Stability of the Haldane phase in anisotropic magnetic ladders

Örs Legeza
Research Institute for Solid State Physics, P.O. Box 49, H-1525 Budapest, Hungary
and Technical University of Budapest, H-1521 Budapest, Hungary

Jenö Sólyom
Research Institute for Solid State Physics, P.O. Box 49, H-1525 Budapest, Hungary
(Received 18 June 1997)

We have considered the properties of anisotropic two-leg ladder models with $S=1/2$ or $S=1$ spins on the rungs, using White's density-matrix renormalization-group method. We have generalized the method by taking into account the symmetries of the model in order to reduce the dimensions of the matrix to be diagonalized, thereby making it possible to consider more states. The boundaries in the parameter space of the extended region, where the Haldane phase exists, are estimated. [S0163-1829(97)05542-2]

I. INTRODUCTION

The properties of magnetic systems where the localized moments form a ladderlike structure,[1–3] have been intensively studied recently. Most of such materials can be described by an isotropic spin Hamiltonian, therefore the theoretical studies were almost exclusively done on isotropic models.[4–10] The question arises as to what effect the anisotropy might have. The answer to the question is not trivial.

It is known that two-leg ladder models with $S=1/2$ spins on both legs behave basically like an $S=1$ spin model if the rung coupling between the spins on the two legs is strong enough. It is also known that integer and half-odd integer spin models have essentially different phase diagrams, when considered as a function of the anisotropy of the exchange. Beside the ferromagnetic, antiferromagnetic, and planar phases an additional phase, the Haldane phase[11] appears for a finite range of anisotropy. Our aim in this paper is to study, how this phase appears in anisotropic ladder models for intermediate values of the interchain couplings.

For this purpose we have determined the low-lying part of the energy spectrum of an anisotropic Heisenberg ladder model by using the density-matrix renormalization-group (DMRG) method proposed recently by White.[12] We have generalized the method in such a way that together with any spin configuration that is kept after the truncation of the Hilbert space, the other configurations related to it by the symmetries of the ladder model are also automatically taken into account. This allows us to consider more states without increasing the size of the matrices and thereby to improve the accuracy.

The layout of the paper is as follows. In Sec. II we give a short description of the ladder model and show what phase diagrams are expected, if the value of the spins on the legs is $S=1/2$ or $S=1$. The symmetry considerations introduced in the application of the DMRG procedure are briefly discussed in Sec. III. Section IV presents the numerical results. Finally Sec. V contains a brief discussion of the results.

II. LADDER MODELS AND THEIR EXPECTED PHASE DIAGRAM

In a two-leg ladder model the spins at rung i will be denoted by σ_i and τ_i. The length of the spin can be arbitrary. In most of the calculations we will take $S=1/2$ spins, but a comparison with the $S=1$ case will also be considered.

When the coupling between the legs is neglected, the Hamiltonian of two decoupled anisotropic Heisenberg chains is recovered. It can be written in the form

$$\mathcal{H}_0=\sum_i \left[\frac{1}{2}J_{xy}(\sigma_i^+\sigma_{i+1}^- + \sigma_i^-\sigma_{i+1}^+) + J_z\sigma_i^z\sigma_{i+1}^z\right] + \sum_i \left[\frac{1}{2}J_{xy}(\tau_i^+\tau_{i+1}^- + \tau_i^-\tau_{i+1}^+) + J_z\tau_i^z\tau_{i+1}^z\right]. \quad (1)$$

The xy part of the exchange is written in terms of the raising and lowering operators, and its coupling is allowed to differ from that of the zz part.

Introducing now the couplings between the chains, different kinds of ladder models can be constructed depending of the choice of this coupling. Usually this coupling is assumed to act between spins on the same rung only. In an anisotropic model this would mean a coupling of the form

$$\mathcal{H}_1=\sum_i \left[\frac{1}{2}J'_{xy}(\sigma_i^+\tau_i^- + \sigma_i^-\tau_i^+) + J'_z\sigma_i^z\tau_i^z\right]. \quad (2)$$

In the limit when this coupling is ferromagnetic and strong, the two spins on the same rung couple into a single larger spin. That is the reason why a spin-1/2 ladder can behave like a spin-1 chain, or a spin-1 ladder like a spin-2 chain.

Assuming that the diagonally situated nearest-neighbor spins are also coupled, it was shown[13] that this coupling makes the hidden topological long-range order characteristic for the Haldane phase even stronger.

An alternative way to introduce interchain coupling is to choose the following form for the interaction:

$$\mathcal{H}_1=\sum_i \left[\frac{1}{2}J'_{xy}(\sigma_i^+\tau_{i+1}^- + \sigma_i^-\tau_{i+1}^+) + J'_z\sigma_i^z\tau_{i+1}^z\right] + \sum_i \left[\frac{1}{2}J'_{xy}(\tau_i^+\sigma_{i+1}^- + \tau_i^-\sigma_{i+1}^+) + J'_z\tau_i^z\sigma_{i+1}^z\right]. \quad (3)$$

In this paper we look at the properties of the model defined by Eqs. (1) and (3). In a special case this is equivalent to one of the models studied by White,[13] but we will consider a larger parameter space, although the anisotropy ratio will be taken to be the same for the intrachain and interchain couplings

$$J_z/J_{xy}=J'_z/J'_{xy}, \quad (4)$$

and therefore a single parameter

$$\lambda=\frac{J'_{xy}}{J_{xy}}=\frac{J'_z}{J_z} \quad (5)$$

will be used to characterize the strength of the interchain couplings.

An interesting feature of our model is that by interchanging the spins between the two legs on every even or odd site, the intrachain and interchain couplings change their role. At $\lambda=1$, where the intrachain and interchain couplings are equal, the model is transformed into itself. For other values of λ, the energy scale has to be changed. Taking this into account, we find that for $\lambda>0$ all energy levels satisfy a simple self-duality relationship[14]

$$E(\lambda)=\lambda E(1/\lambda). \quad (6)$$

This allows us to connect the weak- and strong-coupling limits of the model. For $\lambda<0$ the model would include ferromagnetic and antiferromagnetic interchain couplings, which requires the modification[15] of Eq. (6).

The self-dual $\lambda=1$ point plays a special role in other respects as well. At this point, with our choice of the couplings, the Hamiltonian of a single chain with composite spin is recovered

$$\mathcal{H}=\sum_i [J_{xy}(S_i^xS_{i+1}^x+S_i^yS_{i+1}^y)+J_zS_i^zS_{i+1}^z], \quad (7)$$

where $\vec{S}_i=\vec{\sigma}_i+\vec{\tau}_i$. It is obvious that if both σ and τ are spin-1/2 operators, this model is not a true $S=1$ Heisenberg model, since the two spins can form not only the triplet, but also the singlet combination. It has been shown,[14] however, that the low-lying levels of the Hamiltonian in Eq. (7) and that of the true $S=1$ Heisenberg model are identical, and therefore they have the same phase diagram.

The phase diagram expected for the model in the plane spanned by the anisotropy, J_z/J_{xy} and λ, is shown schematically in Fig. 1. In drawing the phase boundaries we have taken into account that the ferromagnetic phase appears for $J_z/J_{xy}\geq 1$, independently of λ. On the other hand, the boundary between the Haldane and antiferromagnetic phases is expected to depend on λ. At $\lambda=0$ the ladder model consists of two decoupled spin-1/2 chains, and therefore the Haldane phase does not exist. At $\lambda=1$, according to previous finite-size calculations[16–19] on the equivalent $S=1$ chain, the massive Haldane phase exists in a finite range of anisotropy. The numbers obtained for the critical values of the anisotropy are somewhat different in the different calculations, but the best estimates give the range

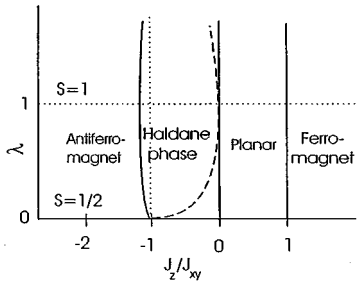

FIG. 1. Schematic phase diagram of the $S=1/2$ ladder model in the $(\lambda, J_z/J_{xy})$ plane. The dashed line shows an alternative phase boundary between the Haldane and planar phases, as discussed in the text.

$$-1.18<J_z/J_{xy}<0. \quad (8)$$

The value of the critical anisotropy, $(J_z/J_{xy})_{c1}\simeq -1.18$, where the transition from the Haldane phase with singlet ground state to the doubly degenerate antiferromagnetic state occurs, is not determined by any symmetry. It is an Ising-type transition. Close to it, on both sides of the transition point, the gap opens linearly.

It follows from the duality relationship for the energy levels that if λ_c is a critical point, then $1/\lambda_c$ should also be a critical coupling. The phase boundary of the antiferromagnetic phase should therefore start from $(J_z/J_{xy})_{c1}=-1$ at $\lambda=0$, returning to this value when $\lambda\to\infty$, and passing through $(J_z/J_{xy})_{c1}\simeq -1.18$ at $\lambda=1$.

Looking at the boundary between the Haldane and planar phases, the massive phase appears from the critical planar phase via a Kosterlitz-Thouless-type transition. In the continuum limit of the $S=1$ chain the value $(J_z/J_{xy})_{c2}=0$ is obtained[20] for the critical anisotropy. This particular value suggests that it is determined by a hidden symmetry of the model, and therefore it is expected that this same critical value could be found in the $S=1/2$ spin-ladder model at any λ. This would mean that for $-1\leq J_z/J_{xy}<0$ the interchain coupling is a relevant perturbation. An arbitrarily small coupling will already generate a Haldane gap. The corresponding phase boundary is shown in Fig. 1 by a vertical straight line at $J_z/J_{xy}=0$.

This natural assumption becomes questionable, however, if we compare this phase diagram with that of the spin-1 ladder. Based on similar considerations we can argue that at $\lambda=0$ the behavior is that of two decoupled spin-1 chains, while at $\lambda=1$ the properties of the spin-2 Heisenberg model should be recovered. Since both are integer spin models, the Haldane phase exists in both cases in an extended range of anisotropy around the isotropic antiferromagnetic point. In the spin-2 model this range is, however, much narrower[21] than in the spin-1 case, so clearly the boundaries of the Haldane phase to both the planar and the antiferromagnetic phases should strongly depend on the interchain coupling, as shown in Fig. 2.

Moreover the value of the Haldane gap is much smaller in the $S=2$ spin chain than for $S=1$. This is known reliably for

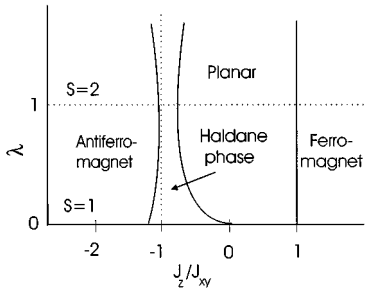

FIG. 2. Schematic phase diagram of the $S=1$ ladder model in the $(\lambda, J_z/J_{xy})$ plane.

the isotropic antiferromagnetic model only,[12,22] but should be true in the anisotropic case as well. We show schematically in Fig. 3 how the antiferromagnetic and Haldane gaps depend on the anisotropy for the spin-1/2, spin-1, and spin-2 Heisenberg models. In all cases the antiferromagnetic state has a doubly degenerate ground state with a finite energy gap to the spin-wave excitations. For $S=1/2$ the transition into this state is of Kosterlitz-Thouless type, and the gap opens exponentially slowly. For spin-1 and spin-2 chains the transition from the Haldane phase is of second order, so the gap opens linearly on both sides. The vanishing of the Haldane gap at $(J_z/J_{xy})_{c2}$ happens again in a Kosterlitz-Thouless-like manner.

By coupling now two spin-1 chains into a spin-1 ladder, the effect of the interchain coupling is expected to be opposite to that discussed above. The Haldane gap decreases or it might even vanish when this coupling is switched on. This raises the question whether in the spin-1/2 ladder model the

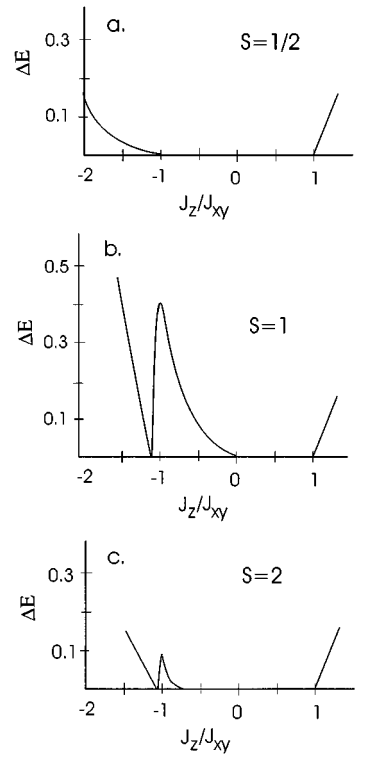

FIG. 3. The energy gap of the $S=1/2,1$, and 2 Heisenberg chains as a function of the anisotropy J_z/J_{xy}.

interchain coupling is in fact a relevant perturbation for $-1 \leqslant J_z/J_{xy} < 0$, and perhaps the phase boundary between the Haldane and planar phases does not go in the way discussed above. An alternative possibility is shown in Fig. 1 by a dashed line.

III. NUMERICAL PROCEDURE

In this paper we try to elucidate this problem by looking at the degeneracy of the ground state and the generation or disappearance of gaps when the interchain couplings are switched on. In order to do this we have applied the DMRG method[12] to the model defined by Eqs. (1) and (3) using the anisotropy J_z/J_{xy} and the relative strength of the interchain coupling, λ as the two parameters.

It has been found earlier in various applications that the DMRG method gives better results for systems with open boundary condition (OBC) than for periodic boundary condition (PBC). On the other hand, when OBC is used, the free spins remaining at the ends in the valence-bond-like state of the ladder model introduce extra energy-level degeneracies, and therefore the analysis of the spectrum becomes somewhat more difficult. In that region of the couplings, where the gap is very small, in order to get more accurate results, we have used OBC, otherwise we have done calculations with both boundary conditions.

The major limiting factor in the application of the DMRG method is that only a subset of all possible states is kept, and the eigenvalue matrix is diagonalized in this subspace only. The accuracy can be improved, if first the Hilbert space is block diagonalized by taking into account the natural symmetries of the Hamiltonian, and the DMRG procedure is applied to the blocks separately, considering the same fixed number of states in each block. When using OBC, translational symmetry is lost, so the total momentum is not a good quantum number. In the anisotropic model we also lose the SU(2) symmetry. Therefore only the z component of the total spin, S_T^z can be used to classify the energy levels.

It is easily seen that the ladder model Hamiltonian has two further symmetries, two mirror planes that are perpendicular to the plane of the ladder. One goes across the middle of the rungs of the ladder. It transforms the σ and τ spins into each other (σ-τ symmetry). The other cuts the legs of the ladder in the middle, reflecting the spins on the left onto spins on the right (left-right symmetry). Moreover, the $S_T^z=0$ subspace, which will be of particular interest for us, has an additional symmetry, the spin reversal or up-down symmetry. The corresponding operators will be denoted as $\mathcal{P}_{\sigma-\tau}$, $\mathcal{P}_{l-r}$, and $\mathcal{P}_{\uparrow\downarrow}$. The eigenstates of the system can be either symmetric or antisymmetric under these operations. An even-parity state will be labeled by $+$, while an odd-parity state by $-$.

It is advantageous to include these symmetries in the DMRG procedure by choosing wave functions that are eigenstates of the parity operators. Using the notation of White,[23] the superblock wave function $\psi(\alpha_l s_{l+1} s_{l+2} \beta_{l+3})$ is formed out of the states α_l and β_{l+3} of the two blocks and the states s_{l+1} and s_{l+2} of the two added spins,

$$|\psi_{\pm}\rangle = \sum_{\substack{\alpha_l s_{l+1} \\ s_{l+2}\beta_{l+3}}} A_{\alpha_l s_{l+1} s_{l+2} \beta_{l+3}} \{\psi(\alpha_l s_{l+1} s_{l+2} \beta_{l+3}) \pm \mathcal{P}\psi(\alpha_l s_{l+1} s_{l+2} \beta_{l+3})\}. \quad (9)$$

$A_{\alpha_l s_{l+1} s_{l+2} \beta_{l+3}}$ is a normalization constant which takes the value 1/2 or $1/\sqrt{2}$, depending on whether the state obtained by the symmetry operation is identical with the original one or not.

The σ-τ and spin-reversal operations are products of local operators that act on the spin states of a single rung, so they can be used even if the left and right blocks are not of equal length. The four states $|\downarrow\downarrow\rangle$, $|\downarrow\uparrow\rangle$, $|\uparrow\downarrow\rangle$, and $|\uparrow\uparrow\rangle$ of the σ and τ spins on the same rung span a basis on which

$$\mathcal{P}^1_{\sigma-\tau} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad \mathcal{P}^1_{\uparrow\downarrow} = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}. \quad (10)$$

In each iteration cycle of building larger blocks the operators are renormalized as $P^{l+1} = OP^l O^\dagger$ and they are stored with the other block operators. The O matrix contains the new truncated basis states of the subsequent iteration cycles. A local operator acting on a block state gives

$$P^l|\alpha_l\rangle = a_{\alpha_l}|\alpha_l'\rangle, \quad (11)$$

where the coefficient a_{α_l} is 1 or -1 for the symmetric or antisymmetric combination, respectively.

In the first step of the infinite algorithm, when the block consists of the states of a single rung, $|\alpha_1\rangle = |s_{l+1}\rangle$ and $a_{\alpha_l} = 1$. The iterated matrix P^{l+1} has one element in each row and that value gives a_{l+1}. Therefore, the local symmetries simply give

$$\mathcal{P}^l_{\text{local}}\psi(\alpha_l s_{l+1} s_{l+2} \beta_{l+3}) = a_{\alpha_l} a_{\beta_{l+3}} \psi(\alpha_l' s_{l+1}' s_{l+2}' \beta_{l+3}'). \quad (12)$$

On the other hand, the operator $\mathcal{P}^l_{l-r}$ mixes the states of different rungs and can be used only when the two blocks are of equal length. When acting on a superblock wave function, it gives

$$\mathcal{P}^l_{l-r}\psi(\alpha_l s_{l+1} s_{l+2} \beta_{l+3}) = \psi(\beta_{l+3} s_{l+2} s_{l+1} \alpha_l). \quad (13)$$

The total parity of the wave function is the product of the left-right, $\uparrow\downarrow$ and σ-τ parities. In what follows, unless otherwise specified, only the total parity will be given. It is worth mentioning that if several symmetries are used, the factor $A_{\alpha_l s_{l+1} s_{l+2} \beta_{l+3}}$ has to be included for each symmetry. This ensures that every configuration is taken into account only once.

All these symmetry operations reduce the size of the Hilbert space of the superblock Hamiltonian by a factor of about 2. This decreases the memory requirements and allows us to keep more spin configurations, which improves the accuracy of the DMRG method. The local symmetries can be included into both the infinite- and finite-system algorithms. The left-right symmetry can be used in the infinite-system method only, but by keeping more states it would produce better starting vectors[23] for the diagonalization procedure in the finite-system method.

Using these symmetry considerations the Hilbert space is split into subspaces characterized by the z component of the total spin and the parity. In order to obtain the ground state and some low-lying states of the ladder, in principle, one has to determine a few low-lying eigenstates of all subspaces. For a finite chain with N sites the nth energy level of the $S^z_T = s$ sector with parity p will be denoted by $E_{s,n,p}(N)$. Similarly the energy gap between the states with energies $E_{s',n',p'}$ and $E_{s,n,p}$ will be denoted by $\Delta_{s,n,p;s',n',p'}(N)$.

Except for the ferromagnetic regime, in the spin-1/2 chain the lowest-lying energy level belongs to the $S^z_T = 0$ sector and it has odd parity under left-right and spin reflection symmetries for $N \bmod 4 = 0$, while it has even parity for chains with $N \bmod 4 = 2$. The parity of the first excited state is opposite to that of the ground state and the parity changes for every higher lying level. Therefore, in the infinite-lattice algorithm of the DMRG method the parity has to be changed in every iteration cycle.

This difficulty does not arise either in the spin-1 chain or in the ladder models. In the spin-1 chain the ground state was found to be in the $S^z_T = 0$ sector with even parity under left-right reflection for all chain lengths N. In the ladder model beside the left to right reflection we also have the σ-τ symmetry. The ground state of this model has positive parity under both reflections for all non-negative values of λ. The excited states also preserve their parity as a function of λ. Therefore in this case the same symmetry combination has to be used in every successive step of the DMRG algorithm.

Because the energy gaps are expected to be rather small close to the phase boundaries, we have used the finite-lattice method version of the DMRG with two or three iteration cycles. We calculated the energy gaps for ladders with $N = 16,32,48,64,82,100,128$ sites, and used a finite-size scaling procedure to extrapolate to infinite system. Due to our restricted computational facility the number of states M representing the block in the DMRG method could be chosen between $M = 100$ and 200 states. The truncation error was the worst close to the critical points. For the second and higher excited states it was about $10^{-6} - 10^{-7}$, corresponding to a real error of about 10^{-3}.

Several formulas have been proposed to extrapolate the finite-size results to the thermodynamic limit. When a finite gap is expected, the $N \to \infty$ limit of the gap can be obtained by fitting the energy difference of the various $E_{s,n,p}$ energy levels to the form[4] $\Delta(N) = \Delta + A\exp(-N/\xi)$. On the other hand, for open systems, where the finite-size effects are more pronounced, the form[22] $\Delta(N) = \Delta + A/N$ or an inverse squared dependence[24] $\Delta(N) = \Delta + A/N^2$ should be used. The former one is known to give a lower-bound estimate of the gap.

In most cases we have used the formulas with $1/N$ or $1/N^2$. The exponential dependence was assumed when neither the N^{-1} nor the N^{-2} fit gave satisfactory result.

IV. NUMERICAL RESULTS

In this section we present the results of our numerical calculations. Since the gaps are expected to be rather small,

resulting in relatively large errors in the extrapolation to infinite systems, we are not able to locate exactly the phase boundaries, where the gaps vanish. We will therefore restrict ourselves to a qualitative check of how the phase diagram may look.

Because nothing particularly interesting is expected on the $J_z/J_{xy}>0$ side, the system is ferromagnetic if $J_z/J_{xy}>1$ and planar if $0<J_z/J_{xy}<1$ independently of λ, in what follows we will consider the $J_z/J_{xy}<0$ region only. We have chosen four different values of the anisotropy, namely $J_z/J_{xy}=-2,-1.1,-0.8,-0.5$ and varied λ from 0 to 1, to see how the character of the ground state changes. The energies will always be measured in units of J_{xy}.

A. The $\lambda=0$ and $\lambda=1$ lines

As mentioned above, at $\lambda=0$ the properties of two decoupled spin-1/2 chains should be recovered, while at $\lambda=1$ at least the low-energy part of the spectrum is identical to that of the spin-1 chain. Our calculations along these lines aimed to test the accuracy of the method and to find the relevant subspaces of the Hilbert space.

Let us consider first the case $\lambda=0$. When $J_z/J_{xy}<-1$, the antiferromagnetic chains give a 2×2-fold degenerate ground state in the $S_T^z=0$ subspace. Accordingly the gap $\Delta_{02-,01+}$ and two other gaps in the $S_T^z=0$ sector should go to zero in the limit $N\to\infty$. In fact our calculation gives an extrapolated value of the order of 10^{-3}. This shows the real accuracy of the numerical calculations.

The next levels above this fourfold degenerate ground state have one or two spins flipped. The corresponding gaps, $\Delta_{11-,01+}$ and $\Delta_{21+,01+}$ were found to be finite, opening slowly as the anisotropy increases. Above this gap a continuum of states is found as shown by the vanishing of the gap $\Delta_{12+,11-}$.

In the planar phase all these gaps should vanish. In fact in the range $-1<J_z/J_{xy}<0$ the gaps $\Delta_{11-,01+}$ and $\Delta_{21+,01+}$ were found to be of the order of 10^{-3}, which we consider to be zero.

Along the line $\lambda=1$ the antiferromagnetic phase appears for $J_z/J_{xy}<-1.18$. The twofold degeneracy of the ground state is in fact recovered, since the gap $\Delta_{02-,01+}$ scales to values of the order of 10^{-3}. The antiferromagnetic gap $\Delta_{11-,01+}$ remains finite.

In the Haldane phase, $-1.18<J_z/J_{xy}<0$, we have again a fourfold degenerate ground state, if the ladder has free ends, but here the gaps $\Delta_{02-,01+}$ and $\Delta_{11-,01+}$ should scale to zero exponentially. The values obtained for the gap are of the order of 10^{-4}. The next levels above them are E_{21+} and E_{12+}, which cross each other at $J_z/J_{xy}=-1$. Therefore the real gap above the ground state is $\Delta_{21+,01+}$ for $J_z/J_{xy}>-1$, while it is $\Delta_{12+,01+}$ for $J_z/J_{xy}<-1$. This gap was found to be 0.147(1), 0.4105(3), 0.223(1), 0.096(3) for $J_z/J_{xy}=-1.1,-1,-0.8,-0.5$. Our result at $J_z/J_{xy}=-1$ agrees quite well with the best estimate[12] for the Haldane gap of the isotropic $S=1$ model.

B. The antiferromagnetic regime

Taking now intermediate values for λ, we consider first the transition from the Haldane phase to the antiferromagnetic phase for $J_z/J_{xy}<-1$. Since the phase boundary is not determined by any symmetry, it is expected that for $-1.18<J_z/J_{xy}<-1$ the antiferromagnetic gap, $\Delta_{11-,01+}$ which is finite at $\lambda=0$, should vanish for a finite λ_c, and then for larger λ the Haldane gap $\Delta_{12+,01+}$ should open up. Since the values of the gaps are very small, it is difficult to determine accurately the value λ_c, where this happens.

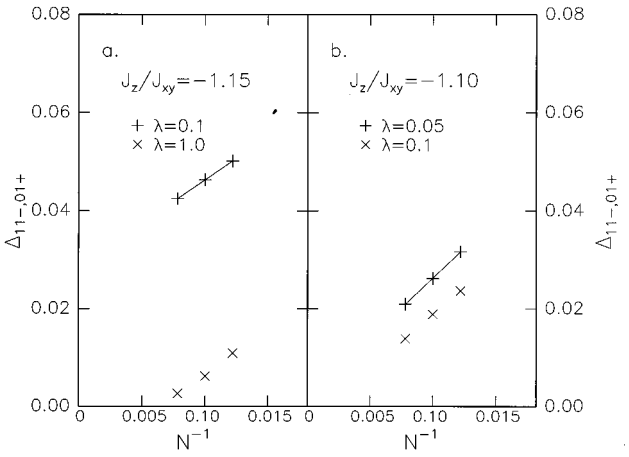

FIG. 4. The antiferromagnetic gap $\Delta_{11-,01+}$ as a function of N^{-1} at (a) $J_z/J_{xy}=-1.15$, $\lambda=0.1$ and $\lambda=1$ and (b) $J_z/J_{xy}=-1.1$, $\lambda=0.05$, and $\lambda=0.1$.

As a first attempt, we have investigated the closing of the antiferromagnetic and the opening of the Haldane gap as a function of λ at $J_z/J_{xy}=-1.1$. The thermodynamic limit of the Haldane gap could be determined very well using the N^{-2} dependence for $\lambda>0.1$. In this region this gap is finite. At the same time the antiferromagnetic gap is found to vanish. For $\lambda\leqslant0.1$, however, no reliable extrapolation procedure was found and therefore we can only claim that the transition from the antiferromagnetic to the Haldane phase occurs at a very small value of λ, between $\lambda=0$ and $\lambda=0.05$. This indicates that due to the smallness of the antiferromagnetic gap of the spin-1/2 chain a very small, although finite, interchain coupling is sufficient to drive the system into the Haldane phase. This means that the phase boundary starts from the $J_z/J_{xy}=-1$, $\lambda=0$ point with an almost horizontal slope.

Taking a somewhat larger anisotropy, $J_z/J_{xy}=-1.15$, the antiferromagnetic state survives to a larger value of λ, as shown in Fig. 4. The lower bound estimate of the gap $\Delta_{11-,01+}$ at $\lambda=0.1$ is 0.030(3). This point, therefore, belongs to the antiferromagnetic phase. Moving up in the phase diagram with λ to $J_z/J_{xy}=-1.15$, $\lambda=1$ or to the right to the point $J_z/J_{xy}=-1.1$, $\lambda=0.1$, this same antiferromagnetic gap clearly scales to zero, indicating that these points are already in the Haldane phase. The phase boundary should therefore have the shape indicated in Fig. 1.

C. The planar phase

Next we considered the stability of the planar phase in the $-1<J_z/J_{xy}<0$ regime. We have measured the gap $\Delta_{21+,01+}$, which should vanish at $\lambda=0$, as a function of λ for several values of the anisotropy.

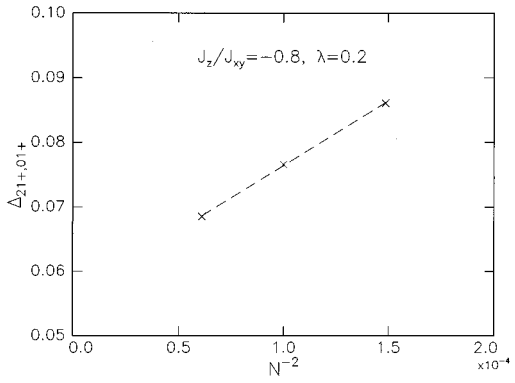

FIG. 5. The energy gap $\Delta_{21+,01+}$ as a function of N^{-2} at $\lambda=0.2$, $J_z/J_{xy}=-0.8$.

The accuracy of our calculations was checked by comparing the energy values calculated for $\lambda<1$ and $\lambda>1$, using the self-duality relationship of Eq. (6). We have got the same energies to at least 6 or 8 digits. We show in Fig. 5 the results obtained for $J_z/J_{xy}=-0.8$. At $\lambda=0$ the gap scales to $0.008(2)$ as $1/N$. At $\lambda=0.2$ an excellent fit can be obtained by the $1/N^2$ fit for $N=128,100,82$. The extrapolated gap was found to be $0.057(2)$.

The finite-size scaling procedure is not that clear for $\lambda=0.1$. Neither a $1/N$ nor a $1/N^2$ fit is satisfactory. This indicates that the available chain lengths are still not long enough to determine Δ accurately. The estimated value of the gap is between $0.025(3)$ and $0.035(3)$. Comparing this with the gap at $\lambda=0.2$, we could conclude that in the thermodynamic limit the gap opens linearly with $\lambda_c=0$, in the same way[15] as for $J_z/J_{xy}=-1$.

For J_z/J_{xy} closer to zero, the Haldane gap is too small even at $\lambda=1$. At $J_z/J_{xy}=-0.5$ the extrapolated value of the gap is about $0.096(3)$. For small values of λ of the order of 0.1 the error of the DMRG method becomes comparable to the value of the gap and no reliable extrapolation procedure was found. The results are, however, in agreement with the assumption that $\lambda_c=0$.

These results indicate that the interchain coupling is relevant in the whole $-1\leqslant J_z/J_{xy}<0$ region. An arbitrarily weak interchain coupling of this type would drive the spin-1/2 ladder into the Haldane phase.

D. The spin-1 ladder model

The spin-1 ladder model is constructed in the same way as the spin-1/2 model except that the σ_i and τ_i operators in Eq. (1) and (3) are now spin-1 operators. In the $\lambda=0$ limit, which in this case corresponds to two decoupled spin-1 chains, the Haldane phase exists for a wide range of anisotropy, namely for $-1.18<J_z/J_{xy}<0$. At $\lambda=1$ this model should behave like a spin-2 chain, in which the Haldane phase is squeezed into a very narrow region around the isotropic point. The gap itself is also small. According to the best estimate[22] it is $\Delta=0.085(5)$ at the isotropic point.

Therefore, as shown in Fig. 2, the Haldane gap is expected to vanish at a finite value of the interchain coupling when J_z/J_{xy} is not too close to -1. In order to see this, we have looked at the gap $\Delta_{21+,01+}$, which is finite in the Haldane phase, but vanishes in the planar one. It was found that at $J_z/J_{xy}=-0.7,\lambda=0.5$ this gap was already zero. Although we could not locate the boundary precisely, it is clear that, taking into account again the self-duality relationship, the phase boundary should be perpendicular to the anisotropy axis at $\lambda=1$ and have the shape shown in Fig. 2.

V. DISCUSSION

In this paper we have studied the stability of the Haldane phase in a magnetic ladder model. Our special choice of the coupling between the chains allowed us to investigate and smoothly interpolate between both the half-odd integer and integer spin Heisenberg models. We have applied the DMRG method which was improved to reduce the computational time and to increase the accuracy.

We have found that for the $S=1/2+1/2$ composite spin model the phase boundary between the antiferromagnetic and the Haldane phase is a smooth curve and the value of λ_c is a function of the anisotropy parameter, J_z/J_{xy}. For the boundary between the Haldane and planar phases our results indicate that it is at $J_z/J_{xy}=0$ independently of λ. For $0\leqslant J_z/J_{xy}<1$ the system remains in the planar phase, while for $-1\leqslant J_z/J_{xy}<0$ the interchain coupling is relevant. The critical value where the Haldane gap starts to open up is $\lambda_c=0$.

This is, however, not the only possibility. Our results are not in contradiction with the assumption that λ_c is finite, although small, except when J_z/J_{xy} is rather close to 0, as shown by the dashed line in Fig. 1.

We should also mention that since the point $\lambda=1,J_z/J_{xy}=0$ on the boundary between the Haldane and planar phases was obtained in the continuum limit, it cannot be excluded that in the lattice model this boundary at $\lambda=1$ is not exactly at $J_z/J_{xy}=0$, but at a small negative value. In this case the boundary between the Haldane and planar phases should be slightly deformed from that shown in Fig. 1.

On the basis of our calculations, unfortunately, we are unable to decide, which scenario takes place. The argument that gave $(J_z/J_{xy})_{c2}=0$ at $\lambda=1$ would give a phase boundary which is independent of λ, meaning that the interchain coupling is relevant for any J_z/J_{xy} in the range $-1\leqslant J_z/J_{xy}<0$. The same reasoning might then indicate that the interchain coupling is relevant also in the case when four $S=1/2$ chains are coupled. With an appropriate choice of the couplings this would, however, generate a four-leg ladder that behaves like an $S=2$ chain. In this model the phase boundary between the planar and Haldane phases cannot be independent of λ, in the same way as in the two-leg $S=1$ ladder. Further calculations, keeping probably close to 1000 states in the DMRG procedure, are necessary to decide between these possible scenarios and to determine the precise shape of the phase boundaries.

ACKNOWLEDGMENTS

This research was supported in part by the Hungarian Research Fund (OTKA) under Grant No. 15870 and by the U.S.-Hungarian Joint Fund under Grant No. 555.

[1] D. C. Johnston, J. W. Johnson, D. P. Goshorn, and A. J. Jacobson, Phys. Rev. B **35**, 219 (1987); R. S. Eccleston, T. Barnes, J. Brody, and J. W. Johnson, Phys. Rev. Lett. **73**, 2626 (1994).
[2] Z. Hiroi, M. Azuma, M. Takano, and Y. Bando, J. Solid State Chem. **95**, 230 (1991); M. Azuma, Z. Hiroi, M. Takano, K. Ishida, and Y. Kitaoka, Phys. Rev. Lett. **73**, 3463 (1994).
[3] R. J. Cava *et al.*, J. Solid State Chem. **94**, 170 (1991).
[4] K. Hida, J. Phys. Soc. Jpn. **60**, 1347 (1991).
[5] E. Dagotto, J. Riera, and D. Scalapino, Phys. Rev. B **45**, 5744 (1992); T. Barnes, E. Dagotto, J. Riera, and E. S. Swanson, *ibid.* **47**, 3196 (1993); T. Barnes and J. Riera, *ibid.* **50**, 6817 (1994).
[6] H. Watanabe, K. Nomura, and S. Takada, J. Phys. Soc. Jpn. **62**, 2845 (1993).
[7] K. Okamoto, D. Nishino, and Y. Saika, J. Phys. Soc. Jpn. **62**, 2587 (1993).
[8] T. Hsu and J. C. Angles̀ d'Auriac, Phys. Rev. B **47**, 14 291 (1993).
[9] R. M. Noack, S. R. White, and D. J. Scalapino, Phys. Rev. Lett. **73**, 882 (1994).
[10] S. Gopalan, T. M. Rice, and M. Sigrist, Phys. Rev. B **49**, 8901 (1994); M. Sigrist, T. M. Rice, and F. C. Zhang, *ibid.* **49**, 12 058 (1994).
[11] F. D. M. Haldane, Phys. Rev. Lett. **50**, 1153 (1983); Phys. Lett. **93A**, 464 (1983).
[12] S. R. White, Phys. Rev. Lett. **69**, 2863 (1992); Phys. Rev. B **48**, 10 345 (1993).
[13] S. R. White, Phys. Rev. B **53**, 52 (1996).
[14] J. Sólyom and J. Timonen, Phys. Rev. B **38**, 6832 (1988).
[15] Ö. Legeza, G. Fáth, and J. Sólyom, Phys. Rev. B **55**, 291 (1997).
[16] R. Botet and R. Jullien, Phys. Rev. B **27**, 613 (1983); R. Botet, R. Jullien, and M. Kolb, *ibid.* **28**, 3914 (1983).
[17] G. Gómez-Santos, Phys. Rev. Lett. **63**, 790 (1989).
[18] K. Nomura, Phys. Rev. B **40**, 9142 (1989).
[19] T. Sakai and M. Takahashi, Phys. Rev. B **43**, 13 383 (1992).
[20] M. den Nijs, Phys. Rev. B **23**, 6111 (1981); Physica A **111**, 237 (1982).
[21] F. C. Alcaraz and A. Moreo, Phys. Rev. B **46**, 2896 (1992).
[22] U. Schollwöck and T. Jolicoeur, Europhys. Lett. **30**, 493 (1995).
[23] S. R. White, Phys. Rev. Lett. **77**, 3633 (1996).
[24] E. S. Sørensen and I. Affleck, Phys. Rev. Lett. **71**, 1633 (1993).