Phase Diagram of an Asymmetric Spin Ladder

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We investigate an asymmetric zigzag spin ladder with different exchange integrals on both legs using bosonization and renormalization group approaches. When the leg exchange integrals and frustration both are sufficiently small, renormalization group analysis shows that the Heisenberg critical point flows to an intermediate-coupling fixed point with gapless excitations and a vanishing spin velocity. When they are large, a spin gap opens and a dimer liquid is realized. Here, we find a continuous manifold of Hamiltonians with dimer product ground states, interpolating between the Majumdar-Ghosh and sawtooth spin-chain model.

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The interplay of geometric frustration and quantum fluctuations, and eventually broken translational invariance, in low-dimensional spin systems gives rise to novel magnetic phases. Examples include spin chains with interactions beyond nearest neighbors, spin ladders, triangular, and Kagomé systems [1]. Spin ladders, in particular, have attracted much interest and several model problems are well understood [2] and highlight the role played by frustration. Spin-isotropic two-leg ladders with railroad geometry quite generally lead to a singlet ground state separated by a finite excitation gap from the first triplet states [2]. Zigzag ladders are more strongly frustrated and, depending on the ratio of the leg to rung exchange integrals, may have gapless spin liquid ground states or gapped dimer states [3]. Compounds such as $Cu_2(C_5H_{12}N_2)_2Cl_4$ and $CuGeO_3$ have been suggested to be described as railroad and zigzag ladders, respectively [4].

Little work has been done on asymmetric spin ladders where the exchange integrals on both legs differ. Only the extreme case where one leg of a zigzag ladder is missing entirely (sawtooth or Δ chain) has been solved [5,6]. The ground state of this model is a product of nearest-neighbor (NN) singlets and there is a spin gap, as in the Majumdar-Ghosh (MG) model [7]. The properties of the excitations in both models are different, however. Sawtooth chains may describe the material $YCuO_{2.5}$ [5,6]. Here, we perform a systematic study of asymmetric zigzag spin ladders. Important questions concern possible new phases generated by the leg asymmetry, their excitation spectra, and their physical properties, as well as quantitative changes brought about by leg asymmetry to the excitations in the more usual phases found on zigzag ladders (spin liquid, Néel, and dimer states).

We consider a Heisenberg model on the structure shown in Fig. 1, and represent this as a chain with an alternating next-nearest-neighbor (NNN) exchange

$$H = \sum_l \{J_1 \mathbf{S}_l \cdot \mathbf{S}_{l+1} + [J_2 + (-1)^l \delta]\, \mathbf{S}_l \cdot \mathbf{S}_{l+2}\}, \qquad (1)$$

where $J_1 \equiv 1$ and $J_2 \pm \delta$ are the NN and alternating NNN coupling constants, respectively.

$\delta = 0$ is the ordinary zigzag ladder or frustrated spin chain [3], and fixing in addition $J_2 = \frac{1}{2}J_1$ gives the exactly solved MG model [7]. The sawtooth chain has $\delta = J_2 = \frac{1}{2}J_1$ [5,6].

Following the general approach to map the quantum spin model to a continuum field theory [8] and using the standard dictionary of Abelian bosonization [9], we obtain an effective boson Hamiltonian $H = H_0 + H_1$ with

$$H_0 = \int dx\, \frac{u}{2\pi}\left[K(\pi\Pi)^2 + \frac{1}{K}(\partial_x\Phi)^2\right], \qquad (2)$$

$$H_1 = \int dx\left[\frac{g_3}{2(\pi a)^2}\cos 4\Phi + \frac{g_1}{\pi^2 a}(\partial_x\Phi)\cos 2\Phi\right]. \qquad (3)$$

$\Phi(x)$ is a bosonic phase field and $\Pi(x)$ its canonically conjugate momentum. u and K are the effective spin velocity and coupling constants, including the effects of marginal interactions. a is a short-distance cutoff, $g_3 \propto 1 - J_2/J_{2c}$ is the Umklapp-scattering amplitude, and $g_1 \propto \delta$ is the amplitude of the alternating NNN field. In this paper, we consider only the case $J_1/2 \geq J_2 > \delta$, while, for $J_2 > 0.5J_1$, quite different field theory treatments are required [10,11].

For $\delta = 0$, the model (1) is well understood [3]. Its elementary excitations are spinons which are gapless for $J_2 < J_{2c} = 0.2412$ [4] when frustration is irrelevant and the ground state is unique, or gapped for

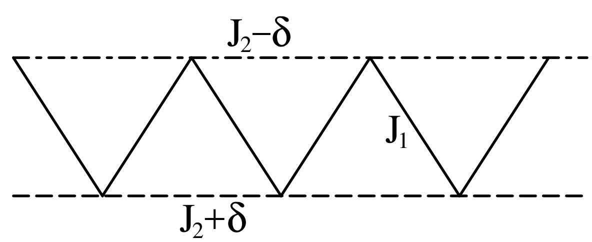

FIG. 1. The asymmetric zigzag spin ladder.

$J_2 > J_{2c}$ when frustration is relevant and the ground state is doubly degenerate. In the field theory (2), (3), this translates into the g_3 term being either marginally irrelevant, leading to the weak-coupling Heisenberg fixed point ($K^{(H)} = 1/2, g_3^{(H)} = 0$) [8], or relevant, yielding a strong-coupling dimer state. When the SU(2) spin symmetry is broken, a Néel state or an easy-plane spin liquid may form. Introducing dimerization, i.e., an alternating J_1, produces an effective confining potential between the spinons. The elementary excitations become a spin triplet and a spin singlet above the unique ground state. In the language of field theory, the external dimerization corresponds to a relevant term $\sin 2\Phi$ which lifts the double degeneracy of the dimer ground state [12].

Qualitative results on the influence of the new interaction (g_1) can be obtained from physical considerations alone. First, the scaling dimensions of the Umklapp and nearest-neighbor alternation terms g_3 and g_1 are

$$d_{g_3} = 4K, \qquad d_{g_1} = K + 1. \tag{4}$$

At the Heisenberg fixed point, g_3 is marginal with $d_{g_3} = 2$, while the g_1 term with $d_{g_1} = 3/2$ is relevant. We conclude that g_1 destabilizes the isotropic Heisenberg fixed point and the spin liquid ground state. On the other hand, there is no standard strong-coupling theory for the g_1 term. Usually (e.g., $g_3 \rightarrow \pm\infty$), the boson field $\Phi(x)$ locks into a constant value with small fluctuations, and an associated excitation gap. Such a phase locking, however, is forbidden by the $\partial_x \Phi$ prefactor to the $\cos(2\Phi)$ term in H_1. Second, the g_1 term, induced by the alternating NNN interaction, does not confine the spinons and plays a role very different from the external dimerization, as can be checked in the dimer state by comparing the sawtooth chain [5,6] with the MG model [7]. Moreover, from differences in the size of the spin gaps in these two models, it follows that the g_1 term quite generally counteracts the Umklapp term while an external NN dimerization would cooperate.

That g_1 opens no spin gap despite being a relevant perturbation of the Heisenberg fixed point is also corroborated by the absence of a magnetization plateau in our model in small magnetic fields [13]. A necessary condition for the formation of a magnetization plateau in the absence of modulated external fields is an alternating component of the exchange integrals [14,15]. For an alternating NN exchange, a magnetization plateau is observed in small magnetic fields, but alternating NNN exchange is observed only in high fields [13,15].

We now perform a perturbative renormalization group (RG) analysis by mapping the model on a modified (by g_1) classical 2D *XY* model [16,17]. Introducing the reduced variables $y_3 = g_3/\pi u$ and $y_1 = g_1/\sqrt{2}\,\pi u$, we obtain the linearized RG equations

$$\frac{dK}{dl} = -y_3^2 K^2 + y_1^2 K^4, \tag{5}$$

$$\frac{dy_3}{dl} = (2 - 4K) y_3 + K^2 y_1^2, \tag{6}$$

$$\frac{dy_1}{dl} = (1 - K) y_1 - 4K^2 y_1 y_3, \tag{7}$$

$$\frac{du}{dl} = -\frac{1}{2} u y_1^2 (1 + K) K^2 \tag{8}$$

under a change of length scale $a \rightarrow a e^{dl}$. These equations, and our solutions to be discussed below, can also accommodate anisotropy in the NN and NNN exchange integrals. The RG equation for the spin velocity u is a consequence of the anisotropy of the g_1 interaction in the classical 2D *XY* model, i.e., its nonretarded but nonlocal character in the quantum field theory (3), and has been discussed before in the 1D electron-phonon problem [18]. For $y_1 = 0$, one finds the three generic phases discussed earlier [3]: (i) a weak-coupling spin liquid phase ($g_3^\star = 0, K^\star \geq 1/2$) terminating at the isotropic Heisenberg fixed point $K^{(H)} = 1/2$; (ii) a strong-coupling Néel phase $g_3^\star \rightarrow \infty$; (iii) a strong-coupling dimer phase $g_3^\star \rightarrow -\infty$. Moreover, u is not renormalized for $y_1 = 0$. Spin-rotation invariant models scale along the separatrix between Néel and spin liquid phases, or along its continuation into the dimer regime.

Taking y_1, the most relevant perturbation, finite, changes this simple picture. Quite generally, the corrections to the RG flow of K and g_3 are *positive,* while those from g_3 are negative. In the spin liquid phase, close to the isotropic Heisenberg fixed point, the alternating NNN exchange will *increase* both K and y_3, and therefore *reverse* the direction of the RG flow, compared to the $y_1 = 0$ situation. The sign of this effect agrees with the spin gap reduction in the dimer phase when going from the MG to the sawtooth model. The magnitude of the effect is a direct consequence of the scaling dimension d_{g_1}. Figure 2 shows a family of solutions of the RG equations, projected on the y_3-K plane, which have been linearized for the purpose of the figure to accurately control spin-rotation invariance (cf. below).

The flow reversal is seen in much of the first quadrant. When K is increased sufficiently by y_1, this perturbation becomes irrelevant, however, and the RG flow bends back to a weak-coupling fixed line ($K^\star \geq 1, y_3^\star = 0, y_1^\star = 0$), describing a spin liquid with an increased easy-plane anisotropy. Its spin velocity u is decreased but remains finite.

More interesting is the spin-rotation invariant line ($y_3 = 4K - 2$ in the linearized RG). While the initial flow towards the Heisenberg fixed point also reverses its direction under the influence of y_1, it reaches a new finite-coupling fixed point ($K^\star \approx 0.578, y_3^\star \approx 0.315, y_1^\star \approx \pm 0.544$), respectively ($K^\star = 0.6, y_3^\star = 0.4, y_1^\star = \pm 0.8$) in the linearized RG. This fixed point is attractive for spin-rotation invariant systems, and repulsive otherwise with a flow into the spin liquid or Néel phases for easy-plane (easy-axis) anisotropy. At the fixed point,

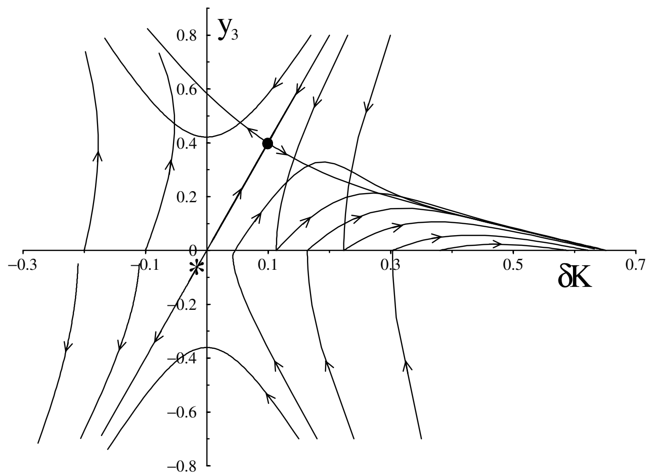

FIG. 2. The scaling trajectories for $y_1(l = 0) = 0.001$ projected on the y_3-δK plane. $\delta K = K - 1/2$, and the dot locates the new intermediate coupling fixed point. The Néel state is realized in the upper left, the dimer state in the lower left, and the spin liquid in the right part of the figure. The star locates the boundary between flows to the new fixed point and into the dimer regime.

the renormalized spin velocity vanishes, $u^\star = 0$. This conclusion follows from Eq. (8) and is independent of the exact value of the fixed point as long as it is located on the RG separatrix with $1/2 < K < \infty$. Consequently, conformal invariance is broken, and we do not expect power-law decay of the correlation functions. Thermodynamic properties will be different from a Heisenberg chain: the specific heat will show nonlinear temperature dependence, and the magnetic susceptibility will depend on temperature. This state is significantly different from the Luttinger-type spin fluid state of the Heisenberg model. The fixed point Hamiltonian can be rewritten as $H^\star = u^\star \mathcal{H}(K^\star, g_1^\star, g_3^\star)$ where $\mathcal{H}$ is independent of $u^\star$. It becomes trivial, $H^\star = 0$, at the fixed point because $u^\star = 0$. We interpret this as our spins effectively decoupling at the lowest energy scales, i.e., a kind of asymptotic freedom in this spin-rotation invariant ladder.

From standard arguments, we find that the elementary excitations in the fixed point, spinon and antispinon, are still gapless. One can also provide a variational argument, based on an effective Hamiltonian H_1, Eq. (3). Minimizing its energy directly produces pairwise kink and antikink solutions corresponding to the elementary excitations with energies proportional to g_3, respectively, g_1. Including the quantum fluctuations from H_0 is expected to delocalize these kinks and reduce their energies further. Using now our fixed point properties $g_{1,3} = y_{1,3}^\star u^\star$, $u^\star \to 0$ makes the excitation gap vanish at the fixed point. Also, the numerical results of Wiessner *et al.* [13] indicate a paramagnetic susceptibility.

A natural question arises here: Is this intermediate fixed point stable against higher-order perturbations? Our answer is positive although we do not attach any particular significance to the numerical values of the coupling constants, which may change as higher-order corrections are included. Its location on the RG separatrix between the Néel state and the easy-plane spin liquid is protected by spin-rotation invariance and it can be pushed neither back to the Heisenberg fixed point nor to strong coupling, $K \to \infty$, by higher-order operators. The first option is inconsistent with the scaling dimensions, the second one would correspond, in the fermion language, to long-range pairing order which is excluded in 1D. Scaling into the dimer regime is inconsistent with the absence of a magnetization plateau [13].

Care should be taken when comparing these predictions to results, e.g., from exact numerical diagonalization on small clusters (size N). The finite system size will stop the RG flow at a scale $l_N = \ln N$, and the fixed point ($l \to \infty$) is *not* reached. However, Eqs. (5)–(8) predict a spin velocity decreased significantly by the alternating component of the NNN exchange, with an unusual size dependence which can be evaluated by integrating the RG equations up to l_N. Because of the scale dependence of the renormalization, the finite-size spectrum likely exhibits significant nonlinear corrections which, again, are size dependent. The velocity renormalization also suggests a scale dependence of the magnetic susceptibility. A direct solution of our model in a magnetic field is rather involved, however, because higher-order terms lead to a field-induced generation of new, relevant operators. This will be reported later.

Of course, when J_2 increases beyond a critical value $J_{2c}(\delta)$ now depending on the exchange alternation, the RG flows to a strong-coupling fixed point, which corresponds to the quantum dimer phase. For $y_1 = 0.001$, this critical point is indicated in (K, y_3) coordinates in Fig. 2 by a star. For small δ and $J_2 > J_{2c}(\delta)$, our RG equations show that the spin gap is decreased by increasing δ, but the system will remain in the universality class of the dimer liquid.

However, we do not expect that the field theory description is very precise for J_2 near the MG point $J_2 = 0.5J_1$. The main reason is that the correlation length, which is proportional to the inverse of the energy gap, decreases quickly when J_2 increases much beyond $J_{2c}(\delta)$. To access this limit, we now discuss the influence of NNN exchange alternation on the ground state and excitations of the Majumdar-Ghosh model. For the MG model [7], the two linearly independent ground states, say, left or right dimer ground state, are products of nearest-neighborly singlets, respectively,

$$|\Phi_L\rangle = \prod_{l=\text{odd}} [l, l+1], \qquad |\Phi_R\rangle = \prod_{l=\text{even}} [l, l+1], \tag{9}$$

where $[i,j] = ([\uparrow]_i[\downarrow]_j - [\downarrow]_i[\uparrow]_j)/\sqrt{2}$ denotes the singlet combinations of spin i and j. Equation (9) also represents the degenerate ground state of the sawtooth model [5,6].

How are these models connected? We notice that NNN exchange alternation does not modify the product states of nearest-neighbor singlets

$$H_\delta \,|\Phi_{L,R}\rangle = \sum (-1)^l \delta \mathbf{S}_l \mathbf{S}_{l+2} \,|\Phi_{L,R}\rangle = 0\,. \tag{10}$$

Furthermore, we can prove that introducing NNN exchange alternation into the MG model, or changing it in the sawtooth chain, will not affect their ground states. There is thus an entire manifold of Hamiltonians, parametrized by δ with $J_1 = 2J_2$ fixed, with doubly degenerate NN-dimer product ground states $|\Phi_{L,R}\rangle$. This kind of ground state attracted much attention recently for the experimental realization of $SrCu_2(BO_3)_2$ as the 2D Shastry-Sutherland model [19,20].

While in these models, the focus is on the ground state, and we also can characterize the elementary excitations as kinks and antikinks with finite excitation energies and different dispersions in the dimer state of our ladder. Starting from the MG model, the kinks can be thought of as domain walls separating the different dimer ground state configurations. From symmetry considerations, the kink and antikink properties are identical in the MG model. With alternating NNN interaction, the symmetry between legs is broken; some properties will differ between kinks and antikinks, in particular, the dispersions. However, they still survive as the elementary excitations of the asymmetric spin ladder system. The alternating NNN interaction does not serve as a confining potential for the kink and antikink, but changes the energy gap of the excitations. Based on the cluster variation method [5,6], our numerical estimates indicate that the gap decreases from 0.234 in the MG model to 0.219 in the sawtooth chain with increasing δ, while the ground state remains invariant. Particularly, for $\delta = J_2$, i.e., the sawtooth chain, the kink excitation is exactly a single spin on an odd site and dispersionless, while an antikink is still a domain wall propagating with an effective mass [5,6].

The preceding results can also be understood from the point of view of the corresponding field model. The presence of the g_1 term $\partial_x \Phi \cos 2\Phi$ does not lift the degeneracy of the dimer ground state, which is the constant solution minimizing the energy of the Hamiltonian with the g_3 term. Near the strong-coupling dimer fixed point, the g_3 term is much more relevant than the g_1 term. In this case, the soliton solutions of the $\cos 4\Phi$ sine-Gordon equation will survive. However, the g_1 term, although it is much less relevant than the g_3 term, gives different masses to the sine-Gordon kink and antikink solutions. This give us a rough explanation of the asymmetric kink and antikink excitations in the presence of alternating NNN coupling. The difference in (numerically determined) gap size between the MG and the sawtooth chains, is consistent with our RG results on the influence of δ for smaller J_2, on the spin gap magnitude.

Spin-isotropic, asymmetric zigzag ladders are described, in the limit of weak frustration, by an intermediate coupling fixed point with gapless excitations and a vanishing spin velocity, likely indicating a decoupling of the spins at low energy scales. For larger frustration, a more usual dimer liquid phase is realized whose spin gap decreases with increasing leg asymmetry. A continuous manifold of Hamiltonians with the same singlet product ground state interpolates between the Majumdar-Ghosh model and the sawtooth spin chain. In addition, we find gapless spin liquid and gapped Néel states with easy-plane and easy-axis anisotropy. Extensions we currently consider include external fields and doping with charge carriers.

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