Topological order, dimerization, and spinon deconfinement in frustrated spin ladders

Eugene H. Kim,¹ Ö. Legeza,² and J. Sólyom²

¹Department of Physics, University of Windsor, Windsor, Ontario, Canada N9B 3P4 ²Research Institute for Solid State Physics and Optics, P.O. Box 49, H-1525 Budapest, Hungary

(Received 17 December 2007; published 22 May 2008)

We consider topological order and dimer order in several frustrated spin ladder models, which are related to higher-dimensional models of current interest; we also address the occurrence of fractionalized phases with deconfined spinon excitations in these models. Combining results obtained with both analytic and numerical methods, we discuss how the occurrence of dimerized or fractionalized phases is dictated by the system's geometry.

DOI: 10.1103/PhysRevB.77.205121

PACS number(s): 71.30.+h, 71.10.Fd

I. INTRODUCTION

Frustrated spin systems give rise to a wealth of interesting behavior; hence, they have attracted considerable attention.¹ Typically, the low-lying excitations in spin systems are magnons. However, there has been particular interest in identifying fractionalized phases, where the magnon "breaks apart" into more fundamental objects. When doped, such phases would give rise to metallic states that do not fall within the Fermi liquid paradigm—the elementary excitations in these phases would not have the quantum numbers of an electron. However, finding systems which exhibit fractionalized phases has proven to be extremely challenging.

Motivated largely by Anderson's original resonating valence-bond² (RVB) suggestions for the high- T_c cuprate superconductors, substantial effort has focused on searching for fractionalized phases in models having short-range RVB ground states.³ A related approach has been to consider dimer models, where only short-ranged valence bonds with specified dynamics are considered.⁴ While lacking longrange order in the conventional sense, i.e., lacking a local order parameter, these short-range valence-bond ground states have a subtle form of order, namely, topological order.⁵ It is now appreciated that a precise characterization of fractionalized phases is via its topological order.⁶ However, whether a fractionalized phase occurs actually strongly depends on the system's geometry. More specifically, the system's geometry must allow for "liquidity" in the spectrum of states.⁷ Many systems with short-range RVB ground states do not exhibit such liquidity-they would prefer to dimerize rather than to exhibit a fractionalized phase.⁸

In this work, we address the occurrence of fractionalized and dimerized phases in several frustrated spin ladder models. Ladder models provide a unique testing ground, as powerful analytic and numerical techniques from onedimensional physics can be utilized. Indeed, ladder models have allowed controlled calculations to investigate topological order,^{9–11} the occurrence of dimer order,¹² and the occurrence of fractionalized excitations¹³ in spin models. Furthermore, ladder models have allowed for controlled calculations, which demonstrate that pairing and, in particular, $d_{x^2-y^2}$ pairs could arise when these spin models are doped.¹⁴ The models we consider are related to higherdimensional systems of current interest; investigations of the one-dimensional analogs are particularly relevant, in light of recent work which showed that the mechanism giving rise to fractionalized excitations is the same in both one and two dimensions.¹⁵ However, besides being a testing ground and illustrating the types of possible behaviors, these ladder models are interesting in their own right, as there are a number of materials that are well described by ladder models.¹⁶

In large regions of parameter space, the models we consider have short-range RVB ground states. More specifically, in large regions of parameter space, these models have ground states that are continuously related to the ground states of the so-called rung-singlet phase or the Haldane phase. (Typical configurations in these ground states are schematically shown in Figs. 2 and 4 in Sec. II.) While these phases have nearly identical properties, their ground states differ in a subtle way, namely, in their topological order. With frustrating interactions, these states could be tuned to become degenerate, and then one has the necessary liquidity for the deconfinement of spinon excitations. However, as will be seen below, depending on the model's spatial symmetries, this liquidity and spinon deconfinement could be preempted by dimerization.

The rest of the paper is organized as follows. In Sec. II, we describe the ladder models considered in this work—the cross-coupled, zigzag, and diagonal ladders—and we recall some of their known properties. In Sec. III, the exact ground states of the models are discussed (along certain lines in parameter space). Section IV contains a discussion of topological order in these models and some comments on the low-energy excitations. In Sec. V, we analyze the models in the limit of weak interchain couplings by using bosonization and renormalization-group (RG) techniques. In Sec. VI, we present numerical results obtained via the density-matrix renormalization-group (DMRG) algorithm; we discuss these numerical results in light of the results from the previous sections. Finally, in Sec. VII, we summarize and present some concluding remarks.

II. MODELS

We begin with two antiferromagnetic spin-1/2 Heisenberg chains, each described by the Hamiltonian



FIG. 1. The ordinary ladder.

$$H_0^{(i)} = \sum_l J_{\parallel} \mathbf{S}_l^{(i)} \cdot \mathbf{S}_{l+1}^{(i)}, \quad i = 1, 2,$$
(1)

where $\mathbf{S}_{l}^{(i)}$ is the spin operator at site *l* on chain *i*. We will be interested in coupling the chains together in various ways, such that the resulting models have different spatial symmetries. In this work, we will consider only antiferromagnetic couplings. We start by coupling the chains together so that the resulting models are not frustrated. We then include frustrating interactions and investigate their influence on the properties of the models.

The simplest way to couple the chains together is by

$$H_{\perp} = \sum_{l} J_{\perp} \mathbf{S}_{l}^{(1)} \cdot \mathbf{S}_{l}^{(2)}, \qquad (2)$$

so that the full Hamiltonian is

$$H_L = \sum_{i=1}^{2} H_0^{(i)} + H_{\perp}, \qquad (3)$$

which is depicted in Fig. 1. We will refer to this as an *ordinary ladder*. This model has received considerable attention. Indeed, it can be thought of as a strip of a two-dimensional square lattice; hence, its properties have been investigated to give clues as to the physics occurring in the high- T_c cuprate superconductors.¹⁷

When J_{\perp} is large $(J_{\perp} \gg J_{\parallel})$, the ground state is essentially a product of rung singlets with a gap to the excited states the gap is due to the energy necessary to break a singlet bond. When $J_{\parallel} \simeq J_{\parallel}$, it has been shown that the energy gap persists; the ground state is well described by a short-range valence-bond state, a typical configuration of which is shown in Fig. 2. It has been established that the entire region $0 < J_{\perp} < \infty$ is, in fact, continuously related.^{18,19} As this entire region of parameter space is related to the regime $J_{\parallel} \gg J_{\parallel}$, where the ground state is a product of rung singlets, it is often referred to as the *rung-singlet phase*. Incidentally, the dominance of rung-singlet bonds can be measured by determining their weight in the ground state, $\rho_s = (1/N) \Sigma_{l=1}^N \langle \Psi | S_l S_l^{\dagger} | \Psi \rangle$, where $| \Psi \rangle$ is the ground-state wave function and $S_l = (1/\sqrt{2})[|\uparrow\rangle_l^{(1)}|\downarrow\rangle_l^{(2)} - |\downarrow\rangle_l^{(1)}|\uparrow\rangle_l^{(2)}]$. A state belongs to the rung-singlet phase if $\rho_s > 1/4$.²⁰

We also consider coupling the spins to their next-nearest neighbors on the opposite leg of the ladder. This coupling is described by



FIG. 2. A typical valence-bond configuration in the rung-singlet ground state of the two-leg ordinary Heisenberg ladder.

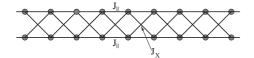


FIG. 3. Ladder with diagonal couplings.

$$H_X = \sum_{l} J_X(\mathbf{S}_l^{(1)} \cdot \mathbf{S}_{l+1}^{(2)} + \mathbf{S}_l^{(2)} \cdot \mathbf{S}_{l+1}^{(1)}), \qquad (4)$$

so that the full Hamiltonian is

$$H_{\rm C} = \sum_{i=1}^{2} H_0^{(i)} + H_X,$$
 (5)

which the resulting model is shown in Fig. 3.

This system is known^{21,22} to have a gapped spectrum of spin-1 magnons. Furthermore, the entire regime $0 < J_X < \infty$ is continuously related to the Haldane phase²³ of the spin-1 chain. This can be understood by considering the point $J_{x}=J_{\parallel}$ —here, the low-energy spectrum of Eq. (5) is equivalent to that of the S=1 Heisenberg spin chain.^{24,25} To see this, we start with the Hamiltonian of a spin-1 chain $H = J_{\parallel} \Sigma_l \mathbf{S}_l \cdot \mathbf{S}_{l+1}$, which is known to be in the Haldane phase. When the spin-1 operator on site l is represented as a sum of two spin-1/2 operators, $\mathbf{S}_l = \mathbf{S}_l^{(1)} + \mathbf{S}_l^{(2)}$, one obtains Eq. (5) with $J_X = J_{\parallel}$. Since the total spin of each rung commutes with the Hamiltonian, the eigenstates can be classified by the total spins on the rungs. It has been shown that in the low-energy part of the spectrum, all rungs are in their triplet (S=1) state, and hence the same Haldane gap appears in the ladder model as well. In this representation, the Haldane state of the spin-1 chain can be described rather well by short-ranged valence bonds between neighboring rungs, with a typical configuration of which is shown in Fig. 4.

Finally, we consider the ladder model shown in Fig. 5(a), where the interchain coupling is given by

$$H_d = \sum_{l} J_2 \mathbf{S}_{2l}^{(1)} \cdot (\mathbf{S}_{2l-1}^{(2)} + \mathbf{S}_{2l+1}^{(2)}).$$
(6)

Previous work has established²⁶ that this model is in the same universality class as the model in Eq. (5). Hence, removing half of the cross couplings in an appropriate way from Eq. (5) does not change the universality class. Part of our motivation for considering this model is because it is a representation of the " N_p =2 diagonal ladder" shown in Fig. 5(b); it is a minimal model to study diagonal stripes, which have been observed in the high- T_c cuprate superconducting material La_{2-x}Sr_xCuO₄ (Ref. 27) and the nickel oxides La₂NiO_{4.125} (Ref. 28) and La_{1-x}Sr_xNiO₄.²⁹

As mentioned above, we are interested in the effect of frustration on these models. In what follows, we analyze three models obtained by introducing frustrating interactions

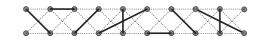


FIG. 4. A typical valence-bond configuration in the ground state of the ladder model shown in Fig. 3.

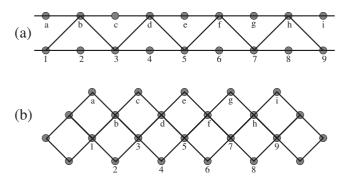


FIG. 5. (a) Ladder with a diagonal coupling between every second spin. (b) $N_p=2$ diagonal ladder.

to the models described above. (Again, we will consider only antiferromagnetic interchain couplings in this work.) Our motivation for doing so is because the resulting models have different spatial symmetries. As will be discussed below, these symmetries play a crucial role in determining the properties of the models.

A. Cross-coupled ladder

The first model we consider has both H_{\perp} and H_X simultaneously present. The resulting model with Hamiltonian

$$H_{\rm CC} = \sum_{i=1}^{2} H_0^{(i)} + H_\perp + H_X \tag{7}$$

is shown in Fig. 6(a). For the rest of this work, we will refer to this model as a cross-coupled ladder. Notice that this spin model is invariant under translation by a single site; it is also invariant if the legs of the ladder are interchanged: leg 1 \leftrightarrow leg 2. Part of our motivation for the study of this model is its relationship to the two-dimensional model with nearest-neighbor and next-nearest-neighbor exchange couplings, which is often referred to as the J_1-J_2 model—Eq. (7) is a one-dimensional strip of this model. Furthermore, Eq. (7) is related to a chain of edge-sharing tetrahedra.³⁰ Indeed, by taking every second rung and rotating it by 90° about its midpoint, one obtains the structure shown in Fig. 6(b); by adding a next-nearest-neighbor coupling (along the

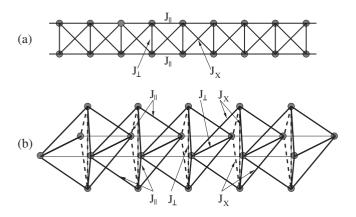


FIG. 6. (a) The *cross-coupled* ladder. (b) The cross-coupled ladder as a chain of edge-sharing tetrahedra.

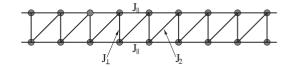


FIG. 7. The zigzag ladder model.

chain) to Eq. (7), a spin model on a chain of edge-sharing tetrahedra is obtained. As there are a number of materials described by spin models on corner-sharing tetrahedra, i.e., pyrochlores,³¹ it is not unreasonable that materials with edge-sharing tetrahedra can be realized.

The model in Eq. (7) has been investigated in a number of works, but its phase diagram and properties are still under debate. When J_{\perp} is the dominant interchain coupling, the system is continuously related to the ordinary ladder (with $J_X=0$; hence, the system is in the rung-singlet phase. On the other hand, when J_X is the dominant interchain coupling, the system is continuously related to Eq. (5), and the system is in the Haldane phase. For weak interchain couplings, previous analytic treatments¹⁰ suggested a first-order transition between the rung-singlet and Haldane phases when $J_{\perp} \simeq 2J_X$. Numerical results on the model^{11,32} were consistent with a first-order transition for both weak and strong interchain couplings. Recent numerical work, however, has suggested that the transition is actually continuous when the interchain coupling is weak, which becomes first-order only for stronger interchain coupling.^{20,33} Furthermore, recent analytical work¹² has argued that there is a spontaneously dimerized phase in between the rung-singlet and Haldane phases, rather than a direct transition between the two phases as observed in previous works.

B. Zigzag ladder

The second ladder model we consider contains again both rung and diagonal couplings, but only half the diagonal couplings of the cross-coupled ladder are present, as shown in Fig. 7. This model is often referred to as a *zigzag ladder*; its Hamiltonian is

$$H_Z = \sum_{i=1}^{2} H_0^{(i)} + H_\perp + H_z, \tag{8}$$

where

$$H_{z} = \sum_{l} J_{2} \mathbf{S}_{l}^{(1)} \cdot \mathbf{S}_{l+1}^{(2)}.$$
 (9)

This spin model is invariant under translation by a single site. However, unlike the cross-coupled ladder that is invariant under the interchange of the legs, this model lacks that symmetry. Part of the motivation for considering this model comes from the two-dimensional triangular lattice—Eq. (8) is a one-dimensional strip of the triangular lattice has been of considerable recent interest, which is motivated largely in part by the discovery of the triangular lattice material Cs_2CuCl_4 and, in particular, to evidence that this material exhibits a two-dimensional fractionalized phase with decon-

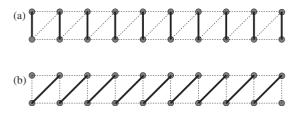


FIG. 8. The two degenerate ground states of the zigzag ladder at the Majumdar–Ghosh point (Ref. 39).

fined spinons.³⁴ However, besides being a toy model for understanding spin systems on a triangular lattice, this model is relevant to the quasi-one-dimensional material SrCuO₂.³⁵

The properties of the zigzag ladder are well known when J_{\perp} or J_2 vanishes and also along the line $J_{\perp}=J_2$. When J_{\perp} or J_2 vanishes, the model reduces to the ordinary ladder. When $J_{\perp}=J_2$, the zigzag ladder is equivalent to the spin-1/2 frustrated Heisenberg chain with nearest-neighbor coupling J_{\perp} and next-nearest-neighbor coupling J_{\parallel} . This chain model is known to be critical for $J_{\perp} > J_{\perp c}$ $(J_{\perp c} = J_{\parallel} / 0.241)$,^{36,37} being in the same universality class as the antiferromagnetic spin-1/2 Heisenberg chain. The spinons of the spin-1/2 chain acquire a gap (but they remain deconfined), and the ground state becomes doubly degenerate for $J_{\perp} = J_2 < J_{\perp c}$.³⁸ At the Majumdar–Ghosh (MG) point³⁹ $J_{\perp} = J_2 = 2J_{\parallel}$, the two degenerate ground states have a simple form in the thermodynamic limit, each consisting of decoupled singlets, as shown in Fig. 8. It has been shown that these two ground states can be continuously related to the rung-singlet and Haldane phases.⁴⁰ For even weaker interchain couplings $J_{\perp} = J_2 < 2J_{\parallel}$, incommensurate oscillations appear in the short-range correlations.41-45

C. Diagonal ladder

Finally, we consider the model obtained when the couplings described both by Eqs. (2) and (6) are simultaneously present. The model is shown in Fig. 9(a) and is described by the Hamiltonian

$$H_D = \sum_{i=1}^{2} H_0 + H_\perp + H_d.$$
(10)

For the rest of this work, we will refer to this ladder model as a *diagonal ladder*. Unlike the previous two ladder models

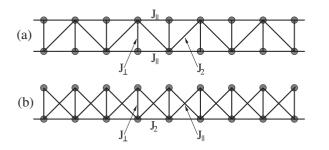


FIG. 9. (a) The diagonal ladder model. (b) Alternative representation of the diagonal ladder, which is obtained by interchanging sites on every second rung.

that were invariant under translation by a single site, Eq. (10) is invariant under translation by two sites. Furthermore, similar to the zigzag ladder, Eq. (10) is not invariant under the interchange of the legs. However, it is invariant under the combined operation of leg interchange followed by a translation by a single site. Interestingly, this ladder model can, in fact, be transformed into one which is invariant under translation by a single site, but lacking inversion symmetry. This is accomplished by interchanging the sites on every second rung of the ladder, $S_{2l}^1 \leftrightarrow S_{2l}^2$; the resulting model is shown in Fig. 9. We are unaware of work which investigated the role of frustrating interactions in this model.

III. EXACT GROUND STATES

An interesting feature of the models considered in this work is that their exact ground states have a simple form for a certain regime of parameters. The key to establishing this is decomposing the system into a set of "triangles."⁴⁶ Here, we review the argument and discuss the ground states that arise.

Consider three s=1/2 spins arranged on a triangle. Suppose the spins on sites 1 and 2 are coupled by an exchange coupling J_1 , these two spins are coupled to the spin on site 3 by an exchange coupling J. The Hamiltonian for the triangle is

$$H_{\text{triangle}} = J_1 \mathbf{S}_1 \cdot \mathbf{S}_2 + J(\mathbf{S}_1 + \mathbf{S}_2) \cdot \mathbf{S}_3. \tag{11}$$

We are interested in the case where both J and J_1 are antiferromagnetic; hence, the ground state is a doublet. There are two ways of achieving this: (a) a singlet across sites 1 and 2 with a free spin-1/2 on site 3 or (b) a triplet across sites 1 and 2 added to the spin-1/2 on site 3 to form a spin-1/2. Let [i,j]denote a singlet between sites *i* and *j*. Then, using

$$(\mathbf{S}_i + \mathbf{S}_j)[i,j] = 0, \tag{12}$$

(13)

the energy of the state in (a) is found to be $E_a = -3J_1/4$; the energy of state in (b) is $E_b = -J + J_1/4$. We see that the state in (a)—the state with a singlet across sites 1 and 2—is the lowest-energy state if $J < J_1$.

Using information from the previous paragraph, we now address the ground states of the ladder models considered in this work. We begin by considering the cross-coupled ladder model. In this model, four triangles can be assigned to each rung; the Hamiltonian can be written as

 $H_{\rm CC} = \sum_l \, (H_{l+}^{(1)} + H_{l-}^{(1)} + H_{l+}^{(2)} + H_{l-}^{(2)}),$

with

$$\begin{split} H_{l+}^{(1)} &= \frac{1}{4} J_{\perp} \mathbf{S}_{l}^{(1)} \cdot \mathbf{S}_{l}^{(2)} + \frac{1}{2} J_{\parallel} \mathbf{S}_{l}^{(1)} \cdot \mathbf{S}_{l+1}^{(1)} + \frac{1}{2} J_{\mathbf{X}} \mathbf{S}_{l}^{(2)} \cdot \mathbf{S}_{l+1}^{(1)}, \\ H_{l-}^{(1)} &= \frac{1}{4} J_{\perp} \mathbf{S}_{l}^{(1)} \cdot \mathbf{S}_{l}^{(2)} + \frac{1}{2} J_{\parallel} \mathbf{S}_{l}^{(1)} \cdot \mathbf{S}_{l-1}^{(1)} + \frac{1}{2} J_{\mathbf{X}} \mathbf{S}_{l}^{(2)} \cdot \mathbf{S}_{l-1}^{(1)}, \\ H_{l+}^{(2)} &= \frac{1}{4} J_{\perp} \mathbf{S}_{l}^{(1)} \cdot \mathbf{S}_{l}^{(2)} + \frac{1}{2} J_{\parallel} \mathbf{S}_{l}^{(2)} \cdot \mathbf{S}_{l+1}^{(2)} + \frac{1}{2} J_{\mathbf{X}} \mathbf{S}_{l}^{(1)} \cdot \mathbf{S}_{l+1}^{(2)}, \\ H_{l+}^{(2)} &= \frac{1}{4} J_{\perp} \mathbf{S}_{l}^{(1)} \cdot \mathbf{S}_{l}^{(2)} + \frac{1}{2} J_{\parallel} \mathbf{S}_{l}^{(2)} \cdot \mathbf{S}_{l-1}^{(2)} + \frac{1}{2} J_{\mathbf{X}} \mathbf{S}_{l}^{(1)} \cdot \mathbf{S}_{l+1}^{(2)}, \\ \end{split}$$

$$(14)$$

When $J_{\parallel}=J_X$, the terms in Eq. (14) can be written in the form of Eq. (11). Then, by using Eq. (12), it follows that the state

TOPOLOGICAL ORDER, DIMERIZATION, AND SPINON...

$$|\psi\rangle = \prod_{l} [l1, l2], \tag{15}$$

where the spins on each rung form a singlet, is an exact eigenstate of the Hamiltonian in Eq. (13) with energy

$$E = -\frac{3}{4}J_\perp N. \tag{16}$$

We would like to determine if and when Eq. (15) is the ground state. To do so, consider each of the triangles in Eq. (14) individually. If $J_{\perp}/2 > J_{\parallel}$, the lowest-energy state of each triangle (when individually considered) has a singlet between the spins on the same rung. It is known that if a Hamiltonian can be written as the sum of terms, the ground-state energy cannot be smaller than the sum of the lowest energies of its constituents. For the ground state of Eq. (13), this gives the inequality

$$E_0 \ge -\frac{3}{4}J_\perp N,\tag{17}$$

where *N* is the number of rungs. Hence, we see that Eq. (16) saturates the bound in Eq. (17) when $J_{\perp}/2 > J_{\parallel}$; Eq. (15) is the ground state for $J_{\parallel}=J_X$ with $J_{\perp}/2 > J_{\parallel}$.^{30,47}

We now consider the zigzag ladder. It can be decomposed into two triangles per rung,

$$H_{Z} = \sum_{l} (H_{l+}^{(2)} + H_{l-}^{(1)}), \qquad (18)$$

where

$$H_{l+}^{(2)} = \frac{1}{2} J_{\perp} \mathbf{S}_{l}^{(1)} \cdot \mathbf{S}_{l}^{(2)} + J_{\parallel} \mathbf{S}_{l}^{(2)} \cdot \mathbf{S}_{l+1}^{(2)} + \frac{1}{2} J_{2} \mathbf{S}_{l}^{(1)} \cdot \mathbf{S}_{l+1}^{(2)},$$

$$H_{l-}^{(1)} = \frac{1}{2} J_{\perp} \mathbf{S}_{l}^{(1)} \cdot \mathbf{S}_{l}^{(2)} + J_{\parallel} \mathbf{S}_{l}^{(1)} \cdot \mathbf{S}_{l-1}^{(1)} + \frac{1}{2} J_{2} \mathbf{S}_{l}^{(2)} \cdot \mathbf{S}_{l-1}^{(1)}.$$
 (19)

When $J_{\parallel}=J_2/2$, the terms in Eq. (19) can be written in the form of Eq. (11); the energy of the state in Eq. (15) saturates the lower bound in Eq. (17) for $J_{\perp}/2 > J_{\parallel}$. Hence, Eq. (15) is the exact ground state for $J_{\parallel}=J_2/2$ with $J_{\perp}/2 > J_{\parallel}$.⁴⁶ Note that another exact ground state of the zigzag ladder follows by symmetry. When $J_{\parallel}=J_{\perp}/2$ and $J_2/2 \ge J_{\parallel}$, the ground state is again a product of singlets, but this time, they are diagonally formed between neighboring rungs,⁴⁶

$$|\psi\rangle = \prod_{l} [l1, (l-1)2].$$
 (20)

We now go on and consider the diagonal ladder. The diagonal ladder can be decomposed into two triangles per rung, but the triangles have different orientations for even and odd rungs,

$$H_D = \sum_{l} \left(H_{(2l)+}^{(2)} + H_{(2l)-}^{(2)} + H_{(2l+1)+}^{(1)} + H_{(2l+1)-}^{(1)} \right), \quad (21)$$

where now

$$\begin{split} H^{(2)}_{(2l)+} &= \frac{1}{2} J_{\perp} \mathbf{S}^{(1)}_{2l} \cdot \mathbf{S}^{(2)}_{2l} + J_{\parallel} \mathbf{S}^{(2)}_{2l} \cdot \mathbf{S}^{(2)}_{2l+1} + \frac{1}{2} J_2 \mathbf{S}^{(1)}_{2l} \cdot \mathbf{S}^{(2)}_{2l+1}, \\ H^{(2)}_{(2l)-} &= \frac{1}{2} J_{\perp} \mathbf{S}^{(1)}_{2l} \cdot \mathbf{S}^{(2)}_{2l} + J_{\parallel} \mathbf{S}^{(2)}_{2l} \cdot \mathbf{S}^{(2)}_{2l-1} + \frac{1}{2} J_2 \mathbf{S}^{(1)}_{2l} \cdot \mathbf{S}^{(2)}_{2l-1}, \\ H^{(1)}_{(2l+1)+} &= \frac{1}{2} J_{\perp} \mathbf{S}^{(1)}_{2l+1} \cdot \mathbf{S}^{(2)}_{2l+1} + J_{\parallel} \mathbf{S}^{(1)}_{2l+1} \cdot \mathbf{S}^{(1)}_{2l+2} + \frac{1}{2} J_2 \mathbf{S}^{(1)}_{2l+1} \cdot \mathbf{S}^{(2)}_{2l+2}, \end{split}$$

$$H_{(2l+1)-}^{(1)} = \frac{1}{2} J_{\perp} \mathbf{S}_{2l+1}^{(1)} \cdot \mathbf{S}_{2l+1}^{(2)} + J_{\parallel} \mathbf{S}_{2l+1}^{(1)} \cdot \mathbf{S}_{2l}^{(1)} + \frac{1}{2} J_2 \mathbf{S}_{2l+1}^{(2)} \cdot \mathbf{S}_{2l}^{(1)}.$$
(22)

When $J_{\parallel} = J_2/2$, the terms in Eq. (22) can be written in the form of Eq. (11), and thus Eq. (15) is the exact ground state for $J_{\parallel} = J_2/2$ with $J_{\perp}/2 \ge J_{\parallel}$.

IV. TOPOLOGICAL ORDER AND SPINONS IN LADDER MODELS

From the discussion in Secs. II and III, the ladder models considered in this work have similar ground-state properties in extended regions of parameter space—their ground states are described by a collection of short-ranged valence bonds, which are separated by a gap to the excited states. However, the ground states of these ladder models, in fact, differ in a subtle way, namely, in their topological order. More specifically, the number of valence bonds crossing an arbitrary vertical line is always even in the rung-singlet phase, while the number is always odd in the Haldane phase. This can be explicitly seen in the configurations shown in Figs. 2, 4, and 8. Hence, a topological number Q can be defined by the parity of the number of short-range valence bonds crossing an arbitrary vertical line.¹⁰ This Q, which is either even or odd, is a good quantum number for short-range valence-bond states since the Hamiltonian has finite matrix elements only between configurations with the same Q. For long-range valence-bond states, however, the Hamiltonian mixes the Q= even and Q = odd configurations; hence, no such topological distinction is possible.

It is worth noting that for open boundary conditions (OBC), Q= odd ground states have spin-1/2 localized at the ends of the ladder, while Q= even states do not. As can be seen from Figs. 8(b), these end spins occur for topological reasons. They are analogous to the edge states in the quantum Hall effect; in general, the presence of such edge excitations is a signal of nontrivial topological order.⁴⁸

It has also been pointed out¹⁰ that the topological order of the valence bonds is related to the "hidden order" present in two-leg Heisenberg spin ladders, namely, *string order*, which is analogous to the string order in antiferromagnetic spin-1 chains.⁴⁹ This string order is detected by the two string order parameters,^{9,10,50}

$$\mathcal{O}_{\text{odd}}^{\alpha} = -\lim_{|i-j| \to \infty} \left\langle (S_{i,1}^{\alpha} + S_{i,2}^{\alpha}) \exp\left(i\pi \sum_{l=i+1}^{j-1} (S_{l,1}^{\alpha} + S_{l,2}^{\alpha})\right) \right\rangle$$
$$\times (S_{j,1}^{\alpha} + S_{j,2}^{\alpha}) \right\rangle,$$
$$\mathcal{O}_{\text{even}}^{\alpha} = -\lim_{|i-j| \to \infty} \left\langle (S_{i+1,1}^{\alpha} + S_{i,2}^{\alpha}) \exp\left(i\pi \sum_{l=i+1}^{j-1} (S_{l+1,1}^{\alpha} + S_{l,2}^{\alpha})\right) \right\rangle$$
$$\times (S_{j+1,1}^{\alpha} + S_{j,2}^{\alpha}) \right\rangle.$$
(23)

In Refs. 10 and 11, it was observed that when $\mathcal{O}_{odd} \neq 0$ in some region of a model's parameter space, \mathcal{O}_{even} vanishes in



FIG. 10. Spinons topologically separating distinct regions.

that region and vice versa. This can, in fact, be rigorously established by using a slightly modified version of these quantities.¹⁹ Indeed, these modified string order parameters can be written in terms of the order and disorder fields of two Ising models— \mathcal{O}_{odd} in terms of the order fields σ_1 and σ_2 , while \mathcal{O}_{even} in terms of the disorder fields μ_1 and μ_2 . Therefore, \mathcal{O}_{odd} and \mathcal{O}_{even} are dual to each other and, hence, cannot be simultaneously nonzero. Moreover, it has been shown¹⁰ that models with Q=even ground states have $\mathcal{O}_{odd} \neq 0$, while models with Q=even ground states have $\mathcal{O}_{even} \neq 0$. Hence, the string order parameters detect the topological order of the valence bonds.

This topological order has important consequences for the excitation spectrum. In these models with short-range valence-bond ground states, the simplest excitation is generated by breaking one of the valence bonds, which promotes it to a triplet. An interesting and important question is how this excited state propagates. More specifically, does the triplet propagate coherently or does it break apart so that the individual spins forming the triplet-referred to as spinonspropagate independently. In both the rung-singlet and Haldane phases, it is known that the triplet coherently propagates. The reason for this can be understood by looking at Fig. 10 and counting the number of valence bonds crossing a vertical line. When a valence bond is broken in a state with Q=even, if this triplet breaks apart, it leaves a string of valence bonds with the "wrong" topology in the intermediate region. This gives rise to an increase in the local energy, which is proportional to the distance between the two spinons; as a result, the spinons are confined into a (gapped) spin-1 magnon. (A similar situation occurs in the Q=odd Haldane phase.)

From Fig. 10, one also sees that if the two topologically distinct ground states can be made degenerate, one can expect spinons to be deconfined. This is because the string of wrong valence bonds between the two spinons would not give an increase in energy. Thus, the degeneracy provides the "liquidity" necessary for spinon deconfinement.⁷ Indeed, as discussed in Sec. II, this is known to happen in the zigzag ladder due to the frustrating interaction. It is reasonable to expect that similar phenomena could generically occurfrustrating interactions could tune the topologically distinct rung-singlet and Haldane ground states to be degenerate, so that spinons are deconfined and propagate as elementary excitations. While this expectation is reasonable, as will be discussed in detail below, there are other possible phasesnamely, dimerized phases-which could intervene. Moreover, we will see that the system's geometry plays a crucial role in determining whether the system may dimerize or not.

V. WEAK-COUPLING ANALYSIS

It is useful to consider the physics in the limit where the interchain coupling is weak, as controlled analytical calculations are possible. More specifically, we start with two decoupled spin-1/2 chains and consider the interchain coupling as a perturbation. Provided that there is no phase transition, the low-energy Hamiltonian deduced in the weak-coupling limit is valid even at strong coupling, although with renormalized parameters. This approach has been utilized in various other works; besides providing a detailed understanding of the properties of the two-leg ladder and its relation to the spin-1 chain,¹⁹ it has been effective at uncovering and elucidating the phenomena that can arise in these systems.^{12,13,51–54}

We begin Sec. V by briefly describing the formalism mainly to establish our conventions. (More detailed accounts can be found, e.g., in Ref. 55.) We go on to deduce the effective low-energy Hamiltonians for the models considered in this work and then discuss the physics contained in these effective Hamiltonians. In particular, we discuss the role of the various irrelevant operators that arise. These operators were ignored in most previous works but were recently argued to affect the physics qualitatively in some situations.¹² As will be elaborated on below, quantum fluctuations can give rise to several different behaviors. To understand the physics of these quantum fluctuations, we use the RG and examine the behavior of the system under a change in scale.

A. Formalism

The low-energy properties of the spin-1/2 chain are described by an $SU(2)_1$ Wess-Zumino-Witten (WZW) model with Hamiltonian

$$H = \frac{\upsilon}{2\pi} \int dx (\mathbf{J}_R \cdot \mathbf{J}_R + \mathbf{J}_L \cdot \mathbf{J}_L), \qquad (24)$$

where the velocity v is related to J_{\parallel} and \mathbf{J}_R and \mathbf{J}_L are currents satisfying the SU(2)₁ Kac–Moody operator product expansion (OPE),

$$:J_{R}^{\alpha}(z)::J_{R}^{\beta}(w):=\frac{\delta_{\alpha,\beta}}{2(z-w)^{2}}+\frac{\mathrm{i}\,\epsilon^{\alpha\beta\gamma}}{2(z-w)}J_{R}^{\gamma}(w),$$
$$:J_{L}^{\alpha}(\bar{z})::J_{L}^{\beta}(\bar{w}):=\frac{\delta_{\alpha,\beta}}{2(\bar{z}-\bar{w})^{2}}+\frac{\mathrm{i}\,\epsilon^{\alpha\beta\gamma}}{2(\bar{z}-\bar{w})}J_{L}^{\gamma}(w),\qquad(25)$$

with $z=v\tau+ix$ and $\overline{z}=v\tau-ix$. The SU(2)₁ WZW model has a single primary (matrix) field $g(z,\overline{z})$ of dimension (1/4, 1/4). (g is the field appearing in the σ -model representation.) Physical operators of the spin-1/2 chain are given by combinations of the components g—the staggered magnetization $n^{\alpha}(z,\overline{z})$ and the dimerization $\epsilon(z,\overline{z})$,

$$n^{\alpha}(z,\overline{z}) = \operatorname{Tr}[\sigma^{\alpha}g(z,\overline{z})], \quad \boldsymbol{\epsilon}(z,\overline{z}) = \operatorname{Tr}[g(z,\overline{z})], \quad (26)$$

where the $\{\sigma^{\alpha}\}$ are the Pauli matrices. The n^{α} and ϵ fields have leading short-distance behavior,

$$:n^{\alpha}(z)::n^{\beta}(w):=\frac{\delta_{\alpha\beta}}{|z-w|},$$
$$:\epsilon(z)::\epsilon(w):=\frac{1}{|z-w|},$$

$$:n^{\alpha}(z)::\epsilon(w):=0. \tag{27}$$

Furthermore, being linear combinations of the components of g, their OPEs with currents are

$$:J_{R}^{\alpha}(z)::n^{\beta}(w):=\frac{i}{2(z-w)}[\epsilon^{\alpha\beta\gamma}n^{\gamma}(w)-\delta_{\alpha\beta}\epsilon(w)],$$
$$:J_{L}^{\alpha}(z)::n^{\beta}(w):=\frac{i}{2(\overline{z}-\overline{w})}[\epsilon^{\alpha\beta\gamma}n^{\gamma}(w)+\delta_{\alpha\beta}\epsilon(w)],$$
$$:J_{R}^{\alpha}(z)::\epsilon(w):=\frac{i}{2(z-w)}n^{\alpha}(w),$$
$$:J_{L}^{\alpha}(z)::\epsilon(w):=\frac{-i}{2(\overline{z}-\overline{w})}n^{\alpha}(w).$$
(28)

[In Eqs. (27) and (28), $n^{\alpha}(z) \equiv n^{\alpha}(z, \overline{z})$ and $\epsilon(z) \equiv \epsilon(z, \overline{z})$.]

At low energies, the spin operator on chain *i*, $\mathbf{S}_{l}^{(i)}$, can be written as

$$\frac{\mathbf{S}_{l}^{(i)}}{a} = \frac{1}{2\pi} [\mathbf{J}_{iR}(x) + \mathbf{J}_{iL}(x)] + (-1)^{l} \frac{M}{2\pi a^{1/2}} \mathbf{n}_{i}(x), \quad (29)$$

where *a* is an ultraviolet regulator ($a \sim$ the lattice spacing) and *M* is a nonuniversal O(1) constant. In what follows, we will need to know the behavior of the fields upon translation by a single site. From the invariance of the spin operator $\mathbf{S}_{l}^{(i)}$ under translation, we deduce how $\mathbf{J}_{iR}(x)$, $\mathbf{J}_{iL}(x)$, and $\mathbf{n}_{i}(x)$ transform. Then, as all of the terms on the right-hand side of Eq. (28) must transform in the same way upon translation, we deduce how $\epsilon_{i}(x)$ transforms. Hence, we arrive at

$$\mathbf{J}_{iR/L}(x) \to \mathbf{J}_{iR/L}(x),$$
$$\mathbf{n}_i(x) \to -\mathbf{n}_i(x), \quad \boldsymbol{\epsilon}_i(x) \to -\boldsymbol{\epsilon}_i(x). \tag{30}$$

B. Operators and phases: Topological order, dimer order, and deconfined spinons

As described above, starting from two spin-1/2 chains, we are interested in the fate of the system upon turning on an interchain coupling. In Sec. V B, we discuss the various operators that can arise in the low-energy Hamiltonian(s); we discuss the physics that these operators give rise to.

The low-energy Hamiltonians are dictated by symmetry. The models we are considering are all SU(2) symmetric; hence, all operators appearing must transform as SU(2) scalars. Therefore, if only relevant and marginal operators are considered, the operators

$$\boldsymbol{\epsilon}_{1} \text{ and } \boldsymbol{\epsilon}_{2}, \quad \boldsymbol{\epsilon}_{1}\boldsymbol{\epsilon}_{2}, \quad \mathbf{n}_{1} \cdot \mathbf{n}_{2}, \quad \mathbf{n}_{1}\partial_{x}\mathbf{n}_{2}, \quad \boldsymbol{\epsilon}_{1}\partial_{x}\boldsymbol{\epsilon}_{2},$$

$$(\mathbf{J}_{1R} + \mathbf{J}_{1L}) \cdot \mathbf{n}_{2}, \quad (\mathbf{J}_{2R} + \mathbf{J}_{2L}) \cdot \mathbf{n}_{1},$$

$$(\mathbf{J}_{1R} \cdot \mathbf{J}_{2L} + \mathbf{J}_{2R} \cdot \mathbf{J}_{1L}), \quad (\mathbf{J}_{1R} \cdot \mathbf{J}_{1L} + \mathbf{J}_{2L} \cdot \mathbf{J}_{2R}) \quad (31)$$

have the potential of appearing in the low-energy Hamiltonians. Furthermore, we will not consider the terms J_{1R} . J_{2R}

and J_{1L} . Even though these terms have two dimensions (and, hence, are marginal), they couple excitations moving in the same direction on both chains and give rise only to small quantitative corrections. As will be discussed below, other symmetries of the various models will further restrict the operators allowed in their low-energy Hamiltonians.

The physics is determined by the operator that flows to strong coupling first under the RG. When the $\mathbf{n}_1 \cdot \mathbf{n}_2$ term determines the physics, the resulting phases have gapped magnons with spinons being confined.¹⁹ (The $\mathbf{n}_1 \cdot \mathbf{n}_2$ term, in fact, gives rise to a strong confining potential that binds spinons together from the two chains to form a gapped magnon.) Furthermore, these phases have topological order; information about this topological order is contained in the sign of the $\mathbf{n}_1 \cdot \mathbf{n}_2$ term's coefficient. Another possibility is if the physics is determined by the $(\mathbf{J}_{1R} \cdot \mathbf{J}_{2L} + \mathbf{J}_{2R} \cdot \mathbf{J}_{1L})$ term. When this occurs, it has been shown that the resulting phase is a fractionalized phase with deconfined spinons.¹³ Finally, if the physics is determined by the ϵ_1 and ϵ_2 or $\epsilon_1 \epsilon_2$ term(s), the result is a spontaneously dimerized phase.

There are other operators in Eq. (31). However, these operators do not determine the phases that arise, although they modify the properties within a particular phase. In particular, $(\mathbf{J}_{1R} \cdot \mathbf{J}_{1L} + \mathbf{J}_{2L} \cdot \mathbf{J}_{2R})$ is the marginally irrelevant operator present in the two spin-1/2 chains.⁵⁶ Furthermore, $\mathbf{n}_1 \cdot \partial_x \mathbf{n}_2$ and $\epsilon_1 \partial_x \epsilon_2$ are believed to give rise to incommensurate correlations.^{13,54} Finally, as will be seen below, the $(\mathbf{J}_{1R} + \mathbf{J}_{1L}) \cdot \mathbf{n}_2$ and $(\mathbf{J}_{2R} + \mathbf{J}_{2L}) \cdot \mathbf{n}_1$ are always subleading to $\mathbf{n}_1 \cdot \mathbf{n}_2$ and $\epsilon_1 \epsilon_2$ and, hence, do not determine the phases that arise.

C. Effective low-energy Hamiltonians

Here, we deduce the effective low-energy Hamiltonians for the frustrated ladder models considered in this work. We then derive RG equations describing how the parameters in the low-energy Hamiltonian evolve under a change in scale. Finally, we derive the initial values of the parameters from the microscopic models in the limit of weak interchain coupling.

1. Cross-coupled ladder

Besides being SU(2) symmetric, the cross-coupled ladder is invariant under translation by one site and also inversion about the center of the ladder: leg 1 \leftrightarrow leg 2. Translation by one site forbids ϵ_1 and ϵ_2 from appearing alone; it also forbids the operators $(\mathbf{J}_{1R}+\mathbf{J}_{1L})\cdot\mathbf{n}_2$ and $(\mathbf{J}_{2R}+\mathbf{J}_{2L})\cdot\mathbf{n}_1$. Inversion about the center forces operators from leg 1 and leg 2 to symmetrically appear; in particular, it forbids the operators $\mathbf{n}_1\partial_x\mathbf{n}_2$ and $\epsilon_1\partial_x\epsilon_2$ from appearing. These symmetries constrain the effective low-energy Hamiltonian to have the form

$$H = \int dx \left[\gamma (\mathbf{J}_{1R} \cdot \mathbf{J}_{1L} + \mathbf{J}_{2L} \cdot \mathbf{J}_{2R}) + \lambda (\mathbf{J}_{1R} \cdot \mathbf{J}_{2L} + \mathbf{J}_{1L} \cdot \mathbf{J}_{2R}) + \frac{g}{a} \mathbf{n}_1 \cdot \mathbf{n}_2 + \frac{\beta}{a} \epsilon_1 \epsilon_2 \right].$$
(32)

To understand the physics contained in Eq. (32), we use the RG and investigate the behavior under a transformation of scale. By using the OPEs in Eqs. (25), (27), and (28), we deduce the RG equations for the parameters to be⁵⁷

$$\frac{d\gamma}{dl} = \gamma^2 - \frac{1}{2}g^2 + \frac{1}{2}\beta^2,$$
$$\frac{d\lambda}{dl} = \lambda^2 + g^2 - g\beta,$$
$$\frac{dg}{dl} = g - \frac{1}{2}\gamma g + \lambda g - \frac{1}{2}\lambda\beta,$$
$$\frac{d\beta}{dl} = \beta + \frac{3}{2}\gamma\beta - \frac{3}{2}\lambda g.$$
(33)

From the structure of the RG equations, we see that if either g or β is nonzero, both $\mathbf{n}_1 \cdot \mathbf{n}_2$ and $\epsilon_1 \epsilon_2$ will be generated upon renormalization. However, if both g=0 and $\beta=0$, these operators will not appear. Hence, one would expect the relevant $\mathbf{n}_1 \cdot \mathbf{n}_2$ or $\epsilon_1 \epsilon_2$ terms to determine the physics under most situations. If both of these terms are suppressed, the physics would be determined by the marginally relevant $(\mathbf{J}_{1R} \cdot \mathbf{J}_{2L} + \mathbf{J}_{1L} \cdot \mathbf{J}_{2R})$.

To deduce the values of the parameters in Eq. (32), we insert Eq. (29) into Eqs. (2) and (4); we obtain

$$H_{\perp} + H_X = \int \frac{dx}{(2\pi)^2} \left[(J_{\perp} - 2J_X) \frac{M^2}{a} \mathbf{n}_1 \cdot \mathbf{n}_2 - 2J_X \frac{M^2}{a} \sum_{m=1}^{\infty} \frac{a^{2m}}{(2m)!} \mathbf{n}_1 \partial_x^{2m} \mathbf{n}_2 + (J_{\perp} + 2J_X) \times (\mathbf{J}_{1R} \cdot \mathbf{J}_{2L} + \mathbf{J}_{1L} \cdot \mathbf{J}_{2R}) \right].$$
(34)

A lattice Hamiltonian gives rise to a continuum field theory with an infinite number of operators.⁵⁶ Here, besides $\mathbf{n}_1 \cdot \mathbf{n}_2$ and $(\mathbf{J}_{1R} \cdot \mathbf{J}_{2L} + \mathbf{J}_{1L} \cdot \mathbf{J}_{2R})$, an infinite number of irrelevant operators of the form $\mathbf{n}_1 \cdot \partial_x^{2m} \mathbf{n}_2$ appear. From Eq. (34), the relevant operator $\mathbf{n}_1 \cdot \mathbf{n}_2$ determines the physics for generic values of J_{\parallel} and J_{\perp} . When the $\mathbf{n}_1 \cdot \mathbf{n}_2$ term is suppressed, it appears that the physics is determined by the $(\mathbf{J}_{1R} \cdot \mathbf{J}_{2L} + \mathbf{J}_{1L} \cdot \mathbf{J}_{2R})$ term. However, things are more subtle—the irrelevant $\mathbf{n}_1 \cdot \partial_x^{2m} \mathbf{n}_2$ can generate the relevant $\mathbf{n}_1 \cdot \mathbf{n}_2$ and $\epsilon_1 \epsilon_2$ when integrated out.¹² Indeed, focusing on the leading irrelevant operator $\mathbf{n}_1 \cdot \partial_x^2 \mathbf{n}_2$, the term

$$(J_{\perp} + 2J_X) \int \frac{d^2 x_1}{(2\pi)^2} (\mathbf{J}_{1R} \cdot \mathbf{J}_{2L} + \mathbf{J}_{1L} \cdot \mathbf{J}_{2R})$$
$$\times J_X M^2 a \int \frac{d^2 x_2}{(2\pi)^2} \mathbf{n}_1 \cdot \partial_x^2 \mathbf{n}_2$$
(35)

appears in the partition function at second order. By using the OPEs in Eq. (28),

$$\frac{J_X(J_\perp + 2J_X)M^2}{(2\pi)^2 a} \left[\frac{1}{2} \mathbf{n}_1 \cdot \mathbf{n}_2 - \frac{3}{4} \boldsymbol{\epsilon}_1 \boldsymbol{\epsilon}_2 \right]$$
(36)

is generated in the low-energy Hamiltonian. Hence, to leading order, we deduce

$$\lambda = \frac{J_{\perp} + 2J_X}{(2\pi)^2}, \quad \beta = -\frac{3}{8\pi} \frac{(J_{\perp} + 2J_X)J_XM^2}{(2\pi)^2},$$
$$g = \frac{(J_{\perp} - 2J_X)M^2}{(2\pi)^2} + \frac{J_XM^2}{4\pi} \frac{J_{\perp} + 2J_X}{(2\pi)^2}.$$
(37)

As mentioned above, the relevant operator $\mathbf{n}_1 \cdot \mathbf{n}_2$ determines the physics for generic values of J_{\parallel} and J_{\perp} . Now, when $g \rightarrow 0$ in Eq. (37), the relevant $\epsilon_1 \epsilon_2$ is present (from integrating out the irrelevant operators); one may expect it to determine the physics. However, its coefficient is significantly smaller than the $(\mathbf{J}_{1R} \cdot \mathbf{J}_{2L} + \mathbf{J}_{1L} \cdot \mathbf{J}_{2R})$ term. Therefore, a subtle competition between the two interactions should be expected. This competition will be investigated in detail in our numerical calculations.

2. Zigzag ladder

Like the cross-coupled ladder, the zigzag ladder is invariant under translation by a single site. However, it lacks the symmetry of inversion about the center of the ladder. Hence, the operators from leg 1 and leg 2 do not have to appear symmetrically—now, the operators $\mathbf{n}_1 \partial_x \mathbf{n}_2$ and $\epsilon_1 \partial_x \epsilon_2$ are allowed. The effective low-energy Hamiltonian has the form

$$H = \int dx \left[\gamma (\mathbf{J}_{1R} \cdot \mathbf{J}_{1L} + \mathbf{J}_{2L} \cdot \mathbf{J}_{2R}) + \lambda (\mathbf{J}_{1R} \cdot \mathbf{J}_{2L} + \mathbf{J}_{1L} \cdot \mathbf{J}_{2R}) + \frac{g}{a} \mathbf{n}_1 \cdot \mathbf{n}_2 + \frac{\beta}{a} \boldsymbol{\epsilon}_1 \boldsymbol{\epsilon}_2 + g_1 \mathbf{n}_1 \cdot \partial_x \mathbf{n}_2 + \beta_1 \boldsymbol{\epsilon}_1 \partial_x \boldsymbol{\epsilon}_2 \right].$$
(38)

As with the cross-coupled ladder, we investigate the physics of Eq. (38) by using the RG. By using the OPEs, we deduce the RG equations for the parameters to be

$$\frac{d\gamma}{dl} = \gamma^{2} - \frac{1}{2}g^{2} + \frac{1}{2}\beta^{2} + \frac{1}{4}g_{1}^{2} - \frac{1}{4}\beta_{1}^{2},$$

$$\frac{d\lambda}{dl} = \lambda^{2} + g^{2} - g\beta + \frac{1}{2}g_{1}^{2} - \frac{1}{2}g_{1}\beta_{1},$$

$$\frac{dg}{dl} = g - \frac{1}{2}\gamma g + \lambda g - \frac{1}{2}\lambda\beta,$$

$$\frac{d\beta}{dl} = \beta + \frac{3}{2}\gamma\beta - \frac{3}{2}\lambda g,$$

$$\frac{dg_{1}}{dl} = -\frac{1}{2}\gamma g_{1} + \lambda g_{1} - \frac{1}{2}\lambda\beta_{1},$$

$$\frac{d\beta_{1}}{dl} = \frac{3}{2}\gamma\beta_{1} - \frac{3}{2}\lambda g_{1}.$$
(39)

As with the cross-coupled ladder, $\mathbf{n}_1 \cdot \mathbf{n}_2$ and $\epsilon_1 \epsilon_2$ will be generated upon renormalization unless both g=0 and $\beta=0$. Similarly, $\mathbf{n}_1 \cdot \partial \mathbf{n}_2$ and $\epsilon_1 \partial \epsilon_2$ will appear unless both $g_1=0$ and $\beta_1=0$. Hence, as with the cross-coupled ladder, one would expect the $\mathbf{n}_1 \cdot \mathbf{n}_2$ or $\epsilon_1 \epsilon_2$ terms to determine the physics under most situations; if they are suppressed, the physics would be determined by $(\mathbf{J}_{1R} \cdot \mathbf{J}_{2L} + \mathbf{J}_{1L} \cdot \mathbf{J}_{2R})$.

To deduce the values of the parameters in Eq. (38), we insert Eq. (29) into Eqs. (2) and (8); we obtain

$$H_{\perp} + H_{z} = \int \frac{dx}{(2\pi)^{2}} \Biggl\{ (J_{\perp} - J_{2}) \frac{M^{2}}{a} \mathbf{n}_{1} \cdot \mathbf{n}_{2} + \frac{M^{2}}{a} \sum_{m=1}^{\infty} \frac{1}{m!} \Biggl(\frac{a}{2} \Biggr)^{m} [J_{\perp}(-1)^{m} - J_{2}] \mathbf{n}_{1} \partial_{x}^{m} \mathbf{n}_{2} + (J_{\perp} + J_{2}) (\mathbf{J}_{1R} \cdot \mathbf{J}_{1L} + \mathbf{J}_{2L} \cdot \mathbf{J}_{2R}) \Biggr\}.$$
 (40)

As we saw with the cross-coupled ladder, the lattice Hamiltonian gives rise to an infinite number of operators in the field theory. Similar to the cross-coupled ladder, the relevant $\mathbf{n}_1 \cdot \mathbf{n}_2$ determines the physics for generic values of J_{\parallel} and J_{\perp} . Furthermore, when the $\mathbf{n}_1 \cdot \mathbf{n}_2$ term is suppressed, the irrelevant operators may generate terms that determine the physics. Interestingly, for this model, all the terms of the form $\mathbf{n}_1 \cdot \partial_x^{2m} \mathbf{n}_2$ have their coefficient proportional to $(J_{\perp} - J_2)$. Hence, all the operators of the form $\mathbf{n}_1 \cdot \partial_x^{2m} \mathbf{n}_2$ are fine tuned away along the line $J_{\perp}=J_2$; only terms of the form $\mathbf{n}_1 \cdot \partial_r^{2m+1} \mathbf{n}_2$ are present. As there are only derivatives of odd power, they are unable to generate terms such as $\mathbf{n}_1 \cdot \mathbf{n}_2$ or $\epsilon_1 \epsilon_2$. Therefore, for this model, the irrelevant operators do not change the physics (although they give rise to small quantitative changes, e.g., in the size of energy gaps); to leading order, we deduce the parameters in Eq. (38) to be

$$\lambda = \frac{J_{\perp} + J_2}{(2\pi)^2}, \quad g = \frac{(J_{\perp} - J_2)M^2}{(2\pi)^2}, \quad \beta = 0,$$

$$g_1 = -\frac{(J_\perp + J_2)M^2}{2(2\pi)^2}, \quad \beta_1 = 0.$$
 (41)

3. Diagonal ladder

Like the previous two models, the diagonal ladder has translation invariance. However, unlike the cross-coupled and zigzag ladders which are invariant under translation by a single site, the diagonal ladder is invariant under translation by two sites. Furthermore, while this model is not invariant under inversion about the center of the ladder (leg $1 \leftrightarrow \log 2$), it is invariant under inversion compounded by translation by one site. Due to the invariance under translation by two sites, the operators ϵ_1 , ϵ_2 and $(\mathbf{J}_{1R}+\mathbf{J}_{1L})\cdot\mathbf{n}_2$, $(\mathbf{J}_{2R}+\mathbf{J}_{2L})\cdot\mathbf{n}_1$ are now allowed. However, the symmetry of inversion compounded by translation by translation by one site constrains them to appear in the combination $(\epsilon_1-\epsilon_2)$ and $[(\mathbf{J}_{1R}+\mathbf{J}_{1L})\cdot\mathbf{n}_2-(\mathbf{J}_{2R}+\mathbf{J}_{2L})\cdot\mathbf{n}_1]$. Hence, the effective low-energy Hamiltonian has the form

$$H = \int dx \left[\frac{\alpha}{a^{3/2}} (\boldsymbol{\epsilon}_1 - \boldsymbol{\epsilon}_2) + \gamma (\mathbf{J}_{1R} \cdot \mathbf{J}_{1L} + \mathbf{J}_{2L} \cdot \mathbf{J}_{2R}) + \lambda (\mathbf{J}_{1R} \cdot \mathbf{J}_{2L} + \mathbf{J}_{1L} \cdot \mathbf{J}_{2R}) + \frac{g}{a} \mathbf{n}_1 \cdot \mathbf{n}_2 + \frac{\beta}{a} \boldsymbol{\epsilon}_1 \boldsymbol{\epsilon}_2 + \frac{\kappa}{a^{1/2}} [(\mathbf{J}_{1R} + \mathbf{J}_{1L}) \cdot \mathbf{n}_2 - (\mathbf{J}_{2R} + \mathbf{J}_{2L}) \cdot \mathbf{n}_1] \right].$$

$$(42)$$

As before, we use the OPEs to deduce the RG equations for the parameters; we find

$$\frac{d\gamma}{dl} = \gamma^2 - \frac{1}{2}g^2 + \frac{1}{2}\beta^2 + \frac{1}{2}\alpha^2,$$
$$\frac{d\lambda}{dl} = \lambda^2 + g^2 - g\beta,$$
$$\frac{dg}{dl} = g - \frac{1}{2}\gamma g + \lambda g - \frac{1}{2}\lambda\beta - \kappa^2,$$
$$\frac{d\beta}{dl} = \beta + \frac{3}{2}\gamma\beta - \frac{3}{2}\lambda g + \alpha^2 - \frac{3}{2}\kappa^2,$$
$$\frac{d\alpha}{dl} = \frac{3}{2}\alpha + \frac{3}{4}\gamma\alpha + \beta\alpha,$$
$$\frac{d\kappa}{dl} = \frac{1}{2}\kappa - \frac{1}{4}\gamma\kappa + \frac{1}{4}\lambda\kappa - g\kappa + \frac{1}{2}\beta\kappa.$$
(43)

For this ladder model, the operator $(\epsilon_1 - \epsilon_2)$ is allowed; if its initial coefficient is zero, this term will never be generated. Furthermore, we must have $\alpha=0$, g=0, $\beta=0$, and $\kappa=0$ in order for all the relevant operators to be vanished. In particular, if any of these are nonzero, the $\mathbf{n}_1 \cdot \mathbf{n}_2$ and $\epsilon_1 \epsilon_2$ terms will be generated.

To deduce the values of the parameters in Eq. (42), we insert Eq. (29) into Eq. (10); we obtain

$$H_{\perp} + H_{d} = \int \frac{dx}{(2\pi)^{2}} \Biggl\{ (J_{\perp} - J_{2}) \frac{M^{2}}{a} \mathbf{n}_{1} \cdot \mathbf{n}_{2} - J_{2} \frac{M^{2}}{a} \sum_{m=1}^{\infty} \frac{a^{2m}}{(2m)!} \mathbf{n}_{1} \cdot \partial_{x}^{2m} \mathbf{n}_{2} + (J_{\perp} + J_{2}) (\mathbf{J}_{1R} \cdot \mathbf{J}_{1L} + \mathbf{J}_{2L} \cdot \mathbf{J}_{2R}) + \frac{J_{2}M}{a^{1/2}} [(\mathbf{J}_{1R} + \mathbf{J}_{1L}) \cdot \mathbf{n}_{2} - (\mathbf{J}_{2R} + \mathbf{J}_{2L}) \cdot \mathbf{n}_{1}] + \frac{J_{2}M}{a^{1/2}} \sum_{m=1}^{\infty} \frac{a^{2m}}{(2m)!} [(\mathbf{J}_{1R} + \mathbf{J}_{1L}) \cdot \partial_{x}^{2m} \mathbf{n}_{2} - (\mathbf{J}_{2R} + \mathbf{J}_{2L}) \cdot \partial_{x}^{2m} \mathbf{n}_{1}] \Biggr\}.$$
(44)

Interestingly, even though the term $(\epsilon_1 - \epsilon_2)$ is allowed, its coefficient is zero. However, the relevant $[(\mathbf{J}_{1R} + \mathbf{J}_{1L}) \cdot \mathbf{n}_2 - (\mathbf{J}_{2R} + \mathbf{J}_{2L}) \cdot \mathbf{n}_1]$ is always present; as mentioned above, it generates both the $\mathbf{n}_1 \cdot \mathbf{n}_2$ and $\epsilon_1 \epsilon_2$ terms. Hence, for this

model, the irrelevant operators give rise only to small quantitative corrections; the physics that can occur is already contained in the relevant operators already present. Therefore, to leading order, we deduce the values of the parameters in Eq. (42) to be

$$\lambda = \frac{J_{\perp} + J_2}{(2\pi)^2}, \quad g = \frac{(J_{\perp} - J_2)M^2}{(2\pi)^2}, \quad \beta = 0,$$

$$\kappa = \frac{J_2 M}{(2\pi)^2}, \quad \alpha = 0.$$
(45)

As mentioned above, the zigzag ladder is expected to have a fractionalized phase when $g \rightarrow 0$; one can expect a subtle competition between $\epsilon_1 \epsilon_2$ and $(\mathbf{J}_{1R} \cdot \mathbf{J}_{2L} + \mathbf{J}_{1L} \cdot \mathbf{J}_{2R})$ in the cross-coupled ladder. For this ladder model, as $\epsilon_1 \epsilon_2$ is generated by the relevant $[(\mathbf{J}_{1R} + \mathbf{J}_{1L}) \cdot \mathbf{n}_2 - (\mathbf{J}_{2R} + \mathbf{J}_{2L}) \cdot \mathbf{n}_1]$ term, it is reasonable to expect a regime of parameter space where $\epsilon_1 \epsilon_2$ flows to strong coupling first and the system dimerizes.

VI. NUMERICAL RESULTS AND DISCUSSION

In this section, we present our numerical results for the phase diagrams of the models introduced in Sec. II; we discuss them in light of the analytical results presented in Secs. III–V.

A. Numerical method

The numerical calculations have been performed on finite ladders with OBC using the DMRG algorithm⁵⁸ with the dynamic block-state selection (DBSS) approach.^{59,60} We have set the threshold value of the quantum information loss χ to 10⁻⁸ and the minimum number of block states $M_{\rm min}$ to 64. All relevant eigenstates have been independently targeted by using four to six DMRG sweeps until the entropy sum rule⁶⁰ has been satisfied. The accuracy of the Davidson diagonalization routine has been set to 10⁻⁷.

Recently, it has been shown that quantum phase transitions (QPTs) can be conveniently studied by calculating some measure of entanglement.⁶¹⁻⁷¹ In particular, the von Neumann entropy of a block containing a finite number of neighboring sites often gives a clear indication of a QPT, as anomalies appear in these quantities at the transition: the entropy exhibits a jump at a first-order transition or develops a cusp (with increasing N) at a continuous transition. Furthermore, even if the entropy is analytic, its extrema are often indicative of changes in the system. Indeed, extrema in the entropy are known to occur in the SU(n) Hubbard model at 1/n filling, where a Kosterlitz–Thouless transition occurs;^{67,72,73} extrema are also known to occur at the valence-bond-solid point of the spin-1 bilinear-biquadratic chain,⁷⁴ where the system's wave function changes character.⁴⁵ Therefore, in what follows, besides looking for discontinuities and cusps in the entropy, we will also scrutinize the regions where the entropies exhibit extrema (without developing a cusp).

It should be noted that, depending on how a first-order transition is realized, one might have difficulty distinguish-

ing it from a continuous transition. More specifically, if the two levels corresponding to the different ground states are already orthogonal in a finite-sized system, the entropy of a block will exhibit a jump when the two levels cross (in a finite-sized system). However, if the two levels are not orthogonal in a finite-sized system, the wave function, energy, and consequently the entropy of a block will continuously vary in any finite-sized system. In this case, the level crossing develops only asymptotically, and the jump in the entropy appears only in the $N \rightarrow \infty$ limit.

In this work, we consider (i) s_l , the entropy of the *l*th rung, (ii) $s_{l,l+1}$, the two-rung entropy of the neighboring *l*th and (l+1)st rungs, (iii) $s_{l,l+1}^{(i)}$, the two-site entropy of the spins $\mathbf{S}_l^{(i)}$ and $\mathbf{S}_{l+1}^{(i)}$ on chain *i*, and also (iv) $s_N(l)$, the entropy of a block formed by the left *l* rungs of a ladder with *N* rungs. To avoid end effects, we compute s_l , $s_{l,l+1}$, and $s_{l,l+1}^{(i)}$ in the middle of the ladder for l=N/2 or l=N/2+1. As discussed above, one of our primary interests is to identify dimerized phases that may arise and the concomitant breaking of translational symmetry. The appearance of a columnar dimerized phase can be detected by considering the difference of two-rung entropies,

$$D_s = s_{l+1,l+2} - s_{l,l+1}, \quad l = N/2.$$
(46)

Alternatively, taking the block entropy $s_N(l)$ of the left l rungs, one can consider

$$\tilde{D}_s = s(l) - s(l+1), \quad l = N/2,$$
(47)

which tells how the block entropy of the left half changes when an extra rung is added. The appearance of staggered dimerization can be detected by considering the difference of two-site entropies on the two chains,

$$P_s = (s_{l+1,l+2}^{(1)} - s_{l,l+1}^{(1)}) - (s_{l+1,l+2}^{(2)} - s_{l,l+1}^{(2)}), \quad l = N/2.$$
(48)

Further information about the phases that arise can be deduced by studying the length dependence of $s_N(l)$.^{75–79} For noncritical, gapped models, this quantity saturates to a finite value when l is far from the boundaries, while for critical systems,

$$s_N(l) = \frac{c}{6} \ln \left[\frac{2N}{\pi} \sin \left(\frac{\pi l}{N} \right) \right] + g, \qquad (49)$$

where *c* is the central charge.^{75,80} Moreover, if the system's ground state is spatially inhomogeneous, oscillations appear in $s_N(l)$.⁴⁵ Hence, the Fourier spectrum

$$\widetilde{s}(k) = \frac{1}{N} \sum_{l=0}^{N} e^{-ikl} s_N(l)$$
(50)

carries information⁴⁵ about the spatial inhomogeneity: if the amplitude of a peak at a nonzero wave number k^* remains finite in the thermodynamic limit, this indicates a periodic spatial modulation of the ground state with wavelength $\lambda = 2\pi/k^*$.

In what follows, we will often need to know the large-*N* behavior of various quantities. For any quantity *A*, the finite-size scaling ansatz

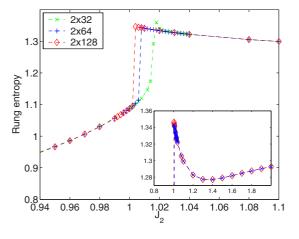


FIG. 11. (Color online) Single-rung entropy as a function of J_2 for $J_{\perp}+J_2=2J_{\parallel}$ with $J_{\parallel}=1$ for three different lengths of the ladder.

$$A(N) = A_0 + a/N^\beta \tag{51}$$

has been used, where A_0 , a, and β are free parameters determined by a least-squares fitting procedure.

B. Results and discussion

1. Zigzag ladder

We first present results for the zigzag ladder. Since the phase diagram and properties of this model are well known, it serves as a test case for the other models. The J_{\perp} , J_2 parameter space was explored by calculating various entropy functions for J_{\perp} and J_2 satisfying

$$J_{\perp} + J_2 = C J_{\parallel} \tag{52}$$

for several values of *C*. In the numerical calculations, the energy scale was set by taking J_{\parallel} to be unity.

We first show results obtained for C=2. As seen in Fig. 11, s_l in the middle of the ladder is discontinuous at $J_{\perp}=J_2=J_{\parallel}$, which indicates a first-order transition. Besides the discontinuity, the inset of Fig. 11 shows a minimum in the entropy at $J_2 \simeq 1.36 J_{\parallel}$. Moreover, there is also a minimum in $\tilde{s}(k)$ at an incommensurate k^* in the region $0.5 < J_2/J_{\parallel}$ < 1.36. On physical grounds, there is no reason to expect another transition in the zigzag ladder since any deviation from the $J_{\perp} = J_2$ line drives the system into the rung-singlet or Haldane phase. Indeed, this minimum is a finite-size effect-it originates from the two end spins of the Haldane phase. To substantiate this, notice that there is no sign of this minimum in the rung-singlet phase, while we know that the phase boundaries must be symmetric under the interchange of J_{\perp} and J_2 . Furthermore, by attaching spin 1/2 to the ends of the ladder with a strong anitferromagnetic coupling, the end spins can be eliminated.⁸¹ When the calculations are repeated with these extra spin 1/2 attached to the ends, the minimum in $\tilde{s}(k)$ at an incommensurate k^* disappears.

Performing the calculations for couplings satisfying Eq. (52) with other values of *C*, a behavior similar to Fig. 11 was observed whenever the line $J_{\perp}=J_2$ was crossed at $J_{\perp} < J_{\parallel}/0.241$. That indicates that the system undergoes a first-order transition (along the line $J_{\perp}=J_2$) for

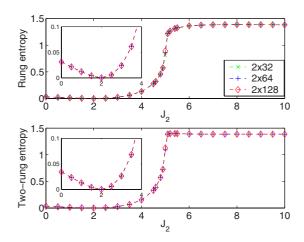


FIG. 12. (Color online) Single-rung and block entropies for $J_{\perp}+J_2=10J_{\parallel}$ as a function of J_2 for ladders with 32, 64, and 128 rungs. The insets show the behavior near $J_2=2J_{\parallel}$, where the entropies vanish.

 $J_{\parallel} < J_{\parallel}/0.241$. Different behaviors in the entropies were observed, however, for stronger interchain couplings. Figure 12 shows s_l (top panel) and $s_{l,l+1}$ (bottom panel) in the middle of the ladder for $J_{\perp} + J_2 = 10J_{\parallel}$. In the rung-singlet phase, s_l is small, as the spins on a rung are predominantly in a singlet state; in the Haldane-type phase, s_l is close to $\ln 4 \approx 1.386$, since the valence bonds are predominantly formed between neighboring rungs. Notice, however, that s_l has no longer a jump at $J_{\perp} = J_2 = C J_{\parallel}/2$ (as it did in Fig. 11); rather, s_l and $s_{l,l+1}$ have a discontinuity in their slope. When $s_N(l)$ was computed at the point $J_{\perp}=J_2$, it was found that it could fit well with the form given in Eq. (49) with c=1. These results are consistent with a continuous transition between the rungsinglet and Haldane-type phases in this regime. They are consistent with the fact that if the zigzag ladder is written as a single chain with nearest- and next-nearest-neighbor couplings, the chain is critical in this regime with the low-energy physics being described by Eq. (24).

The insets of Fig. 12 show s_l and $s_{l,l+1}$ in a region about $J_2=2J_{\parallel}$; we see that the entropy functions vanish at $J_2=2J_{\parallel}$ for any length of the ladder. This is because the exact ground state is a product of rung singlets [see Eq. (15)] for $J_2=2J_{\parallel}$. In fact, the entropies vanish along the entire line $J_2=2J_{\parallel}$ when $J_{\perp} \ge 2J_{\parallel}$, as Eq. (15) is the exact ground state. Furthermore, computing the entropy of the two spins coupled along the diagonal by J_2 , $\mathbf{S}_l^{(1)}$ and $\mathbf{S}_{l+1}^{(2)}$, this entropy was found to vanish for $J_{\perp}=2J_{\parallel}$ when $J_2 \ge 2J_{\parallel}$. This is because Eq. (20) is the exact ground state along this line. More generally, due to the symmetry of the model, one obtains the same results presented in Figs. 11 and 12 if J_{\perp} and J_2 are interchanged; instead of considering rung entropies, one must consider the entropies of diagonally coupled spins.

Setting together these results, we arrive at the phase diagram in Fig. 13. The transition line at $J_{\perp}=J_2$ is of first order in the weak-coupling limit, which becomes of second order at strong couplings. The entire region above (below) the line $J_{\perp}=J_2$ is continuously related to the exactly solvable line $J_2=2J_{\parallel}$ ($J_{\perp}=2J_{\parallel}$) and, hence, is in the rung-singlet (Haldane) phase. In terms of the effective low-energy Hamiltonian dis-

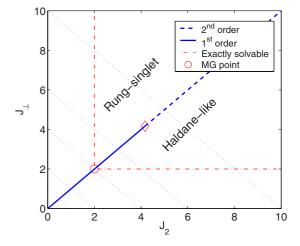


FIG. 13. (Color online) Phase diagram of the zigzag ladder. The first- and second-order transitions between the rung-singlet and Haldane phases are denoted by solid and dashed lines, respectively. The ground state along the dashed-dotted line is an exact rung-singlet or diagonal-singlet valence-bond state. The dotted lines indicate the parameter values where the DMRG calculation were done.

cussed in Sec. V C 2, the physics in these phases is determined by the $\mathbf{n}_1 \cdot \mathbf{n}_2$ term; in the rung-singlet (Haldane) phase, its coefficient is positive (negative). As discussed in Sec. IV, the rung-singlet (Haldane) phase has Q=even (Q=odd) topological order, and the elementary excitations are gapped magnons with spinons being confined. Along the $J_{\perp} = J_2$ line, the two topologically distinct ground states become degenerate and spinons are deconfined, with domain walls between the two topologically distinct (and energetically degenerate) ground states. As mentioned in Sec. VII, at weak coupling, the physics is determined by the $(\mathbf{J}_{1R} \cdot \mathbf{J}_{2L})$ + \mathbf{J}_{2R} · \mathbf{J}_{1L}) term (with the $\mathbf{n}_1 \cdot \partial_x \mathbf{n}_2$ and $\epsilon_1 \partial_x \epsilon_2$ terms giving rise to incommensuration). Looking at Eq. (40), this fractionalized phase occurs because the geometry of the zigzag ladder fine tunes away an infinite number of operators which could cause dimerization.

2. Cross-coupled ladder

As with the zigzag ladder, we calculated s_l and $s_{l,l+1}$ for J_{\perp} and J_X satisfying Eq. (52) with various values of *C*. Figure 14 shows results obtained for intermediate values of the interchain couplings, C=2 and C=3. Here, we see that the entropy functions display a finite jump, indicating a first-order transition. The inset shows that s_l vanishes (independent of the ladder's length) at $J_X=J_{\parallel}$. This occurs because Eq. (15) is the exact ground state for $J_X=J_{\parallel}$ with $J_{\perp} \ge 2J_{\parallel}$. It was shown in Ref. 32 that Eq. (15) is, in fact, the ground state for $J_X=J_{\parallel}$ and $J_{\perp} \ge 1.401J_{\parallel}$. Our numerical results are in agreement with this prediction.

Besides the finite jump at $J_X=0.8$, Fig. 14 also shows that the two-site entropy possesses a minimum around $J_X\approx 1$; furthermore, weak incommensurate oscillations were found to appear in $s_N(l)$. Similar to the zigzag ladder, these are finite-size effects due to the end spins in the Haldane phase. Indeed, when calculations are repeated for a system in which

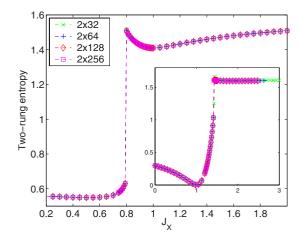


FIG. 14. (Color online) Two-rung entropy of the cross-coupled ladder as a function of J_X for $J_{\perp}=2J_{\parallel}-J_X$ for various system sizes. The dashed line is a guide for the eyes. The inset shows the same but for the $J_{\perp}=3J_{\parallel}-J_X$.

spin 1/2's are attached to the ends of the ladder (to freeze the end spins), the block entropy $s_N(l)$ saturates for shorter chains and the minimum in $\tilde{s}(k)$ at an incommensurate k^* disappears. The amplitude of the remaining negative peak in $\tilde{s}(k)$ at $k^* = \pi$ was found to vanish in the thermodynamic limit. Hence, no spatial inhomogeneity develops along the transition line.

The numerical results show a different behavior when C < 1.3. s_l as a function of J_X is shown in Fig. 15 for C=1. The ground-state wave function continuously evolves in the weak-coupling regime; as longer and longer ladders are considered, s_l exhibits a sharper and sharper maximum (bounded from above by ln 4), developing into a cusp at $J_{Xc}/J_{\parallel}=0.355(3)$. Such behavior is suggestive of a continuous transition. Recent numerical works reported a continuous transition in the weak-coupling regime, ^{20,33} which is in disagreement with analytic results¹⁰ as well as previous numerical calculations.¹¹ However, the analytic results are expected to be reliable in the weak-coupling regime. As was checked

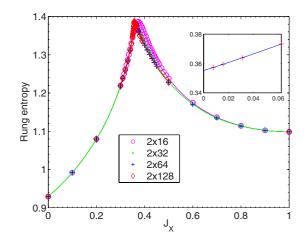


FIG. 15. (Color online) One-rung entropy of the cross-coupled ladder model for $J_{\perp}+J_X=J_{\parallel}$ for several system sizes. The solid line is a polynomial fit. The inset shows the finite-size scaling of the position of the maximum of the entropy.

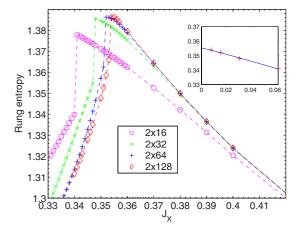


FIG. 16. (Color online) Same as Fig. 15 but with spin-1/2 particles attached to the two ends of the ladder with strong antiferromagnetic couplings. The inset shows the finite-size scaling of the position of the jump in the entropy.

by the DBSS procedure, a reliable extrapolation of the gap requires calculations on longer ladders and keeping a significantly larger number of block states than was available in Ref. 20. The same holds for the entropy. Moreover, as was shown above, spurious effects can arise due to end spins. Indeed, when the calculations were repeated by attaching spin 1/2 to the ends of the ladder, s_l behaves somewhat differently. As shown in Fig. 16, instead of an abrupt change in slope, a jump now seems to develop; its position scales to the same value of J_{Xc} obtained in Fig. 15. This behavior suggests that the transition is of first order. Based on these considerations, we believe that the transition is, in fact, first order. Although the singlet ground-state wave function continuously evolves in the weak-coupling regime for finite-sized systems, a crossing with the next singlet level is expected to develop in the $N \rightarrow 8$ limit (as per the discussion in Sec. VI A); the asymmetric cusp in Fig. 15 is expected to develop into a jump.

A further interesting feature of the model for weak interchain coupling is shown in Fig. 17. More specifically, the two-rung entropy $s_{l,l+1}$ measured for l=N/2 exhibits two well separated peaks at $J_{Xc_1}(N)$ and $J_{Xc_2}(N)$, but it exhibits a single peak for l=N/2+1. The difference $D_s(N)$ is also finite in the region between J_{Xc_1} and J_{Xc_2} . This could suggests the existence of a columnar dimer phase in a narrow range of couplings, as predicted in Ref. 12. However, the two peaks merge in the $N \rightarrow \infty$ limit and the width of the putative dimer phase shrinks to zero. As shown in the inset of Fig. 17, a finite-size scaling analysis gives the same critical value as the one-rung entropy. The same behavior was observed in the calculation along the line $J_X=0.2J_{\parallel}$ confirming the findings of Ref. 33.

We have also computed $s_N(l)$ and its Fourier transform $\tilde{s}(k)$. $|\tilde{s}(k)|$ was found to have an extra peak at $k^* = \pi$, besides the one at k=0. However, $|\tilde{s}(k^*=\pi)|$ was found to vanish in the large-*N* limit, which indicates that the ground state is always spatially homogeneous. Similar behavior was found for other values of J_{\perp} and J_X in the weak-coupling regime. Furthermore, we computed the staggered dimerization [see Eq. (48)] and we found that it also vanishes in the $N \rightarrow 0$

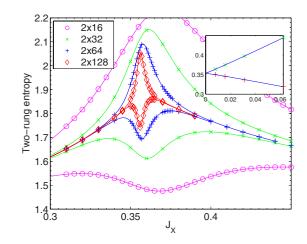


FIG. 17. (Color online) Two-rung entropy of the cross-coupled ladder model for $J_{\perp} + J_X = J_{\parallel}$ for various system sizes. The solid line is a polynomial fit. The inset shows the finite-size scaling of the positions of the peaks of the entropy.

limit. This provides strong evidence that, at least for weak interchain coupling, there is no intermediate columnar or staggered dimer phase between the rung-singlet and Haldane phases.

Setting together these results, we obtain the phase diagram for the cross-coupled ladder, as shown in Fig. 18. The entire region above the transition line is continuously related to the exactly solvable line $J_X/J_{\parallel}=1$ and, hence, is in the rung-singlet phase. The entire region below the transition line is continuously related the point $J_X=1$ and $J_{\perp}=0$ and, hence, is in the Haldane phase. As with the zigzag ladder, the physics in these phases is determined by the $\mathbf{n}_1 \cdot \mathbf{n}_2$ term in the low-energy Hamiltonian—these phases have topological order and confined spinons. As discussed in Sec. V C 1, at the transition, there is a subtle competition between the $(\mathbf{J}_{1R} \cdot \mathbf{J}_{2L} + \mathbf{J}_{1L} \cdot \mathbf{J}_{2R})$ and $\epsilon_1 \epsilon_2$ terms, which give rise to a fractionalized and dimerized phase, respectively. However, the entire transition line appears to be of first order, with no

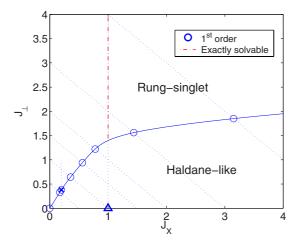


FIG. 18. (Color online) Phase diagram of the cross-coupled ladder. The symbol \times denotes the transition point calculated in Ref. 33. \triangle denotes the point where the ladder model is equivalent to a spin-1 chain. The ground state is an exact rung-singlet state along the dashed-dotted line.

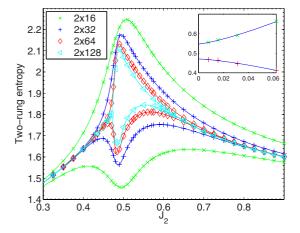


FIG. 19. (Color online) Two-rung entropy of the diagonal ladder model for $J_{\perp}+J_2=J_{\parallel}$ for various system sizes. The solid line is a polynomial fit. The inset shows the finite-size scaling of the positions of the peaks of the entropy.

evidence for an intermediate dimerized phase being found. Hence, our results suggest that a dimerized phase does not appear in this model. In constructing the phase diagram, we made use of a duality relationship of the model. Similar to what was described for the diagonal ladder in Sec. II, one can interchange the spins on every second rung: $S_{2l}^1 \leftrightarrow S_{2l}^2$. When this is done for this ladder model, another crosscoupled ladder is obtained but with J_{\parallel} and J_X interchanged. This implies that energies and, in particular, energy gaps satisfy

$$E(J_{\parallel}, J_{\perp}, J_X) = E(J_X, J_{\perp}, J_{\parallel}).$$
⁽⁵³⁾

Scaling by J_{\parallel} , one obtains

$$E(J_{\perp}/J_{\parallel}, J_X/J_{\parallel}) = (J_X/J_{\parallel})E(J_{\perp}/J_X, J_{\parallel}/J_X).$$
(54)

3. Diagonal ladder

As with the other models, we computed s_l and $s_{l,l+1}$ for J_{\perp} and J_2 which satisfy Eq. (52) with various values of *C*. Here, in contrast to the other two models, we find a dimerized phase intervening between the rung-singlet and Haldane phases.

Figure 19 shows $s_{l,l+1}$ for $J_{\perp} + J_2 = J_{\parallel}$. While the behavior appears similar to Fig. 17, the $N \rightarrow \infty$ limit is drastically different. Indeed, while a single transition was found for the cross-coupled ladder, the inset of Fig. 19 shows that the two peaks do not collapse in this model. Hence, Fig. 19 suggests the system undergoes two distinct transitions at J_{2c_1}/J_{\parallel} =0.459 and J_{2c_2}/J_{\parallel} =0.563, with a columnar dimerized phase between the two transition lines. To substantiate this, we have computed $s_N(l)$ and subsequently $|\tilde{s}(k^* = \pi)|$, with the entropy difference between neighboring plaquettes D_s (shown in Fig. 20) and also the energy difference between neighboring plaquettes. All of these quantities were found to scale to a finite value in the region between J_{2c_1} and J_{2c_2} . Similar behavior was found for other values of the parameters in the weak-coupling limit. Hence, we conclude that a columnar dimerized phase does, in fact, exist between the

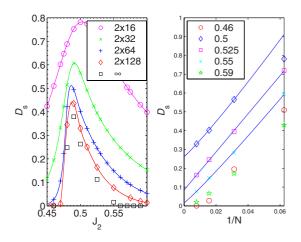


FIG. 20. (Color online) The dimerization entropy of the diagonal ladder model for $J_{\perp}+J_2=J_{\parallel}$ for various system sizes. The solid line is a polynomial fit. The left panel shows the finite-size scaling of the D_s for various J_2 values.

rung-singlet and Haldane phases in this model.

When the calculations were repeated for $J_{\perp}+J_2>2J_{\parallel}$, a single first-order transition was obtained. It is worth noting that due to the rather small values of the gap, the asymptotic behavior can be seen only for long ladders. As before, convergence can be accelerated in the Haldane phase by attaching spin 1/2 to the ends of the ladder (to pin the end spins).

Figure 21 summarizes our finding for the phase diagram of the diagonal ladder. The entire region above the transition line is continuously related to the exactly solvable line $J_2/J_{\parallel}=2$ and, hence, is in the rung-singlet phase. The entire region below the transition line is in the Haldane phase. As with the previous two ladder models, these phases have topological order with confined spinons; the physics in these phases is determined by the $\mathbf{n}_1 \cdot \mathbf{n}_2$ term in the low-energy Hamiltonian. However, contrary to what was found for the cross-coupled and zigzag ladders, from the discussion in Sec. V C 3, it is reasonable to expect a regime in between the rung-singlet and Haldane phases where the diagonal ladder

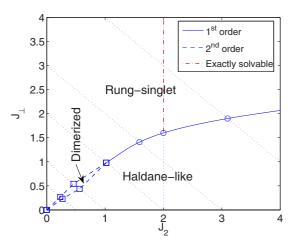


FIG. 21. (Color online) Phase diagram of the diagonal ladder. The first- and second-order phase transition points are indicated by the circle and square symbols, respectively. The exact rung-singlet ground state is indicated by a dashed-dotted line.

dimerizes (i.e., where the physics is determined by the $\epsilon_1 \epsilon_2$ term). This is, indeed, found to be the case—a narrow but extended region is found where the ground state is dimerized. The first-order transition is replaced in the weak-coupling regime by two second-order transitions.

VII. CONCLUDING REMARKS

In this work, we considered several frustrated spin ladder models, which are related to higher-dimensional models of current interest. In large regions of parameter space, these models have short-range RVB ground states with topological order; they are adiabatically related to the ground states of the rung-singlet or Haldane phase. We investigated the role of frustrating interactions on the models, addressing, in particular, how the transition between phases with different topological orders occurs. In the simplest case, a direct transition takes place along the line where the even- and oddtopology phases become degenerate. While the elementary excitations of the topologically ordered phases are gapped magnons, spinons become deconfined along the transition line and a fractionalized phase is obtained. Alternatively, the transition may occur in two steps, with an intermediate phase having broken translational symmetry. In this case, spinons always remain confined.

An important observation from our analysis is the strong "desire" for broken-symmetry phases to arise at the transition between the rung-singlet and Haldane phases. Indeed, we saw that spin models typically give rise to an infinite number of operators that could cause dimerization.¹² These operators arose in the diagonal ladder, and a dimerized phase was seen to appear in the phase diagram. These operators also arose in the cross-coupled ladder; nevertheless, in agreement with

Ref. 33, we found no evidence for dimerized phases in our numerics. The RG equations suggest that this occurs due to a subtle interplay and/or competition of quantum fluctuations. Although no dimerized phase appears in the cross-coupled ladder studied in this paper, in this delicate situation even small perturbations are likely to drive the cross-coupled model into dimerized phases, as shown in Ref. 82. The zig-zag ladder was an exception—the model's geometry fine tunes away the infinite number of operators which could cause dimerization.

We believe these results give an outlook into the physics of higher-dimensional systems. In particular, our results show the importance of a system's geometry in achieving the necessary liquidity for fractionalized excitations to occur. Hence, our results illustrate why fractionalized phases are hard to come by—fractionalized phases are delicate objects, which require some level of fine tuning. Even on lattices where the necessary fine tuning occurs (such as the triangular lattice), small perturbations due to, e.g., spin-phonon coupling⁵¹ or ring exchanges, are likely to drive the system into a dimerized phase.

ACKNOWLEDGMENTS

E.H.K. gratefully acknowledges the warm hospitality of the Research Institute for Solid State Physics and Optics (Budapest, Hungary), where parts of this work were performed. This work was supported by the NSERC (E.H.K.), SHARCNET (E.H.K. and J.S.), the Hungarian Research Fund OTKA under Grants No. K 68340, No. F 46356, and No. NF 61726 (O.L. and J.S.), and the János Bolyai Research Fund (O.L.). The authors acknowledge computational support from Dynaflex Ltd. under Grant No. IgB-32.

- ¹For reviews, see *Frustrated Spin Systems*, edited by H. T. Diep (World Scientific, Singapore, 2004); *Quantum Magnetism*, edited by U. Schollwock, J. Richter, D. J. Farnell, and R. F. Bishop, Lectures Notes in Physics Vol. 645 (Springer, Berlin, 2004).
- ²P. W. Anderson, Science **235**, 1196 (1987).
- ³S. Sachdev, in *Low Dimensional Quantum Field Theory for Condensed Matter Physicists*, edited by Y. Lu, S. Lundqvist, and G. Morandi (World Scientific, Singapore, 1995).
- ⁴E. Fradkin, *Field Theories of Condensed Matter Systems* (Addison-Wesley, New York, 1991).
- ⁵N. E. Bonesteel, Phys. Rev. B **40**, 8954 (1989).
- ⁶X. G. Wen, Phys. Rev. B **44**, 2664 (1991); T. Senthil and M. P. A. Fisher, *ibid.* **61**, 9690 (2000).
- ⁷R. Moessner, S. L. Sondhi, and E. Fradkin, Phys. Rev. B **65**, 024504 (2001).
- ⁸F. D. M. Haldane, Phys. Rev. Lett. **61**, 1029 (1988); N. Read and S. Sachdev, Phys. Rev. B **42**, 4568 (1990).
- ⁹S. R. White, Phys. Rev. B 53, 52 (1996).
- ¹⁰E. H. Kim, G. Fáth, J. Sólyom, and D. J. Scalapino, Phys. Rev. B 62, 14965 (2000).
- ¹¹G. Fáth, Ö. Ligeza, and J. Sólyom, Phys. Rev. B **63**, 134403 (2001).

- ¹²O. A. Starykh and L. Balents, Phys. Rev. Lett. **93**, 127202 (2004).
- ¹³D. Allen, F. H. L. Essler, and A. A. Nersesyan, Phys. Rev. B 61, 8871 (2000).
- ¹⁴R. M. Noack, S. R. White, and D. J. Scalapino, Physica C 270, 281 (1996); H. J. Schulz, Phys. Rev. B 53, R2959 (1996); L. Balents and M. P. A. Fisher, *ibid.* 53, 12133 (1996).
- ¹⁵A. Seidel and D.-H. Lee, Phys. Rev. Lett. **97**, 056804 (2006).
- ¹⁶For a review, see E. Dagotto, Rep. Prog. Phys. **62**, 1525 (1999).
- ¹⁷D. J. Scalapino, Nature (London) **377**, 12 (1995); E. Dagotto and T. M. Rice, Science **271**, 618 (1996).
- ¹⁸S. R. White, R. M. Noack, and D. J. Scalapino, Phys. Rev. Lett. 73, 886 (1994).
- ¹⁹D. G. Shelton, A. A. Nersesyan, and A. M. Tsvelik, Phys. Rev. B 53, 8521 (1996).
- ²⁰X. Wang, Mod. Phys. Lett. B **14**, 327 (2000).
- ²¹Ö. Legeza, G. Fáth, and J. Sólyom, Phys. Rev. B 55, 291 (1997).
- ²²Ö. Legeza and J. Sólyom, Phys. Rev. B 56, 14449 (1997).
- ²³F. D. M. Haldane, Phys. Rev. Lett. 50, 1153 (1983); Phys. Lett. 93A, 464 (1983).
- ²⁴J. Sólyom and J. Timonen, Phys. Rev. B **38**, 6832 (1988).
- ²⁵Y. Xian, Phys. Rev. B **52**, 12485 (1995).
- ²⁶G. Sierra, M. A. Martín-Delgado, S. R. White, D. J. Scalapino,

and J. Dukelsky, Phys. Rev. B **59**, 7973 (1999); M. A. Martín-Delgado, J. Rodriguez-Laguna, and G. Sierra, *ibid.* **72**, 104435 (2005).

- ²⁷S. Wakimoto, G. Shirane, Y. Endoh, K. Hirota, S. Ueki, K. Yamada, R. J. Birgeneau, M. A. Kastner, Y. S. Lee, P. M. Gehring, and S. H. Lee, Phys. Rev. B **60**, R769 (1999); S. Wakimoto, R. J. Birgeneau, M. A. Kastner, Y. S. Lee, R. Erwin, P. M. Gehring, S. H. Lee, M. Fujita, K. Yamada, Y. Endoh, K. Hirota, and G. Shirane, *ibid.* **61**, 3699 (2000).
- ²⁸J. M. Tranquada, D. J. Buttrey, V. Sachan, and J. E. Lorenzo, Phys. Rev. Lett. **73**, 1003 (1994).
- ²⁹ V. Sachan, D. J. Buttrey, J. M. Tranquada, J. E. Lorenzo, and G. Shirane, Phys. Rev. B **51**, 12742 (1995).
- ³⁰M. P. Gelfand, Phys. Rev. B **43**, 8644 (1991).
- ³¹ J. S. Gardner, S. R. Dunsiger, B. D. Gaulin, M. J. P. Gingras, J. E. Greedan, R. F. Kiefl, M. D. Lumsden, W. A. MacFarlane, N. P. Raju, J. E. Sonier, I. Swainson, and Z. Tun, Phys. Rev. Lett. **82**, 1012 (1999); A. S. Wills, N. P. Raju, and J. E. Greedan, Chem. Mater. **11**, 1510 (1999); M. J. Harris, M. P. Zinkin, Z. Tun, B. M. Wanklyn, and I. P. Swainson, Phys. Rev. Lett. **73**, 189 (1994); R. De Pape and G. Ferey, Mater. Res. Bull. **21**, 971 (1986).
- ³²Zheng Weihong, V. Kotov, and J. Oitmaa, Phys. Rev. B 57, 11439 (1998).
- ³³H.-H. Hung, C.-D. Gong, Y.-C. Chen, and M.-F. Yang, Phys. Rev. B **73**, 224433 (2006).
- ³⁴R. Coldea, D. A. Tennant, A. M. Tsvelik, and Z. Tylczynski, Phys. Rev. Lett. **86**, 1335 (2001); R. Coldea, D. A. Tennant, and Z. Tylczynski, Phys. Rev. B **68**, 134424 (2003).
- ³⁵M. Matsuda and K. Katsumata, J. Magn. Magn. Mater. **140-144**, 1671 (1995); Z. Hiroi, M. Azuma, M. Takano, and Y. Bando, J. Solid State Chem. **95**, 230 (1991); N. Motoyama, H. Eisaki, and S. Uchida, Phys. Rev. Lett. **76**, 3212 (1996); M. Matsuda, K. Katsumata, K. M. Kojima, M. Larkin, G. M. Luke, J. Merrin, B. Nachumi, Y. J. Uemura, H. Eisaki, N. Motoyama, S. Uchida, and G. Shirane, Phys. Rev. B **55**, R11953 (1997).
- ³⁶K. Okamoto and K. Nomura, Phys. Lett. A **169**, 433 (1992).
- ³⁷S. Eggert, Phys. Rev. B **54**, R9612 (1996).
- ³⁸F. D. M. Haldane, Phys. Rev. B **25**, 4925 (1982); **26**, 5257(E) (1982).
- ³⁹C. K. Majumdar and D. K. Ghosh, J. Math. Phys. **10**, 1388 (1969); **10**, 1399 (1969).
- ⁴⁰A. K. Kolezhuk and H.-J. Mikeska, Phys. Rev. B 56, R11380 (1997).
- ⁴¹T. Tonegawa and I. Harada, J. Phys. Soc. Jpn. 56, 2153 (1987);
 T. Tonegawa, I. Harada, and M. Kaburagi, *ibid.* 61, 4665 (1992).
- ⁴²R. Chitra, S. Pati, H. R. Krishnamurthy, D. Sen, and S. Ramasesha, Phys. Rev. B **52**, 6581 (1995).
- ⁴³S. R. White and I. Affleck, Phys. Rev. B **54**, 9862 (1996).
- ⁴⁴A. A. Aligia, C. D. Batista, and F. H. L. Essler, Phys. Rev. B 62, 3259 (2000).
- ⁴⁵Ö. Legeza, J. Sólyom, L. Tincani, and R. M. Noack, Phys. Rev. Lett. **99**, 087203 (2007).
- ⁴⁶B. S. Shastry and B. Sutherland, Phys. Rev. Lett. **47**, 964 (1981).
- ⁴⁷I. Bose, Phys. Rev. B **45**, 13072 (1992); I. Bose and S. Gayen, *ibid.* **48**, 10653 (1993).
- ⁴⁸X.-G. Wen, *Quantum Field Theory of Many-Body Systems* (Oxford University Press, New York, 2004).
- ⁴⁹M. P. M. den Nijs and K. Rommelse, Phys. Rev. B 40, 4709

(1989).

- ⁵⁰ Y. Nishiyama, N. Hatano, and M. Suzuki, J. Phys. Soc. Jpn. 64, 1967 (1995).
- ⁵¹A. A. Nersesyan and A. M. Tsvelik, Phys. Rev. Lett. **78**, 3939 (1997).
- ⁵²A. A. Nersesyan, A. O. Gogolin, and F. H. L. Essler, Phys. Rev. Lett. **81**, 910 (1998).
- ⁵³E. Orignac and T. Giamarchi, Phys. Rev. B 56, 7167 (1997).
- ⁵⁴D. C. Cabra, A. Honecker, and P. Pujol, Eur. Phys. J. B **13**, 55 (2000).
- ⁵⁵P. Di Francesco, P. Mathieu, and D. Senechal, *Conformal Field Theory* (Springer-Verlag, New York, 1997).
- ⁵⁶I. Affleck, in *Fields, Strings, and Critical Phenomena*, edited by E. Brézin and J. Zinn-Justin (North-Holland, Amsterdam, 1990).
- ⁵⁷J. Cardy, *Scaling and Renormalization in Statistical Physics* (Cambridge University Press, Cambridge, 1996).
- ⁵⁸S. R. White, Phys. Rev. Lett. **69**, 2863 (1992); Phys. Rev. B **48**, 10345 (1993).
- ⁵⁹Ö. Legeza, J. Röder, and B. A. Hess, Phys. Rev. B 67, 125114 (2003).
- ⁶⁰Ö. Legeza and J. Sólyom, Phys. Rev. B **70**, 205118 (2004).
- ⁶¹W. K. Wootters, Phys. Rev. Lett. **80**, 2245 (1998).
- ⁶²P. Zanardi, Phys. Rev. A **65**, 042101 (2002).
- ⁶³T. J. Osborne and M. A. Nielsen, Phys. Rev. A **66**, 032110 (2002).
- ⁶⁴A. Osterloh, L. Amico, G. Falci, and R. Fazio, Nature (London) 416, 608 (2002).
- ⁶⁵S.-J. Gu, H.-Q. Lin, and Y.-Q. Li, Phys. Rev. A **68**, 042330 (2003).
- ⁶⁶ J. Vidal, G. Palacios, and R. Mosseri, Phys. Rev. A **69**, 022107 (2004); J. Vidal, R. Mosseri, and J. Dukelsky, *ibid.* **69**, 054101 (2004).
- ⁶⁷S.-J. Gu, S.-S. Deng, Y.-Q. Li, and H.-Q. Lin, Phys. Rev. Lett. **93**, 086402 (2004).
- ⁶⁸L.-A. Wu, M. S. Sarandy, and D. A. Lidar, Phys. Rev. Lett. **93**, 250404 (2004).
- ⁶⁹M.-F. Yang, Phys. Rev. A **71**, 030302(R) (2005).
- ⁷⁰Ö. Legeza and J. Sólyom, Phys. Rev. Lett. **96**, 116401 (2006).
- ⁷¹S.-S. Deng, S.-J. Gu, and H.-Q. Lin, Phys. Rev. B **74**, 045103 (2006).
- ⁷²K. Buchta, Ö. Legeza, E. Szirmai, and J. Sólyom, Phys. Rev. B 75, 155108 (2007).
- ⁷³D. Larsson and H. Johannesson, Phys. Rev. Lett. **95**, 196406 (2005); Phys. Rev. A **73**, 042320 (2006).
- ⁷⁴I. Affleck, T. Kennedy, E. H. Lieb, and H. Tasaki, Phys. Rev. Lett. **59**, 799 (1987).
- ⁷⁵P. Calabrese and J. Cardy, J. Stat. Mech.: Theory Exp. 2004, P06002.
- ⁷⁶G. Vidal, J. I. Latorre, E. Rico, and A. Kitaev, Phys. Rev. Lett. 90, 227902 (2003).
- ⁷⁷V. E. Korepin, Phys. Rev. Lett. **92**, 096402 (2004).
- ⁷⁸I. Affleck and A. W. W. Ludwig, Phys. Rev. Lett. **67**, 161 (1991).
- ⁷⁹N. Laflorencie, E. S. Sørensen, M.-S. Chang, and I. Affleck, Phys. Rev. Lett. **96**, 100603 (2006).
- ⁸⁰C. Holzhey, F. Larsen, and F. Wilczek, Nucl. Phys. **B424**, 443 (1994).
- ⁸¹S. R. White and D. A. Huse, Phys. Rev. B 48, 3844 (1993).
- ⁸²T. Vekua and A. Honecker, Phys. Rev. B **73**, 214427 (2006).