Antiferromagnetic spin ladders: Crossover between spin $S=1/2$ and $S=1$ chains

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We study a model of two weakly coupled isotropic spin-1/2 Heisenberg chains with an antiferromagnetic coupling along the chains (spin ladder). It is shown that the system always has a spectral gap and the lower lying excitations are triplets. For the case of identical chains the model in the continuous limit is shown to be equivalent to four decoupled noncritical Ising models with the $Z_2\times SU(2)$ symmetry. For this case we obtain the *exact* expressions for asymptotics of spin-spin correlation functions. It is shown that when the chains have different exchange integrals $J_1\gg J_2$ the spectrum at low energies is described by the O(3)-nonlinear σ model. We discuss the topological order parameter related to the gap formation and give a detailed description of the dynamical magnetic susceptibility.

I. INTRODUCTION

It has been widely recognized that one-dimensional antiferromagnets with half-integer and integer spins have dramatically different excitation spectra. The original theoretical prediction by Haldane[1] that Heisenberg chains with half-integer spin are gapless, whereas those with integer spin are gapped, has been confirmed experimentally.[2] To gain insight into the physics underlying this result, one may study systems intermediate between spin $S=1/2$ and $S=1$. The simplest of these is the "Heisenberg spin ladder," which has isotropic couplings $J_{||}$ along the chains and $J_\perp$ between them. Although such systems with both antiferromagnetic[3–8] and ferromagnetic[9–12] interchain couplings have been the subject of considerable recent theoretical interest, certain problems remain unresolved leaving room for our contribution. A very remarkable fact about the spin $S=1/2$ Heisenberg chain is that its excitation spectrum consists of spin-1/2 particles (spinons). Physically such excitations can be created only in pairs because upon flipping one spin the total spin projection is changed by one: $\Delta S_z=1$. Thus, in the $S=1/2$ Heisenberg chain, the conventional magnons carrying spin 1 are deconfined into spin-1/2 spinons. Putting two $S=1/2$ chains together one can observe how spinons are confined back into magnons by measuring the dynamical susceptibility $\chi''(\omega,q)$. The interchain exchange $J_\perp$ serves here as a control parameter: at $|J_\perp|\ll J_{||}$ there is a wide energy range where χ'' is dominated by incoherent multiparticle processes, and a narrow region at low energies where χ'' exibits a single-magnon peak around $q=\pi$.

One can obtain a qualitative understanding of the spinon confinement by considering the strong-coupling limit of the spin-ladder problem. As frequently happens in one-dimensional models, the strong-coupling limit gives a correct qualitative picture of the low-lying excitations. One should, however, be careful to define this limit properly. The proper definition assumes that it is possible to perform a perturbative expansion about the strong-coupling fixed point in negative powers of the coupling constant. In the spin-ladder problem there are two candidates for the strong-coupling fixed point: the limits of strong antiferromagnetic ($J_\perp\gg J_{||}$) and ferromagnetic ($-J_\perp\gg J_{||}$) interchain coupling, respectively. It is clear that only the former case constitutes the correctly defined strong-coupling limit. At $J_\perp/J_{||}\to+\infty$ the spin ladder is decomposed into an array of decoupled rungs, each rung representing a "molecule" whose singlet ground state is separated from the triplet excited state by a large gap of the order of $J_\perp$. When one makes $J_{||}$ finite, the triplet excitations form a band with bandwidth $\sim J_{||}$. The properties of such a system can be analyzed perturbatively, with $J_{||}/J_\perp$ being the small parameter.

On the other hand, strong ferromagnetic interchain coupling leads to the formation of local spins $S=1$ associated with each rung of the ladder, thus producing a conventional spin $S=1$ Heisenberg antiferromagnet with a nonzero Haldane gap in the excitation spectrum. In contrast to the previous case, the bandwidth of the triplet excitations and the spectral gap are of the same order of magnitude, $\sim J_{||}$. This problem lacks a small parameter and cannot be analyzed by perturbation theory. A variety of approximate methods have been suggested to study the $S=1$ antiferromagnetic spin chain (see Ref. 13 and references therein); however, it is not our purpose to review them here.

In this paper we present our analysis of a weakly coupled spin ladder $J_{||}\gg|J_\perp|$. We have found this limit more interesting from the theoretical point of view, for it allows us to start out with a well-defined picture of gapless spinon excitations on each spin-1/2 Heisenberg chain. By switching on a weak interchain exchange interaction, we then study the crossover between the gapless regime of two decoupled $S=1/2$ Heisenberg chains and the strong-coupling limit, taking place on lowering the energy scale. Despite the fact that

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our results have only qualitative validity for the presently available experimental realizations of double chain ladders [$Sr_{n-1}Cu_{n+1}O_{2n}$ (Ref. 14) and $(VO)_2P_2O_7$ (Ref. 15)] where both exchange integrals are of the same order, we hope that weakly interacting spin ladders will be synthesized in the future.

An interesting fact about the weak-coupling limit is that the emerging physical picture is independent of the sign of $J_\perp$. As follows from the above discussion, this universality is not so obvious at $|J_\perp| \gg J_{||}$. Therefore comparing our results with the strong-coupling analysis one can see that the main universal features of the spectrum are its symmetry and the persistence of the gap. As we have mentioned above, the low-lying excitations turn out to be triplets in all limits and for all signs of $J_\perp$.

The paper is organized as follows. In Sec. II we derive the continuous version of the spin-ladder Hamiltonian for the case of identical chains. To achieve this we employ the bosonization approach, but the resulting effective theory is most simply represented in terms of fermions. In this representation the effective Hamiltonian of the spin ladder contains four species of weakly interacting real fermions. [The difference between ordinary (Dirac) and real (Majorana) fermions is that the latter ones have only positive energies $\epsilon(p) = \sqrt{p^2+m^2}$. Therefore one can always describe one Dirac fermion as a superposition of two Majorana fermions.] Three of these modes comprise a degenerate triplet and the remaining one lies above having a mass approximately three times as big. The magnitude of the mass gaps is of the order of the interchain exchange. As we have mentioned above, for any sign of the interchain coupling, the leading asymptotics of the correlation functions are determined by the triplet of Majorana fermions as for the $S=1$ chain.[13] This means that at $J_\perp < 0$ our description remains qualitatively valid even when $J_\perp$ is not small. The fact that the low-energy sector of the model is essentially a free theory makes it possible to obtain nonperturbative expressions for asymptotics of all correlation functions. This is done in Sec. III. In Sec. IV we discuss a situation where the ladder consists of inequivalent chains. It is shown that, in the limit when exchange integrals on the chains strongly differ, the low-lying excitations are described by the O(3)-nonlinear σ model. The adequacy of this treatment is guaranteed by the fact that this σ model has a small bare coupling constant.

The fact that the excitation spectrum of the O(3)-nonlinear σ model consists of massive triplets provides further support for our conclusion that the spectral gap and the symmetry of the low-lying excitation branch are the most universal features of the model.

The appearance of a spectral gap in the $S=1$ Heisenberg chain is known to be associated with the breakdown of a hidden discrete symmetry characterized by a nonlocal (string) order parameter.[16,17] A similar topological string order has been recently shown to exist in the related $S=1/2$ spin chain with alternating exchange couplings J and J'.[18] On changing the ratio J'/J from $-\infty$ to 1 with J kept positive, this model continuously interpolates between the $S=1$ chain and gapless Heisenberg $S=1/2$ chain, thus displaying properties of the gapful Haldane phase in whole range $J'/J<1$. In Sec. V we derive the string order parameter for the spin-ladder model, following essentially the same procedure as that suggested for the bond-alternating chain,[18,19] and identify the corresponding hidden symmetry. The paper has a Conclusion and two Appendices where we provide technical details about bosonization and string order parameters.

II. COUPLING OF IDENTICAL CHAINS: ABELIAN BOSONIZATION

In this section we apply the Abelian bosonization method to the spin-ladder model

$$H = J_\parallel \sum_{j=1,2} \sum_n \mathbf{S}_j(n) \cdot \mathbf{S}_j(n+1) + J_\perp \sum_n \mathbf{S}_1(n) \cdot \mathbf{S}_2(n) \tag{1}$$

describing two antiferromagnetic ($J_\parallel > 0$) spin-1/2 Heisenberg chains with a weak interchain coupling ($|J_\perp| \ll J_\parallel$) of arbitrary sign. Abelian bosonization is a well-known procedure, but for the sake of completeness we briefly overview it in the Appendix A. In the continuum limit, the critical properties of isolated $S=1/2$ Heisenberg chains are described in terms of massless Bose fields $\phi_j(x) (j=1,2)$:

$$H_0 = \frac{v_s}{2} \sum_{j=1,2} \int dx [\Pi_j^2(x) + (\partial_x \phi_j(x))^2], \tag{2}$$

where the velocity $v_s \sim J_\parallel a_0$ and Π_j are the momenta conjugate to ϕ_j. The interchain coupling

$$H_\perp = J_\perp a_0 \int dx [\mathbf{J}_1(x) \cdot \mathbf{J}_2(x) + \mathbf{n}_1(x) \cdot \mathbf{n}_2(x)] \tag{3}$$

is expressed in terms of the operators $\mathbf{J}_j(x)$ and $\mathbf{n}_j(x)$ which represent, respectively, the slowly varying and staggered parts of the local-spin-density operator and are defined in the Appendix A. According to (A19), the current-current term in (3) is marginal, while interaction of the staggered parts of the spin densities is strongly relevant. So we start our analysis by dropping the former term (its role will be discussed later). Using then bosonization formulas (A18) for $\mathbf{n}_j(x)$, we get

$$H_\perp = \frac{J_\perp \lambda^2}{\pi^2 a_0} \int dx \left[-\frac{1}{2} \cos\sqrt{2\pi}(\phi_1 + \phi_2) + \frac{1}{2} \cos\sqrt{2\pi}(\phi_1 - \phi_2) + \cos\sqrt{2\pi}(\theta_1 - \theta_2) \right],$$

where $\theta_j(x)$ is the field dual to $\phi_j(x)$. Denote

$$m = \frac{J_\perp \lambda^2}{2\pi} \tag{4}$$

and introduce linear combinations of the fields ϕ_1 and ϕ_2:

$$\phi_\pm = \frac{\phi_1 \pm \phi_2}{\sqrt{2}}. \tag{5}$$

The total (ϕ_+) and relative (ϕ_-) degrees of freedom decouple, and the Hamiltonian of two identical Heisenberg chains transforms to a sum of two independent contributions:

$$H = H_+ + H_-, \tag{6}$$

$$H_+(x)=\frac{v_s}{2}(\Pi_+^2+(\partial_x\phi_+)^2)-\frac{m}{\pi a_0}\cos\sqrt{4\pi}\phi_+ , \quad (7)$$

$$H_-(x)=\frac{v_s}{2}(\Pi_-^2+(\partial_x\phi_-)^2)+\frac{m}{\pi a_0}\cos\sqrt{4\pi}\phi_- + \frac{2m}{\pi a_0}\cos\sqrt{4\pi}\theta_- . \quad (8)$$

In the above derivation, the $\mathbf{J}_1\cdot\mathbf{J}_2$ term has been omitted as being only marginal, as opposed to the retained, relevant $\mathbf{n}_1\cdot\mathbf{n}_2$ term. It is worth mentioning that there are modifications of the original two-chain lattice model for which the $\mathbf{J}_1\cdot\mathbf{J}_2$ term does not appear at all in the continuum limit, and mapping onto the model (6) becomes exact. In two such modifications, the interchain coupling is changed to

$$H_\perp^{(A)}=\frac{J_\perp}{2}\sum_n \mathbf{S}_1(n)\cdot[\mathbf{S}_2(n)-\mathbf{S}_2(n+1)] \quad (9)$$

or

$$H_\perp^{(B)}=\frac{J_\perp}{4}\sum_n [\mathbf{S}_1(n)-\mathbf{S}_1(n+1)]\cdot[\mathbf{S}_2(n)-\mathbf{S}_2(n+1)]. \quad (10)$$

The structure of these models explains why the low-energy physics of two *weakly* coupled Heisenberg chains must not be sensitive to the sign of the interchain coupling $J_\perp$. This conclusion is in agreement with recent results of Ref. 8.

Let us turn back to Eqs. (7) and (8). One immediately realizes that the critical dimension of all the cosine terms in Eqs. (7), (8) is 1; therefore the model (6) is a theory of free massive fermions. The Hamiltonian H_+ describes the sine-Gordon model at $\beta^2=4\pi$; so it is equivalent to a free massive Thirring model. Let us introduce a spinless Dirac fermion related to the scalar field ϕ_+ via identification

$$\psi_{R,L}(x)\simeq(2\pi a_0)^{-1/2}\exp(\pm i\sqrt{4\pi}\phi_{+;R,L}(x)) \quad (11)$$

Using

$$\frac{1}{\pi a_0}\cos\sqrt{4\pi}\phi_+(x)=i[\psi_R^\dagger(x)\psi_L(x)-\text{H.c.}]$$

we get

$$H_+(x)=-iv_s(\psi_R^\dagger\partial_x\psi_R-\psi_L^\dagger\partial_x\psi_L)-im(\psi_R^\dagger\psi_L-\psi_L^\dagger\psi_R). \quad (12)$$

For future purposes, we introduce two real (Majorana) fermion fields

$$\xi_\nu^1=\frac{\psi_\nu+\psi_\nu^\dagger}{\sqrt{2}}, \quad \xi_\nu^2=\frac{\psi_\nu-\psi_\nu^\dagger}{\sqrt{2}i}, \quad (\nu=R,L) \quad (13)$$

to represent H_+ as a model of two degenerate massive Majorana fermions

$$H_+=H_m[\xi^1]+H_m[\xi^2], \quad (14)$$

where

$$H_m[\xi]=-\frac{iv_s}{2}(\xi_R\partial_x\xi_R-\xi_L\partial_x\xi_L)-im\xi_R\xi_L . \quad (15)$$

Now we shall demonstrate that the Hamiltonian H_- in (8) reduces to the Hamiltonian of two *different* Majorana fields. As before, we first introduce a spinless Dirac fermion

$$\chi_{R,L}(x)\simeq(2\pi a_0)^{-1/2}\exp(\pm i\sqrt{4\pi}\phi_{-;R,L}(x)), \quad (16)$$

$$\frac{1}{\pi a_0}\cos\sqrt{4\pi}\phi_-(x)=i[\chi_R^\dagger(x)\chi_L(x)-\text{H.c.}],$$

$$\frac{1}{\pi a_0}\cos\sqrt{4\pi}\theta_-(x)=-i[\chi_R^\dagger(x)\chi_L^\dagger(x)-\text{H.c.}].$$

Apart from the usual mass bilinear term (charge-density-wave pairing), the Hamiltonian H_- also contains a "Cooper pairing" term originating from the cosine of the dual field:

$$H_-(x)=-v_s(\chi_R^\dagger\partial_x\chi_R-\chi_L^\dagger\partial_x\chi_L)+im(\chi_R^\dagger\chi_L-\chi_L^\dagger\chi_R) + 2im(\chi_R^\dagger\chi_L^\dagger-\chi_L\chi_R). \quad (17)$$

We introduce two Majorana fields

$$\xi_\nu^3=\frac{\chi_\nu+\chi_\nu^\dagger}{\sqrt{2}}, \quad \rho_\nu=\frac{\chi_\nu-\chi_\nu^\dagger}{\sqrt{2}i}, \quad (\nu=R,L). \quad (18)$$

The Hamiltonian H_- then describes two massive Majorana fermions, $\xi_{R,L}^3$ and $\rho_{R,L}$, with masses m and $-3m$, respectively:

$$H_-=H_m[\xi^3]+H_{-3m}[\rho]. \quad (19)$$

Now we observe that $\xi^a, a=1,2,3,$ form a triplet of Majorana fields with the same mass m. There is one more field ρ with a larger modulus of mass, $3|m|$. So, the total Hamiltonian

$$H=H_m[\vec{\xi}]+H_{-3m}[\rho] \quad (20)$$

with

$$H_m[\vec{\xi}]=\sum_{a=1,2,3}\left\{-\frac{iv_s}{2}(\xi_R^a\partial_x\xi_R^a-\xi_L^a\partial_x\xi_L^a)-im\xi_R^a\xi_L^a\right\}. \quad (21)$$

The O(3)-invariant model $H_m[\vec{\xi}]$ was suggested as a description of the $S=1$ Heisenberg chain by Tsvelik.[13] This equivalence follows from the fact that, in the continuum limit, the integrable $S=1$ chain with the Hamiltonian

$$H=\sum_n [(\vec{S}_n\vec{S}_{n+1})-(\vec{S}_n\vec{S}_{n+1})^2] \quad (22)$$

is described by the critical Wess-Zumino model on the SU(2) group at the level $k=2$, and the latter is in turn equivalent to the model of three massless Majorana fermions, as follows from the comparison of conformal charges of the corresponding theories:

$$C_{\text{SU}(2),k=2}^{\text{WZW}}=\frac{3}{2}=3C_{\text{Major fermion}}.$$

The $k=2$ level, SU(2) currents expressed in terms of the fields ξ^a are given by

$$I^a_{R,L}=-\frac{i}{2}\epsilon^{abc}\xi^b_{R,L}\xi^c_{R,L}. \tag{23}$$

When small deviations from criticality are considered, no single-ion anisotropy $[\sim D(S^z)^2, S=1]$ is allowed to appear due to the original SU(2) symmetry of the problem. So, the mass term in (21) turns out to be the only allowed relevant perturbation to the critical SU(2), $k=2$ Wess-Zumino-Witten (WZW) model.

Thus, the fields ξ^a describe triplet excitations related to the effective spin-1 chain. Remarkably, completely decoupled from them are singlet excitations described in terms of the field ρ. Another feature is that this picture is valid for *any* sign of $J_\perp$, in agreement with the effective lattice models (9) and (10) which we actually are dealing with.

Since the spectrum of the system is massive, the role of the so far neglected (marginal) part of the interchain coupling (3) is exhausted by renormalization of the masses and velocity. Neglecting the latter effect, this interaction can be shown to have the following invariant form:

$$\begin{aligned}H_{\rm marg}&=\frac{1}{2}J_\perp a_0\int dx[(I^a_R I^a_L)-(\xi^a_R\xi^a_L)(\rho_R\rho_L)]\\&=\frac{1}{2}J_\perp a_0\int dx[(\xi^1_R\xi^1_L)(\xi^2_R\xi^2_L)+(\xi^2_R\xi^2_L)(\xi^3_R\xi^3_L)\\&\quad+(\xi^3_R\xi^3_L)(\xi^1_R\xi^1_L)-(\xi^1_R\xi^1_L+\xi^2_R\xi^2_L+\xi^3_R\xi^3_L)(\rho_R\rho_L)].\end{aligned} \tag{24}$$

In a theory of N massive Majorana fermions, with masses $m_a(a=1,2,\dots,N)$ and a weak four-fermion interaction

$$H_{\rm int}=\frac{1}{2}\sum_{a\neq b}g_{ab}\int dx(\xi^a_R\xi^a_L)(\xi^b_R\xi^b_L), \quad (g_{ab}=g_{ba})$$

renormalized masses $\tilde{m}_a$ estimated in the first order in g are given by

$$\tilde{m}_a=m_a+\sum_{b(\neq a)}\frac{g_{ab}}{2\pi v}m_b\ln\frac{\Lambda}{|m_b|}. \tag{25}$$

Using (24) and (25), we find renormalized values of the masses of the triplet and singlet excitations:

$$m_t=m\left(1+\frac{5J_\perp a_0}{4\pi v}\ln\frac{\Lambda}{|m|}\right), \tag{26}$$

$$m_s=3m\left(1+\frac{J_\perp a_0}{4\pi v}\ln\frac{\Lambda}{|m|}\right). \tag{27}$$

III. CORRELATION FUNCTIONS FOR THE IDENTICAL CHAINS

Since the singlet excitation with mass $m_s\simeq 3m$ does not carry spin, its operators do not contribute to the slow components of the total magnetization. The latter is expressed in terms of the $k=2$ SU(2) currents (23):

$$M^a\sim I^a_R+I^a_L. \tag{28}$$

Therefore the two-point correlation function of spin densities at small wave vectors ($|q|\ll\pi/a_0$) is given by the simple fermionic loop. A simple calculation gives the following expression for its imaginary part:

$$\mathrm{Im}\chi^{(R)}(\omega,q)=\frac{2q^2m^2v^2}{s^3\sqrt{s^2-4m^2}} \tag{29}$$

for $s^2=\omega^2-v^2q^2>4m^2$ (the imaginary part is zero for $s^2<4m^2$). Thus the dynamical magnetic susceptibility at small wave vectors has a threshold at $2m$.

It turns out that it is possible to calculate exactly the two-point correlation functions of the staggered magnetization. This is due to the fact that the corresponding operators of the Heisenberg chains are related (in the continuum limit) to the order and disorder parameter fields of $2d$ Ising models;[20,21] the correlation functions of the latter operators are known exactly even out of criticality.[22]

Using formulas (A18) of Appendix A, the components of the total ($\mathbf{n}^{(+)}=\mathbf{n}_1+\mathbf{n}_2$) and relative ($\mathbf{n}^{(-)}=\mathbf{n}_1-\mathbf{n}_2$) staggered magnetization can be represented as

$$\begin{aligned}&n_x^{(+)}\sim\cos\sqrt{\pi}\theta_+\cos\sqrt{\pi}\theta_-, \quad n_x^{(-)}\sim\sin\sqrt{\pi}\theta_+\sin\sqrt{\pi}\theta_-,\\&n_y^{(+)}\sim\sin\sqrt{\pi}\theta_+\cos\sqrt{\pi}\theta_-, \quad n_y^{(-)}\sim\cos\sqrt{\pi}\theta_+\sin\sqrt{\pi}\theta_-,\\&n_z^{(+)}\sim\sin\sqrt{\pi}\phi_+\cos\sqrt{\pi}\phi_-, \quad n_z^{(-)}\sim\cos\sqrt{\pi}\phi_+\sin\sqrt{\pi}\phi_-.\end{aligned} \tag{30}$$

The fields ϕ_+,θ_+ and ϕ_-,θ_- are governed by the Hamiltonians (7) and (8), respectively. Let us first consider exponentials $\exp(\pm i\sqrt{\pi}\phi_+)$, $\exp(\pm i\sqrt{\pi}\theta_+)$. Their correlation functions have been extensively studied in the context of the *noncritical* Ising model (see, for example, Ref. 22). It has been shown that these bosonic exponents with scaling dimension 1/4 are expressed in terms of the order (σ) and disorder (μ) parameters of two Ising models as follows:

$$\begin{aligned}&\cos(\sqrt{\pi}\phi_+)=\mu_1\mu_2, \quad \sin(\sqrt{\pi}\phi_+)=\sigma_1\sigma_2,\\&\cos(\sqrt{\pi}\theta_+)=\sigma_1\mu_2, \quad \sin(\sqrt{\pi}\theta_+)=\mu_1\sigma_2.\end{aligned} \tag{31}$$

Let us briefly comment on this correspondence.

As already discussed, the $\beta^2=4\pi$ sine-Gordon model H_+, Eq. (7), is equivalent to a model of two degenerate massive Majorana fermions, Eqs. (14), (15). As is well known (see, e.g., Ref. 24), a theory of massive Majorana fermion describes long-distance properties of $2d$ Ising model, the fermionic mass being proportional to $m\sim t=(T-T_c)/T_c$. So, H_+ is equivalent to two decoupled $2d$ Ising models. Let σ_j and μ_j ($j=1,2$) be the corresponding order and disorder parameters. At criticality (zero fermionic mass), four products $\sigma_1\sigma_2$, $\mu_1\mu_2$, $\sigma_1\mu_2$, and $\mu_1\sigma_2$ have the same critical dimension 1/4 as that of the bosonic exponentials $\exp(\pm i\sqrt{\pi}\phi_+)$, $\exp(\pm i\sqrt{\pi}\theta_+)$. Therefore there must be some correspondence between the two groups of four operators which should also hold at small deviations from criticality. To find this correspondence, notice that, as follows from (7), at $m>0\langle\cos\sqrt{\pi}\phi_+\rangle\neq 0$, while $\langle\sin\sqrt{\pi}\phi_+\rangle=0$. Since the case $m>0$ corresponds to the disordered phase of the Ising systems ($t>0$), $\langle\sigma_1\rangle=\langle\sigma_2\rangle=0$, while $\langle\mu_1\rangle=\langle\mu_2\rangle\neq 0$. At $m<0$ (ordered Ising systems, $t<0$) the situation is inverted: $\langle\cos\sqrt{\pi_+}\phi\rangle=0$, $\langle\sin\sqrt{\pi}\phi_+\rangle\neq 0$, $\langle\sigma_1\rangle=\langle\sigma_2\rangle\neq 0$, $\langle\mu_1\rangle=\langle\mu_2\rangle=0$. This explains the first two formulas of Eq. (31).

Clearly, the exponentials of the dual field θ_+ must be expressed in terms of $\sigma_1\mu_2$ and $\mu_1\sigma_2$. To find the correct correspondence, one has to take into account the fact that a local product of the order and disorder operators of a single Ising model results in the Majorana fermion operator, i.e.,

$$\xi^1\sim\cos\sqrt{\pi}(\phi_+ +\theta_+)\sim\sigma_1\mu_1,$$

$$\xi^2\sim\sin\sqrt{\pi}(\phi_+ +\theta_+)\sim\sigma_2\mu_2.$$

This leads to the last two formulas of Eq. (31).

To derive similar expressions for the exponents of ϕ_- and θ_-, the following facts should be taken into account: (i) the Hamiltonian (17) describing "$-$" modes is diagonalized by the same transformation (18) as the Hamiltonian (12) responsible for the "$+$" modes; (ii) the Majorana fermions now have different masses, and (iii) one fermionic branch has a negative mass. In order to take a proper account of these facts one should recall the following:

(a) A negative mass means that we are below the transition.

(b) It follows from (ii) that "$-$" bosonic exponents are also expressed in terms of order and disorder parameters of two Ising models, the latter, however, being characterized by different t's. We denote these operators as σ_3,μ_3 (mass m) and σ,μ (mass $-3m$).

(c) Operators corresponding to a negative mass can be rewritten in terms of the ones with the positive mass using the Kramers-Wannier duality transformation

$$t\rightarrow -t,\quad \sigma\rightarrow\mu,\quad \mu\rightarrow\sigma. \tag{32}$$

Taking these facts into account we get the following expressions for the "$-$" bosonic exponents:

$$\cos(\sqrt{\pi}\phi_-)=\mu_3\sigma,\quad \sin(\sqrt{\pi}\phi_-)=\sigma_3\mu,$$

$$\cos(\sqrt{\pi}\theta_-)=\sigma_3\sigma,\quad \sin(\sqrt{\pi}\theta_-)=\mu_3\mu. \tag{33}$$

Combining Eqs. (31) and (33), from (30) we get the following, manifestly SU(2) invariant, expressions:

$$n_x^+\sim\sigma_1\mu_2\sigma_3\sigma,\quad n_y^+\sim\mu_1\sigma_2\sigma_3\sigma,\quad n_z^+\sim\sigma_1\sigma_2\mu_3\sigma, \tag{34}$$

$$n_x^-\sim\mu_1\sigma_2\mu_3\mu,\quad n_y^-\sim\sigma_1\mu_2\mu_3\mu,\quad n_z^-\sim\mu_1\mu_2\sigma_3\mu. \tag{35}$$

It is instructive to compare them with two possible representations for the staggered magnetization operators for the $S=1$ Heisenberg chain which can be derived from the $SU(2)_2$ WZW model:[23,13]

$$S^x\sim\sigma_1\mu_2\sigma_3,\quad S^y\sim\mu_1\sigma_2\sigma_3,\quad S^z\sim\sigma_1\sigma_2\mu_3 \tag{36}$$

or

$$S^x\sim\mu_1\sigma_2\mu_3,\quad S^y\sim\sigma_1\mu_2\mu_3,\quad S^z\sim\mu_1\mu_2\sigma_3. \tag{37}$$

Agreement is achieved if the singlet excitation band is formally shifted to infinity. This implies substitutions $\sigma\simeq\langle\sigma\rangle\neq 0$, $\mu\simeq\langle\mu\rangle\simeq 0$ for ferromagnetic interchain coupling ($m\sim J_\perp<0$), or $\sigma\simeq\langle\sigma\rangle\simeq 0$, $\mu\simeq\langle\mu\rangle\neq 0$ for antiferromagnetic interchain coupling ($m\sim J_\perp>0$). Thus, we observe that, as expected, for ferromagnetic (antiferromagnetic) interchain interaction the staggered $S=1$ magnetization is determined by the total (relative) staggered magnetization of the two-chain system.

A more precise meaning of this approximation becomes apparent when one considers asymptotic behavior of the corresponding two-point correlation functions in the two limits $r\rightarrow 0$ and $r\rightarrow\infty$.[25] In the limit $r\rightarrow\infty$ they are as follows:

$$\langle\sigma_a(r)\sigma_a(0)\rangle=G_\sigma(\tilde{r})=\frac{A_1}{\pi}K_0(\tilde{r})+O(e^{-3\tilde{r}}), \tag{38}$$

$$\begin{aligned}\langle\mu_a(r)\mu_a(0)\rangle&=G_\mu(\tilde{r})\\&=A_1\left\{1+\frac{1}{\pi^2}\left[\tilde{r}^2[K_1^2(\tilde{r})-K_0^2(\tilde{r})]\right.\right.\\&\qquad\left.\left.-\tilde{r}K_0(\tilde{r})K_1(\tilde{r})+\frac{1}{2}K_0^2(\tilde{r})\right]\right\}+O(e^{-4\tilde{r}}),\end{aligned} \tag{39}$$

where $\tilde{r}=rM$ ($M=m$ or $3m$), A_1 is a nonuniversal parameter, and it has been assumed that M is positive. If M is negative the correlation functions are obtained by simply interchanging σ and μ, and putting $M\rightarrow -M$ [the duality transformation (32)]. Therefore, as might be expected, at large distances, a difference between the ladder and the $S=1$ chains appears only in $\exp(-3mr)$ terms due to the contribution of the excitation branch with $M=3m$ absent in the $S=1$ chain.

In the limit $\tilde{r}\rightarrow 0$ the correlation functions are of power-law form:

$$G_\sigma(\tilde{r})=G_\mu(\tilde{r})=\frac{A_2}{\tilde{r}^{1/4}} \tag{40}$$

plus nonsingular terms. The ratio of the constants A_1 and A_2 is a universal quantity involving Glaisher's constant (A):

$$\frac{A_2}{A_1}=2^{-1/6}A^{-3}\exp\frac{1}{4}, \tag{41}$$

$$A=1.282\,427\,129\ldots. \tag{42}$$

We conclude this section by writing down the exact expression for the staggered magnetization two-point correlation functions. The correlation function for spins on the same chain is given by

$$\begin{aligned}\langle n_1^a(\tau,x)n_1^a(0,0)\rangle&=G_\sigma^2(mr)G_\mu(mr)G_\sigma(3mr)\\&\quad+G_\mu^2(mr)G_\sigma(mr)G_\mu(3mr).\end{aligned} \tag{43}$$

The interesting asymptotics are

$$\langle n_1^a(\tau,x)n_1^a(0,0)\rangle=\frac{1}{2\pi r}\tilde{Z}\quad\text{at}\quad mr\ll 1, \tag{44}$$

$$\frac{m}{\pi^2} Z K_0(mr)\Bigg(1+\frac{2}{\pi^2}\Big\{(mr)^2[K_1^2(mr)-K_0^2(mr)] - mrK_0(mr)K_1(mr)+\frac{1}{2}K_0^2(mr)\Big\}\Bigg)+O(e^{-5mr}); \quad mr \gg 1, \quad (45)$$

where $r^2=\tau^2+v^2x^2$ and

$$\frac{\tilde{Z}}{Z}=\frac{2^{4/3}e}{3^{1/4}}A^{-12}\approx 0.264. \quad (46)$$

The complete expressions for the functions $G_{\sigma,\mu}(\tilde{r})$ are given in Ref. 25. For the interchain correlation function we get

$$\langle n_1^a(\tau,x)n_2^a(0,0)\rangle = G_\sigma^2(mr)G_\mu(mr)G_\sigma(3mr) - G_\mu^2(mr)G_\sigma(mr)G_\mu(3mr). \quad (47)$$

At $mr \ll 1$ it decays as $(mr)^{-2}$; the leading asymptotics at $mr \gg 1$ is the same as (45) (up to the -1 factor). The difference appears only in terms of order of $\exp(-5mr)$. The important point is that at $mr \gg 1$ the contribution from the singlet excitation appears only in the fifth order in $\exp(-mr)$. Therefore it is unobservable by neutron scattering at energies below $5m$.

Using the above expressions we can calculate the imaginary part of the dynamical spin susceptibility in two different regimes. For $|\pi-q|\ll 1$ we have

$$\mathrm{Im}\chi^{(R)}(\omega,\pi-q;q_\perp)=Z\begin{cases} 2\cos q_\perp\left[\frac{m}{|\omega|}\delta(\omega-\sqrt{v^2q^2+m^2})+F(\omega,q)\right], & \omega<5m \\ (1+\cos q_\perp)\frac{0.264}{\sqrt{\omega^2-v^2q^2}}, & \omega\gg 5m, \end{cases} \quad (48)$$

where the transverse "momentum" $q_\perp$ takes values 0 and π. The factor Z is assumed to be m independent so that at $m\to 0$ we reproduce the susceptibility of noninteracting chains. We have calculated the function $F(\omega,q)$ only near the $3m$ threshold where it is equal to

$$F(\omega,q)\approx \frac{144}{\pi m^2}\sqrt{\omega^2-v^2q^2-9m^2}. \quad (49)$$

For $|q|\ll 1$ we have

$$\mathrm{Im}\chi^{(R)}(\omega,q;q_\perp)=[1+\cos^2(q_\perp/2)]f(s,m), \quad (50)$$

where $f(s,m)$ is given by Eq. (29).

IV. INEQUIVALENT CHAINS: NON-ABELIAN BOSONIZATION

In this section we consider two interacting spin $S=1/2$ chains with different intrachain exchange integrals $J_{||}^1\neq J_{||}^2$. It turns out that the most adequate approach in this case is non-Abelian bosonization. The reason for this is that non-Abelian bosonization explicitly preserves the SU(2) symmetry present in the Hamiltonian. The Abelian bosonization approach which does not respect this symmetry encounters difficulties.

As shown by Affleck,[26] by a mapping from a fermionic theory, the $S=\frac{1}{2}$ Heisenberg antiferromagnet can be described by a $k=1$, SU(2) Wess-Zumino-Witten (WZW) model with the following action:

$$S_k=kW(\mathbf{g}), \quad W(\mathbf{g})=\frac{1}{16\pi}\int \mathrm{Tr}(\partial_\mu \mathbf{g}^+\partial_\mu \mathbf{g})d^2x+\Gamma(\mathbf{g}),$$

$$\Gamma(\mathbf{g})=\frac{i}{24\pi}\int d^3X\,\epsilon^{\alpha\beta\gamma}\mathrm{Tr}(\mathbf{g}^+\partial_\alpha \mathbf{g}\mathbf{g}^+\partial_\beta \mathbf{g}\mathbf{g}^+\partial_\gamma \mathbf{g}), \quad (51)$$

where matrix $\mathbf{g}\in$ SU(2). There can in general be marginally irrelevant perturbations to this theory, which generate logarithmic corrections to the correlation function exponents, but do not change their qualitative behavior (i.e., power law). In general this model describes not just the spin $S=1/2$ Heisenberg chain, but any (1+1)-dimensional system of fermions with the charge degree of freedom frozen out and no gap in the spin sector.

The WZW model may look unfamiliar, but it is not so difficult to deal with since its operators and their exact correlation functions are already known from the application of conformal field theory[27] (see also Ref. 28). As we have mentioned above, the great advantage of the WZW model is that it explicitly possesses the SU(2)×SU(2) symmetry of the massless fermion spin sector, and is also critical (massless). In (1+1) dimensions the distinction between relativistic fermions and bosons is illusory; one can choose to think about a system in either representation (this has been known for some time; hence the "Luttinger liquid"). The WZW model is therefore just a way of thinking about the spin sector in terms of bosons; just as in Abelian bosonization, one can represent operators from the fermionic theory in terms of those of the bosonic theory and vice-versa. From a practical point of view, these relations between the two sets of operators can be thought of as ready made tools. It is not necessary to worry about their slightly exotic appearance or their justification in order to apply them. (But those seeking a deeper appreciation are referred to the papers cited above.)

The bosonized expression for the spin operator of the Heisenberg chain is given by[26]

$$\vec{S}_n = \vec{J}_R + \vec{J}_L + \text{const}(-1)^n \, \text{Tr}(\mathbf{g}^+ \vec{\sigma} - \mathbf{g}\vec{\sigma}), \tag{52}$$

where the currents are given by

$$J_R^a = -\frac{i}{2\pi} \text{Tr}(\partial_- \mathbf{g})\mathbf{g}^+ T^a, \quad J_L^a = \frac{i}{2\pi} \text{Tr}\mathbf{g}^+ \partial_+ \mathbf{g} T^a. \tag{53}$$

[T^a are the Pauli matrices—generators of the SU(2) group.] These currents satisfy the SU(2) Kac-Moody algebra described in the Appendix A.

Consider two Heisenberg chains coupled by an antiferromagnetic nearest-neighbor interaction. It can be represented like this:

$$S = W_1(\mathbf{h}) + W_2(\mathbf{g}) + \lambda_1[\vec{H}_R + \vec{H}_L][\vec{G}_R + \vec{G}_L] + \lambda_2 \text{Tr}[(\mathbf{g} - \mathbf{g}^+)\vec{\sigma}]\text{Tr}[(\mathbf{h} - \mathbf{h}^+)\vec{\sigma}], \tag{54}$$

where the dynamics of one chain is represented by the matrix $\mathbf{g}$ and the currents $\vec{G}_{R,L}$ and the other by $\mathbf{h}$ and $\vec{H}_{R,L}$. The indices 1,2 distinguish between different spin-wave velocities. Without a loss of generality we can put $v_1 > v_2$.

The currents have conformal dimensions (1,0) and (0,1); using the formula for the conformal dimensions of the matrices for the SU(n) group derived in Ref. 27:

$$\Delta = \frac{n^2 - 1}{2n(n+k)} \tag{55}$$

we get that for $n=2$, $k=1$, $\mathbf{g}$ and $\mathbf{h}$ both have conformal dimensions $(\frac{1}{4}, \frac{1}{4})$. The λ_2 term is therefore the relevant interaction, whereas the current couplings are only marginal. For this reason, the current interaction will be neglected at this stage. Then the interaction can be written as

$$\text{Tr}[(\mathbf{g} - \mathbf{g}^+)\vec{\sigma}] \cdot \text{Tr}[(\mathbf{h} - \mathbf{h}^+)\vec{\sigma}] = \frac{1}{2}\{ \text{Tr}[(\mathbf{g} - \mathbf{g}^+)(\mathbf{h} - \mathbf{h}^+)] - \text{Tr}[(\mathbf{g} - \mathbf{g}^+)] \, \text{Tr}[(\mathbf{h} - \mathbf{h}^+)]\}. \tag{56}$$

Making the substitution $\alpha = \mathbf{g}\mathbf{h}^+$, which leaves the measure invariant, and using the remarkable identity[27]

$$W(\alpha \mathbf{h}^+) = W(\alpha) + W(\mathbf{h}) + \frac{1}{2\pi}\int \text{Tr}\alpha^+ \partial_- \alpha \mathbf{h}^+ \partial_+ \mathbf{h} d^2x, \tag{57}$$

we arrive at the following expression for the action:

$$S = [W_1(\mathbf{h}) + W_2(\mathbf{h})] + \frac{1}{2\pi}\int \text{Tr}\alpha^+ \partial_- \alpha \mathbf{h}^+ \partial_+ \mathbf{h} d^2x + W_1(\alpha) + \lambda_2[\text{Tr}(\alpha + \alpha^+) - \text{Tr}(\alpha^+ \mathbf{h}^{+2} + \text{H.c.}) + \text{Tr}(\mathbf{h}^+ - \mathbf{h}) \, \text{Tr}(\mathbf{h}^+ \alpha^+ - \alpha \mathbf{h})] \tag{58}$$

[here $\partial_\pm = \frac{1}{2}(\partial_\tau \mp i\partial_x)$].

The identity (57) is nothing very mysterious. It is simply a generalization of an identity familiar from Abelian bosonization. To see this, consider substituting explicitly for the special case of Abelian bosonization, the $U(1)$ fields $e^{i\beta\phi_1}$ and $e^{i\beta\phi_2}$ for the matrices α and $\mathbf{h}$, respectively. Then the WZW action, $W(\alpha)$ reduces to the action for free scalar bosons as we would expect:

$$W(\alpha = e^{i\beta\phi_1}) = \frac{\beta^2}{4\pi}\int \partial_+ \phi_1 \partial_- \phi_1 d^2x = \frac{\beta^2}{16\pi}\int [(\partial_x \phi_1)^2 + (\partial_\tau \phi_1)^2] d^2x \tag{59}$$

and the interaction term in (57) becomes

$$\frac{1}{2\pi}\int \text{Tr}\alpha^+ \partial_- \alpha \mathbf{h}^+ \partial_+ \mathbf{h} d^2x = \frac{-\beta^2}{4\pi}\int (\partial_+ \phi_1 \partial_- \phi_2 + \partial_+ \phi_2 \partial_- \phi_1) d^2x. \tag{60}$$

The field $\alpha\mathbf{h}^+$ is $e^{i\beta(\phi_1 - \phi_2)} = e^{i\beta\phi_-}$, and so the identity (57) becomes

$$\frac{\beta^2}{4\pi}\int \partial_+ \phi_- \partial_- \phi_- d^2x = \frac{\beta^2}{4\pi}\left[\int \partial_+ \phi_1 \partial_- \phi_1 d^2x + \int \partial_+ \phi_2 \partial_- \phi_2 d^2x - \int (\partial_+ \phi_1 \partial_- \phi_2 + \partial_+ \phi_2 \partial_- \phi_1) d^2x\right]. \tag{61}$$

Therefore the identity (57) is just an analog of the following simple statement:

$$[\nabla(\phi_1 - \phi_2)]^2 = (\nabla\phi_1)^2 + (\nabla\phi_2)^2 - 2\nabla\phi_1 \cdot \nabla\phi_2, \tag{62}$$

where the last term is the "interaction term."

We shall consider the most relevant interaction, $\text{Tr}(\alpha + \alpha^+)$ first. The effective action for α is in this approximation:

$$S = W_1(\alpha) + \lambda \, \text{Tr}(\alpha + \alpha^+). \tag{63}$$

From the first-order renormalization-group equation we get

$$\frac{d\lambda}{d \ln L} \simeq \left(2 - \frac{1}{2}\right)\lambda. \tag{64}$$

Integrating up to a scale where the coupling becomes of order 1 and taking this to give some estimate of the dynamically generated mass, one gets $M\sim\lambda^{2/3}$. Much more information can be found by realizing that the model (63) is equivalent to the $\beta^2=2\pi$ sine-Gordon model (see, for example, Ref. 26).

Thus on the scale $|x|\gg M^{-1}$ the fluctuations of the α field are frozen and we can approximate

$$\mathrm{Tr}(\alpha\mathbf{h}^+)\mathrm{Tr}(\mathbf{h})\approx\langle\mathrm{Tr}\alpha\rangle:[\mathrm{Tr}(\mathbf{h})]^2:. \tag{65}$$

At this large scale the cross term containing derivatives of h and α gives the irrelevant contribution

$$S_{\mathrm{int}}\sim M^{-2}\partial_+\partial_-\mathbf{h}^+\partial_+\partial_-\mathbf{h}. \tag{66}$$

Therefore the asymptotic behavior at large distances is governed by the following action:

$$S=W_1(h)+W_2(h)+c_2:[\mathrm{Tr}(\mathbf{h})]^2: \tag{67}$$

where $c_2\sim\lambda^{4/3}$ and which can be further modified by the coordinate rescaling:

$$x_0=\sqrt{v_1v_2}\tau,\quad x_1=x \tag{68}$$

such that we finally have

$$S=S_0+S_1, \tag{69}$$

$$S_0=\frac{1}{2c_1}\int d^2x\ \mathrm{Tr}(\partial_\mu\mathbf{h}^+\partial_\mu\mathbf{h})d^2x+2\Gamma(\mathbf{h}), \tag{70}$$

$$S_1=\int d^2x\tilde{c}_2\{:[\mathrm{Tr}\mathbf{h}^2]:+:[\mathrm{Tr}(\mathbf{h}^+)^2]:-:[\mathrm{Tr}(\mathbf{h}-\mathbf{h}^+)]^2:\}, \tag{71}$$

where

$$1/c=\sqrt{v_1/v_2}+\sqrt{v_2/v_1}.$$

The model with action (69) is not critical; coupling constants c_1,c_2 undergo further renormalization. Let us show that the coupling c_2 renormalizes faster to strong coupling. To show this we shall suppose that this is the case and check that the obtained result is self-consistent. It is easy to check that the effective potential (71) vanishes if $\mathbf{h}$ is a traceless matrix and has a fixed determinant:

$$\mathbf{h}\approx i(\vec{\sigma}\vec{n}),\quad \vec{n}^2=1. \tag{72}$$

Excitations, which correspond to configurations where $\mathrm{Tr}\mathbf{h}\neq\mathbf{0}$, acquire a gap. The estimate for this gap is

$$M_0^2\sim c\sqrt{v_1v_2}c_2\sim\min(v_1,v_2)\lambda^{4/3}\sim\frac{v_2}{v_1}M^2. \tag{73}$$

On energies smaller than the gap one can treat the $\mathbf{h}$ matrix as traceless. Substituting expression (72) into Eq. (69) we get the O(3)-nonlinear σ model as an effective action for small energies:

$$S=\frac{1}{2\tilde{c}}\int d^2x(\partial_\mu\vec{n})^2,\quad \vec{n}^2=1, \tag{74}$$

$$\frac{1}{\tilde{c}}=(\sqrt{v_1/v_2}+\sqrt{v_2/v_1})(1-\langle n_0^2\rangle). \tag{75}$$

The reason why the Wess-Zumino term effectively disappears from the action is the following. After substituting Eq. (72) into the expression for $\Gamma(\mathbf{h})$ the Wess-Zumino term reduces to the topological term:

$$2\Gamma(i\vec{\sigma}\vec{n})=\frac{i}{4}\int d^2x\epsilon_{\mu\nu}(\vec{n}[\partial_\mu\vec{n}\times\partial_\nu\vec{n}])=2\pi ik, \tag{76}$$

where k is an integer number. The factor in front of the topological term is such that its contribution to the action is always a factor of $2\pi i$ and therefore does not affect the partition function. The mass gap of the model (74) is given by

$$\begin{aligned}M&=M_0\tilde{c}^{-1}\exp(-2\pi/\tilde{c})\\&\approx M\left[1-\frac{c}{2\pi}\ln(M/M_0)\right]\exp(-2\pi/c).\end{aligned} \tag{77}$$

As long as this gap is much smaller than M_0, the adopted approach is self-consistent. The latter is achieved for any appreciable difference between the velocities.

Excitations of the O(3)-nonlinear σ model are $S=1$ triplets.[29] Thus, the spectrum is qualitatively the same as for identical chains. That is what one might expect because the model of Majorana fermions is a strong-coupling limit of the O(3)-nonlinear σ model (see Ref. 13).

The correlation functions of the O(3)-nonlinear σ model are known only in the form of the Lehmann expansion:[30]

$$\langle\vec{n}(\tau,x)\vec{n}(0,0)\rangle\sim K_0(mr)+O[\exp(-3mr)]. \tag{78}$$

Note that the first term in the expansion coincides with the one for identical chains. Therefore a difference in dynamical magnetic susceptibilities for both cases will become manifest only at energies $\omega>3m$. The lowest feature in $\mathrm{Im}\chi^{(R)}(\omega,q)$ is in both cases the sharp peak

$$\mathrm{Im}\chi^{(R)}(\omega,q)\sim\frac{m}{\sqrt{q^2+m^2}}\delta(\omega-\sqrt{q^2+m^2}) \tag{79}$$

corresponding to the triplet excitation. Such a peak has been observed in $(\mathrm{VO})_2\mathrm{P}_2\mathrm{O}_7$.[15]

V. STRING ORDER PARAMETER IN THE SPIN-LADDER MODEL

Den Nijs and Rommelse[16] (see, also, Ref. 17) have argued that the gapful Haldane phase of the $S=1$ spin chain is characterized by a topological order measured by the string order parameter

$$\langle O^\alpha\rangle=\lim_{|n-m|\to\infty}\left\langle S_n^\alpha\exp\left(i\pi\sum_{j=n+1}^{m-1}S_j^\alpha\right)S_m^\alpha\right\rangle,$$

$$(S=1,\alpha=x,y,z). \tag{80}$$

The nonzero value of $\langle O^\alpha\rangle$ has been related to the breakdown of a hidden $Z_2\times Z_2$ symmetry.[19] In this section we use the Abelian bosonization method (Sec. II) to construct the string operator in the continuum limit of the $S=1/2$ spin-ladder model and identify the corresponding discrete symmetry with that of the related Ising models.

Since spin-rotational invariance remains unbroken, the string order parameter must respect this symmetry. However, Abelian bosonization is not an explicitly SU(2) invariant procedure. For this reason, it turns out that it is the z component of the string operator that acquires a simple form in the continuum limit. On the other hand, due to the unbroken SU(2) symmetry, the very choice of the quantization (z-) axis is arbitrary; therefore the expectation values for all components of the string operator will coincide.

To construct a string order parameter $O^z(n,m)$ for the spin-ladder model, we shall follow the same route as that previously used for the bond-alternating $S=1/2$ chain[19] (technical details are given in Appendix B). We start from the lattice version of the model, construct a product of two spin-1/2 operators belonging to the jth rung, $S_1^z(j)S_2^z(j)$, and then take a product over all rungs between $j=n$ and $j=m$:

$$O^z(n,m)=\prod_{j=n}^{m}\,[-4S_1^z(j)S_2^z(j)]$$
$$=\exp\left(i\pi\sum_{j=n}^{m}\,[S_1^z(j)+S_2^z(j)]\right). \tag{81}$$

Assuming that $|m-n|\gg 1$, we pass to the continuum limit in the exponential and retain only the smooth parts of the spin operators expressing them in terms of the spin currents $J^z_{a;R,L}(x),(a=1,2)$:

$$O^z(x,y)=\exp\left(\pm i\pi\sum_{a=1,2}\int_x^y dx' S_a^z(x')\right)$$
$$=\exp\left(\pm i\pi\sum_{a=1,2}\int_x^y dx'[J^z_{a;R}(x')+J^z_{a;R,L}(x')]\right). \tag{82}$$

Using Eqs. (5) and (A10), we find that the exponential is expressed in terms of the field ϕ_+ only. Thus we find a very transparent representation for the string operator:

$$O^z(x,y)=\exp\{i\sqrt{\pi}[\phi_+(x)-\phi_+(y)]\}. \tag{83}$$

Using Eq. (31),

$$\exp(i\sqrt{\pi}\phi_+(x))\sim\mu_1\mu_2+i\sigma_1\sigma_2, \tag{84}$$

we find that the string operator is expressed in terms of the Ising order and disorder operators. For either sign of $J_\perp$, we find that, in the limit $|x-x'|\to\infty$, the vacuum expectation value of $O^z(x,y)$ is indeed nonzero:

$$\lim_{|x-x'|\to\infty}\langle O^z(x,y)\rangle\sim\langle\sigma_1\rangle^2\langle\sigma_2\rangle^2=\langle\sigma\rangle^4\neq 0,\quad J_\perp<0, \tag{85}$$

$$\lim_{|x-x'|\to\infty}\langle O^z(x,y)\rangle\sim\langle\mu_1\rangle^2\langle\mu_2\rangle^2=\langle\mu\rangle^4\neq 0,\quad J_\perp>0. \tag{86}$$

As in the case of the bond-alternating spin chain, the nonvanishing expectation value of the string order parameter in the limit of infinite string manifests breakdown of a discrete $Z_2\times Z_2$ symmetry. This is the symmetry of two decoupled Ising models described by the Hamiltonian H_+ in the Majorana fermion representation (14): $H_+=H_m[\xi^1]+H_m[\xi^2]$ remains invariant with respect to sign inversion of both chiral components of each Majorana spinor, $\xi^a_{R,L}\to-\xi^a_{R,L}$, $(a=1,2)$. Under these transformations, the Ising order and disorder parameters change their signs. On the other hand, since the two Majorana fermions are massive, this symmetry is broken in the *ground state* of H_+: the mass terms break the duality symmetry $\xi^a_L\to-\xi^a_L$, $\xi^a_R\to\xi^a_R$. This amounts to finite expectation values of the Ising variables σ_1 and σ_2 (or μ_1 and μ_2), which in turn results in a nonzero string order parameter, as shown in Eqs. (85) and (86).

VI. CONCLUSIONS

As the reader can see the spin ladder presents an exciting opportunity to study the formation of massive spin $S=1$ and $S=0$ particles which appear as bound states of the spin $S=1/2$ excitations of individual Heisenberg chains. At small interchain coupling $|J_\perp|\ll J_{||}$ the masses of these particles are of the order of $|J_\perp|$. The $S=1$ branch is always lower independently of the sign of $J_\perp$. At $J_\perp/J_{||}\to 0$ the singlet spectral gap is three times as large as the triplet one. The imaginary part of the dynamical spin susceptibility $\chi''(\omega,q;q_\perp)$ calculated in Sec. III contains essential information about particle dynamics. The smallness of the interchain coupling in comparison with the spinon bandwidth allows us to see many multiparticle resonances developing in χ''. At small energies the susceptibility exhibits a sharp peak around $q=\pi$ corresponding to the stable $S=1$ massive particle; at energies $\omega>3m$ $\chi''(\omega,q)$ has an incoherent tail originating from multiparticle processes. Below the $5m$ threshold the singlet branch does not contribute to $\chi''(\omega,q)$ and the latter coincides with the susceptibility of a $S=1$ chain. The contribution from the singlet mode becomes essential at energies much greater than the spectral gap and the susceptibility asymptotically approaches its value for a spin-1/2 chain. We emphasize that the described picture holds only in the ideal limit $J_\perp/J_{||}\to 0$. We suppose that in real systems it will be difficult to make this ratio less than 0.1.

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APPENDIX A: BASIC FACTS ABOUT BOSONIZATION

Antiferromagnetic spin-chain Hamiltonians, such as the Heisenberg Hamiltonian

$$H=J\sum_{n=1}^{N}\mathbf{S}_n\cdot\mathbf{S}_{n+1}\quad(S=1/2,\quad J>0) \tag{A1}$$

can be mapped onto fermionic theories. Using bosonization, these can be recast as generalized Sine-Gordon or WZW models. This is useful because a great deal is known about these theories, such as correlation functions, scaling dimensions of operators, etc. A brief summary of this approach is given below.

Following Refs. 26, we start from a *symmetry preserving* fermionization of the spin operators

$$\mathbf{S}_n = \psi^\dagger_{n\alpha} \frac{\vec{\sigma}_{\alpha\beta}}{2} \psi_{n\beta}. \tag{A2}$$

To eliminate the redundant zero- and double-occupancy states, the constraint $\Sigma_\alpha \psi^\dagger_{n\alpha}\psi_{n\alpha}=1$ for all lattice sites n should be imposed. Such a constraint will effectively work, if one considers a 1/2-filled, $U>0$ Hubbard model for the field $\psi_{n\alpha}$. In this model, a Mott-Hubbard charge gap m_c is known to exist for *any* positive U. Therefore, at low energies, $|E| \ll m_c$, only spin excitations remain; those describe universal dynamical properties of the spin-chain model (A1) in the continuum limit.

Assuming that $U \ll t$, we linearize the free-particle spectrum near two Fermi points, $\pm k_F (k_F = \pi/2a_0)$, and decompose the Fermi field into right-moving and left-moving chiral components:

$$\psi_{n\alpha} \to \sqrt{a_0}\psi_\alpha(x), \quad \psi_\alpha(x) = (-i)^n \psi_{R\alpha}(x) + i^n \psi_{L\alpha}(x). \tag{A3}$$

We then introduce the scalar [U(1)] and vector [SU(2)] currents (the local charge and spin densities)

$$J_{R,L} = :\psi^\dagger_{R,L;\alpha}\psi_{R,L;\alpha}:, \quad \mathbf{J}_{R,L} = :\psi^\dagger_{R,L;\alpha}\frac{\vec{\sigma}_{\alpha\beta}}{2}\psi_{R,L;\beta}: \tag{A4}$$

satisfying anomalous [U(1) and SU(2)] Kac-Moody algebras:

$$[J_R(x), J_R(x')] = \frac{1}{i\pi}\delta'(x-x'), \tag{A5}$$

$$[J^a_R(x), J^b_R(x')] = i\epsilon^{abc} J^c_R(x)\delta(x-x') - \frac{i}{4\pi}\delta^{ab}\delta'(x-x') \tag{A6}$$

(with similar relations for the left components). These algebras lead to fermion-boson duality which allows us to represent the Hamiltonian of free fermions as a sum of two independent (commuting) contributions of gapless charge and spin collective modes (Sugawara form):

$$\begin{aligned} H^0 &= H^0_{\mathrm{U}(1)} + H^0_{\mathrm{SU}(2)} \\ &= \int dx \bigg[\frac{\pi v_F}{2}(:J_R J_R: + :J_L J_L:) \\ &\quad + \frac{2\pi v_F}{3}(:\mathbf{J}_R\cdot\mathbf{J}_R: + :\mathbf{J}_L\cdot\mathbf{J}_L:)\bigg]. \end{aligned} \tag{A7}$$

The charge part is equivalently described in terms of a massless scalar field ϕ_c. Under identifications $J_R + J_L = (1/\sqrt{\pi})\partial_x\phi_c$, $J_R - J_L = -(1/\sqrt{\pi})\Pi_c$, where Π_c is the momentum conjugate to the field ϕ_c, one obtains

$$H^0_{\mathrm{U}(1)} = \frac{v_s}{2}\int dx [\Pi^2_c(x) + (\partial_x\phi_c(x))^2]. \tag{A8}$$

The spin part $H^0_{\mathrm{SU}(2)}$ represents the level $k=1$ SU(2)-symmetric critical Wess-Zumino-Witten (WZW) model.

A weak Hubbard interaction preserves the important property of charge-spin separation, $H_{\mathrm{Hubbard}} = H_c + H_s$. Umklapp processes relevant at 1/2-filling transform $H^0_{U(1)}$ to a quantum sine-Gordon model

$$H_c = \int dx \left(\frac{v_c}{2}[\Pi^2_c + (\partial_x\phi_c)^2] + \text{const } g \cos\beta_c\phi_c \right), \tag{A9}$$

which at $g \sim U/t > 0$ occurs in its strong-coupling, massive phase ($\beta^2 < 8\pi$), with the single-soliton mass m_c being just the the Mott-Hubbard commensurability gap.

In the spin sector, interaction $-2g\mathbf{J}_R\cdot\mathbf{J}_L$ is added to $H^0_{\mathrm{SU}(2)}$. This interaction is marginally *irrelevant* (since $g>0$). Therefore, the universal scaling properties of the Heisenberg $S=1/2$ spin chain (A1) are described by the level $k=1$ WZW model $H^0_{\mathrm{SU}(2)}$.[26]

The possibility of an Abelian bosonization of the Heisenberg chain (A1) stems from the fact that conformal charges of the $k=1$ SU(2) WZW models and free massless Bose field coincide: $C^{\mathrm{WZW}}_{\mathrm{SU}(2),k=1} = C_{\mathrm{boson}} = 1$. Using relations $(1/3)\mathbf{J}_{R(L)}\cdot\mathbf{J}_{R(L)} = J^z_{R(L)}J^z_{R(L)}$, $H^0_{\mathrm{SU}(2)}$ can be expressed in terms of J^z currents only; introducing then a pair of canonical variables, ϕ_s and Π_s, via

$$J^z_R + J^z_L = \frac{1}{\sqrt{2\pi}}\partial_x\phi_s, \quad J^z_R - J^z_L = -\frac{1}{\sqrt{2\pi}}\Pi_s, \tag{A10}$$

one finds

$$H^0_{\mathrm{SU}(2)} \to H_B = \frac{v_s}{2}\int dx [\Pi^2_s(x) + (\partial_x\phi_s(x))^2]. \tag{A11}$$

The price we pay for this simplification is the loss of spin rotational invariance in the bosonized structure of the spin currents: the J^x and J^y cannot be represented as simply as J^z, and require bosonization of the Fermi fields:

$$\psi_{R,L;\alpha}(x) \simeq (2\pi a_0)^{-1/2}\exp(\pm i\sqrt{4\pi}\varphi_{R,L;\alpha}(x)). \tag{A12}$$

Linear combinations

$$\Phi_\alpha = \varphi_{R\alpha} + \varphi_{L\alpha}, \quad \Theta_\alpha = -\varphi_{R\alpha} + \varphi_{L\alpha}$$

constitute scalar fields Φ_α and their dual counterparts Θ_α introduced for each spin component. The fields describing the charge and spin degrees of freedom are defined as follows:

$$\phi_c = \frac{\Phi_\uparrow + \Phi_\downarrow}{\sqrt{2}}, \quad \theta_c = \frac{\Theta_\uparrow + \Theta_\downarrow}{\sqrt{2}},$$

$$\phi_s = \frac{\Phi_\uparrow - \Phi_\downarrow}{\sqrt{2}}, \quad \theta_s = \frac{\Theta_\uparrow - \Theta_\downarrow}{\sqrt{2}}, \tag{A13}$$

where $\partial_x\theta_{c,s} = \Pi_{c,s}$.

To bosonize $J^\pm_{R,L}$, use (A12) to obtain:

$$J_R^+ = \psi_{R\uparrow}^\dagger \psi_{R\downarrow} = \frac{1}{2\pi a_0} \exp(-i\sqrt{2\pi}(\phi_s - \theta_s)),$$

$$J_L^+ = \psi_{L\uparrow}^\dagger \psi_{L\downarrow} = \frac{1}{2\pi a_0} \exp(i\sqrt{2\pi}(\phi_s + \theta_s)). \quad \text{(A14)}$$

Note that, as expected, the charge field ϕ_c does not contribute to the spin SU(2) currents. Moreover, despite the fact that the definitions (A14) contain cutoff a_0 explicitly, the current-current correlation functions are cutoff independent and reveal the underlying SU(2) symmetry:

$$\langle J^a(x) J^b(x')\rangle = -\frac{\delta^{ab}}{4\pi^2} \frac{1}{(x-x')^2}. \quad \text{(A15)}$$

The SU(2) currents $\mathbf{J}_R(x)$, $\mathbf{J}_L(x)$ determine the smooth parts of the spin operators in the continuum limit. Namely, at $a_0 \to 0$

$$\mathbf{S}_n \to a_0 \mathbf{S}(x), \quad \mathbf{S}(x) = \mathbf{J}_R(x) + \mathbf{J}_L(x) + (-1)^n \mathbf{n}(x), \quad \text{(A16)}$$

where

$$\mathbf{n}(x) = \psi_{R\alpha}^\dagger(x) \frac{\vec{\sigma}_{\alpha\beta}}{2} \psi_{L\beta}(x) + \text{H.c.} \quad \text{(A17)}$$

is the staggered part of the local-spin density.

When bosonizing (A17), the (redundant) charge excitations emerge, since off-diagonal bilinears like $\psi_R^\dagger \psi_L$ and $\psi_L^\dagger \psi_R$ describe particle-hole *charge* excitations with momentum transfer $\pm 2k_F$. We find

$$n^z = -\frac{1}{\pi a_0} \cos\sqrt{2\pi}\phi_c \sin\sqrt{2\pi}\phi_s,$$

$$n^\pm = \frac{1}{\pi a_0} \cos(\sqrt{2\pi}\phi_c) \exp(\pm i\sqrt{2\pi}\theta_s).$$

Being interested in the energy range $|E| \ll m_c$, one can replace the charge operator $\cos(\sqrt{2\pi}\phi_c)$ by its nonzero vacuum expectation value; we denote this (nonuniversal) value by $\lambda = \langle \cos(\sqrt{2\pi}\phi_c)\rangle$ and arrive at bosonization formulas for $\mathbf{n}(x)$:

$$n^z(x) = -\frac{\lambda}{\pi a_0} \sin\sqrt{2\pi}\phi_s(x),$$

$$n^\pm(x) = \frac{\lambda}{\pi a_0} \exp[\pm i\sqrt{2\pi}\theta_s(x)]. \quad \text{(A18)}$$

This completes the bosonization of the spin operators for the isotropic Heisenberg chain. Notice that the critical dimensions of the smooth and staggered parts of the spin densities are different:

$$\dim J^a = 1, \quad \dim n^a = 1/2. \quad \text{(A19)}$$

APPENDIX B: HIDDEN $Z_2 \times Z_2$ SYMMETRY AND STRING ORDER PARAMETER IN THE BOND-ALTERNATING $S=1/2$ HEISENBERG CHAIN

In addition to the $S=1/2$ spin-ladder model, there is another system which is related to the $S=1$ spin chain—the spin-1/2 chain with alternating ferromagnetic and antiferromagnetic bonds:

$$H = 4J \sum_{j=1}^{N/2} [(\mathbf{S}_{2j-1} \cdot \mathbf{S}_{2j}) - \beta(\mathbf{S}_{2j} \cdot \mathbf{S}_{2j+1}]. \quad \text{(B1)}$$

This model is instructive in the sense that the string order parameter, whose nonzero expectation value signals breakdown of a hidden discrete symmetry, can be easily constructed.[19] The analogous construction is then directly generalized for the spin-ladder model.

A gap in the excitation spectrum of the model (B1) persists in the whole range $0 < \beta < \infty$. At $\beta = 0$ the ground state of model represents an array of disconnected singlets. At $\beta \gg 1$, strong ferromagnetic coupling between the spins on the $\langle 2j, 2j+1\rangle$ bonds leads to the formation of local triplets, and the model (B1) reduces to a $S=1$ Heisenberg chain. Using a nonlocal unitary transformation, Kohmoto and Tasaki[19] have demonstrated equivalence of the model (B1) to a system of two coupled quantum Ising chains, i.e., two coupled $2d$ Ising models. This transformation provides an exact representation of the spin operators S_n^α as products of two Ising-like order (σ, τ) and disorder $(\tilde{\sigma}, \tilde{\tau})$ operators, essentially a lattice version of relations (31) and (33) (see, e.g., Ref. 31). Nearest-neighbor bilinears of the original spin operators take the form

$$4S_{2j}^x S_{2j+1}^x = -\sigma_j^z \sigma_{j+1}^z, \quad 4S_{2j-1}^x S_{2j}^x = -\tau_j^x,$$

$$4S_{2j}^y S_{2j+1}^y = -\tau_j^z \tau_{j+1}^z, \quad 4S_{2j-1}^y S_{2j}^y = -\sigma_j^x,$$

$$4S_{2j}^z S_{2j+1}^z = -\sigma_j^z \sigma_{j+1}^z \tau_j^z \tau_{j+1}^z, \quad 4S_{2j-1}^z S_{2j}^z = -\sigma_j^x \tau_j^x, \quad \text{(B2)}$$

where

$$\sigma_j^x = \tilde{\sigma}_{j-1/2}^z \tilde{\sigma}_{j+1/2}^z, \quad \tau_j^x = \tilde{\tau}_{j-1/2}^z \tilde{\tau}_{j+1/2}^z, \quad \text{(B3)}$$

$$\tilde{\sigma}_{j+1/2}^z = \prod_{l=j+1}^{N/2} \sigma_l^x, \quad \tilde{\tau}_{j+1/2}^z = \prod_{l=1}^{j-1} \tau_l^x. \quad \text{(B4)}$$

Relations (B2) make the Hamiltonian (B1) equivalent to two coupled quantum Ising chains:

$$H = -J \sum_{j=1}^{N/2} [(\beta\sigma_j^z \sigma_{j+1}^z + \sigma_j^x) + (\beta\tau_j^z \tau_{j+1}^z + \tau_j^x) + (\beta\sigma_j^z \sigma_{j+1}^z \tau_j^z \tau_{j+1}^z + \sigma_j^x \tau_j^x)]. \quad \text{(B5)}$$

The model (B5) is invariant under independent rotations of the σ and τ spins by angle π about the spin x axis which comprise a $Z_2 \times Z_2$ group. Since this group is discrete, it can be spontaneously broken, in which case the spectrum of the system would be massive. It is easily understood from (B5) that, in the limit of large positive β when the model reduces to the $S=1$ chain, the $Z_2 \times Z_2$ symmetry is broken, with

$$\langle \sigma_j^z \rangle = \langle \tau_j^z \rangle = \langle \sigma_j^z \tau_j^z \rangle \neq 0. \quad \text{(B6)}$$

[It has been used in Eq. (B6) that, under transformation $\mu_j^z = \sigma_j^z \tau_j^z$ to a new pair of variables, μ_j^z and τ_j^z, the two-chain Hamiltonian (B5) preserves its form.]

Representation (B2) hints to the way how an order parameter measuring breakdown of the $Z_2 \times Z_2$ symmetry should be constructed out of the spin operators S_n^α. Following Kohmoto and Tasaki, consider a product

$$\prod_{l=2k}^{2n-1} 2S_l^x=\prod_{j=k}^{n-1} 4S_{2j}^x S_{2j+1}^x=\prod_{j=k}^{n-1}(-\sigma_j^z\sigma_{j+1}^z)$$
$$=(-1)^{n-k}(\sigma_k^z\sigma_{k+1}^z)(\sigma_{k+1}^z\sigma_{k+2}^z)\cdots(\sigma_{n-1}^z\sigma_n^z)$$
$$=(-1)^{n-k}\sigma_k^z\sigma_n^z. \tag{B7}$$

Using the relation $i\sigma_j^\alpha=\exp(i\pi\sigma_j^\alpha/2)$, we find that

$$O^x(k,n)\equiv\exp\left(i\pi\sum_{l=2k}^{2n-1}S_l^x\right)=\sigma_k^z\sigma_n^z. \tag{B8}$$

This is the x component of the string order operator. According to (B6), in the limit $|k-n|\to\infty$, its vacuum expectation value is nonzero:

$$\langle O^x(k,n)\rangle\to\langle\sigma\rangle^2\neq 0. \tag{B9}$$

It is important that the string always contains an even number of sites, starting at an even site and ending at an odd site. For a string starting at an odd site and ending at an even site, the corresponding string operator is expressed in terms of disorder operators and therefore has zero expectation value:

$$\prod_{l=2k+1}^{2n} 2S_l^x=\prod_{j=k+1}^{n} 4S_{2j-1}^x S_{2j}^x=(-1)^{n-k}(\tilde\tau_{k+1/2}^z\tilde\tau_{k+3/2}^z)$$
$$\times(\tilde\tau_{k+3/2}^z\tilde\tau_{k+5/2}^z)\cdots(\tilde\tau_{n-1/2}^z\tilde\tau_{n+1/2}^z)$$
$$=(-1)^{n-k}\tilde\tau_{k+1/2}^z\tilde\tau_{n+1/2}^z.$$

The y and z components of the string operator are constructed in a similar manner:

$$O^y(k,n)=\exp\left(i\pi\sum_{l=2k}^{2n-1}S_l^y\right)$$
$$=\prod_{l=2k}^{2n-1}2iS_l^y=\prod_{j=k}^{n-1}(-4S_{2j}^yS_{2j+1}^y)$$
$$=\prod_{j=k}^{n-1}\tau_j^z\tau_{j+1}^z=\tau_k^z\tau_n^z, \tag{B10}$$

$$O^z(k,n)=\exp\left(i\pi\sum_{l=2k}^{2n-1}S_l^z\right)=\sigma_k^z\tau_k^z\sigma_n^z\tau_n^z. \tag{B11}$$

The SU(2) invariance of the expectation value of the string order parameter

$$O^\alpha(k,n)=\exp\left(i\pi\sum_{l=2k}^{2n-1}S_l^\alpha\right),\quad (S=1/2,\quad \alpha=x,y,z) \tag{B12}$$

follows from (B6).

Notice that in the limiting case $\beta\gg 1$, the string order parameter (B12) for the $S=1/2$ bond-alternating chain automatically transforms to the exponential of the string order parameter (80) for the $S=1$ chain.

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