, $2.0J$, $1.0J$, $0.4J$, and finally $J_\perp=0$. The first peak, corresponding to a single spin-

TABLE III. Lanczos results for energies of the spin-triplet excitations on the 2×12 Heisenberg ladder. $E_1(k_x)/J$ is tabulated.

k_x \ $J_\perp/J$	0	1	2	5	10
0	−10.063 087	−12.619 443	−17.919 331	−39.889 180	−79.422 570
$\pi/6$	−9.956 765	−12.520 234	−17.847 870	−39.996 306	−79.543 654
$\pi/3$	−9.331 725	−11.968 225	−17.711 982	−40.303 395	−79.882 488
$\pi/2$	−9.048 185	−11.912 299	−18.052 517	−40.762 449	−80.366 087
$2\pi/3$	−9.178 838	−12.305 865	−18.545 818	−41.279 251	−80.876 938
$5\pi/6$	−9.685 079	−12.917 365	−19.076 675	−41.706 050	−81.270 789
π	−10.418 934	−13.366 148	−19.342 940	−41.875 333	−81.419 644

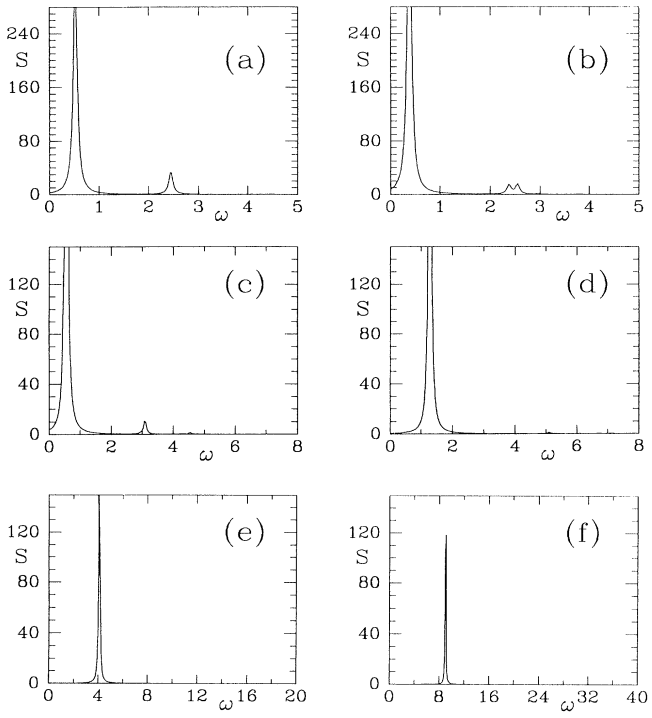

FIG. 4. The dynamical structure factor $S(k_x=\pi,\omega)$ for a 2×8 cluster as a function of frequency ω, at momentum $k_x=\pi$. (a), (b), (c), (d), (e), and (f) are for $J_\perp/J=0.0$, 0.4, 1.0, 2.0, 5.0, and 10.0, respectively. The δ functions appearing in Eq. (19) are regularized with a width of $\varepsilon=0.1J$. The vertical-axis units are arbitrary, but the same units were used in all six cases.

triplet excitation, remains clear in all cases. Note that the offset of the first peak, at $\omega\approx 0.5J$ in Fig. 4(a), is a finite-size artifact; this separation is the singlet-triplet gap, and will approach zero in the bulk limit. Finite size effects should be much less important in Figs. 4(c)–4(f); in Fig. 2 one sees that the singlet-triplet gap on the 2×8 lattice is not far from the bulk limit for $J_\perp \gtrsim J$. It should be possible to determine the values of the model parameters J and $J_\perp$ with some certainty if neutron scattering experiments on candidate materials such as $(VO)_2P_2O_7$ can be used to determine $S(k,\omega)$.

IV. SUMMARY AND CONCLUSIONS

We have used several analytical and numerical techniques to study the ground-state and low-lying excitations of the Heisenberg antiferromagnetic spin ladder. Our results suggest a nonzero energy gap between the spin-singlet ground state and spin-triplet excited states for all cross-ladder couplings $J_\perp > 0$.

The behavior of the gap may be due to the critical point of the one-dimensional Heisenberg chain, which is characterized by power-law spin correlations without long-range order. The absence of a broken symmetry in a gapless system may imply that the model is sensitive to small perturbations such as an infinitesimal $J_\perp$. If the absence of a broken symmetry is indeed the crucial feature of the ladder which allows a gap for all $J_\perp$, we might expect in contrast that two coupled Heisenberg planes would require a nonzero $J_\perp$(crit) to develop a gap, due to the broken rotational symmetry in isolated planes represented by the staggered magnetization. It should be feasible to test this possibility in future investigations through numerical simulations of coupled Heisenberg planes.

The spin-triplet states of the ladder form a band of excitations; the bandwidth is determined primarily by the coupling J along the ladder, whereas the singlet-triplet gap is sensitive to both J and $J_\perp$. The spin-wave velocity for fixed J is suppressed by the interchain coupling $J_\perp$, and in the limit $J_\perp \to \infty$ is reduced to zero. Many of our results for the excitations of the Heisenberg ladder are reminiscent of results for the dimerized chain. These include a gap for any departure from the pure Heisenberg chain limit, and a band of spin-triplet excitations above the gap. The close resemblance of these two systems was noted previously in studies of $Cu(NO_3)_2\cdot\frac{5}{2}H_2O$;[10] both ladder and dimer-chain models were proposed for this material, and their thermodynamic properties were found to be very similar.

The similarity to copper nitrate suggests that the experimental techniques which proved effective in clarifying its magnetic properties should also be useful in the study of vanadyl pyrophosphate. The techniques which allowed the selection of a particular dimerized chain model from several competing chain and ladder models were proton resonance measurements,[16] and more definitively, neutron scattering studies.[17] Thermodynamic measurements in external magnetic fields were also useful in establishing the presence of a gap and in confirming contributions due to the spin-triplet states. In addition to these approaches, a measurement of the spin-triplet dispersion relation in vanadyl pyrophosphate may be possible using inelastic neutron scattering, which would allow a test of the folded band of excitations and the suppressed spin-wave velocity predicted by the ladder model.

ACKNOWLEDGMENTS

We are grateful to J. Cooke, H. Q. Lin, S. H. Liu, G. D. Mahan, and A. Moreo for useful discussions relating to this work. The numerical studies were primarily carried out on a Cray-YMP computer at the Florida State University Computing Center and a VAX-9000 computer at the University of Tennessee Computing Center, and we thank them for their support. We also acknowledge the support of Martin Marietta Energy Systems, Inc., through Oak Ridge National Laboratory Project No. 3210-0427; the Center for Theoretical Physics of the Massachusetts Institute of Technology; the Natural Sciences and Engineering Research Council of Canada; and the United States Department of Energy under Contract Nos. DE-FG05-91ER40627 with the Physics Department of the University of Tennessee and DE-AC05-840R21400 managed by Martin Marietta Energy Systems, Inc.

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