Non-Haldane Spin-Liquid Models with Exact Ground States

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We present a family of spin-ladder models which can be solved exactly for the ground state and exhibit non-Haldane spin-liquid properties as predicted recently by Nersesyan and Tsvelik [Phys. Rev. Lett. **78**, 3939 (1997)], and study their excitation spectra using a simple variational *Ansatz*. The elementary excitation is neither a magnon nor a spinon, but a pair of propagating triplet or singlet solitons connecting two spontaneously dimerized ground states. Second-order phase transitions separate this phase from the Haldane phase and the rung-dimer phase. [S0031-9007(98)05634-8]

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It is well known that one-dimensional (1D) Heisenberg antiferromagnets can exhibit several types of disordered "quantum spin liquid" phases. The spin-$\frac{1}{2}$ chain has a unique disordered gapless ground state with power-law decay of spin correlations, and its elementary excitations are pairs of spinons carrying spin $\frac{1}{2}$ [1]. The ground state of the frustrated $S=\frac{1}{2}$ chain with sufficiently strong next-nearest neighbor interaction is doubly degenerate, the excitations are also spinon pairs, but the spectrum is "gapful" [2–4]; in presence of any finite exchange alternation along the chain the spinon pairs get confined into well defined magnon excitations [5]. The spin-1 (Haldane) chain has a unique spin-liquid ground state with a gap above it formed by a triplet of magnons carrying spin $S=1$ [6]. The two-leg $S=\frac{1}{2}$ ladder, i.e., two Heisenberg $S=\frac{1}{2}$ chains coupled by a transverse exchange, also has a disordered gapful ground state with magnons as elementary excitations [7], and is believed to be essentially in the same phase as the Haldane chain, as well as frustrated $S=\frac{1}{2}$ chain with alternating exchange [8–10].

Recently, Nersesyan and Tsvelik [11] have proposed an interesting example of a 1D *"non-Haldane spin liquid"* which has a gapped spectrum but whose excitations are neither spinons nor magnons. Using field-theoretical arguments, they have shown that under certain conditions a two-leg $S=\frac{1}{2}$ Heisenberg ladder with additional leg-leg biquadratic interaction enters a spontaneously dimerized phase with the excitation spectrum determined by the two-particle continuum, and identified the elementary excitations as pairs of singlet and triplet domain walls connecting the two dimerized ground states.

In this Letter we present a set of models which exhibit non-Haldane spin-liquid properties as predicted by Nersesyan and Tsvelik, and whose ground state can be found *exactly*. We study their excitation spectrum within a simple variational approach, and discuss phase transitions into the Haldane and other phases.

We start from a more general ladder Hamiltonian which includes also transverse interaction along the ladder diagonals and two additional biquadratic interactions. The model is described by the Hamiltonian

$$\begin{aligned}\hat{H} = \sum_i & J(\mathbf{S}_{1,i}\mathbf{S}_{1,i+1} + \mathbf{S}_{2,i}\mathbf{S}_{2,i+1}) + J_r\mathbf{S}_{1,i}\mathbf{S}_{2,i} \\ & + V(\mathbf{S}_{1,i}\mathbf{S}_{1,i+1})(\mathbf{S}_{2,i}\mathbf{S}_{2,i+1}) \\ & + J_d(\mathbf{S}_{1,i}\mathbf{S}_{2,i+1} + \mathbf{S}_{2,i}\mathbf{S}_{1,i+1}) \\ & + K\{(\mathbf{S}_{1,i}\mathbf{S}_{2,i+1})(\mathbf{S}_{2,i}\mathbf{S}_{1,i+1}) \\ & - (\mathbf{S}_{1,i}\mathbf{S}_{2,i})(\mathbf{S}_{1,i+1}\mathbf{S}_{2,i+1})\}, \end{aligned} \tag{1}$$

where the indices 1 and 2 distinguish lower and upper legs, respectively, and i labels rungs. The model considered by Nersesyan and Tsvelik corresponds to $J_d = K = 0$. To construct the ground state Ψ_0 for the Hamiltonian (1), we will use the technique of matrix-product (MP) states [12,13]. We start from the following *Ansatz:*

$$\begin{aligned}\Psi_0 &= \mathrm{tr}\{g_1(\tilde{u})\cdot g_2(u)\cdots g_{2N-1}(\tilde{u})\cdot g_{2N}(u)\}, \\ g_i(u) &= u\cdot\hat{\mathbb{1}}|s\rangle_i + \sigma^{+1}|t_{+1}\rangle_i + \sigma^{-1}|t_{-1}\rangle_i + \sigma^0|t_0\rangle_i\,. \end{aligned} \tag{2}$$

Here $|s\rangle_i$ and $|t_\mu\rangle_i$ are, respectively, the singlet and triplet states of the ith rung, $2N$ is the total number of rungs (periodic boundary conditions are assumed), $\hat{\mathbb{1}}$ is the 2×2 unit matrix, σ^μ are the Pauli matrices, and u, $\tilde{u}$ are free parameters. A simpler version of this *Ansatz* with $u=\tilde{u}$ describes several known examples of valence bond type states, e.g., at $u=0$ the wave function Ψ_0 is the ground state of the effective Affleck-Kennedy-Lieb-Tasaki chain [14] whose $S=1$ spins are composed from pairs of $S=\frac{1}{2}$ spins of the ladder rungs,

$$\hat{H} = \sum_n \mathbf{S}_n\mathbf{S}_{n+1} - \beta(\mathbf{S}_n\cdot\mathbf{S}_{n+1})^2, \tag{3}$$

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at $\beta = -\frac{1}{3}$, and for $u = 1$ or $u = \infty$ one obtains two degenerate ground states of the Majumdar-Ghosh chain [2]. Originally (2) with $u = \tilde{u}$ was proposed in Ref. [15] as a variational wave function, and recently it was used by us [10] to construct another class of exact ground states for a more general ladder model. In the following, we set $u \neq \tilde{u}$, then the state Ψ_0 is dimerized and the translation for one rung leads to a different state with the same energy. The *Ansatz* (2) obeys rotational symmetry, i.e., Ψ_0 is a global singlet [15,16].

The Hamiltonian (1) can be rewritten as a sum of identical local terms coupling neighboring rungs, $\hat{H} = \sum_i (\hat{h}_{i,i+1} - E_0)$. Let us demand that the wave function (2) is a zero-energy ground state of $\hat{H}$ (which can always be achieved by the appropriate choice of E_0), then the following requirements have to be fulfilled [13]: (i) The local Hamiltonian $\hat{h}_{i,i+1}$ has to annihilate Ψ_0, which, due to the product property of (2), means that all elements of the two matrix products $g_i(u)g_{i+1}(\tilde{u})$, $g_i(\tilde{u})g_{i+1}(u)$ should be zero-energy eigenstates of $\hat{h}_{i,i+1}$; (ii) the other eigenstates of $\hat{h}_{i,i+1}$ should have positive energy. Those two conditions fix the structure of the local Hamiltonian as follows:

$$\hat{h}_{i,i+1} = \sum_{J=0,1,2} \sum_{M=-J}^{J} \lambda_J |\psi_{JM}\rangle\langle\psi_{JM}|, \qquad (4)$$

where the eigenvalues $\lambda_J > 0$, and $|\psi_{JM}\rangle$ are the components of the positive-energy multiplets constructed from the states of the four-spin plaquette $(i, i + 1)$:

$$\begin{aligned} |\psi_{00}\rangle &= [3 + (u\tilde{u})^2]^{-1/2}\{\sqrt{3}|ss\rangle + u\tilde{u}|tt\rangle_{J=0}\}, \\ |\psi_1\rangle &= [2 + f^2]^{-1/2}\{f|tt\rangle_{J=1} + |st\rangle + |ts\rangle\}, \\ |\psi_2\rangle &= |tt\rangle_{J=2}, \qquad f \equiv (u + \tilde{u})/\sqrt{2}. \end{aligned} \qquad (5)$$

Here we use the notation $|tt\rangle_{J=1}$ for the triplet of states with the total spin $J = 1$ constructed, in turn, from two triplets on rungs i and $i + 1$, etc.

Now we demand that the structure (4) is compatible with the desired form of the Hamiltonian (1), which yields the connection between the parameters J, J_r, J_d, V, K on one hand, and the local eigenvalues λ_J and singlet weight parameters u, $\tilde{u}$ of the ground state wave function on the other. Those solutions can be classified into the following three types:

(A) "Checkerboard-dimer" model with $K = 0$, $J_d \neq 0$.—

$$\begin{gathered} u = \pm 1, \quad \tilde{u} = \mp 1, \quad V = 4J/3, \quad K = 0, \\ \lambda_1 = 1, \quad \lambda_0 = 3x/8, \quad \lambda_2 = 3(1 - x), \\ 0 \leq x \leq 1, \quad J_r = (8J/3)(2 - 3x)/(4 - 3x), \\ J_d = J_r/2, \quad J > 0, \end{gathered} \qquad (6)$$

the ground state energy density per rung is $E_0 = -\frac{3}{4}J$, and x is an arbitrary parameter. Two degenerate ground states are simply checkerboard-type products of singlet bonds along the ladder legs. A generic example from this family is the model at $x = \frac{2}{3}$ with a purely biquadratic interchain interaction:

$$J_r = J_d = K = 0, \qquad J = 3V/4 > 0. \qquad (7)$$

This "generic" model lies within the class of Hamiltonians considered by Nersesyan and Tsvelik. At $x = 1$ the eigenvalue λ_2 vanishes, indicating a first-order transition into the fully polarized ferromagnetic state.

(B) Multicritical model.—

$$\begin{gathered} u = -\tilde{u}, \quad \lambda_0 = 0, \quad \lambda_2 = 3\lambda_1, \\ J_r = V = 4J/3, \quad J_d = J_r/2, \quad K = 0, \quad J > 0. \end{gathered} \qquad (8)$$

This model has a remarkable property: *any* wave function $\Psi_0(u)$ of the form (2) with $u = -\tilde{u}$ is a ground state with the same energy per rung $E_0 = -\frac{3}{4}J$. One can show that two ground state (g.s.) wave functions with different values of u are *asymptotically orthogonal* in thermodynamic limit $N \to \infty$: $\langle\Psi_0(u)|\Psi_0(u')\rangle = z^N$, $z(u, u') \leq 1$, so that the degeneracy of the ground state is exponentially large. It is easy to observe that the model (8) is a particular case of (6) at $x = 0$, so that the model (6) has another phase transition point at $x = 0$; below we will argue that this transition is of the first order.

(C) Model with two second-order phase boundaries with $J_d = 0$, $K \neq 0$.—

$$\begin{aligned} u = -\tilde{u}, \quad K = J_r &= \lambda_0(u^2 - 1)(u^2 + 3)/2, \\ J_d = 0, \quad V &= \lambda_0(5u^4 + 2u^2 + 9)/4, \\ J &= 3\lambda_0(u^4 + 10u^2 + 5)/16, \\ \lambda_1 &= \lambda_0(3u^4 + 14u^2 + 15)/8, \\ \lambda_2 &= \lambda_0(5u^4 + 18u^2 + 9)/8, \end{aligned} \qquad (9)$$

the g.s. energy per rung is $E_0 = -\frac{3}{64}\lambda_0(7u^4 + 22u^2 + 19)$. This is a one-parametric family of models since u is arbitrary (the parameter λ_0 just sets the energy scale and thus is irrelevant). A particular case $u = \pm 1$ again leads to the generic model (7). One can readily observe that at $u = 0$ or $u = \infty$ the ground state is no more dimerized. The state with $u = 0$ describes the ground state of an effective $S = 1$ chain (3) with $\beta = -\frac{1}{3}$; the state with $u = \infty$ corresponds to a product of singlet bonds on the rungs. It is easy to calculate spin-spin and dimer-dimer correlation functions $C_S(n) = \langle S^z_{1,i} S^z_{1,i+n}\rangle$ and $C_D(n) = \langle D_i D_{i+n}\rangle$; here $D_i = \mathbf{S}_{1,i} \cdot (\mathbf{S}_{1,i+1} - \mathbf{S}_{1,i-1})$:

$$\begin{aligned} C_S(n) &= (u^2 + 3)^{-1}(z_+ z_-)^n(\delta_{n,2k} - z_-\delta_{n,2k+1}), \\ C_D(n) &= 144u^2/(u^2 + 3)^4, \\ z_\pm &= (u \pm 1)^2/(u^2 + 3). \end{aligned} \qquad (10)$$

One can see that the dimer correlations exhibit long-range order vanishing for $u \to 0, \infty$, but remarkably there is no exponential tail. The spin correlation length goes through zero at $u = 1$ and diverges at $u \to \infty$; however, there is no long-range spin order at $u \to \infty$ since the amplitude of spin correlations vanishes in this limit. Thus, one can conclude that the model (C) exhibits two second-order phase transitions: into the Haldane phase at $u = 0$ and into the rung-dimer phase at $u = \infty$. We will show below that those transitions are characterized by vanishing singlet and triplet gaps, respectively.

By induction with respect to the ladder length one can prove that in cases (A) and (C) the two ground states given by the MP *Ansatz* are the only ground states of the system.

Elementary excitations of the model (A) can be easily visualized as singlet or triplet diagonal bonds separating the two ground states and thus being solitons in the dimer order (see Fig. 1). Since solitons can be created only in pairs, the excitation spectrum is a two-particle continuum. To study the scattering soliton states, one may consider the ladder with $2N + 1$ rungs and periodic boundary conditions, and write down a simple single-soliton variational state with a certain value of momentum p and parity $\zeta = \pm 1$:

$$|p\rangle_{t,s}^{\zeta} = \sum_n e^{ip(2n+1)}|n\rangle_{t,s}^{\zeta}, \qquad (11)$$

Here the momenta are defined in terms of the Brillouin zone of nondimerized ladder, so that $p \in [0, \pi]$. The states $|n\rangle_{t,s}^{\zeta}$ are shown in Fig. 1; in a MP formulation they can be written as

$$|n\rangle_{s,t}^{\zeta} = \prod_{i=1}^{n}[g_{2i-1}(\widetilde{u})g_{2i}(u)]g_{2n+1}^{(s,t)}\prod_{i=n+1}^{N} g_{2i}(\widetilde{u})g_{2i+1}(u),$$
$$g_{\zeta}^{s} = g(u) - \zeta g(\widetilde{u}), \quad g_{\zeta,\mu}^{t} = \sigma^{\mu}g(u) + \zeta g(\widetilde{u})\sigma^{\mu}. \qquad (12)$$

Here $\mu = 0, \pm 1$ denotes the z projection of spin of the triplet excitation. Another candidate for the role of the elementary excitation is a magnon (the Haldane triplet); the corresponding variational wave function can be again written in the form (11) with

$$|n\rangle_{H}^{\zeta} = \prod_{i=1}^{n-1}[g_{2i-1}(\widetilde{u})g_{2i}(u)]g_{\zeta}^{H}\prod_{i=n+1}^{N} g_{2i-1}(\widetilde{u})g_{2i}(u),$$
$$g_{\zeta,\mu}^{H} = \sigma^{\mu}g_{2n-1}(\widetilde{u})g_{2n}(u) + \zeta g_{2n-1}(\widetilde{u})\sigma^{\mu}g_{2n}(u). \qquad (13)$$

The variational dispersion laws have the following form:

$$\varepsilon(p) = e_0/[1 + 2c_0A(z,p)],$$
$$A(z,p) = [\cos(2p) - z]/[1 + z^2 - 2z\cos(2p)], \qquad (14)$$

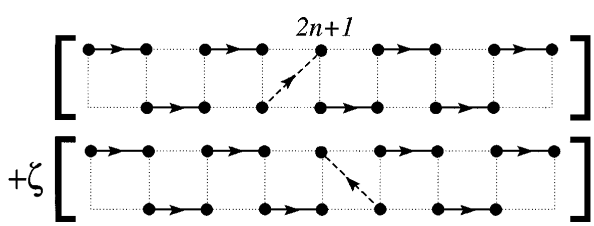

FIG. 1. The states $|n\rangle_{t,s}^{\zeta}$ used in Eq. (11), in a special case of the model (7). Thick solid lines indicate singlet bonds, and thick dashed lines can be either singlets or triplets. Arrows indicate the "direction" of the singlet bonds [i.e., $|s_{1\to 2}\rangle = 2^{-1/2}(|\uparrow_1\downarrow_2\rangle - |\downarrow_1\uparrow_2\rangle)$].

and for the model (6) one has, in J units,

$$c_0^{s,t} = z_{s,t}(1/2 - \zeta), \quad z_{s,t} = 1/4, \quad z_H = c_0^H = 0,$$
$$e_0^H = 1, \quad e_0^s = \frac{4 + 3x}{(4 - 2\zeta)(4 - 3x)}, \qquad (15)$$
$$e_0^t = \frac{44 - 39x}{6(2 - \zeta)(4 - 3x)}.$$

One can see that the lowest energy is always reached for the odd-parity states ($\zeta = -1$). The Haldane triplet is in this case dispersionless, and has a high energy equal to 1. The elementary excitation is a soliton-antisoliton pair, and for the scattering states its energy is given by

$$\widetilde{E}(k,q) = \varepsilon_{s,t}[(k+q)/2] + \varepsilon_{s,t}[(k-q)/2], \qquad (16)$$

where k and q are the total and relative momentum. For $x = \frac{2}{3}$ [i.e., for the generic model (7) with zero transverse exchange] the energies of triplet and singlet solitons coincide. The lowest boundary $E(k)$ of the continuum described by (16) at $x = \frac{2}{3}$ is shown in Fig. 2. The gap is given by $E(0) = E(\pi) = \frac{1}{2}J$, and the lowest excitation has a 16-fold degeneracy because the states of a soliton pair can be classified into two singlets (ss) and $(tt)_{J=0}$, three triplets (st), (ts), and $(tt)_{J=1}$, and one quintuplet $(tt)_{J=2}$. The energy of the Haldane triplet is lower than the continuum boundary in the vicinity of the zone center $k = \frac{\pi}{2}$, indicating the possible presence of bound soliton-antisoliton states. If the transverse exchange is switched on (i.e., $x \neq \frac{2}{3}$), the singlet-triplet degeneracy is lifted, and for $x < \frac{2}{3}$ ($x > \frac{2}{3}$) the lowest excitation is determined by singlet (triplet) solitons, respectively. Behavior of the corresponding gaps is shown in Fig. 3(a); one can see that for both phase transition points $x = 0$ and $x = 1$ the gaps remain finite, which suggests that the transition to the "multicritical" state at $x = 0$ is of the first order.

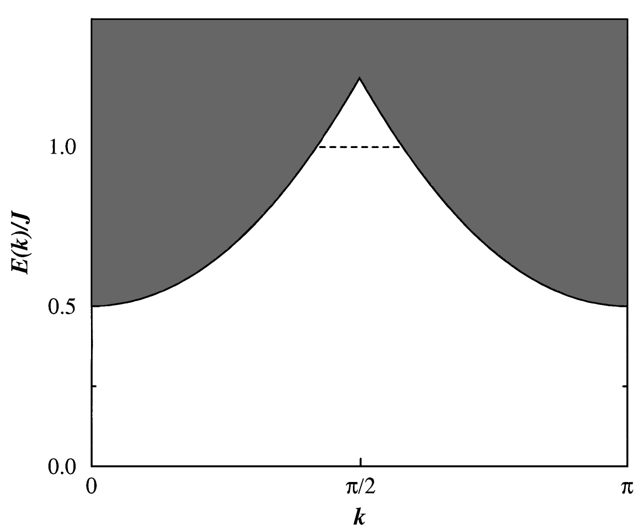

FIG. 2. The excitation spectrum of the model (7). The continuum is determined by free two-soliton states; its lowest boundary is 16-fold degenerate. The dashed line is determined by the Haldane triplet excitation (13) and indicates a variational estimate for bound soliton-antisoliton states.

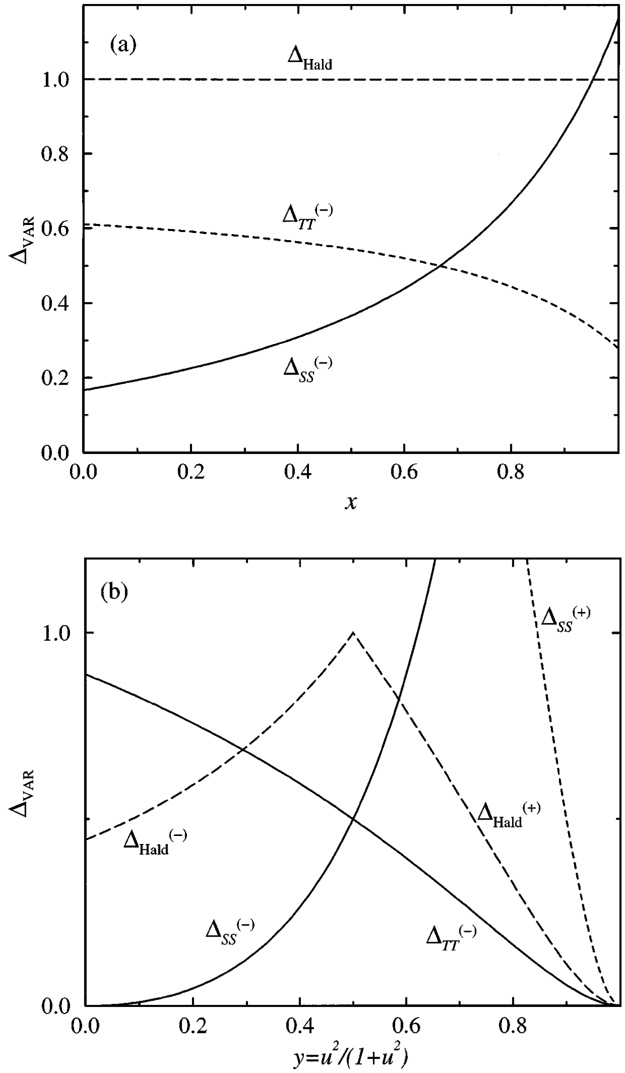

FIG. 3. (a) The gaps of different variational excitations for the model (6); (b) the same for model (9). Here Δ_{SS}^{ζ}, Δ_{TT}^{ζ}, and Δ_{H}^{ζ} denote the gaps of singlet-singlet, triplet-triplet soliton pairs, and the Haldane triplet, respectively, and $\zeta = \pm 1$ is the parity.

The *Ansätze* (12) and (13) can be used for the model (C) as well. One again obtains the dispersion laws of the form (14), with

$$\begin{gathered}
c_0^s = z_s(1 + \zeta z_s^{-1/2})/2, \quad c_0^t = z_t(1 - \zeta z_t^{-1/2})/2, \\
e_0^s = 12u^2/\{(u^2+3)^2(1+\zeta z_s^{1/2})\}, \\
e_0^t = 4(u^2+2)/\{(u^2+3)^2(1-\zeta z_t^{1/2})\}, \\
c_0^H = z_H + \frac{\zeta z_H^{1/2}(1-z_H)}{2(1+\zeta z_H^{1/2})}, \\
e_0^H = \frac{8 z_t^{1/2}}{(u^2+3)(1+\zeta z_H^{1/2})}, \quad z_s^{1/2} = \frac{u^2-3}{u^2+3}, \\
z_t^{1/2} = \frac{u^2+1}{u^2+3}, \quad z_H^{1/2} = \frac{u^2-1}{u^2+3}.
\end{gathered} \tag{17}$$

Behavior of the gaps is shown in Fig. 3(b) as a function of parameter $y = u^2/(1+u^2)$. Again, the lowest excitations are always soliton pairs. At $y \to 0$ the odd-singlet soliton gap goes to zero, indicating the second-order transition to the Haldane phase. At $y \to 1$ three gaps (of even-singlet and odd-triplet solitons and of the even Haldane triplet) vanish, signaling another second-order transition into the rung-dimer phase. Actually, it follows from (17) that at $y \to 0$ (1) the whole continuum of singlet (triplet) soliton pairs collapses to zero.

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