Real-space renormalization-group study of the phase diagram of two coupled quantum spin-1/2 chains

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We investigate the phase diagram of two coupled quantum spin-1/2 chains, a square ladder, allowing for anisotropies both in the interchain and intrachain coupling, using the recently introduced density-matrix renormalization-group (DMRG) algorithm. We consider open chains up to a length of 2×200, while retaining up to 120 states in the truncated basis of the Hilbert space. The phase diagram is discussed in connection with exact results and bosonization analysis. Numerically, we show that the crossover from the critical behavior of the uncoupled disordered spin-1/2 chain to a gapped quantum liquid sets in for infinitesimal interchain coupling, both for ferromagnetic and antiferromagnetic interchain coupling. The Haldane phase of the coupled chains is, even for small interchain couplings, generically described by the Affleck-Kennedy-Lieb-Tasaki model. We also discuss typical shortcomings of the DMRG for some choices of the interaction parameters.

I. INTRODUCTION

In recent years, marked by the general revival of interest in one-dimensional antiferromagnetic quantum spin systems due to Haldane's conjecture[1] in 1983, the topic of two (or more) coupled antiferromagnetic quantum spin-1/2 chains has been investigated in several papers.[2–10] The interest in the problem has several origins. There exist experimental systems, vanadyl pyrophosphate $(VO)_2P_2O_7$ (Refs. 11–13) and $Sr_2Cu_4O_6$,[14] which are quantum spin ladders and allow one to check some of the theoretical predictions.[9] Furthermore, the problem of two coupled chains links up to several other problems of physical interest: on increasing the coupling between chains from zero to a strong ferromagnetic coupling, spin-1/2 pairs with adjacent spins on each chain are forced into their triplet spin-1 state; we therefore recover the physics of a spin-1 chain, which is fundamentally different from that of a spin-1/2 chain.[1] One question that arises naturally is whether the crossover from one regime to the other happens at some finite coupling strength or is immediate for an infinitely small interchain coupling; this question has been addressed by Refs. 2,4,6,7, with contradicting results. Increasing the coupling between chains from zero to a strong antiferromagnetic coupling, the problem reduces to the problem of an Ising chain with a transverse magnetic field, solved by Pfeuty.[4,7,15] Again, the question of the crossover from one regime to the other arises; whether the crossover from a critical behavior typical of a spin-1/2 chain to a gapped spin liquid which is found for large interchain couplings happens for infinitesimal couplings or not, is under dispute, though strong evidence in favor of an infinitesimal coupling strength at the transition is available.

At the same time, for a coupling between chains equal to the intrachain coupling, one is investigating the first step towards a two-dimensional spin-1/2 square lattice. There is now a general consensus that this lattice shows Néel order at zero temperature;[16] what remains to be investigated is how this behavior emerges from an increasing number of coupled critical and disordered spin-1/2 chains, in particular, whether there is a fundamental difference in the behavior of an even and of an odd number of coupled chains.[8] Furthermore, bosonization techniques[17] linked to exactly known limiting results have allowed Strong and Millis to propose a phase diagram for the isotropically coupled spin chains,[4,7] which shows a rather rich competition between magnetic ordering and "quenching" of magnetic momenta in the singlet states.

In this work, we are going to investigate the phase diagram of two coupled spin-1/2 chains in a rather general coupling space, investigating both intrachain *and interchain coupling anisotropies*, using the density matrix renormalization-group (DMRG) algorithm introduced by White.[19,20] Two aims are pursued by this study: on the one hand, we are interested in verifying the analytical predictions, which sometimes rest on poorly controlled approximations. On the other hand, relatively little is known about the general behavior of the DMRG algorithm. Studies so far have been mainly concentrated on high-precision studies of single points in the phase diagram of a physical system away from phase transition lines; for exceptions see Refs. 10,21,22. It is therefore also worthwhile to report the effectiveness of the DMRG in the various parts of the phase diagram.

II. BOSONIZATION RESULTS

To start with, we recapitulate the main results obtained by the bosonization technique,[4,7] extending them at the same time to anisotropic interchain couplings. The complete Hamiltonian for the two coupled chains reads

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$$H=J\sum_n \frac{1}{2}(S^+_{1,n}S^-_{1,n+1}+S^-_{1,n}S^+_{1,n+1})+J^z\sum_n S^z_{1,n}S^z_{1,n+1}+J\sum_n \frac{1}{2}(S^+_{2,n}S^-_{2,n+1}+S^-_{2,n}S^+_{2,n+1})+J^z\sum_n S^z_{2,n}S^z_{2,n+1}$$
$$+J_\perp\sum_n \frac{1}{2}(S^+_{1,n}S^-_{2,n}+S^-_{1,n}S^+_{2,n})+J^z_\perp\sum_n S^z_{1,n}S^z_{2,n}, \tag{1}$$

with 1,2 being the chain index. We assume in the following $J=1$. The procedure is as follows: using a Jordan-Wigner transformation, the Hamiltonian is rewritten in terms of a half-filled system of spinless fermions; these in their turn are replaced by two sets of relativistic massless fermions, moving with the Fermi momentum $\pm\pi/2$ on the chain. Those can be expressed by scalar bosonic fields; quartic interaction terms simplify in part to quadratic terms.

For the bosonization of the two chains, we introduce two sets of anticommuting spinless fermionic operators for the upper and lower chain, c_1 and c_2, to carry out a Jordan-Wigner transformation. The bosonization of the two single chains can therefore be taken directly from the literature (e.g., Ref. 23):

$$H^B=\frac{1}{2}\left(1+\frac{\gamma}{\pi}\right)\int dx\Big[\Pi^2(x)+(\partial_x\phi)^2(x) - \frac{4\gamma}{\pi^2\alpha^2}\cos\sqrt{16\pi/(1+2\gamma/\pi)}\,\phi\Big], \tag{2}$$

where α is a short-wavelength cutoff, which is typically of the order of the lattice spacing; $\phi\equiv\phi_1,\phi_2$ for the upper (lower) chain; Π is the associated canonical momentum. The interchain term can be separated in an *exchange term* (in $J_\perp$) and an *interaction term* (in $J^z_\perp$).

Let us first consider the interaction term $V_2=J^z_\perp\Sigma_n S^z_{1,n}S^z_{2,n}$. Applying the Jordan-Wigner transformation gives a model of spinless fermions at half-filling, which in terms of relativistic fermions reads

$$V_2=aJ^z_\perp\int dx[:j_{01}::j_{02}:+(\psi^\dagger_{1,L}(x)\psi_{1,R}(x)\psi^\dagger_{2,R}(x)\psi_{2,L}(x) + \text{H.c.})+(\psi^\dagger_{1,L}(x)\psi_{1,R}(x)\psi^\dagger_{2,L}\psi_{2,R}+\text{H.c.})]. \tag{3}$$

The last term is the umklapp term present due to the half-filling ($k_F=\pi/2$). The arrows indicate the upper and lower chain, L and R stand for left and right movers. The current j_{0i} is defined by $\psi^\dagger_{i,R}\psi_{i,R}+\psi^\dagger_{i,L}\psi_{i,L}$. Bosonization gives

$$V_2=aJ^z_\perp\int dx\,\frac{1}{4\pi}[(\partial_x\phi_\uparrow+\partial_x\phi_\downarrow)^2-(\partial_x\phi_\uparrow-\partial_x\phi_\downarrow)^2] + \frac{aJ^z_\perp}{2\pi^2\alpha^2}\int dx\,\cos\sqrt{4\pi}(\phi_\uparrow-\phi_\downarrow) + \frac{aJ^z_\perp}{2\pi^2\alpha^2}\int dx\,\cos\sqrt{4\pi}(\phi_\uparrow+\phi_\downarrow). \tag{4}$$

The exchange term $V_1=J_\perp\Sigma_n 1/2(S^+_{1,n}S^-_{2,n}+S^-_{1,n}S^+_{2,n})$ is more complicated in that it contains a nonvanishing string operator because of the presence of different sets of Fermi operators. Bosonization gives

$$S^+_n=\sqrt{\frac{1}{2\pi}}\,[1+(-1)^{x/a}\cos\sqrt{4\pi}\phi]e^{i\sqrt{\pi}\tilde\phi}, \tag{5}$$

$$S^-_n=\sqrt{\frac{1}{2\pi}}\,[1+(-1)^{x/a}\cos\sqrt{4\pi}\phi]e^{-i\sqrt{\pi}\tilde\phi}, \tag{6}$$

where $\tilde\phi=\phi_R-\phi_L$. The leading contribution to S^+S^- will come from those products of exponentials which have *lowest* dimension. Passing to the continuum limit and resubstituting chain indices one finds

$$V_1=J_\perp\frac{1}{2\pi a}\,dx\,\cos\sqrt{\pi}(\tilde\phi_1-\tilde\phi_2) \tag{7}$$

as the leading contribution. One puts together

$$H=H_1+H_2+V_1+V_2 \tag{8}$$

and introduces operators (anti)symmetric under the exchange of the chains:

$$\Psi_\pm=\frac{1}{\sqrt2}(\phi_1\pm\phi_2), \tag{9}$$

$$\chi_\pm=\frac{1}{\sqrt2}(\tilde\phi_1\pm\tilde\phi_2). \tag{10}$$

Using

$$\partial_x\tilde\phi_{1,2}(x)=\Pi_{1,2}(x), \tag{11}$$

one finds ($\alpha\to a$, the lattice spacing)

$$H=\frac{a}{2}\int dx\left[\left(1-\frac{J^z}{\pi}\right)(\partial_x\chi_+)^2+\left(1+\frac{3J^z}{\pi}\right)(\partial_x\Psi_+)^2+\frac{J_\perp^z}{\pi}(\partial_x\Psi_+)^2\right]+\int dx\,\frac{J_\perp^z}{2\pi^2 a}\cos\sqrt{8\pi}\Psi_+ +\frac{a}{2}\int dx\left[\left(1-\frac{J^z}{\pi}\right)\right.$$
$$\left.\times(\partial_x\chi_-)^2+\left(1+\frac{3J^z}{\pi}\right)(\partial_x\Psi_-)^2-\frac{J_\perp^z}{\pi}(\partial_x\Psi_+)^2\right]+\int dx\,\frac{J_\perp^z}{2\pi^2 a}\cos\sqrt{8\pi}\Psi_-+\int dx\,\frac{J_\perp}{2\pi^2 a}\cos\sqrt{2\pi}\chi_-. \quad (12)$$

The Hamiltonian therefore splits into two parts, acting on different sectors, one symmetric and the other antisymmetric under chain exchange: $H=H_++H_-$. One drops mixed symmetry terms like

$$-\frac{J^z}{2\pi^2 a^2}\cos\sqrt{8\pi}\Psi_+\cos\sqrt{8\pi}\Psi_-,$$

as there are always more relevant operators present in the renormalization-group sense. To bring the Hamiltonian into the form of a normal free bosonic Hamiltonian plus interaction one rescales. Introducing spin wave velocities

$$c_+=1+\frac{J^z}{\pi}+\frac{J_\perp^z}{2\pi}, \quad (13)$$

$$c_-=1+\frac{J^z}{\pi}-\frac{J_\perp^z}{2\pi} \quad (14)$$

and rescaling the (anti)symmetric operators as

$$\sqrt{c_{\Psi\pm}}\Psi_\pm\to\Psi_\pm, \quad (15)$$

$$\sqrt{c_{\chi\pm}}\chi_\pm\to\chi_\pm, \quad (16)$$

where

$$c_{\Psi\pm}=1+\frac{2J^z}{\pi}\pm\frac{J_\perp^z}{2\pi}, \quad (17)$$

$$c_{\chi\pm}=1-\frac{2J^z}{\pi}\mp\frac{J_\perp^z}{2\pi}, \quad (18)$$

one obtains, setting $a=1$,

$$H_+=\frac{1}{2}c_+\int dx\left[(\partial_x\chi_+)^2+(\partial_x\Psi_+)^2+\frac{J_\perp^z}{\pi^2 c_+}\cos\sqrt{8\pi/c_{\Psi_+}}\Psi_+\right], \quad (19)$$

$$H_-=\frac{1}{2}c_-\int dx\left[(\partial_x\chi_-)^2+(\partial_x\Psi_-)^2+\frac{J_\perp^z}{\pi^2 c_-}\cos\sqrt{8\pi/c_{\Psi_-}}\Psi_-+\frac{J_\perp}{\pi^2 c_-}\cos\sqrt{2\pi/\chi_-}\chi_-\right]. \quad (20)$$

The rescaling relations, for *small* interactions, conserve the commutation relations between fields and momenta. Analyzing this Hamiltonian, we first consider the breakdown of bosonization, the onset of ferromagnetism. One criterion is that the spin wave velocity becomes negative in either of the Hamiltonians H_+ or H_-. The first condition, $c_+<0$, leads to

$$J^z<-\pi-\frac{J_\perp^z}{2}. \quad (21)$$

In that case H_+ becomes ferromagnetic, which means there is ferromagnetic order on both chains, and the two neighboring spins on the upper and lower chain will have the same magnetization (which we call "symmetric"). Alternatively, $c_-<0$ leads to

$$J^z<-\pi+\frac{J_\perp^z}{2}. \quad (22)$$

In this case H_- becomes ferromagnetic, and the order on the chains is such that spins on the same ladder step show opposite magnetization ("antisymmetric"). For increasingly ferromagnetic J^z the nonferromagnetic region is squeezed out; for $J^z=\pi$ the lower portion shows symmetric ferromagnetism, the upper portion antisymmetric ferromagnetism.

Bosonization results indicate that the phase transition is *independent* of $J_\perp$. Alternatively, we have mapped the coupled spin chain problem in the limit of strongly antiferromagnetic coupling between chains and strong J^z coupling on the chains to an Ising model in a transversal field (using conventional Pauli matrices)

$$H=\sum_i\frac{J^z}{2}\sigma_i^x\sigma_{i+1}^x+\frac{J_\perp}{2}\sigma_i^z, \quad (23)$$

which has been solved exactly by Pfeuty.[15] One finds that in the strong coupling limit the phase transition to singlet ferromagnetism takes place for $|J_\perp|=J^z$ (there is a symmetry under sign change) and is therefore dependent on $J_\perp$ only. This obvious contradiction finds its resolution in the fact that the range of validity of the two approaches is different. We will interpolate between these regimes using numerical methods later.

In the regime of validity of bosonization, one studies the dimension d of the potentially relevant operators in H_+ and H_-, using $d[\cos\beta\phi]=\beta^2/4\pi$,

$$\cos\sqrt{8\pi/c_{\Psi_+}}\Psi_+:\quad d=\frac{2}{1+\frac{2J^z}{\pi}+\frac{J_\perp^z}{2\pi}}, \quad (24)$$

$$\cos\sqrt{8\pi/c_{\Psi-}}\Psi_-:\quad d=\frac{2}{1+\frac{2J^z}{\pi}-\frac{J_\perp^z}{2\pi}}\equiv d_1, \quad (25)$$

$$\cos\sqrt{2\pi/c_{\chi^-}}\chi_-: \quad d=\frac{1}{2(1-2J^z/\pi+J_\perp^z/2\pi)}\equiv d_2. \tag{26}$$

This means that for each operator the condition for relevance is

$$\cos\sqrt{8\pi/c_{\Psi+}}\Psi_+: \quad J^z>-\frac{J_\perp^z}{4}, \tag{27}$$

$$\cos\sqrt{8\pi/c_{\Psi-}}\Psi_-: \quad J^z>\frac{J_\perp^z}{4}, \tag{28}$$

$$\cos\sqrt{2\pi/c_{\chi^-}}\chi_-: \quad J^z<\frac{3}{8}\pi+\frac{J_\perp^z}{4}. \tag{29}$$

We see that for H_- there is always a relevant operator: For small interactions, we have $d_1=1/d_2$. In such a case it matters which is the dominant, i.e., most relevant, operator. The condition for $d_2<d_1$ (the χ_- term more relevant than the Ψ_- term) is

$$J^z<\frac{1}{4}J_\perp^z+\frac{3}{10}\pi. \tag{30}$$

Considering the relevance conditions, we are left with *three* possible phases: (i) a phase where the Ψ_+ and Ψ_- operators are relevant; (ii) a phase where the Ψ_+ and the χ_- operators are relevant (respectively dominant); (iii) a phase where only the χ_- operator is relevant (or, rather, dominant).

Analyzing the correlation functions, one finds that for region (i) both Ψ fields will lock, that is the nonalternating part of the S^z operator will vanish and antiferromagnetic long-range order set in. This phase borders on region (ii) where Ψ_+ and χ_- will lock; considering the operator expressions, one sees that this will not induce order, but the massive terms will make the decay of the correlation functions exponential; a gap over a disordered ground state will be found. This is the behavior as predicted for isotropic integer spins by Haldane. Actually, for very strong ferromagnetic coupling between the chains, we obtain an effective spin-1 chain Hamiltonian, because all spins will be bound in triplet $S=1$ states. In region (iii) there is no relevant operator in H_+, as in region (ii) the chains will be disordered. However, the correlation functions will behave differently. There will be power-law-like contributions to the correlation functions; that means the spectrum will be gapless and the region *critical*. Using these results, it is possible to obtain the phase diagram for *isotropic* interchain coupling shown in Fig. 1. (Note that we differ from Refs. 4,7, in that we have changed their prediction of the transition line from the Haldane to the XY phase such that it is described by $J^z=0$, following results by den Nijs and Rommelse on the transitions in a spin-1 chain[18].) An interesting prediction is that of the existence of a multicritical point: bosonization predicts that the critical phase exists also for antiferromagnetic interchain couplings for ferromagnetic $J^z<0$. As this phase does not exist in the strong coupling limit,[15] it has to terminate in a multicritical point somewhere.

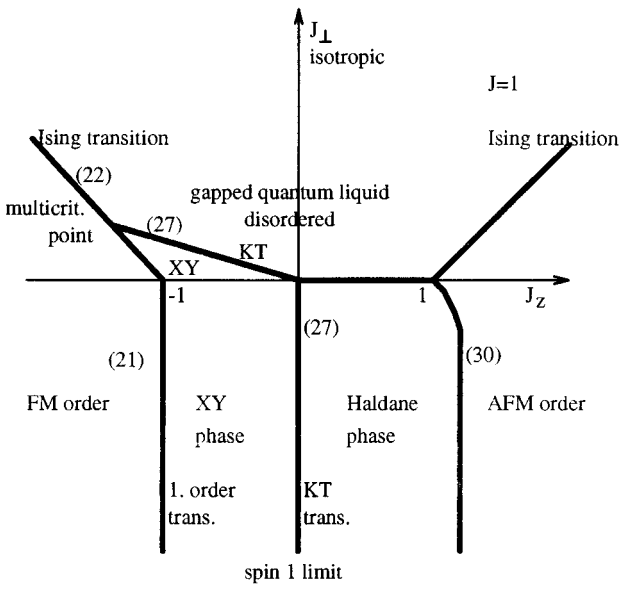

FIG. 1. Schematical phase diagram of two coupled anisotropic spin-1/2 chains for an isotropic interchain coupling; cf. Refs. 4,7.

Before discussing the numerical results guided by the bosonization predictions, we will first give a brief description of the numerical method used.

III. THE DENSITY-MATRIX RENORMALIZATION GROUP

The choice of the density-matrix renormalization-group algorithm was determined by the fact that this method allows one to treat very long chains by comparison to exact diagonalization methods while retaining good precision for energies and expectation values where other methods capable of attacking large systems fail, such as quantum Monte Carlo algorithms. The DMRG is, however, special in that the systematic nature of its approximations leads, on the same system, to results which may vary several orders of magnitude in their precision, like energies per bond, which are extremely well obtained, and correlation lengths, which are consistently underestimated. The precision will also be found to be extremely sensitive to the choice of the interaction parameters.

We do not aim at a complete description of the DMRG; for this the reader is referred to Refs. 19,20. We will just briefly outline the method and highlight the possible shortcomings.

Imagine the following rather general one-dimensional problem: a short-range interaction Hamiltonian H on a chain of length L with N states per site and arbitrary boundary conditions. The low-temperature (especially $T=0$) physics will be well captured by the ground state and the lowest excited states. These can be obtained by diagonalizing a matrix of length N^L using techniques like the Lanczos iterative diagonalization algorithm. The tractable chain lengths are severely limited by the geometrical increase of the matrix size. The DMRG surmounts this difficulty by diagonalizing chains of linearly increasing length, till the desired system size is reached, while retaining only a fixed number M of the states in the growing Hilbert space after each diagonalization, thus

giving an approximate description of the chains. In the standard version, chains are composed out of a left block of spins, which have already been renormalized and which is described by M states, two sites in the center, and a right block of spins. This hybrid system is diagonalized, or more precisely speaking, the targeted state (ground state, first excited state) determined. New blocks are now formed from the old blocks plus the adjacent site. The new block has initially MN states, of which M states are retained. The M states to be retained are those which contribute most to the projection of the targeted state on the new blocks, i.e. the eigenvectors of the reduced density matrix obtained from this projection associated with the M largest eigenvalues of the reduced density matrix. As $\sum_{i=1}^{MN}\lambda_i=1$, the truncation error $P(M)=1-\sum_{i=1}^{M}\lambda_i$ is a good measure of the precision of the results: it tells us how much of the projection of the targeted state we are losing by the truncation. As do other authors, we find a proportionality between errors in chain energies and the truncation error. For other quantities, the connection is more intricate, and has to be determined each time by extrapolations in M. The next chain is formed from the new blocks and two sites added in the center, thus $L\rightarrow L+2$, and the procedure repeats. After the chain has grown to the desired length, one may calculate expectation values of observables relative to the targeted state, for which purpose one has to keep matrix elements of the desired observables in the basis of the truncated Hilbert space, which have to be updated at each truncation. In our application, we have added one ladder rung (i.e., two sites) on each chain half. This allows for a more precise treatment of the interactions as compared to the use of a dimerized and frustrated spin-1/2 chain.[10]

We want to outline two major problems that one may encounter in the application of the DMRG. The system considered is an open system, which, while interesting in its own respect, does not allow for straightforward finite size scaling analysis as would a periodic chain. As has been shown in Ref. 20, periodic (in general closed) systems are tractable, but the precision obtained is largely inferior. Manipulating the coupling strengths at the chain ends while retaining the bulk couplings may change the open boundary conditions such that certain properties of systems with periodic boundary conditions are imitated.

Furthermore, the errors introduced by the DMRG have systematic, not statistical, character. While this is useful to give error estimates and control the algorithm, this may lead to serious problems if results are not extrapolated carefully; unless the precision obtained is such that numerical results for a given M are more or less the exact ones, it is not correct to extrapolate results in L for a given M. The systematic errors may introduce artifacts into the convergence behavior which may be difficult to separate from the real convergence behavior (an example given below, the gap for weak interchain coupling, is extremely sensitive to this problem). It is therefore in general necessary to extrapolate first, for a given L, carefully in M to $M\rightarrow\infty$ (equivalent to the exact result for L) and only then in L to $L\rightarrow\infty$. Any other result is *a priori* untrustworthy.

IV. DMRG RESULTS FOR THE TWO COUPLED SPIN CHAINS

A. Excitation gap in the weak-interchain-coupling limit

A question related to the quantum spin ladder is the behavior of the spectrum for a small interchain coupling $J_\perp=J_\perp^z\rightarrow 0$ (we are only going to consider isotropic interchain coupling here) between two critical spin-1/2 chains with antiferromagnetic anisotropy ($0\leqslant J^z\leqslant 1$). Bosonization predicts that the coupled system is gapped for all nonvanishing interchain couplings. There are numerical and analytical studies which seem to indicate that this is not the case and that there is a critical interchain coupling strength below which the spectrum is essentially that of the underlying spin-1/2 chains, gapless, and the ladder critical.[2,3] Stronger evidence seems to be available in favor of the bosonization prediction, though this question cannot be considered settled.[5,10] The use of Monte-Carlo and exact diagonalization studies is problematic for very small interchain couplings; the results due to the DMRG have not been subject to a critical discussion of possible artifacts, which we will discuss below.

We have tried to elucidate this question using the density-matrix renormalization-group algorithm, which at least allows one to treat much longer chains than the exact diagonalization routines used so far, and give a critical discussion of the artifacts introduced by the DMRG.

It is important to note that for a fixed number M of states kept, one will always, for any $J_\perp\neq 0$, find a finite gap, if one takes as gap the energy difference between the lowest energy states in the $S^z_{\text{total}}=0$ and $S^z_{\text{total}}=1$ subspaces, and extrapolates the results to $L\rightarrow\infty$. This is due to the fact that the effective variational character of the DMRG leads to an overestimation of both the ground state and first exited energy:

$$E_0(L)=E_0^{\text{exact}}(L)+\delta_0(L),$$

$$E_1(L)=E_1^{\text{exact}}(L)+\delta_1(L),$$

where $\delta_i(L)>0$ and monotonously increasing. Furthermore, $\delta_1(L)>\delta_0(L)$ for all $L>L_0$, L_0 being the size of the system that was still done exactly (i.e., before any truncation). The reason for the relative loss of precision for the first excited state relative to the ground state is given by the privileged position of the ground state at the end of the spectrum, which makes it more easily accessible.

The gap is therefore systematically overestimated and thus always finite. For long chains the ground state and excited state energy *per site* will both converge to a fixed value. This does not imply any convergence or precision criterion for the gap; it is just due to the fact that for large L, the newly added spins see effectively infinite chains and truncation produces again and again the same basis states. The converged value will be a variational overestimation of the true energy per site, more overestimated for the excitation than the ground state. For long chains, effectively a finite error $\delta=[\delta_1(L+1)-\delta_1(L)]-[\delta_0(L+1)-\delta_0(L)]$ ($\rightarrow$const for $L\rightarrow\infty$) will be added to the gap for each site added, eventually overwhelming any (physical) decrease of the gap for long chains.

The problem is further enhanced by the fact that the truncation error $1-\Sigma\lambda_i$ (the λ_i being the M retained eigenvalues), which is proportional to the errors in energy added per site,[19,20] $[\delta_1(L+1)-\delta_1(L)]$ and $[\delta_0(L+1)-\delta_0(L)]$, increases dramatically for $J_\perp \to 0$, where the gap is supposedly going to zero. This may be understood as follows: in the strong interchain coupling limit the chains are acting in a strongly correlated way, such that one "compound" chain is described in a basis of M states. In the weak coupling limit, the chains act independently; considering the noninteracting case, the ground state wave function is $\Psi=\psi_1\otimes\psi_2$, the product of two one-chain wave functions. This implies that the M states become the basis of a product space, and effectively (in a crude approximation) of the order of $\sqrt{M}$ states will describe each chain. The spin-1/2 chain can be dealt with very precisely for M of the order of 30; if we consider in our problem $M\approx 100$, we are left with about 10 states for each chain in the weak coupling limit. For $M=10$, even the spin-1/2 chain is not dealt with very precisely. We actually find that for very weak interchain coupling our truncation errors are in good agreement with those for a spin-1/2 chain described by $\sqrt{M}$ states.

The truncation errors are of the order 10^{-5}; the errors in the energies per site are typically of the order of 10 (ground state) or 20 to 30 (excited state) bigger, such that for a chain of length 2×100, the error in the gap is of the order 10^{-2}. At the same time, Barnes found for $J_\perp=0.2$ a gap of the order 0.07(3). Assuming a linear behavior of the gap as $\Delta\approx 0.5 J_\perp$, which seems good at least for large interchain coupling, we may estimate that for $J_\perp=0.05$ we have to show the existence of a gap of the order 0.025, which, together with a spin wave velocity $\pi/2$ (which we take from the uncoupled spin-1/2 chain[24]) leads to a correlation length of about 60. From our experience with the DMRG for spin-2 chains (see Ref. 25) we suspect that chains of length $L>200$ would have to be considered to establish the gap value properly. This, however, would also double the error in the gap, which then by far exceeds the quantity looked for. To reduce the error substantially, we would have to increase $\sqrt{M}$ to about 20, and thus use $M\approx 400$, which exceeds our means.

We are therefore not able to establish a reliable *quantitative* behavior of the gap for small interchain couplings, but have tried instead to estimate the error by comparing carefully results for $M=60$, 80, 100, 120 for chains up to length 2×140 to see whether a gapless spectrum can be excluded without doubt for $J_\perp=\pm 0.05$. This is to substitute the adequate and in principle only correct approach, to extrapolate all energies in M first and then in L.

As already mentioned, we calculate the gap from the difference in the lowest energies of the $S^z_{\text{total}}=0$ and $S^z_{\text{total}}=1$ subspaces. We consider *open* chains, as the precision is even further reduced for closed chains. In the case of *ferromagnetic* interchain couplings this approach must be modified: it gives results showing a gapless spectrum for all interchain couplings. The results in Table I are the gaps for coupled chains of length 100, calculated at $M=75$, $J^z=0.5$. The results have not been extrapolated, and are thus overestimations. The error is of the order 0.01 for the first and of the order 0.001 for the last result. The longer correlation lengths for small couplings lead to a slower decay of the remaining gap. These results are perfectly consistent with a vanishing gap, though a massive phase is expected. This can be understood from the strong coupling limit, the spin-1 chain. It is known that open spin-1 chains have a low-lying excitation triplet which degenerates with the singlet ground state in the thermodynamic limit. This behavior is due to effective free spin-1/2 states at the chain ends, which interact weakly through the chain, and form a singlet or a triplet.[26,20] The Affleck-Kennedy-Lieb-Tasaki (AKLT) valence-bond-solid (VBS) model,[27] which expresses each spin-1 as two symmetricized spin-1/2 particles, which link to other spin-1/2 particles on neighboring sites by singlet bonds, gives an understanding of that phenomenon: one of the 2 spin-1/2 particles on each end site cannot link up and is effectively free. It is by now agreed that the VBS model is generic for the Haldane (i.e., disordered and gapped) phase of the spin-1 chain. Our results show that it is also generic for the Haldane phase of the spin ladder in the weak coupling limit. The degeneracy can be lifted by adding a spin-1/2 to each end of the spin ladder and couple it to the first two (last) spins of the ladder. Then the gap can be found in the standard approach.

TABLE I. Gap for $L=2\times 100$, $M=75$, $J^z=0.5$ for various $J_\perp$ in open *unmodified* chains.

$J_\perp$	Δ
−0.05	0.0206
−0.10	0.0174
−0.20	0.0141
−0.50	0.0096
−1.00	0.0070

For a ferromagnetic coupling $J_\perp=0.05$, we find the gap curves as given in Fig. 2 for $M=60$, 80, 100, and 120 using the infinite length algorithm.[20] The convergence of the gap curves is obvious, and if one extrapolates the gap curves towards $L=\infty$ using a L^{-1} behavior, one obtains a lower boundary of the gap of ≈ 0.014. To find out whether the slight inflection upwards of the gap curves is due to the truncation error or reflects a true physical behavior, we extrapolate the gaps for $L=100$, using the linear dependence of the error in the energies on the truncation error. The results are shown in Table II. We find an extrapolated gap $\Delta=0.039(2)$ for $L=100$, which is just above the straight-line fit to the gap curve. The inflection is thus in part physical. We expect from the $S=1$ chain that the excitations of the ferromagnetically coupled spin chains are generically described by the nonlinear sigma model and the AKLT model, as is indicated by our finding of low-lying end excitations even for very small interchain couplings. In that case the dispersion relation of the chain is for low energies that of a massive relativistic particle. As the chain is open, the momentum is not a good quantum number and one expects a gap equation

$$\Delta(L)=\Delta_\infty+\frac{c^2\pi^2}{2\Delta_\infty L^2}+O(L^3) \tag{31}$$

and therefore a crossover to a parabolic gap curve for $L\gg\xi$.[28] Assuming that for small interchain couplings the spin wave velocity c is essentially that of an uncoupled spin-1/2 chain $c\approx\pi/2$, we may estimate that for a gap ≈ 0.025, $\xi\approx 60$,

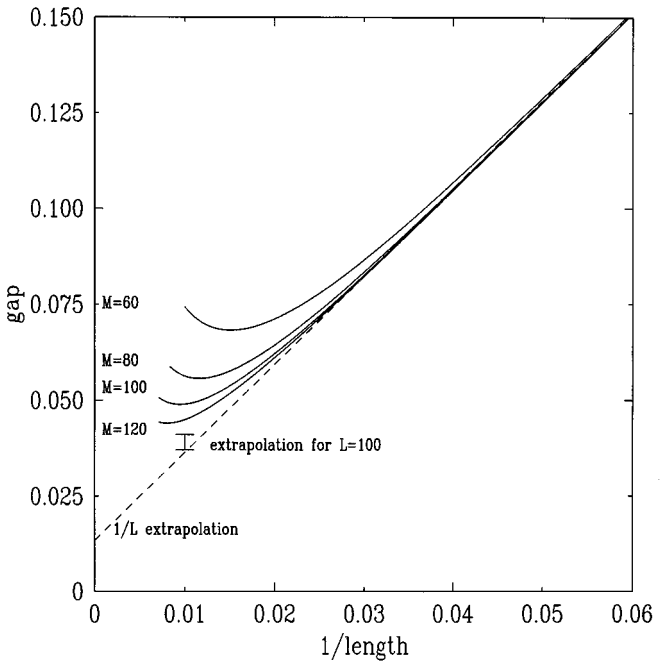

FIG. 2. Results for the gap of two isotropic spin-1/2 chains coupled by an isotropic ferromagnetic interchain coupling $J_\perp=-0.05$ for various numbers M of states retained in the DMRG. Note the increase in the gap for short chain lengths which is an artifact of the DMRG. The dashed line is a linear extrapolation of the part of the gap curve converged in M and thus a lower bound on the gap which is thus found to be nonzero. For $L=100$, the gap value was extrapolated in M to obtain the inclination of the gap curve.

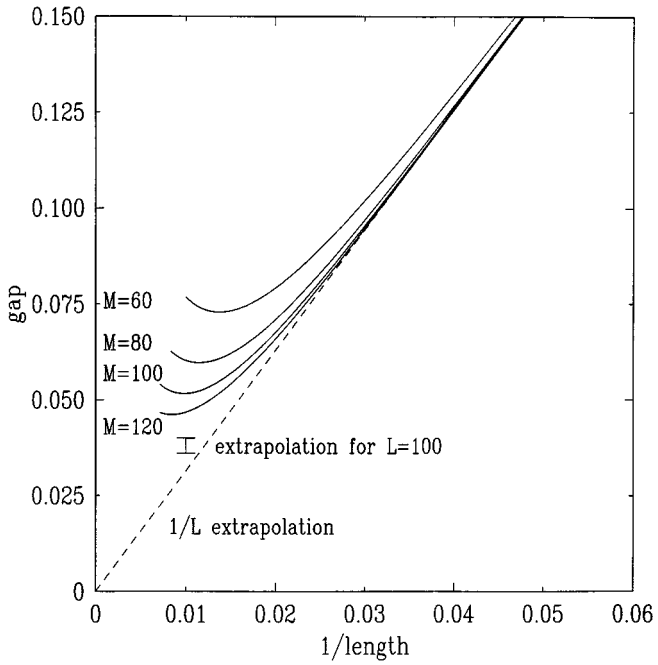

FIG. 3. Results for the gap of two isotropic spin-1/2 chains coupled by an isotropic antiferromagnetic interchain coupling $J_\perp=0.05$ for various numbers M of states retained in the DMRG. Note the increase in the gap for short chain lengths which is an artifact of the DMRG. The dashed line is a linear extrapolation of the part of the gap curve converged in M and thus a lower bound on the gap which is thus found to be nonzero. For $L=100$, the gap value was extrapolated in M to obtain the inclination of the gap curve. There is a clear deviation from the linear extrapolation, which indicates the existence of a finite gap.

which is consistent with the observed small deviation from a mainly L^{-1} dominated gap behavior for the L considered.

The gap is expected to open for stronger interchain couplings and to saturate eventually to the infinite coupling limit of the spin-1 chain gap $\Delta=0.41050(2)$. This convergence is slow: for $J_\perp=0.5$ we find $\Delta=0.106(2)$ and for $J_\perp=1.0$ $\Delta=0.137(2)$.

For antiferromagnetic coupling $J_\perp=0.05$, we find for $M=60$, 80, 100, and 120 gap curves as in Fig. 3. Again, the convergence of the gap curves is obvious. A linear extrapolation of the (converged part of the) gap curve to $L\to\infty$ gives a vanishing gap. To establish whether the gap is nonvanishing, we extrapolate the gap results for $L=100$ to $M=\infty$ to show an upward inclination of the gap curve. The gap is then nonvanishing for $J_\perp=0.05$. The results are given in Table III. The extrapolation is again based on the linear dependence of the errors of the energies on the truncation error. The gap is then found to be 0.038(2) for $L=100$, well above the linear extrapolation to a vanishing gap. We therefore conclude the existence of a nonvanishing gap for small antiferromagnetic couplings.

In agreement with other authors,[5,9] we find a near linear dependence of the gap on $J_\perp$ with $\Delta\approx 0.5J_\perp$ for intermediate interchain coupling strengths. We find the same gap and correlation length as White, Noack, and Scalapino[8] for $J_\perp=1.0$: $\Delta=0.506$ and $\xi=3.2$, which we take as corroboration of the numerical correctness of our program. From this follows that the spin wave velocity in the antiferromagnetically coupled chains changes only slightly from its value for uncoupled chains: for $J_\perp=1$, $c=1.60$ as opposed to $c=1.57$ for the uncoupled chains. We understand the excitations as

TABLE II. Ground state and first excitation energies, associated truncation errors, and the gap for various M for the ground state and the first excited state. $J_\perp=-0.05$ (ferromagnetic interchain coupling).

M	E_0	$\rho_1(M)$	E_1	$\rho_1(M)$	Δ
60	−87.93567	0.45×10^{-4}	−87.86138	0.80×10^{-4}	0.0743
80	−87.94471	0.22×10^{-4}	−87.88843	0.40×10^{-4}	0.0563
100	−87.94824	0.13×10^{-4}	−87.89928	0.22×10^{-4}	0.0490
120	−87.95025	0.83×10^{-5}	−87.90535	0.13×10^{-4}	0.0449
∞	−87.953(1)		−87.914(1)		0.039(2)

TABLE III. Ground state and first excitation energies, associated truncation errors, and the gap for various M for the ground state and the first excited state. $J_\perp=0.05$ (antiferromagnetic interchain coupling).

M	E_0	$\rho_1(M)$	E_1	$\rho_1(M)$	Δ
60	−88.37658	0.47×10^{-4}	−88.29979	0.78×10^{-4}	0.0768
80	−88.38652	0.23×10^{-4}	−88.32628	0.37×10^{-4}	0.0602
100	−88.39087	0.13×10^{-4}	−88.33923	0.22×10^{-4}	0.0516
120	−87.39285	0.83×10^{-5}	−88.34608	0.14×10^{-4}	0.0468
∞	−88.396(1)		−88.358(1)		0.038(2)

the excitation of one ladder rung from its singlet to its triplet state, which sets the energy scale $J_\perp$ for the gap. The excitation then travels on *one* chain alone, like a wandering defect, which sets the spin wave velocity to a value close to that of the uncoupled chain (see also Ref. 5). This picture is in agreement with the resonating valence bond picture introduced by White, Noack, and Scalapino[8] and the results of Barnes *et al.* using a strong coupling expansion.[5]

B. Identification of the phases

The DMRG has allowed us to identify all phases predicted by bosonization, though in one case, the identification is only indirect. We have considered of the order of 100 points of the phase diagram, calculating chains up to $M=120$ and $L=2\times200$. The magnetically ordered phases are well identified, in particular the ferromagnetic phase. The DMRG profits from the fact that the ordered ground state can be expressed from very few states in the S_i^z basis of the Hilbert space. The singlet phase, i.e., the gapped quantum liquid with singlet coupling between adjacent spins, is also well calculated by the DMRG.

We were not able to calculate the properties of the XY phase using the DMRG. This was due to a convergence problem of the underlying diagonalization algorithm. We observed (Fig. 4) a steep increase in the number of iterations needed to diagonalize the system with increasing total length, before this number saturated for very long chains; by comparison, in gapped phases, the number of iterations rarely exceeds 100 and is fairly constant with the chain length. This tells us something about the validity range of the DMRG: it always works reasonably well for gapped spectra, if the point in the phase diagram is not too close to a phase boundary. For a critical system, the behavior seems to depend crucially on the nature of the critical spectrum. The DMRG works very well for the spin-1/2 chain, which is critical. The spectrum, however, is given by $\omega=ck$ and thus the density of states at the ground state energy is finite. The DMRG works also well for excited states of integer spin chains, which are at the bottom of a *band* of excitations with a diverging density of states. We suspect that the XY phase has a *continuous* (due to vortex-vortex interactions) spectrum limited by $\omega=ck^2$ surviving from the ferromagnetic spectrum. For increasing chain length (and thus smaller $\delta k\propto1/L$) the diagonalization algorithm takes more and more time to separate the ground state. The saturation of the number of iterations for very long chains is explained by the fact that in that limit the truncation algorithm leads to a repetitive diagonalization of the infinite-size limit of the chain. In addition to the time problem, Lanczos results obtained by a very high number of iterations lose precision for the eigenstates, as the orthogonality between the Lanczos vectors is numerically more and more lost.

C. The phase transition to ferromagnetism

It should be clear from the above that the exact location of phase boundaries is hard to determine in the DMRG algorithm, both because of the increase in M needed and because of the open boundary conditions which forbid finite-size scaling. We found only one phase transition where already for small M the truncation error was very small and where one can therefore concentrate on an extrapolation of results in L. This is the transition to ferromagnetism for $J^z<0$, where for $M=50$ the truncation error was typically below 10^{-9} (cf. for the transition to antiferromagnetism, we find for the same M typically truncation errors of 10^{-5}). This is

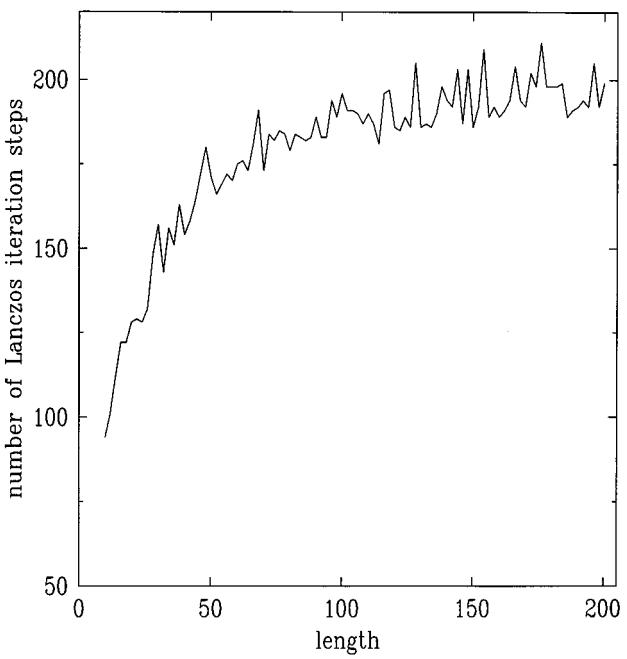

FIG. 4. For $J^z=-0.3$ and $J_\perp=J_\perp^z=-4$ (XY phase) we show for $M=55$ the number of Lanczos iterations needed at each step of the DMRG to obtain convergence of the ground state energy. The oscillations are due to the random starting vector used by the Lanczos algorithm. We expect that ground state vector results have to be handled with caution if the number of iterations sensibly exceeds 100.

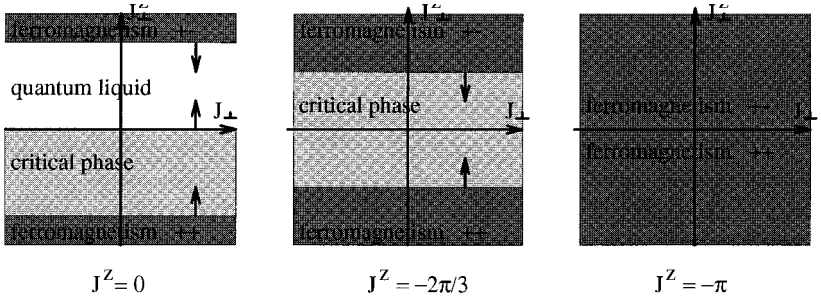

FIG. 5. Schematic representation of the phase diagram predicted by bosonization for an anisotropic interchain coupling $J_\perp$, $J_\perp^z$, in its dependence on a ferromagnetic J^z ($J=1$). Arrows indicate the motion of the transition lines for a more ferromagnetic J^z. The quantum liquid phase disappears for sufficiently negative J^z. $+-$ and $++$ indicate the type of ferromagnetic order found. As these predictions are qualitative, no values are given for the axes.

because the ferromagnetic ground state is described by very few states in the Hilbert space in the S_i^z basis (as opposed to the antiferromagnetic state), which also reduces the number of states necessary for a good description of the ground state in the adjacent disordered phase, which in its correlation is already dominated by the adjacent ferromagnetic phase.

We are going to investigate the phase transition to ferromagnetism for general anisotropic interchain couplings $J_\perp$, $J_\perp^z$. Following the predictions of bosonization, we have to distinguish between two cases: (i) ferromagnetic $J_\perp^z<0$: a first order phase transition from a ferromagnetic phase with ferromagnetically aligned adjacent spins on the two chains to the critical XY phase, and (ii) antiferromagnetic $J_\perp^z>0$: here one should find either a first order phase transition from a ferromagnetic phase with antiferromagnetically aligned adjacent spins on the two chains to the critical XY phase or a second order phase transition of the Ising universality class in two dimensions to a gapped quantum spin liquid.

Before presenting the numerically found results, we want to extend the analytical results to anisotropic interchain coupling. For the bosonization, we have done this in Sec. II, and recapitulate that for *small* J^z, $J_\perp$, and $J_\perp^z$ one expects that the phase transition is driven by $J_\perp^z$ only, with the two ferromagnetical phases driving out the two disordered phases in between, the gapped phase in its turn being driven out by the XY phase (Fig. 5). It may already be expected that for strong $|J_\perp|$ (the Hamiltonian is invariant under the operation $J_\perp \to -J_\perp$, which can be seen from a rotation of the spins of one chain by π around the z axis) the phase boundaries to the ferromagnetic phases curve to give more place to the disordered phases which are favored by the spin-flipping $J_\perp$.

On the other hand, for very strong interchain coupling, information can be obtained from exact mappings. In the strong ferromagnetic interchain coupling limit, the adjacent spins on the two chains will form spin triplets with total $S^z=\pm 1,0$, where, for an anisotropic interchain coupling, the energy of the $S^z=\pm 1$ triplet states is higher than that of the $S^z=0$ triplet state by $1/2(J_\perp^z+|J_\perp|)$. This gives an effective spin-1 with easy-plane single-ion anisotropy term $D(S^z)^2$ where $D=1/2(J_\perp^z+|J_\perp|)$. The interaction along the chain ladder gives an effective interaction for a spin-1 chain for $|J_\perp^{(z)}| \gg |J^{(z)}|$:

$$H=\sum_i \frac{1}{2}\frac{J}{2}(S_i^+ S_{i+1}^- + \text{H.c.}) + \frac{J^z}{2} S_i^z S_{i+1}^z + \frac{1}{2}(J_\perp^z + |J_\perp|)(S^z)^2. \tag{32}$$

For a given J and J^z the transition of the spin-1 chain from the disordered phase to ferromagnetism will depend on D only. This means that for strong interchain coupling we may expect a phase boundary $J_{\perp;\text{crit}}^z = J_{\perp;\text{crit}} + \text{const}$, where the constant is given by J^z. Considering the phase diagram for $S=1$ in the presence of D and J^z anisotropies,[18] one finds that there are two disordered phases adjacent to the ferromagnetic phase: for $|J^z|$ small, one finds the XY phase predicted by bosonization, for $|J^z|$ big, a large-D singlet phase. In both cases, the transition is first order. For the J^z considered, the disordered phase is the XY phase.

In the limit of strong antiferromagnetic interchain coupling the spin pairs on adjacent sites on the two chains will be forced into total $S^z=0$ states. It can be shown, extending a proof given by Strong and Millis[7] to anisotropic interchain couplings, that in the limit of strong interchain coupling and strong J^z, the spin ladder has a ground state where the total S^z spin component per spin ladder rung is conserved and zero. In this limit the spin ladder can be mapped to an Ising spin chain in a transverse magnetic field as treated by Pfeuty:

$$H=\frac{J_\perp}{2}\sigma_i^z + \frac{J^z}{2}\sigma_i^x \sigma_{i+1}^x, \tag{33}$$

where the standard Pauli spin matrices have been used ($+1$ is the triplet and -1 the singlet state with total magnetization 0). Taking the results of Pfeuty, one expects a second order phase transition of the Ising universality class in two classical dimensions for $J^z>|J_\perp|$ from a paramagnetic (i.e., our quantum spin liquid) to a ferromagnetic phase. Generalizing the mapping of the spin ladder to the Ising model to *anisotropic* interchain couplings reveals an interesting crossover of the quantity driving the phase transition: whereas in the weak coupling limit it is $J_\perp^z$ according to bosonization, in the strong coupling limit it is $J_\perp$.

The interest of a numerical study of this phase transition is of course to determine the precise nature of the crossover,

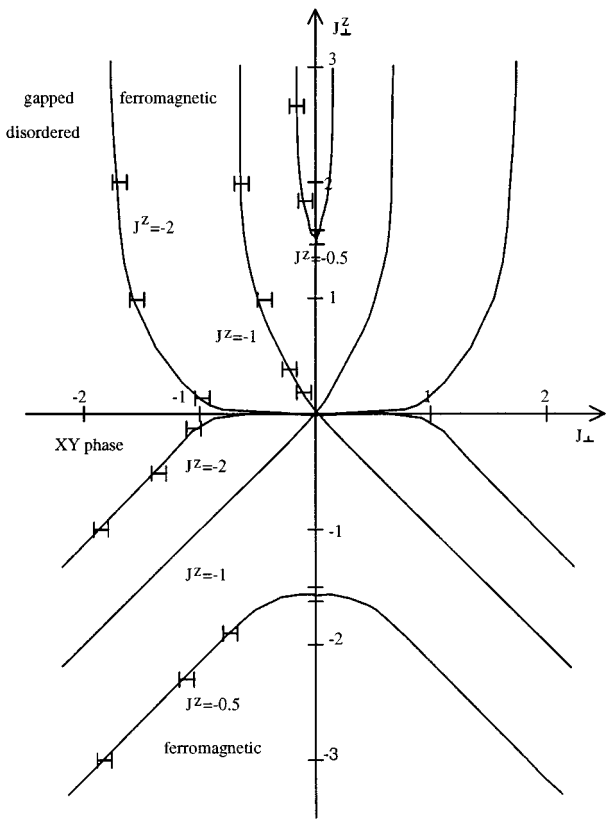

FIG. 6. Transition lines between ferromagnetic and adjacent paramagnetic phases in dependence of the single-chain anisotropy J^z and the anisotropic interchain coupling $J_\perp$ and $J_\perp^z$. The inner phase is for any line the ferromagnetic phase; the outer phase the XY phase in the lower portion of the diagram and the gapped quantum liquid phase in the upper portion. The phase boundary between the XY phase and the gapped phase could not be determined by our means. Error bars indicate limits to within which transition points were determined.

in particular in the weak and intermediate coupling limit, which are the physically most interesting cases. Our results are presented in Fig. 6.

The transition lines in the lower portion of the phase diagram were easily obtained with $M=50$ and chains up to length 50. We could observe (except for extremely short chains) *no* finite size effects, i.e., the localization of the transition remained stable with the length of the considered chains. The transition lines obey for large interchain coupling very well the predicted limiting behavior, where the large interchain coupling limit seems to be reached for already rather small coupling values.

In the upper part of the phase diagram, the situation depends strongly on J^z. For increasing J^z, the ferromagnetic phase appears for smaller $J_\perp^z$, as predicted by bosonization. The regime where the transition is dominated by $J_\perp^z$ predicted by bosonization must be so small that we could not observe it: the transition line curves very quickly upwards to become dominated by $J_\perp$. For $J^z=1$, the transition line touches the no-interchain-coupling point at the origin. For larger J^z, the transition line is first dominated by $J_\perp^z$ (as predicted by bosonization), before curving abruptly upwards to be dominated by $J_\perp$. The critical $J_\perp$ is systematically smaller than J^z (the prediction), but approaches this value for strong J^z: for $J^z=3$, we find a critical $J_\perp\approx 2.8$. In the strong coupling regime, the nature of the disordered phase can be clearly established as the gapped quantum liquid phase. The residual presence of the disordering J interaction limits the ferromagnetic phase.

Establishing the transition lines in this part of the phase diagram was more difficult, as severe finite size effects occur, whereas for $M=60$ finite precision effects on the transition line were already negligible (tested by repeating calculations for various M). We considered chains up to a length of 2×200 to locate the transition down to 0.1. The results were found to obey well a linear dependence in L^{-1}, which allowed extrapolation to the thermodynamic limit. The L^{-1} behavior is to be expected from the critical exponent $\nu=1$ of the Ising transition in two dimensions; scaling theory predicts $J(L)-J(\infty)\propto L^{-1/\nu}$. The effect of the open boundary conditions is mitigated by the great length of the chains considered and by the fact that the boundary terms should typically also contribute as L^{-1}. We can therefore not distinguish whether our chains are long enough to do a sort of (not too precise) finite size scaling or whether the coincidence that $\nu=1$ allowed a reasonable extrapolation.

V. CONCLUSION

Using the DMRG algorithm, we could investigate large parts of the phase diagram of coupled spin-1/2 chains. As was to be expected from the nature of this algorithm, the quality of the results depends sensibly on the phase under study. Phase boundaries could be located precisely only in the case of the transitions to ferromagnetism. We have provided a careful study of the gap behavior for small interchain coupling, both ferromagnetic and antiferromagnetic and find that the gap persists down to small couplings of the order of 0.05. We think that our results are conclusively showing the existence of the gap down to infinitesimal couplings. We also show that the Haldane phase is generically described by the AKLT model. Our findings are in good agreement with the bosonization results, which therefore seems to provide the adequate description of the problem of the coupled spin chains.

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