# Fate of spinons in spontaneously dimerized spin- $\frac{1}{2}$ ladders

Dave Allen and Fabian H. L. Essler

Department of Physics, Theoretical Physics, Oxford University, 1 Keble Road, Oxford, OX1 3NP, United Kingdom

Alexander A. Nersesyan

ICTP, P.O. Box 586, 34100 Trieste, Italy and The Andronikashvili Institute of Physics, Tamarashvili 6, GE-380077 Tbilisi, Georgia

(Received 5 August 1999; revised manuscript received 17 November 1999)

We study a weakly coupled, frustrated two-leg spin-1/2 Heisenberg ladder. For vanishing coupling between the chains, elementary excitations are deconfined, gapless spin-1/2 objects called *spinons*. We investigate the fate of spinons for the case of a weak interchain interaction. We show that despite a drastic change in ground state, which becomes spontaneously dimerized, spinons survive as elementary excitations but acquire a spectral gap. We furthermore determine the *exact* dynamical structure factor for several values of momentum transfer.

## I. INTRODUCTION

The role of frustration in quasi-one-dimensional magnetic materials has attracted much experimental and theoretical attention in recent years. On the theoretical side, the simplest example of a frustrated quantum magnet is the spin-1/2 Heisenberg antiferromagnetic chain with nearest-neighbor-exchange  $\delta J$  and next-nearest-neighbor exchange J. This model is equivalent to a two-leg ladder (see Fig. 1), where the coupling along (between) the legs of the ladder is equal to  $J(\delta J)$ .

The zig-zag ladder model is believed to describe the quantum magnet SrCuO<sub>2</sub> (Refs. 1,2) above the magnetic ordering transition, which takes place at about  $T\approx 2$  K. The exchange constants are estimated to be  $J\approx 1800$  K,  $|\delta J/J|\approx 0.1-0.2$ .<sup>2</sup> A second material with zig-zag structure that has recently attracted much interest is Cs<sub>2</sub>CuCl<sub>4</sub>.<sup>3</sup> However, in Cs<sub>2</sub>CuCl<sub>4</sub> all neighboring chains are coupled by a zig-zag interaction and no pronounced ladder structure exists.

In Refs. 4–6 it was argued that a weak antiferromagnetic zig-zag coupling between the chains drives the model to a massive phase, characterized by spontaneous dimerization (see, also Ref. 7). Let us briefly review some important parts of the derivations of Refs. 5,6. The lattice Hamiltonian of the zig-zag ladder is

$$H = J \sum_{j=1,2} \sum_{n} \mathbf{S}_{j,n} \cdot \mathbf{S}_{j,n+1} + \delta J \sum_{n} (\mathbf{S}_{1,n} + \mathbf{S}_{1,n+1}) \cdot \mathbf{S}_{2,n},$$
(1)

where we assume that  $\delta \leq 1$ . The low-energy effective action for Eq. (1) is now obtained as follows. For  $\delta \rightarrow 0$  one is dealing with two decoupled Heisenberg chains, which can be bosonized in terms of two Wess-Zumino-Novikov-Witten (WZNW) models by using the standard relation between the spin density on chain *j* and the fields of the WZNW model (see, e.g., Ref. 8)

$$\frac{S_j^a(x)}{a_0} = [J_j^a(x) + \overline{J}_j^a(x)] + (-1)^{x/a_0} n_j^a(x).$$
(2)

Here  $a_0$  is the lattice spacing, and the fields  $J_j^a$  and  $\bar{J}_j^a$  are the right and left currents of the WZWN model corresponding to chain *j*. They parametrize the smooth component of the magnetization. Finally,  $\vec{n_j}$  is the staggered component of the magnetization on chain *j*. Using Eq. (2), the zig-zag interchain interaction can be expressed in terms of the WZNW fields. In this way one straightforwardly obtains the current-current interaction<sup>5,6</sup>

$$\mathcal{H}_{c} = \lambda_{1} (J_{1}^{a} + \bar{J}_{1}^{a}) (J_{2}^{a} + \bar{J}_{2}^{a}) - \lambda_{0} (J_{1}^{a} \bar{J}_{1}^{a} + J_{2}^{a} \bar{J}_{2}^{a}), \qquad (3)$$

where  $\lambda_1 \propto \delta J$ . A standard renormalization-group (RG) analysis then shows that the antiferromagnetic interchain interaction  $\lambda_1$  leads to a spontaneously dimerized ground state.<sup>5,6</sup> In Ref. 9 it was shown that, in addition to the current-current interaction (3), a "twist" term arises

$$\mathcal{H}_t = \rho(n_1^a \partial_x n_2^a - n_2^a \partial_x n_1^a). \tag{4}$$

In the presence of exchange anisotropies the twist term induces incommensurabilities in the spin correlations.<sup>9</sup> We expect this to hold true even in the SU(2) symmetric case (no exchange anisotropies) we are interested in here. In the latter case it can be shown that the twist term and current-current interaction are equally important in the RG sense: they diverge (i.e., reach strong coupling) simultaneously, with a fixed ratio.<sup>10</sup> As far as the SU(2) symmetric zig-zag ladder is concerned, it is therefore not possible to separate the effects of the twist and current-current interactions in a simple way.

However, from a purely theoretical point of view it clearly is desirable to develop a thorough understanding of the physics due to isolated current-current and twist interactions. Their effects can be disentangled by introducing an



FIG. 1. Heisenberg zig-zag ladder.

8871

exchange anisotropy,<sup>9</sup> which makes the twist more and the current-current interaction less relevant in the RG sense. Using this trick, a pure twist interaction was studied in Ref. 9.

The role of an isolated current-current interaction has been previously investigated in connection with the zig-zag ladder in Refs. 7,5,6. In particular, the spectrum of elementary excitations and the dynamical structure factor were calculated in Ref. 6 using large-N techniques. It is known that extrapolation of large-N results to small values of N can lead to incorrect results.<sup>11</sup> Having this in mind, we carry out an *exact* calculation in order to determine the spectrum and structure factor. We find that the large-N results are indeed qualitatively incorrect.

As explained above, in the zig-zag ladder both twist and current-current interactions are present; therefore, strictly speaking, our results cannot be directly applied to this model. Nevertheless, we believe that many of our findings presented below remain qualitatively correct when applied to model (1). We discuss this point in more detail in Sec. VII.

In order to connect our results to a microscopic model, we consider a frustrated spin ladder modified in such a way that only current-current interactions emerge in the low-energy effective action.

The outline of this paper is as follows: in Sec. II we introduce a frustrated spin-ladder model giving rise to the desired low-energy effective field theory. In Sec. III we show that the resulting field theory is essentially equivalent to an O(4) Gross-Neveu model.<sup>12</sup> Sections IV and V are concerned with the description of the ground state(s) and elementary excitations. In Sec. VI we determine the exact dynamical structure factor for several values of momentum transfer and show that there are no coherent contributions to the structure factor. We conclude with a summary and discussion of our results.

## **II. A FRUSTRATED LADDER WITHOUT TWIST**

The model we consider is a generalization<sup>13</sup> of the standard two-leg spin ladder which, apart from the on-rung coupling  $J_{\perp}$ , also includes an interaction  $J_{\times}$  across both diagonals of the plaquettes. The Hamiltonian reads

$$H = J \sum_{j=1,2} \sum_{n} \mathbf{S}_{j,n} \cdot \mathbf{S}_{j,n+1} + J_{\perp} \sum_{n} \mathbf{S}_{1,n} \cdot \mathbf{S}_{2,n}$$
$$+ J_{\times} \sum_{n} [\mathbf{S}_{1,n} \cdot \mathbf{S}_{2,n+1} + \mathbf{S}_{1,n+1} \cdot \mathbf{S}_{2,n}].$$
(5)

We assume that

$$J, J_{\perp}, J_{\times} > 0, \qquad J \gg J_{\perp}, J_{\times}.$$
 (6)

The low-energy effective action can be derived by non-Abelian bosonization in the usual way. The Hamiltonian density is found to be of the form

$$\mathcal{H}(x) = \mathcal{H}_1(x) + \mathcal{H}_2(x) + \mathcal{H}_{\text{int}}(x), \tag{7}$$

where  $\mathcal{H}_{1,2}$  are critical SU<sub>1</sub>(2) WZNW models with a marginally irrelevant current-current perturbation ( $\lambda_0 > 0$ ):

$$\mathcal{H}_{j} = \frac{2 \pi v_{s}}{3} (: \overline{\mathbf{J}}_{j} \cdot \overline{\mathbf{J}}_{j} : + : \mathbf{J}_{j} \cdot \mathbf{J}_{j} :) - \lambda_{0} \overline{\mathbf{J}}_{j} \cdot \mathbf{J}_{j}, \quad j = 1, 2.$$
(8)



FIG. 2. The twistless ladder model.

The interaction part is given by

$$\mathcal{H}_{\text{int}} = \lambda_1 (\mathbf{J}_1 + \overline{\mathbf{J}}_1) \cdot (\mathbf{J}_2 + \overline{\mathbf{J}}_2) + \lambda_2 \mathbf{n}_1 \cdot \mathbf{n}_2, \qquad (9)$$

with the coupling constants

$$\lambda_1 = (J_\perp + 2J_\times)a_0, \quad \lambda_2 = (J_\perp - 2J_\times)a_0.$$
 (10)

No marginal perturbation with the twist-term structure arises because the staggered magnetization operators add rather than subtract due to the geometry of the problem (see Fig. 2). The absence of such term can also be deduced from the existence of discrete (reflection) symmetries of the lattice Hamiltonian (5). If  $J_{\perp} = 2J_{\times}$  only the marginal (currentcurrent) interaction survives. This is the case we study in the remainder of this paper.

We note that for generic values of  $J_{\perp}$  and  $J_{\times}$  the interaction of staggered magnetizations dominates and the resulting physics is essentially the same as for the standard ladder  $(J_{\times}=0)^{14}$  (see also chapter 21 of Ref. 15).

## **III. DUALITY TRANSFORMATION**

The low-energy effective action (8) and (9) can be recast as a theory of four massive, interacting, real (Majorana) fermions, or equivalently, four weakly coupled Ising models<sup>6</sup>

$$\mathcal{H} = \frac{i}{2} \sum_{\alpha=0}^{3} v_{\alpha} (\psi_{\alpha} \partial_{x} \psi_{\alpha} - \bar{\psi}_{\alpha} \partial_{x} \bar{\psi}_{\alpha}) + \frac{\lambda_{1} - \lambda_{0}}{2} \sum_{j>i=1}^{3} \psi_{i} \bar{\psi}_{i} \psi_{j} \bar{\psi}_{j} - \frac{\lambda_{1} + \lambda_{0}}{2} \psi_{0} \bar{\psi}_{0} \sum_{i=1}^{3} \psi_{i} \bar{\psi}_{i}.$$

$$(11)$$

Here  $v_1 = v_2 = v_3 = v_s \neq v_0$  are the velocities of the four Majorana fermions. The lattice spin operators are expressed in terms of the Majorana fields and order and disorder operators of the four Ising models as

$$S^{z}_{+}(x) \propto -i(\psi_{1}\psi_{2} + \bar{\psi}_{1}\bar{\psi}_{2}) - \mathcal{A}(-1)^{x/a_{0}}\mu_{1}\mu_{2}\sigma_{3}\sigma_{0},$$
  
$$S^{z}_{-}(x) \propto i(\psi_{3}\psi_{0} + \bar{\psi}_{3}\bar{\psi}_{0}) + \mathcal{A}(-1)^{x/a_{0}}\sigma_{1}\sigma_{2}\mu_{3}\mu_{0}, \quad (12)$$

where  $S_{\pm}^{z}(x) = S_{1}^{z}(x) \pm S_{2}^{z}(x)$  and  $\mathcal{A}$  is a nonuniversal constant. Analogous expressions are available for the other components of the spin operators.<sup>6</sup> A standard one-loop RG analysis shows that the coupling  $\lambda_{0}$  flows to zero, so we will ignore it in what follows. In order to further simplify the problem, we also neglect the small difference between the velocities  $v_{s}$  and  $v_{0}$ , and finally perform a duality transformation on the 0-Majorana

ι

$$\psi_0 \rightarrow \psi_4, \quad \overline{\psi}_0 \rightarrow -\overline{\psi}_4, \quad \sigma_0 \rightarrow \mu_4, \quad \mu_0 \rightarrow \sigma_4.$$
 (13)



FIG. 3. Qualitative picture of the two degenerate dimerized ground states: spins connected by the solid (dotted) lines have a tendency to form singlets (triplets).

This yields the Hamiltonian of the O(4) Gross-Neveu model<sup>12</sup>

$$\mathcal{H} = \frac{iv_s}{2} \sum_{i=1}^{4} \psi_i \partial_x \psi_i - \bar{\psi}_i \partial_x \bar{\psi}_i + \frac{\lambda_1}{2} \sum_{j>i=1}^{4} \psi_i \bar{\psi}_i \psi_j \bar{\psi}_j.$$
(14)

Under Eq. (13) the spin densities transform to

$$S_{+}^{z}(x) \propto -i(\psi_{1}\psi_{2} + \bar{\psi}_{1}\bar{\psi}_{2}) - \mathcal{A}(-1)^{x/a_{0}}\mu_{1}\mu_{2}\sigma_{3}\mu_{4},$$
  
$$S_{-}^{z}(x) \propto i(\psi_{3}\psi_{4} - \bar{\psi}_{3}\bar{\psi}_{4}) + \mathcal{A}(-1)^{x/a_{0}}\sigma_{1}\sigma_{2}\mu_{3}\sigma_{4}.$$
 (15)

### **IV. GROUND STATE**

In order to proceed, it is convenient to use the representation of Eq. (14) in terms of two sine-Gordon models.<sup>18</sup> Ignoring terms that only renormalize the velocity we find that Eq. (14) is equivalent to

$$\mathcal{H} = \sum_{i=\pm} \frac{v_s}{2} [(\partial_x \varphi_i)^2 + (\partial_x \theta_i)^2] + 2\lambda_1 \left[ \frac{1}{8\pi} [(\partial_x \varphi_i)^2 - (\partial_x \theta_i)^2] - \frac{1}{(2\pi a_0)^2} \cos\sqrt{8\pi} \varphi_i \right],$$
(16)

where  $\theta_i$  are the dual fields. The two sine-Gordon models (16) occur on the SU(2) invariant strong-coupling separatrix of the Kosterlitz-Thouless phase diagram and are thus in the massive regime.

#### A. Twistless ladder

The low-energy effective model (16) exhibits a local  $Z_2$  symmetry related to *independent* translations by one lattice spacing on each chain  $(\varphi_{\pm} \rightarrow \varphi_{\pm} + \sqrt{\pi/2})$ . This symmetry is spontaneously broken in the ground state and leads to a non-vanishing dimerization (see Fig. 3). Notice that the  $Z_2$  symmetry appears to be a feature of the low-energy sector only and follows from the fact that spin currents  $\vec{J}_{1,2}$  are translationally invariant objects. The transformation  $\mathbf{S}_1(n) \rightarrow \frac{1}{2}[\mathbf{S}_{1,n+1} + \mathbf{S}_{1,n-1}]$ , or a similar one with  $\mathbf{S}_{1,k} \rightarrow \mathbf{S}_{2,k}$ , changes the lattice Hamiltonian but leaves the low-energy effective field theory invariant and maps the two ground states onto one another.

In order to characterize the dimerization patterns of the two ground states, we determine the expectation values



FIG. 4. Qualitative picture of the spin configuration in the dimerised ground states: spins along the thick diagonal bonds have a tendency to form singlets.

$$\langle \vec{S}_{1,n} \cdot \vec{S}_{2,n} \rangle \propto \langle \vec{J}_1(x) \cdot \vec{J}_2(x) \rangle + \langle \vec{n}_1(x) \cdot \vec{n}_2(x) \rangle,$$

$$\langle \vec{S}_{1,n} \cdot \vec{S}_{2,n+1} \rangle \propto \langle \vec{J}_1(x) \cdot \vec{J}_2(x) \rangle - \langle \vec{n}_1(x) \cdot \vec{n}_2(x) \rangle,$$

$$\langle \vec{S}_{2,n} \cdot \vec{S}_{1,n+1} \rangle \propto \langle \vec{J}_1(x) \cdot \vec{J}_2(x) \rangle - \langle \vec{n}_1(x) \cdot \vec{n}_2(x) \rangle.$$

$$(17)$$

After performing the duality transformation to the O(4) Gross-Neveu model and bosonizing, we obtain

$$\langle \vec{n}_1(x) \cdot \vec{n}_2(x) \rangle \propto \langle \cos\sqrt{2\pi}\varphi_+ \cos\sqrt{2\pi}\varphi_- \rangle = \pm \operatorname{const} m,$$
  
$$\langle \vec{J}_1(x) \cdot \vec{J}_2(x) \rangle \propto \langle (\cos\sqrt{2\pi}\varphi_+ \cos\sqrt{2\pi}\varphi_-)^2 \rangle = \operatorname{const} m^2,$$
  
(18)

where  $m \propto \exp(-\operatorname{const} J/J_{\perp})$  is the (exponentially small) soliton mass in the sine-Gordon model. Due to the smallness of *m*, the  $\langle \vec{n}_1(x) \cdot \vec{n}_2(x) \rangle$  expectation value dominates in Eq. (17), so that within the exponential accuracy the dimerization is proportional to the quantum soliton mass. The  $Z_2$  symmetry of the low-energy effective Hamiltonian (16), that manifests itself in the degeneracy of the two ground states corresponding to different signs in Eq. (18), is spontaneously broken, implying the existence of massive  $Z_2$  kinks. It turns out (see below) that these kinks are elementary excitations of the model.

#### **B.** Zig-zag ladder

Let us discuss the implications of the emergence of spontaneous dimerization for the case of the zig-zag ladder if we ignore the twist term. For the zig-zag ladder the appropriate definition for the dimerization is

$$d = \langle \vec{S}_1(x) \cdot (\vec{S}_2(x + a_0/2) - \vec{S}_2(x - a_0/2)) \rangle.$$
(19)

In the continuum limit we find

$$d \propto \langle \cos \sqrt{2 \pi} \varphi_{+} \cos \sqrt{2 \pi} \varphi_{-} \rangle = \pm \operatorname{const} m.$$
 (20)

The resulting dimerization patterns are shown in Fig. 4. We believe that taking into account the twist term will not qualitatively change this picture.

### **V. EXCITATIONS**

From the exact solution of the sine-Gordon models (16) we infer that there are only four elementary excitations corresponding to solitons and antisolitons in the  $\pm$  sectors. We denote these by  $s_{\pm}$  and  $\bar{s}_{\pm}$ . The elementary excitation have



FIG. 5. A two-spinon state in the twistless ladder. Spinons correspond to kinks between domains with different sign of the dimerization. Solid lines depict bonds along which there is a tendency to form singlets.

a simple interpretation in terms of *dimerization kinks*, i.e., domain walls separating regions of dimerization with opposite sign. It can be shown along the lines of Ref. 16 that these particles carry spin  $\pm 1/2$ . In terms of the low-energy effective theory of two sine-Gordon models (16), the total spin density is given by

$$S_{1}^{z}(x) + S_{2}^{z}(x) = \frac{1}{\sqrt{2\pi}} [\partial_{x}\varphi_{+}(x) + \partial_{x}\varphi_{-}(x)].$$
(21)

Kinks interpolate between asymptotic values of the fields  $\varphi_i$ differing by  $\pm \sqrt{\pi/2}$  as is most easily deduced from the fact that the classical vacua of Eq. (16) are located at

$$\langle \varphi_i \rangle_{\text{class}} = \sqrt{\frac{\pi}{2}} n_i, \quad i = \pm, \qquad (22)$$

where  $n_i$  are arbitrary integers. Integration of Eq. (21) then yields that a single kink carries spin

$$S^{z} = \pm \frac{1}{\sqrt{2\pi}} \sqrt{\frac{\pi}{2}} = \pm \frac{1}{2}.$$
 (23)

The results presented below for the dynamical structure factor are consistent with the interpretation of these kinks as *gapped spinons*. Altogether there are two spin-1/2 multiplets, corresponding to one multiplet for each leg of the ladder. The emerging physical picture is quite simple and pretty: the two-spinon states observed in the structure factor simply correspond to the kinks related to the spontaneous breakdown of the discrete  $Z_2$  symmetry. Simple visualizations of this picture are shown in Fig. 5 for the twistless ladder and in Fig. 7 for the zig-zag ladder.

For the twistless ladder the kinks correspond to vertical domain walls between regions with different signs of dimerization. There is a spin-1/2 associated with each domain wall, although this is not immediately obvious from Fig. 5. In order to get a feeling why a spin-1/2 might be associated with each kink, let us think of the translationally invariant, "double-zig-zag" ground state shown in Fig. 3 as a symmetric superposition of two dimerized states. Each such state represents a sequence of plaquettes with ideal singlet bonds across the plaquette diagonals (with each spin involved in one bond only), has a period  $2a_0$  and is shifted with respect to the other state by one lattice spacing. If the "double-zigzag'' phase occupies a finite domain of the ladder, for the two  $2a_0$ -periodic dimerized states to resonate, the number of rungs within such a domain should be odd. Then the twokink configuration in Fig. 5 can equivalently be viewed as the superposition of states shown in Fig. 6. The intuitive



FIG. 6. "Resonating" ideal dimer configurations.

picture one obtains from Fig. 6 is then that on average there is indeed a spin-1/2 associated with each kink.

For the zig-zag case a much nicer picture emerges. The  $Z_2$  symmetry corresponds to a reflection symmetry on the lattice and kinks look like left over spin-1/2's as shown in Fig. 7. The intuitive picture of Fig. 7 fits well to the identification of a spinon in a spin-1/2 chain as a bare spin insertion into the ground state.<sup>17</sup>

## VI. DYNAMICAL STRUCTURE FACTOR

The long-distance asymptotics of the spin-spin correlation functions are dominated by the soft modes at  $q=0,\pi,q_{\perp}=0,\pi$ , where q and  $q_{\perp}$  denote the wave numbers along and perpendicular to the two chains, respectively. In what follows we will determine the dynamical structure factor for wave numbers in the vicinity of the above four points in  $\vec{q}$ space. Due to the spin-rotational symmetry the dynamical structure factor is given by

$$S(\omega, q, q_{\perp}) \propto \operatorname{Im} i \int_{-\infty}^{\infty} dx \int_{0}^{\infty} dt e^{-i\omega t + iqx} \\ \times \langle [\{S_{1}^{z}(t, x) \pm S_{2}^{z}(t, x)\}, \{S_{1}^{z}(0, 0) \pm S_{2}^{z}(0, 0)\}] \rangle,$$
(24)

where the positive (negative) sign corresponds to  $q_{\perp} = 0$   $(q_{\perp} = \pi)$ .

#### A. Summary of large-N results

The dynamical structure factor has been previously calculated in the framework of a large-*N* approach.<sup>6</sup> The limit  $N \rightarrow \infty$  of Eq. (14) is equivalent to a theory of free massive Majorana fermions



FIG. 7. Physical picture of a two-spinon state. Spinons correspond to kinks connecting domains with different sign of the dimerization.

$$\mathcal{H} = \frac{iv_s}{2} \sum_{i=1}^{N} \psi_i \partial_x \psi_i - \overline{\psi}_i \partial_x \overline{\psi}_i + im \psi_i \overline{\psi}_i \,. \tag{25}$$

The presence of the mass term reflects the spontaneous breakdown of parity, which in turn implies the existence of two degenerate ground states. The sign of the mass terms, as well as the expectation values  $\langle \sigma_a \rangle$  and  $\langle \mu_a \rangle$ , depend on the choice of ground state. In the case where  $\langle \sigma_a \rangle \neq 0$  (the mass of the triplet is positive), the structure factor for  $q_{\perp} = 0$  and q around 0,  $\pi$  was shown to be<sup>6</sup>

$$S(\omega, q \approx \pi, 0) \propto \frac{m}{|\omega|} \,\delta(\omega - \sqrt{v_s^2(q - \pi)^2 + m^2}),$$
$$S(\omega, q \approx 0, 0) \propto \frac{m^2 q^2}{s^3 \sqrt{s^2 - 4m^2}},$$
(26)

where  $s^2 = \omega^2 - v_s^2 q^2$ . The explicit expressions for the structure factor around  $(q,q_{\perp}) = (0,\pi), (\pi,\pi)$  are complicated, but reveal the presence of incoherent two- and three-particle continua, respectively. We will now show that the results obtained in the large-*N* limit are qualitatively incorrect. The reason for this failure of the large-*N* approach is that it entirely neglects the existence of topological kinks interpolating between the two degenerate ordered ground states. Extrapolation of the large-*N* results to lower values of *N* should be done with caution because the spectrum of the O(N) Gross-Neveu model is very sensitive to the value of N.<sup>11</sup>

### **B.** Exact results

We now determine the dynamical structure factor using exact results on form factors in the sine-Gordon model.<sup>19–21</sup> We start with the case  $q_{\perp}=0$ ,  $q\approx 0$ . The smooth component of the sum of the two spin densities is expressed in terms of the sine-Gordon models as follows:

$$S_1^z(x) + S_2^z(x) \big|_{\text{smooth}} \propto \partial_x \varphi_+ + \partial_x \varphi_- \,. \tag{27}$$

This is nothing but the sum of the temporal components of the current operators in the two sine-Gordon models  $(j^0_+ + j^0_-)$ . We are interested in the structure factor, i.e.,

$$S(\omega, q \approx 0, 0) \propto \operatorname{Im} \sum_{\sigma = \pm} i \int_{-\infty}^{\infty} dx \int_{0}^{\infty} dt \times e^{i(\omega + i\varepsilon)t - ivqx} \langle [j_{\sigma}^{0}(x, t), j_{\sigma}^{0}(0, 0)] \rangle,$$
(28)

where  $v_s$  is the velocity of the excitations. We express Eq. (28) in the spectral representation using our knowledge of a complete set of states in terms of (anti) soliton scattering states. Energy and momentum are parametrized in terms of the rapidity variable  $\theta$  as

$$p = m \sinh \theta, \quad \epsilon = m \cosh \theta,$$
 (29)

where m is the mass of the four elementary excitations. The resolution of the identity is given by

$$1 = \sum_{n=0}^{\infty} \sum_{\alpha_i} \int \frac{d\theta_1 \cdots d\theta_n}{(2\pi)^n n!} \\ \times |\theta_n \cdots \theta_1\rangle_{\alpha_n \cdots \alpha_1} {}^{\alpha_1 \cdots \alpha_n} \langle \theta_1 \cdots \theta_n |, \qquad (30)$$

where *n* is the number of particles and  $\alpha_i \in \{s_{\pm}, \overline{s}_{\pm}\}$  specifies their respective "flavor" (soliton or antisoliton in + or – sector). Inserting Eq. (30) in Eq. (28) and using Poincaré invariance yields

$$S(\omega,q\approx0,0)\propto-2\pi\operatorname{Im}\sum_{n=0}^{\infty}\sum_{\alpha_{i}}\int\frac{d\,\theta_{1}\cdots d\,\theta_{n}}{(2\,\pi)^{n}n!}$$

$$\times|F_{j^{0}}(\theta_{1}\cdots\theta_{n})_{\alpha_{1}\cdots\alpha_{n}}|^{2}$$

$$\times\left[\frac{\delta\left(v_{s}q-m\sum_{j}\sinh\theta_{j}\right)}{\omega-m\sum_{j}\cosh\theta_{j}+i\varepsilon}-\frac{\delta\left(v_{s}q+m\sum_{j}\sinh\theta_{j}\right)}{\omega+m\sum_{j}\cosh\theta_{j}+i\varepsilon}\right],\qquad(31)$$

where  $F_{j^0}(\theta_1 \cdots \theta_n)_{\alpha_1 \cdots \alpha_n}$  is the sine-Gordon current form factor

$$F_{j^0}(\theta_1\cdots\theta_n)_{\alpha_1\cdots\alpha_n} \equiv \langle 0|j^0(0,0)|\theta_n\cdots\theta_1\rangle_{\alpha_n\cdots\alpha_1}.$$
(32)

We note that an *n*-particles state only contributes to Eq. (31) above the *n*-particle threshold, i.e.,  $s^2 = \omega^2 - v_s^2 q^2 \ge n^2 m^2$ . Thus, at low energies  $s^2 \le 16m^2$  only two-particle states contribute. The corresponding form factor is<sup>19</sup>

$$F_{j^0}(\theta_1,\theta_2)_{s\bar{s}} = -2m \sinh\left(\frac{\theta_1+\theta_2}{2}\right) f(\theta_1-\theta_2),$$

$$f(\theta) = i \frac{\sinh \theta/2}{2\pi} \times \exp\left(\int_0^\infty d\kappa \frac{\sin^2\left(\frac{\kappa}{2}(\theta - \pi i)\right)}{\kappa \sinh(\pi\kappa)} \left[ th\left(\frac{\pi\kappa}{2}\right) - 1 \right] \right).$$
(33)

After performing the  $\theta$  integrations we obtain

$$S(\omega, q \approx 0, 0) \propto \frac{m^2 v_s^2 q^2 |f(2\,\theta(s))|^2}{s^3 \sqrt{s^2 - 4m^2}},$$
(34)

where  $\theta(s) = \operatorname{arccosh}(s/2m)$  and  $4m^2 < s^2 < 16m^2$ . As we already mentioned, the result (34) is exact as long as  $s^2 < 16m^2$ . For larger energy transfers there are (small) corrections due to four, six, eight, etc., particle states. These can be calculated in the same way as the two-particle contribution. Approaching the threshold s = 2m from above, Eq. (34) goes to zero like  $\sqrt{s-2m}$ .

The result (34) has the same structure as the one obtained in the large-*N* approximation. We note that the vanishing of the structure factor for  $q=0[S(\omega,0,0)=0]$  reflects the fact that the *z* component of spin is a conserved quantity.

Next, we consider the structure factor at  $(q \approx 0, \pi)$ . The smooth component of the difference of spin densities is

$$S_1^z(x) - S_2^z(x) \big|_{\text{smooth}} \propto \partial_\tau \varphi_+ - \partial_\tau \varphi_- \,. \tag{35}$$

This is precisely the difference of the spatial components of the currents in the two sine-Gordon models  $(j_+^1 - j_-^1)$ . Using the exact two-particle form factor we obtain the leading contribution to the structure factor

$$S(\omega, q \approx 0, \pi) \propto \frac{m^2 \omega^2 |f(2\theta(s))|^2}{s^3 \sqrt{s^2 - 4m^2}},$$
 (36)

where  $f(\theta)$  is given by Eq. (33) and again  $4m^2 < s^2 < 16m^2$ . Note that the structure factor does not vanish for  $q \rightarrow 0$  as the magnetization difference between chains is not conserved. This is due to the fact that our starting point does *not* have O(4) symmetry: after the duality transformation we obtain an O(4) symmetric Lagrangian, but correlation functions transform nontrivially. This result is of course expected, since the interchain interaction must break the O(4)~SU(2) ×SU(2) down to SU(2).

Finally, we examine the structure factor at  $(q \approx \pi, 0)$  and  $(q \approx \pi, \pi)$ . The bosonized forms for the staggered components of the sum and difference of the spin densities are found to be

$$S_{1}^{z}(x) + S_{2}^{z}(x)|_{\text{stagg}} \propto \cos\sqrt{\pi}\Phi \cos\sqrt{\pi}\Theta,$$
  
$$S_{1}^{z}(x) - S_{2}^{z}(x)|_{\text{stagg}} \propto \sin\sqrt{\pi}\Phi \sin\sqrt{\pi}\Theta,$$
 (37)

where  $\Phi = (\varphi_+ + \varphi_-)/\sqrt{2}$  and  $\Theta = (\theta_+ - \theta_-)/\sqrt{2}$ . At present it is not known how to calculate form factors for the operators appearing in Eq. (37) as they involve both the field and the dual field. However, it is still possible to determine the qualitative behavior of the structure factor. From Eq. (37) it is clear that the structure factor involves the calculation of form factors of operators

$$\left[\cos \operatorname{or} \sin \right] \left( \sqrt{\frac{\pi}{2}} \varphi_{+} \right) \left[\cos \operatorname{or} \sin \right] \left( \sqrt{\frac{\pi}{2}} \theta_{+} \right)$$
$$\left[\cos \operatorname{or} \sin \right] \left( \sqrt{\frac{\pi}{2}} \varphi_{-} \right) \left[\cos \operatorname{or} \sin \right] \left( \sqrt{\frac{\pi}{2}} \theta_{-} \right). \quad (38)$$

These form factors are obviously products of form factors in the two sine-Gordon models. Let us therefore concentrate on the + sector for the time being. It was shown in Ref. 22 that the operators  $\cos\sqrt{\pi/2}\theta_+$  and  $\sin\sqrt{\pi/2}\theta_+$  in the sine-Gordon model with coupling constant  $\beta = \sqrt{8\pi}$  have fermionic character and thus have nontrivial form factors with one-soliton states. On the other hand, we know from Ref. 19 that  $\cos\sqrt{\pi/2}\varphi_+$  and  $\sin\sqrt{\pi/2}\varphi_+$  are of bosonic character. We, therefore, conclude that + part of the operator (38) has fermionic character. This implies that it couples only to states with at least one (anti) soliton. An analogous statement holds true for the – sector, so that the leading contribution to the structure factor comes from two-particle states. In other words no coherent one-particle excitation exists.

From the above results for the dynamical structure factor we deduce that the low-lying excitations are described in terms of a gapped two-particle scattering continuum. As we have mentioned above, the elementary excitations carry spin-1/2. This leads us to identify them as *massive spinons*.

## VII. SUMMARY

We have studied the effects of pure current-current interactions in a frustrated two-leg spin ladder. We have shown that *spinons*, which are gapless topological excitations propagating along decoupled Heisenberg chains, survive as elementary excitations in the frustrated ladder, but acquire a finite mass gap. We have given an interpretation of these massive spinons as quantum dimerization kinks. The kinks are deconfined and, in all physical states, appear only in pairs. As a result their contribution to the dynamical structure factor is entirely incoherent. Our findings bear a strong resemblance to those of (Ref. 23).

We believe that our results not only apply to the ladder (5), but with some modifications also to the zig-zag ladder (1). As discussed above, in the zig-zag case there is a twist term in addition to the current-current interaction. We conjecture that the effect of the twist term is merely to shift the minimum of the two-spinon continua at  $(q = \pi, 0)$  and  $(q = \pi, \pi)$  to incommensurate wave numbers, i.e., to  $(q = \pi + \delta, 0)$  and  $(q = \pi + \delta, \pi)$ , where  $|\delta| \leq 1$ . Such a picture is consistent with what is known from numerical studies<sup>5,24–26</sup> and also fits well to what one would expect on the basis of an (uncontrolled) extrapolation of the results for  $\delta = O(1)$  (Refs. 27,28) to  $|\delta| \leq 1$ .

Coming back to the twistless chain (5), it should be pointed out that its ground state and excitations have been previously studied for the special case  $J_{\times}=J$  (Refs. 29,30) ("Bose-Gayen model"). In this case, the Hamiltonian (5) exhibits an enlarged (local) symmetry, related to the interchange  $S_1(n) \leftrightarrow S_2(n)$  at *arbitrary* rung *n*, and decouples into two commuting parts describing either an array of entirely decoupled on-rung singlets or an effective S=1chain.<sup>30</sup> In both cases, the ground state belongs to the universality class of the (undimerized) Haldane spin liquids with the spin-1 massive magnons being coherent elementary excitations.<sup>14,23</sup> This is in marked contrast with our findings for  $J_{\times} = \frac{1}{2}J_{\perp} \ll J$  and implies the existence of a crossover between the two regimes at some intermediate coupling.

It should be understood that the region where the marginally perturbed ladder ( $\lambda_2=0$ ) and the Bose-Gayen model start overlapping, i.e., the vicinity of the point  $J_{\perp}=2J_{\times}$ =2J, is not accessible within our continuum approach, based on the assumption that  $J_{\perp}$ ,  $J_{\times} \ll J$ . Staying on the line  $J_{\perp}=2J_{\times}$  and increasing  $J_{\times}$  would enforce the amplitude of the current-current perturbation ( $\lambda_1$ ) to increase, in which case no reliable conclusions are available. On the other hand, one can start approaching the Bose-Gayen regime by keeping  $J_{\perp}$  fixed and increasing  $J_{\times}$ . In this case one inevitably deviates from the line  $J_{\perp}=2J_{\times}$ , and that gives rise to the appearance of the strongly relevant perturbation  $\lambda_2 \mathbf{n}_1 \cdot \mathbf{n}_2$ . The latter introduces an extra potential

$$\mathcal{U} \sim \lambda_2 [2 \cos \sqrt{2} \pi (\varphi_+ - \varphi_-) - \cos \sqrt{2} \pi (\varphi_+ + \varphi_-) \\ \times \cos \sqrt{2} \pi (\theta_+ - \theta_-)], \tag{39}$$

that couples the two sine-Gordon models (16), removes the  $Z_2$  degeneracy between the two dimerized ground states, and thus leads to soliton confinement. The soliton-antisoliton pairs start forming triplet and singlet massive bound states and transform to coherent single-particle excitations. If the deviation from the line  $J_{\perp} = 2J_{\times}$  is large enough, the  $\lambda_2$  perturbation takes over, and the effective low-energy field theory becomes that of four Majorana fermions, with a mass term

$$\propto i\lambda_2 \left(\sum_{a=1}^3 \psi_a \overline{\psi}_a - 3\psi_0 \overline{\psi}_0\right)$$

as it is the case for the standard (nonfrustrated) ladder.<sup>14</sup> It is, therefore, tempting to speculate that the two massive

Haldane phases on the both sides of the line  $J_{\perp} = 2J_{\times}$  can be smoothly connected with those of the Bose-Gayen model. This, however, does not exclude the existence of other phases in the three-parameter space of the model (5).

As discussed in Refs. 31 and 28, a similar soliton confinement scenario is realized if one adds an explicit dimerization to the zig-zag Hamiltonian (1).

#### ACKNOWLEDGMENTS

We thank Armando Aligia, Vladimir Rittenberg, and Alexei Tsvelik for useful discussions. F.H.L.E. and A.A.N. are grateful to the Physikalisches Institut der Universität Bonn, where part of this work was carried out, for financial support and hospitality. F.H.L.E. is supported by the EPSRC under Grant No. AF/98/1081. D.A. would like to thank le Fonds FCAR du Québec for financial support.

- <sup>1</sup>M. Matsuda and K. Katsumata, J. Magn. Magn. Mater. **140**, 1617 (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).
- <sup>2</sup>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, R11 953 (1997).
- <sup>3</sup>R. Coldea, D.A. Tennant, R.A. Cowley, D.F. McMorrow, B. Dorner, and Z. Tylczynski, Phys. Rev. Lett. **79**, 151 (1997).
- <sup>4</sup>F.D.M. Haldane, Phys. Rev. B 25, 4925 (1982).
- <sup>5</sup>S.R. White and I. Affleck, Phys. Rev. B **54**, 9862 (1996).
- <sup>6</sup>D. Allen and D. Sénéchal, Phys. Rev. B 55, 299 (1997).
- <sup>7</sup>R. Julien and F.D.M. Haldane, Bull. Am. Phys. Soc. 28, 34 (1983); K. Okamoto and K. Nomura, Phys. Lett. A 169, 433 (1992); J. Phys. A 27, 5773 (1994); S. Eggert, Phys. Rev. B 54, R9612 (1996).
- <sup>8</sup>I. Affleck, *Field Theory Methods and Quantum Critical Phenomena*, Les Houches, session XLIX (Elsevier, New York, 1989).
- <sup>9</sup>A.A. Nersesyan, A.O. Gogolin, and F.H.L. Essler, Phys. Rev. Lett. **81**, 910 (1998).
- <sup>10</sup>F.H.L. Essler, A.O. Gogolin, and A.A. Nersesyan (unpublished).
- <sup>11</sup>M. Karowski and H.J. Thun, Nucl. Phys. B 190, 61 (1981).
- <sup>12</sup>D. Gross and A. Neveu, Phys. Rev. D 10, 3235 (1974).
- <sup>13</sup>Z. Weihong, V. Kotov, and J. Oitmaa, Phys. Rev. B **57**, 11439 (1998); X. Wang, cond-mat/9803290 (unpublished); A.K. Kolezhuk and H.-J. Mikeska, Int. J. Mod. Phys. B **5**, 2325 (1998).
- <sup>14</sup>D.G. Shelton, A.A. Nersesyan, and A.M. Tsvelik, Phys. Rev. B 53, 8521 (1996).

- <sup>15</sup>A.O. Gogolin, A.A. Nersesyan, and A.M. Tsvelik, *Bosonization and Strongly Correlated Systems* (Cambridge University Press, Cambridge, 1998).
- <sup>16</sup>A.J. Niemi and G.W. Semenoff, Phys. Rep. **135**, 99 (1986); A.O. Gogolin, A.A. Nersesyan, A.M. Tsvelik, and L. Yu, Nucl. Phys. B **540**, 705 (1999).
- <sup>17</sup>J.C. Talstra and S.P. Strong, Phys. Rev. B 56, 6094 (1997).
- <sup>18</sup>E. Witten and R. Shankar, Nucl. Phys. B **141**, 349 (1978).
- <sup>19</sup>M. Karowski and P. Weisz, Nucl. Phys. B 139, 455 (1978).
- <sup>20</sup>F.A. Smirnov, Form Factors in Completely Integrable Models of Quantum Field Theory (World Scientific, Singapore, 1992).
- <sup>21</sup>S. Lukyanov, Mod. Phys. Lett. A 12, 2911 (1997).
- <sup>22</sup>G. Delfino, Phys. Lett. B **450**, 196 (1999).
- <sup>23</sup>A.A. Nersesyan and A.M. Tsvelik, Phys. Rev. Lett. **78**, 3939 (1997).
- <sup>24</sup>R. Bursill, G.A. Gehring, D.J.J. Farnell, J.B. Parkinson, T. Xiang, and C. Zeng, J. Phys.: Condens. Matter 7, 8605 (1995).
- <sup>25</sup>A.A. Aligia, C.D. Batista, and F.H.L. Essler (unpublished).
- <sup>26</sup>D. Cabra, A. Honecker, and P. Pujol, cond-mat/9902112) (unpublished); A. Honecker (unpublished).
- <sup>27</sup>B.S. Shastry and B. Sutherland, Phys. Rev. Lett. 47, 964 (1981).
- <sup>28</sup>S. Brehmer, A.K. Kolezhuk, H.-J. Mikeska, and U. Neugebauer, J. Phys.: Condens. Matter **10**, 1103 (1998).
- <sup>29</sup>I. Bose and S. Gayen, Phys. Rev. B 48, 10 653 (1993).
- <sup>30</sup>Y. Xian, Phys. Rev. B **52**, 12485 (1995).
- <sup>31</sup>I. Affleck, in Dynamical Properties of Uncoventional Magnetic Systems, Vol. 349 of NATO Advanced Study Institute, Series E: Applied Sciences, edited by A. Skjeltorp and D. Sherrington (Kluwer, Dordrecht, 1998).