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# Models with exact ground states connecting smoothly the $S=\frac{1}{2}$ dimer and $S=1$ Haldane phases of one-dimensional spin chains

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We investigate the isotropic two-leg $S=\frac{1}{2}$ ladder with general bilinear and biquadratic exchange interactions between spins on neighboring rungs, and determine the Hamiltonians that have a matrix-product wave function as an exact ground state. We demonstrate that a smooth change of parameters leads one from the $S=\frac{1}{2}$ dimer and Majumdar-Ghosh chains to the $S=1$ chain with biquadratic exchange, which proves that these model systems are in the same phase. The family of Hamiltonians also includes a set of models of isotropic $S=\frac{1}{2}$ chains with only bilinear nearest- and next-nearest-neighbor interactions. The ground state for these models becomes unstable at a line of first-order phase transitions to the ferromagnetic state. [S0163-1829(97)50342-0]

Low-dimensional quantum antiferromagnets have attracted a large amount of both theoretical and experimental interest in recent years. Theoretically, the results of calculations for model systems in one dimension (1D) clearly show the difference between systems with a gapless spectrum of excitations and power-law decay of spin correlations and gapped systems with exponentially decaying correlation functions. The main representatives of these two classes are, respectively, the $S=\frac{1}{2}$ chain with isotropic nearest-neighbor (NN) exchange interaction[1] and the isotropic $S=1$ (Haldane) chain.[2] Gapped elementary excitation spectra are also found in more complicated low-dimensional $S=\frac{1}{2}$ systems such as chains with sufficiently strong additional next-nearest-neighbor (NNN) exchange or with alternating exchange (with noninteracting dimers as the simplest limit) and also isotropic spin ladders with an even number of legs.[3]

Many of these models are realized to a high degree of accuracy in simple compounds, as demonstrated by the following examples: $KCuF_3$ (1D isotropic $S=\frac{1}{2}$ antiferromagnet[4]), $CaCuGe_2O_6$ (weakly interacting dimers[5]), $(VO_2)P_2O_7$ (Ref. 6) and $SrCu_2O_3$ (Ref. 7) (two-leg spin ladder), and $Ni(C_2H_8N_2)_2NO_2ClO_4$ (commonly called NENP, 1D $S=1$ antiferromagnet[8]). Although the precise spin Hamiltonians of these substances are not known, the study of the simple theoretical models mentioned above has contributed in an essential way to the understanding of the behavior of the real materials and these are believed to be in the same phase as the simple models.

In recent years arguments and numerical evidence have been presented stating that the various models with a gapped excitation spectrum, in particular the $S=\frac{1}{2}$ dimer chain, the gapped nearest- and next-nearest-neighbor exchange chain, the two-legged $S=\frac{1}{2}$ spin ladder, and the $S=1$ (Haldane) chain are all in the same phase.[9–14] In this paper we present the following proof for this conjecture: We describe a class of Hamiltonians with exactly known nondegenerate ground states and show that it is possible, by a continuous change of parameters within this class, to connect smoothly the Hamiltonians of the 1D dimer chain, the Majumdar-Ghosh chain, a generalized spin ladder (which includes biquadratic interactions), and the $S=1$ antiferromagnetic chain with additional biquadratic exchange. Given the relevance of these model systems with exactly known ground states for the traditional model systems and for the real quasi-1D compounds, this proves the existence of a single phase for the gapped low-dimensional spin systems above. As a ''byproduct'' of this investigation, we also present a set of models of frustrated $S=\frac{1}{2}$ spin chains (including only bilinear NN and NNN interactions) whose ground states can be found exactly.

Our approach starts from the observation[13] that the exactly known ground states of the Shastry-Sutherland $S=\frac{1}{2}$ chain[15]

$$H=\sum_n \left(1+(-1)^n\delta\right)\mathbf{S}_n\cdot\mathbf{S}_{n+1}+\frac{1}{2}(1-\delta)\mathbf{S}_n\cdot\mathbf{S}_{n+2}, \quad (1)$$

which includes the Majumdar-Ghosh ($\delta=0$) (Ref. 16) and dimer ($\delta=1$) limits as special cases, and the $S=1$ chain with biquadratic exchange,

$$H=\sum_n \mathbf{S}_n\cdot\mathbf{S}_{n+1}-\beta(\mathbf{S}_n\cdot\mathbf{S}_{n+1})^2 \quad (2)$$

at $\beta=-\frac{1}{3}$ [the Affleck, Kennedy, Lieb, and Tasaki (AKLT) model,[17] which is believed to be in the same phase as the Haldane chain with $\beta=0$)] have very similar structures: both ground states can be written as matrix-product (MP) wave functions,

$$|\psi_0\rangle=\prod_i g_i, \quad g_i=\begin{pmatrix} b|s\rangle_i+a|t_0\rangle_i & -\sqrt{2}a|t_{+1}\rangle_i \\ \sqrt{2}a|t_{-1}\rangle_i & b|s\rangle_i-a|t_0\rangle_i \end{pmatrix}. \quad (3)$$

 

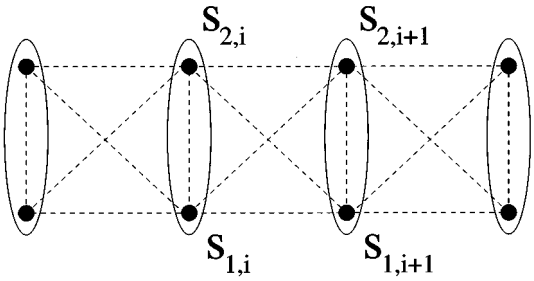


FIG. 1. Generalized spin-$\frac{1}{2}$ ladder with all possible isotropic exchange interactions between nearest-neighbor rungs. Ovals show spin pairs whose states are involved in the elementary matrix $g_i$ defined by Eq. (3). Couplings are described in the text; see Eq. (4).

The ground state of the Shastry-Sutherland chain is obtained setting $a=b=\frac{1}{2}$, where $|s\rangle_i$ and $|\vec{t}\rangle_i$ are the singlet, respectively, triplet formed by two spins $S=\frac{1}{2}$ on adjacent sites $n$ and $n+1$ [$n$ even for $\delta>0$ in Eq. (1)]. The ground state of the AKLT chain is obtained by setting $a=1/\sqrt{3}$, $b=0$, and identifying the remaining triplet with the three states of the spin $S=1$ at site $i$. The matrix elements of the MP wave function $|\psi_0\rangle$ are related to boundary effects for open boundary conditions whereas for periodic boundary conditions the trace should be taken.[17] Matrix-product (or finitely correlated) wave functions were first introduced by Fannes *et al.*[18] a decade ago and have since then found widespread applications in exact and variational calculations.[19–23] These wave functions are characterized by finite (and typically rather short) correlation lengths and are therefore tailored to deal with gapped systems.

It should be emphasized that our MP ansatz for the ladder (3), in contrast to that used in Ref. 22, respects rotational symmetry of the Hamiltonian (4), i.e., the wave function $|\psi_0\rangle$ under periodic boundary conditions is a global singlet.[13,24] The ansatz used by Su[22] has a ''built-in'' broken rotational symmetry and thus can access only states of a ferromagnetic type.

We generalize the models of Eqs. (1) and (2) by considering the following spin ladder Hamiltonian (see Fig. 1): $\hat{H}=\Sigma_i \hat{h}_{i,i+1}$, where

$$\begin{aligned}\hat{h}_{i,i+1}=&C_0+(J_0/2)\mathbf{S}_{1,i}\cdot\mathbf{S}_{2,i}+(J_0'/2)\mathbf{S}_{1,i+1}\cdot\mathbf{S}_{2,i+1}\\&+J_1\mathbf{S}_{1,i}\cdot\mathbf{S}_{1,i+1}+J_1'\mathbf{S}_{2,i}\cdot\mathbf{S}_{2,i+1}+J_2\mathbf{S}_{1,i}\cdot\mathbf{S}_{2,i+1}\\&+J_2'\mathbf{S}_{2,i}\cdot\mathbf{S}_{1,i+1}+K(\mathbf{S}_{1,i}\cdot\mathbf{S}_{1,i+1})(\mathbf{S}_{2,i}\cdot\mathbf{S}_{2,i+1})\\&+K'(\mathbf{S}_{1,i}\cdot\mathbf{S}_{2,i+1})(\mathbf{S}_{2,i}\cdot\mathbf{S}_{1,i+1})\\&+K''(\mathbf{S}_{1,i}\cdot\mathbf{S}_{2,i})(\mathbf{S}_{1,i+1}\cdot\mathbf{S}_{2,i+1}).\end{aligned}\tag{4}$$

This is the general isotropic $S=\frac{1}{2}$ Hamiltonian with exchange interactions restricted to neighboring rungs of the ladder. For periodic boundary conditions, $\frac{1}{2}(J_0+J_0')$ is the coupling on the rungs. In addition there are four pair exchange couplings on the legs and on the diagonals and three biquadratic terms. Together with the constant $C_0$ we have a total of ten parameters. One combination of these is irrelevant since it sets the energy scale. It is essential to include the diagonal interactions as first introduced by White[14] in order to obtain the various limits of interest. These limits include the isotropic spin ladder and also the $S=1$ chain when strongly ferromagnetic exchange on the rungs ($J_0\to-\infty$) is considered to form $S=1$ units with an effective pair interaction $J_{eff}$ and effective biquadratic interaction $K_{eff}$,

$$J_{eff}=(J_1+J_1'+J_2+J_2')/4+(K+K')/8,$$

$$K_{eff}=(K+K')/4.\tag{5}$$

Our procedure in the following is based on the ideas presented in Ref. 20 and generalizes the work for the $S=1$ chain with biquadratic exchange:[17] We start from the MP wave function (3), considering $|s\rangle$ and $|t_\mu\rangle$ as the states of a single rung, and require that the parameters in the Hamiltonian (4) and the free parameter $u=b/a$ in $|\psi_0\rangle$ satisfy the following conditions: (i) $|\psi_0\rangle$ is annihilated by $\hat{H}$, i.e.,

$$\hat{h}_{i,i+1}g_i g_{i+1}=0\,;\tag{6}$$

(ii) all other states of $\hat{H}$ have the energy $E>0$. Then $|\psi_0\rangle$ is the ground state of $\hat{H}$, with the energy density $-C_0$ per rung.

To proceed we write the local Hamiltonian $\hat{h}$ in the alternative formulation[21] using projectors on states with fixed angular momentum of the four spin plaquette $(i,i+1)$ of the ladder:

$$\begin{aligned}\hat{h}=&\lambda_2\sum_M|\Psi_{2,M}\rangle\langle\Psi_{2,M}|+\sum_{k,l=1,2}\lambda_0^{(k,l)}|\Psi_{0,0}^{(k)}\rangle\langle\Psi_{0,0}^{(l)}|\\&+\sum_{k,l=1,2,3}\lambda_1^{(k,l)}\sum_M|\Psi_{1,M}^{(k)}\rangle\langle\Psi_{1,M}^{(l)}|.\end{aligned}\tag{7}$$

Here $|\Psi_{J,M}^{(k)}\rangle$ are the multiplets which can be formed from the four spins $S=\frac{1}{2}$ of one plaquette: one quintuplet, three triplets, and two singlets; the ten parameters $\lambda_J^{(k,l)}=\lambda_J^{(l,k)}$ are linearly related to the ten parameters in the Hamiltonian of Eq. (4). The multiplets $|\Psi_{J,M}^{(k)}\rangle$ are given in terms of the singlets $|s\rangle$ and triplets $|t\rangle$ on rungs $i$ and $i+1$; the plaquette singlets are a linear combination of $|ss\rangle$ and $|(tt)_{J=0}\rangle$, the plaquette triplets are linear combinations of $|ts\rangle$, $|st\rangle$, and $|(tt)_{J=1}\rangle$, and the plaquette quintuplet is $|(tt)_{J=2}\rangle$. It is easily verified that only one singlet and one triplet occur in $g_i g_{i+1}$, namely

$$(3+u^4)^{-1/2}(u^2|ss\rangle-\sqrt{3}|tt\rangle_{J=0})\equiv|\Psi_0^{(1)}\rangle\,,\tag{8}$$

$$(1+u^2)^{-1/2}\left\{\frac{u}{\sqrt{2}}(|ts\rangle+|st\rangle)-|tt\rangle_{J=1}\right\}\equiv|\Psi_1^{(1)}\rangle\,.\tag{9}$$

A convenient choice for the remaining multiplets is

$$\begin{aligned}|\Psi_0^{(2)}\rangle&=(3+u^4)^{-1/2}(\sqrt{3}|ss\rangle+u^2|tt\rangle_{J=0}),\\|\Psi_1^{(2)}\rangle&=(1/\sqrt{2})(|ts\rangle-|st\rangle),\\|\Psi_1^{(3)}\rangle&=(1+u^2)^{-1/2}\{(1/\sqrt{2})(|ts\rangle+|st\rangle)+u|tt\rangle_{J=1}\},\\|\Psi_2\rangle&=|tt\rangle_{J=2}.\end{aligned}\tag{10}$$

Conditions (i) result in five equations, corresponding to

$$\lambda_0^{(1,1)}=\lambda_0^{(1,2)}=\lambda_1^{(1,1)}=\lambda_1^{(1,2)}=\lambda_1^{(1,3)}=0. \quad (11)$$

Thus, in order to lead to MP ground states, the Hamiltonian has to project on the space $|\Psi_0^{(2)}\rangle$, $|\Psi_1^{(2)}\rangle$, $|\Psi_1^{(3)}\rangle$, $|\Psi_2\rangle$ and condition (ii) results in the inequalities

$$\lambda_0^{(2)}>0, \quad \tilde{\lambda}_1^{(\alpha)}>0, \quad \lambda_2>0, \quad (12)$$

where $\tilde{\lambda}_1^{(\alpha)}$ ($\alpha=1,2$) are the two eigenvalues of the matrix $\lambda_1^{(i,j)}$, $(i,j=2,3)$. The inequalities (12) guarantee that the ground state is nondegenerate [apart from the fact that Eq. (3) describes four ground states with different behaviors at the boundaries of open ladders], since it can be shown by induction with respect to the ladder length that the plaquette states [Eqs. (8) and (9)] do not allow any zero energy state different from the MP ground state.

For an explicit discussion of the results we use a somewhat simplified Hamiltonian with less freedom than in the general case. First, we set $J_0=J_0'$, and from one of the conditions (i) we find that this necessarily means $J_1=J_1'$ (which respects the ladder symmetry) and $\lambda_1^{(2,3)}=0$; thus the eigenvalues $\tilde{\lambda}_1^{(\alpha)}$ are identical to the $\lambda_1^{(2,2)}$ and $\lambda_1^{(3,3)}$. Further we set $K-K'=K''=0$ (these combinations are found irrelevant in a more detailed treatment which will be published separately). Then we are left with the six coefficients $C_0$, $J_0$, $J_1$, $J_2$, $J_2'$, $K$ and the conditions (i) take the following form:

$$\begin{aligned}
&2J_1-J_2-J_2'+u^2(4C_0/3-J_0+K/2)=0,\\
&2(2J_1+J_2+J_2')-4C_0-J_0-7K/2+u^2(J_2+J_2'-2J_1)=0,\\
&2(J_2'-J_2)+u(4C_0-J_0+2J_1-J_2-J_2'-K/2)=0,\\
&2J_1+J_2+J_2'+3K/2-4C_0-J_0+2u(J_2-J_2')=0.
\end{aligned} \quad (13)$$

The general solution of these four linear equations contains two arbitrary constants, when the parameter $u=b/a$ of the MP wave function is fixed. We absorb one of the two constants in the energy scale, denote the remaining one by $x$ and define

$$u^2=F$$

to obtain the following family of Hamiltonians with exact MP eigenstates:

$$\begin{aligned}
C_0&=3[9+2x-3(1+x)F+3xF^2]/32,\\
J_0&=3[2-x-(1+x)F+xF^2]/4,\\
2J_1+J_2+J_2'&=[15-9(1+x)F+7xF^2]/4,\\
2J_1-J_2-J_2'&=-xF,\\
2J_2-2J_2'&=F^{1/2}[3(1+x)/2-xF],\\
K&=3(F-1)(xF-1)/4.
\end{aligned} \quad (14)$$

With these definitions the conditions of Eq. (12) become

$$\begin{aligned}
\lambda_0&=x[3+F^2(x)]/4>0,\\
\tilde{\lambda}_1^{(1)}&=[3(1+x)+2xF(x)]/8>0,\\
\tilde{\lambda}_1^{(2)}&=[1+F(x)][3(1+x)-2xF(x)]/8>0,\\
\lambda_2&=[18+8xF^2(x)-9(1+x)F(x)]/8>0.
\end{aligned} \quad (15)$$

The eigenvalues $\lambda_0$ and $\tilde{\lambda}_1^{(1)}$ are positive for $x>0$, $F>0$. The eigenvalues $\tilde{\lambda}_1^{(2)}$ and $\lambda_2$ require a more detailed discussion; it is easily seen that a sufficient (though not necessary) condition for $\lambda_2>0$ is $J_{eff}>0$, and the condition on $\tilde{\lambda}_1^{(2)}$ is equivalent to the requirement $u(J_2-J_2')>0$. We use $F=u^2$ instead of $u$, keeping in mind that changing the sign $u\to-u$ amounts just to interchanging the ladder legs and thus does not bring in any new physics; therefore from now on we assume that $F^{1/2}>0$.

The following illustrative members of this family of Hamiltonians are now easily obtained.

(i) Shastry-Sutherland model:

$$F=1, \quad x=3\delta/(2+\delta), \quad 0<\delta<1. \quad (16)$$

Since the MP wave function with $F=1$, i.e., $a=b$ corresponds to singlets on one type of diagonals,[13] this also covers (after a translation of one of the ladder legs) the case $a=0$. The eigenvalue $\lambda_0$ vanishes for $x=0$, which is to be expected since in the Majumdar-Ghosh limit a second degenerate eigenstate exists (singlets on the alternative bonds).

The solution (16) also applies for partially ferromagnetic interactions, $x>1$, respectively, $(1-\delta)/(1+\delta)<0$. Although the effective interaction between units on the diagonals is ferromagnetic, the Shastry-Sutherland dimer state is the ground state up to $x=9$ (corresponding to $\delta=-3$), since all $\lambda$'s are positive. At the singular point $\delta=-3$ the eigenvalue $\lambda_2$ vanishes and the energy of the dimer ground state coincides with the energy of the fully polarized ferromagnetic configuration. Thus this is the point of the first-order quantum phase transition from dimer to ferromagnetic phase.

(ii) Generalized AKLT model, defined by $F=0$ (i.e., $b=0$, so that only triplets on the rungs can occur):

$$F=0, \quad x \text{ finite}. \quad (17)$$

When choosing a convenient scale factor to render $J_{eff}=1$ this corresponds to the following Hamiltonian:

$$\begin{aligned}
&J_0=4/3-2x/3, \quad J_1=J_2=J_2'=5/6,\\
&K=K'=2/3, \quad K''=0, \quad C_0=3/4+x/3.
\end{aligned} \quad (18)$$

This is essentially the Hamiltonian of Ref. 17, but without requiring explicitly the coupling of two spins $S=\frac{1}{2}$ into a triplet, a result that could be easily obtained directly. The AKLT model in a strict sense is obtained for $x\to+\infty$ and $xF(x)\to0$.

(iii) For $xF(x)=1$ another class of Hamiltonians *without biquadratic terms* is obtained; the condition $\lambda_2>0$ leads to the restriction $x\geq\frac{1}{9}$. A nontrivial case $x=\frac{1}{9}$, when only one

diagonal exchange interaction is present, is equivalent to a chain with NN and NNN exchange:

$$C_0 = 7/12, \quad J_0 = J_0' = 2/3, \quad J_1 = J_1' = J_2' = -1,$$

$$J_2 = K = K' = K'' = 0. \tag{19}$$

This is an $S = \frac{1}{2}$ chain with alternating ferro- and antiferromagnetic exchange and ferromagnetic NNN interactions, a frustrated Heisenberg chain. As in (i), the eigenvalue $\lambda_2$ vanishes and the energy of the fully polarized ferromagnetic state coincides with that of the MP ground state (3). Thus we have obtained two exact points on the line where the chain with NN and NNN interactions[13] undergoes a first-order quantum phase transition to the ferromagnetic state.

(iv) A family of models with exact MP ground states connecting the Majumdar-Ghosh and the AKLT limits is obtained from, e.g.,

$$F(x) = 1/(1+x)^2. \tag{20}$$

Since the Majumdar-Ghosh and dimer chains have identical ground states, Eq. (20) explicitly demonstrates the possibility of transforming the Hamiltonian of the dimer $S = \frac{1}{2}$ chain continuously to the Hamiltonian of the AKLT chain without any singularity (or quantum phase transition) in the ground state.

In summary, we have provided an explicit proof that the gapped $S = \frac{1}{2}$ models listed in the introduction belong to the same phase as the AKLT model for the $S = 1$ chain. Since the latter model is accepted as the simplest representative of gapped isotropic $S = 1$ (Haldane) chains (although its equivalence with the bilinear $S = 1$ chain has not been formally proven so far) our result implies that dimer, Majumdar-Ghosh, and Haldane chains are in the same phase. In addition we have obtained the exact ground state for a new set of frustrated $S = \frac{1}{2}$ chains with alternating ferro- and antiferromagnetic NN and ferromagnetic NNN exchange. The ground state of these new models becomes unstable at a line of first-order phase transitions to the ferromagnetic state.

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