Spontaneous dimerization in quantum-spin chains

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A bosonic approach allowing one to detect a region of a spontaneously dimerized phase in an $S=1$ quantum-spin chain and to develop the critical theories on both phase boundaries is presented. The results obtained agree, in general, with the field-theoretical predictions involving the Wess-Zumino-Witten nonlinear σ model.

I. INTRODUCTION

In the past decade there has been considerable interest in the study of various properties of quantum-spin chains. This interest was, to a great extent, initiated by the intriguing conjecture made by Haldane[1] that the ground state of Heisenberg antiferromagnets with interaction between nearest neighbors depends crucially on the parity of $2S$: for integer S, quantum fluctuations completely restore the symmetry so that the paramagnetic state remains stable at zero temperature as well (and since no symmetry is broken the excitations have a finite gap), while, for half-integer S, the orientational ordering (implying the existence of gapless excitations) survives at $T=0$.

A large amount of effort undertaken just after the appearance of Haldan's paper allowed a number of arguments supporting the conjecture to be found. First of all, the difference between integer and half-integer S (more precisely, between $S=\frac{1}{2}$ and 1) is now clearly seen in numerical experiments for chains of length up to $L=32$.[2-4] The estimated value of the gap for $S=1$ is about 0.4 J. Moreover, the paramagnetic singlet ground state with a finite gap for excitations was recently observed in a rather isotropic and very one-dimensional (1D) $S=1$ antiferromagnet $Ni(C_2H_8N_2)_2NO_2C1O_4$.[5]

From the theoretical point of view, the first question to be answered is which part of the Haldane conjecture is more unexpected, or, equivalently, what is necessary to prove. Really, the naive treatment of a 1D antiferromagnet immediately leads to a theory of the three-component unit vector of antiferromagnetism, $\mathbf{n}(t,x)$, with the Lagrangian

$$L=\frac{1}{2g^2}\partial_\mu n\,\partial^\mu n \ .$$

But this O(3) σ model in $1+1$ dimensions was solved exactly[6] and the expected[7] result is that fluctuations completely restore the symmetry, thus producing a mass gap

$$\Delta\sim\frac{2\pi}{g}\exp(-2\pi/g) \ .$$

According to Affleck,[8] "from this perspective what is more difficult to understand is what was previously taken for granted: the non-existence of a gap for half-integer S."

The first attempts in this direction had a goal to improve the mapping of the quantum antiferromagnetic spin chain onto the O(3) nonlinear σ model.[9-11] As a main discovery, it was established that since the description in terms of the unit vector of antiferromagnetism implies the doubling of the unit cell, then the nonequivalence of the effective distance between neighbors (it is zero or twice the interatomic spacing) ensures an additional so-called ϑ term to appear in the long-wavelength action. Roughly speaking, this term retains a memory about the parity of the site spins since, after doubling, one deals only with the total spin of a pair which is always an integer. This additional term, which enters into the Euclidean action with the coefficient $i\vartheta$, where $\vartheta=2\pi S$, is the integer-valued topological charge (a winding number, measuring the degree of mapping of the order parameter space S_2 onto the real space S_2). Evidently, it plays no role for integer S and does not distinguish between various half-integer spin values (at least for large S since, strictly speaking, the mapping is valid only for $S\gg1$). It was argued[9-13] that this term, although it is a total derivative and, hence, does not appear in the perturbation theory, may stop the increase of the coupling constant g at the scales when g (initially small for $S\gg1$) becomes of the order of unity and nontrivial configurations with nonzero topological charge begin to influence the β function. Strictly speaking, the only thing clearly seen from this approach is that the behavior of all Heisenberg antiferromagnets with different half-integer spin values is universal, at least for large S.

The lack of knowledge of the properties of the σ model with $\vartheta=\pi$ forced one to look for other approaches which could clarify the situation. The first step in this direction was made by Lieb and Affleck.[14] They extended the old $S=\frac{1}{2}$ result of Lieb, Shultz, and Mattis[15] to higher values of S and proved exactly that the ground state of *any* half-integral spin system with a translationally and rotationally invariant Hamiltonian is either degenerate or has a zero gap for excitations. Later Affleck *et al.*[16] exactly solved (after having reformulated the problem in terms of valence bonds) the $S=1$ model with both bilinear and biquadratic interactions present and with the ratio of exchange integrals J and J' (both positive), $J'/J=\frac{1}{3}$. It was rigorously proved (see also Ref. 17) that the ground state is really nondegenerate, all excitations have finite gaps, and the spin-spin correlation function decays exponen-

tially. Since there are absolutely no reasons to expect any principle difference between the model solved and the purely Heisenberg one (except for some fine details, see Ref. 8), then, from the formal point of view, these two results can be considered as a direct proof of the Haldane conjecture.

But apart from the initial discussion on the Heisenberg systems there are another questions to be answered in order to understand the $T=0$ properties of the spin chains. Really, for *any* value of S independently of its parity, a gapless Bethe ansatz solvable "antiferromagnetic" model is known.[18,19] This family of models includes the Heisenberg one for $S=1/2$. Although for general S these models are only the special points in the space of parameters of the generic spin S nearest-neighbor exchange Hamiltonians which, we recall, are the polynomials of the order of $2S$, the existence of massless excitations for integer S needs to be explained since it seems to contradict the mapping onto the σ model with the ϑ term. Formally, this mapping is unsensitive to the switching of the polynomial interactions.[10]

The explanation based on the field-theory approach was given by Affleck and Haldane.[20] They claimed that the integrable models represent the special multicritical transition points into the *spontaneously dimerized* phase where the symmetry with respect to translations by one site is spontaneously broken. These unusual ground states are definitely known to exist in some 1D systems.[21] Roughly speaking, the possibility of the ground state to be dimerized comes from the fact that a separate pair of spins with antiferromagnetic interaction tends to form a spin singlet. Correspondingly, if to combine each spin on an even site with its right (or left) neighbor and to first restrict only with the interactions inside the pairs, then the (twofold degenerate) ground state will be a product of noninteracting singlets. Note that this ground state is ordered: the order parameter Ψ can be defined as[22]

$$\langle \mathbf{S}_i \cdot \mathbf{S}_{i+1} - \mathbf{S}_i \cdot \mathbf{S}_{i-1} \rangle = (-1)^i \Psi \ .$$

The switching of the interactions between pairs gives rise to the zero-point fluctuations which tend to destroy long-range dimer order. However, in some part of a phase diagram the ordering can survive even in the limit of a translationally invariant interaction.

A foregoing discussion will be focused on the case of $S=1$. The most general Hamiltonian contains the bilinear and biquadratic products of nearest neighbors and can be parameterized by a single parameter γ:

$$H = \sum_l \cos\gamma \mathbf{S}_l \cdot \mathbf{S}_{l+1} + \sin\gamma (\mathbf{S}_1 \cdot \mathbf{S}_{l+1})^2 \ , \tag{1}$$

where $0 \le \gamma \le 2\pi$. For $\gamma = 0$ and π it reduces to the usual Heisenberg antiferromagnet and ferromagnet, correspondingly. Below only the lower half-circle $\pi < \gamma < 2\pi$ will be considered. The integrable point mentioned above corresponds to $\gamma = 7\pi/4$ (Fig. 1).

I start with the classical phase diagram of (1). It consists of three phases: the ferromagnetic phase, which is stable at $\gamma < 5\pi/4$, the antiferromagnetic one, stable at $\gamma > 3\pi/2$, and the intermediate so-called spin nematic phase with unbroken time-reversal symmetry $\langle \mathbf{S} \rangle = 0$,

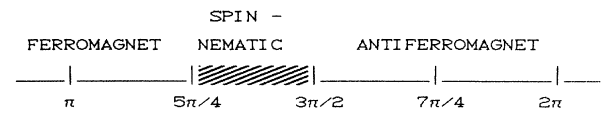

FIG. 1. "Classical" phase diagram of the generic $S=1$ model (1) for $\pi < \gamma < 2\pi$ (Refs. 23 and 24). The ferromagnetic ($\gamma < 5\pi/4$) and antiferromagnetic ($\gamma > 3\pi/2$) phases are separated by the intermediate spin nematic phase with quadruple ordering (shown hatched). $\gamma = 7\pi/4$ is a Bethe ansatz solvable point.

but with the quadrupolar ordering $\langle S_x^2 \rangle = \langle S_y^2 \rangle \neq \langle S_z^2 \rangle$.[23,24]

In one dimension the classical phase diagram is no longer correct in all regions except the ferromagnetic one: fluctuations restore the continuous symmetry. This happens both in the antiferromagnetic phase (as a realization of the Haldane conjecture, hereafter I will refer to this phase as a Haldane one) and in the quantum version of the spin nematic phase. The point, however, is that these two disordered ground states are *qualitatively different*. Roughly speaking, the Haldane phase involves the states of a given pair with the total spin $M=0$ and 1,[16] while the spin nematic phase is formed by the states with $M=0$ and 2.[23] To make this statement more precise, it is worth noticing that the topological "long-range order" in the string correlation function

$$g(l) = -\left\langle S_0^z \prod_{j=1}^{l-1} \exp(i\pi S_j^z) S_l^z \right\rangle \ ,$$

shown by Girvin and Arovas[25] to be present in the Haldane phase does not exist in the spin nematic phase. Moreover, there is no doubling in the spin nematic state (nematic ordering arises on *each* site) and, hence, the corresponding long-wavelength action does not contain the topological ϑ term. Thus, these two different disordered states must be separated by an intermediate phase, which was predicted by Affleck and Haldane[20] to be a dimerized one and to merge with the Haldane phase exactly at the integrable point $\gamma = 7\pi/4$.

Affleck and Haldane also resolved an apparent contradiction between the Bethe ansatz solution for $\gamma = 7\pi/4$ and the mapping onto the σ model with the ϑ term by claiming that the transition to dimerization is governed exactly by the softening of longitudinal fluctuations of what was usually referred to as a "unit" vector of antiferromagnetism n:

$$\mathbf{n} = \frac{\mathbf{L}}{2\sqrt{S(S+1)}}, \quad \mathbf{L} = \mathbf{S}_{2l} - \mathbf{S}_{2l+1} \ . \tag{2}$$

These fluctuations exist since the total spin of a pair may have different values. Correspondingly, just at the transition point, the order-parameter space is isomorphic to SU(2), not to S_2 as inside the Haldane phase. By making use of the knowledge[26] of which Lagrangian describes the conformally invariant SU(2) models, Affleck and Haldane predicted the critical theory at $\gamma = 7\pi/4$ to be given by the $k=2$ (or, generally, $k=2S$) SU(2) Wess-Zumino-Witten model (this proposal was originally formulated in Ref. 27). The shifting from the transition point was

shown to lead to dimerization or to generate a gap in the longitudinal component of the SU(2) matrix (which plays the role of a "unit vector" in the group manifold) which reduces the order parameter space to a surface of a unit sphere S_2 and converts the Wess-Zumino term into the ϑ term of the σ model.

The calculation of the zero-temperature susceptibility[28] and specific heat[29] on the basis of the field-theoretical approach lead to the same results as were obtained from the Bethe ansatz solution. Moreover, recently the prediction of dimerization at $\gamma > 7\pi/4$ was confirmed both by numerical experiments[30–33] and by an exact solution of the purely biquadratic model ($\gamma = 3\pi/4$).[34–36]

The location of the other boundary of the dimerized phase is not known exactly. Solyom[37] proposed this phase to be *the only* intermediate state between the ferromagnetic and Haldane phases. In my opinion, this is very unlikely since completely different symmetries are broken in dimerized and ferromagnetic phases and there are absolutely no reasons to expect a direct transition between them to occur. In a recent paper,[23] I have investigated quantum fluctuations in the spin nematic phase in the vicinity of the ferromagnetic liability point $\gamma = 5\pi/4$, and did not find any trails of instability which might lead to a spontaneous dimerization.

In this article I want to reexamine this issue. I will make use of a direct transformation of spin operators to bosons, suitable to a dimerized state. The standard perturbative analysis of the bosonic version of the original spin Hamiltonian will allow one to detect a stability region of the spontaneously dimerized phase in the $S=1$ generalized translationally invariant spin chain (1) and also in the presence of the imposed staggered interactions. My second aim is to point directly on the mechanism which makes the theory *critical* at the phase boundaries. It is worth noticing that, in the field-theoretical approach to the problem, the additional Wess-Zumino term producing a fixed point of the renormalization-group equations at $\gamma = 7\pi/4$ was introduced by hands namely in order to manifest the conformal invariance.

The paper is organized as follows. I will begin, in Sec. II, with the transformation which allows one to construct a bosonic version of the $S=1$ Hamiltonian supposing the ground state is spontaneously dimerized. In Sec. III the results of the mapping will be presented and the liability lines of the dimerized state as functions of the strength of the staggered interaction will be determined by restricting with only quadratic-order terms in bosons, i.e., in the "spin-wave" approximation. Next, in Sec. IV, I will construct the critical theory on the boundaries and present the arguments favoring that one of the "spin-wave" transition lines, ending at the integrable point $\gamma = 7\pi/4$, is an exact one. The one-loop renormalization-group equation with a nontrivial fixed point present will be derived, though, to some extent, approximately. Finally, Sec. V is devoted to the discussion of the results.

II. BOSONIZATION FOR THE DIMERIZED PHASE

The standard way to bosonize the antiferromagnetic quantum-spin chain is to presume the existence of a short-range Néel order and to introduce *two* types of bosons via the Dyson-Maleev transformation (the latter is more convenient for the isotropic antiferromagnets then the Holstein-Primakoff one). In principle, this procedure is *exact* at zero temperature.[38] In the leading order in $1/S$ when only quadratic terms in the boson operators are retained, the excitations obtained via the diagonilization of the quadratic form are two identical gapless (linear in $\mathbf{k}$) spin-wave modes, which evidently correspond to the *transverse fluctuations of the vector of antiferromagnetism* $\mathbf{L}$. Meanwhile, as was already mentioned in the Introduction, the transition to dimerization is governed by the softening of the longitudinal fluctuations of L — the collective excitations in the framework of the Dyson-Maleev formalism.[39] Thus, the dimerized state can be identified as a state with a finite condensate of collective excitations, which by no doubts makes the standard approach very inconvenient.

Instead, I will take advantage of the fact that, up to zero-point fluctuations, the dimer state is constructed from the singlet configurations of the pairs of neighboring spins and will link first a total spin of each pair with bosons. Since the aim is to find a stability region of the dimerized phase, it is convenient to introduce a separate boson for each excited state of a given pair. The realization of this procedure is elementary: the total spin of a pair

$$\mathbf{M}_l = S_{2l} + \mathbf{S}_{2l+1} \tag{3}$$

is expressed as

$$\begin{aligned} M_l^z &= a_l^\dagger a_l - b_l^\dagger b_l + e_l^\dagger e_l - q_l^\dagger q_l + 2(d_l^\dagger d_l - t_l^\dagger t_l) , \\ M_l^+ &= (M_l^-)^* = \sqrt{2}[a_l^\dagger c_l - c_l^\dagger b_l - \sqrt{2}(d_l^\dagger e_l - q_l^\dagger t_l) \\ &\quad + \sqrt{3}(e_l^\dagger f_l - f_l^\dagger q_l)] . \end{aligned} \tag{4}$$

The analogous transformation for $\mathbf{L}$ is slightly more complicated:

$$\begin{aligned} L_l^z &= -[\sqrt{8/3}(c_l^\dagger U_l + U_l c_l) + (2/\sqrt{3})(c_l^\dagger f_l + f_l^\dagger c_l) \\ &\quad + a_l^\dagger e_l + e_l^\dagger a_l + q_l^\dagger b_l + b_l^\dagger q_l] , \\ L_l^\dagger &= (L_l^-)^* = \sqrt{2}[\sqrt{8/3}(a_l^\dagger U_l + U_l b_l) \\ &\quad - (1/\sqrt{3})(f_l^\dagger b_l + a_l^\dagger f_l) \\ &\quad + (e_l^\dagger c_l + c_l^\dagger q_l) - \sqrt{2}(d_l^\dagger a_l + b_l^\dagger t_l)] , \end{aligned} \tag{5}$$

where

$$\begin{aligned} U_l^2 = [1 &- (a_l^\dagger a_l + b_l^\dagger b_l + c_l^\dagger c_l + e_l^\dagger e_l + q_l^\dagger q_l \\ &+ f_l^\dagger f_l + d_l^\dagger d_l + t_l^\dagger t_l)] . \end{aligned}$$

The analogous transformation for $S = 1/2$ was presented in Ref. 40.

By definition, the physical states correspond to a vacuum state and to eight states with only one boson excited. The excitations created by a, b, and c correspond to $M=1$ and $M^z = 1$, -1 and 0, correspondingly, while those created by e, q, ,f, d, and t represent five different states of $M=2$. One can make sure that all the commutation relations $[M_i, M_j] = i\epsilon_{ijk} M_k$, $[L_i, L_j] = i\epsilon_{ijk} M_k$,

$[M_i, L_j] = i\epsilon_{ijk} L_k$ together with the constraint

$$\mathbf{M}_l^2 + \mathbf{L}_l^2 = 4S(S+1) = 8$$

are satisfied in a physical subspace. Moreover, as the matrix elements between physical and nonphysical subspaces are equal to zero, the transformation is *exact* at zero temperature just as the Holstein-Primakoff transformation for $S = \frac{1}{2}$.

In order to map the initial spin-chain Hamiltonian onto the system of interacting bosonic fields, one must break a chain into pairs and link both spins of a separate pair with the *same* bosons according to

$$\mathbf{S}_{2l} = (\mathbf{M}_l + \mathbf{L}_l)/2, \quad \mathbf{S}_{2l+1} = (\mathbf{M}_l - \mathbf{L}_l)/2 \ . \tag{6}$$

A resulting bosonic Hamiltonian consists of two parts. The first represents an "on-site" interaction $\mathbf{S}_{2l} \cdot \mathbf{S}_{2l+1}$ and is diagonal and quadratic in boson operators. In contrast, the second part — the bosonic version of $\mathbf{S}_{2l} \cdot \mathbf{S}_{2l-1}$—represents the interaction between bosonic fields in different points (with the lattice spacing twice the interatomic distance) and gives rise to the zero-point vibrations.

III. "SPIN-WAVE" THEORY FOR THE DIMERIZED PHASE

I start with the modified version of (1) which also includes staggered interaction ($0 \le \delta \le 1$):

$$H = \cos\gamma \sum_e (\mathbf{S}_{2l} \cdot \mathbf{S}_{2l+1} + \delta \mathbf{S}_{2l} \cdot \mathbf{S}_{2l-1}) + \sin\gamma \sum_e [(\mathbf{S}_{2l} \cdot \mathbf{S}_{2l+1})^2 + \delta(\mathbf{S}_{2l} \cdot \mathbf{S}_{2l-1})^2] \ . \tag{7}$$

The translationally invariant Hamiltonian (1) is a special version of (7) with $\delta = 1$, while for $\delta = 0$ the spin-chain model evidently breaks into a set of separate noninteracting pairs. In the latter case the dimerized state is obviously favorable at $5\pi/4 \le \gamma \le \tan^{-1}\frac{1}{3}$. The nonzero δ gives rise to the interaction between different pairs and evidently diminishes the stability region of the dimerized phase. In order to find the phase boundaries as functions of δ, I will make use of transformations (4)–(6) and map the original model onto the system of eight interacting bosonic fields.

To quadratic order in the bosonic operators and after the transition to momentum space, the Hamiltonian reads

$$H = H_1 + H_2 \ ,$$

where

$$H_1 = \sum_k (a_k^\dagger a_k + b_k^\dagger b_k + c_k^\dagger c_k) \left[\cos\gamma \left(1 - \frac{4\delta}{3} \nu_k \right) - \sin\gamma \left(3 - \frac{2\delta}{3} \nu_k \right) \right] + [a_k^\dagger b_{-k}^\dagger + a_k b_{-k} + \tfrac{1}{2}(c_k^\dagger c_{-k}^\dagger + c_k c_{-k})] \times [\delta \nu_k (2\sin\gamma - 4\cos\gamma)/3] \tag{8}$$

and

$$H_2 = \sum_k (e_k^\dagger e_k + q_k^\dagger q_k + f_k^\dagger f_k + d_k^\dagger d_k + t_k^\dagger t_k) \times \left[3\cos\gamma - \sin\gamma \left[\frac{2\delta}{3} \nu_k \right] \right] + [d_k^\dagger t_{-k}^\dagger + d_k t_{-k} + e^\dagger{}_k q^\dagger{}_{-k} + e_k q_{-k} + \tfrac{1}{2}(f_k^\dagger f_{-k}^\dagger + f_k f_{-k})] \delta \nu_k (2\sin\gamma/3) \ . \tag{9}$$

Here $\nu_k = \cos 2ka$.

Note that, in spite of the apparent breaking of the reflection symmetry (the spin on the right of a given pair interacts only with the spin on the left of the neighboring pair), the bosonic Hamiltonian is invariant under the replacement $k \Longrightarrow -k$ in contrast to the case of Heisenberg antiferromagnetic where the odd in k terms were responsible for the appearance of the ϑ term in the effective action.[11]

The diagonalization of the quadratic form gives two branches of excitations, threefold degenerate and fivefold degenerate, correspondingly:

$$\varepsilon_k^{(1)} = \cos\gamma(1 - 3\tan\gamma) \left[1 - \nu_k \frac{4\delta(2 - \tan\gamma)}{3(1 - 3\tan\gamma)} \right]^{1/2} , \tag{10}$$

$$\varepsilon_k^{(2)} = -3\cos\gamma(\tan\gamma - 1) \left[1 - \nu_k \frac{4\delta\tan\gamma}{9(\tan\gamma - 1)} \right]^{1/2} , \tag{11}$$

The demand of both energies to be positive immediately gives a stability region of the dimerized phase as an interval

$$\gamma_1 \le \gamma \le \gamma_2 \ ,$$

where

$$\gamma_1 = \pi + \tan^{-1}(1 - 4\delta/9)^{-1} \ , \tag{12}$$

$$\gamma_2 = \tan^{-1}[(1 - 8\delta/3)/(3 - 4\delta/3)] \ . \tag{13}$$

At $\delta = 0$, $\gamma_1 = 5\pi/4$ and $\gamma_2 = \tan^{-1}\frac{1}{3}$, as expected. For nonzero δ the stability interval diminishes due to quantum fluctuations but remains *finite* even in the limiting case of the translationally invariant Hamiltonian ($\delta = 1$) when the dimer order arises as a result of a *spontaneous* symmetry breaking (Fig. 2). In the latter case $\gamma_1 = \pi + \tan^{-1}\frac{9}{5}$, while $\gamma_2 = -\pi/4$, which is exactly the Bethe ansatz solvable point.

The dashed line with the error bars in Fig. 2 represents the results of numerical calculations of Singh and Gelfand.[30] The agreement with the present results is rather good, though the theoretical curve (13) is situated slightly lower.

One may ask what the accuracy of the results obtained is since the anharmonic corrections are by no means small even in the limit of small δ. In order to answer to this question I now pass to the anharmonic terms.

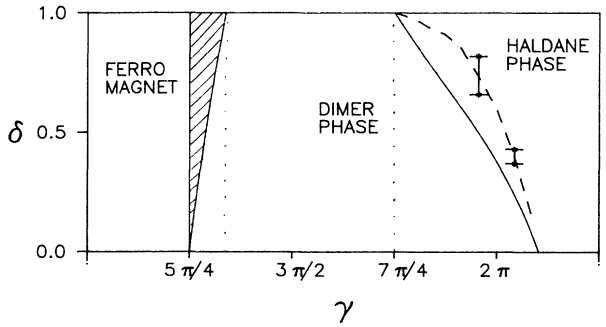

FIG. 2. $T=0$ quantum phase diagram in the γ,δ plane of the modified $S=1$ model (7). Two different disordered phases, 1D versions of antiferromagnetic and spin nematic states, are separated by the dimer phase with broken translational symmetry. The phase boundaries are calculated in the "spin-wave" approximation. The anharmonic corrections are believed not to shift the boundary line ending at the Bethe ansatz solvable point $\gamma=7\pi/4$. The dashed line is a result of numerical calculations of Ref. 30.

IV. CRITICAL THEORIES FOR THE PHASE BOUNDARIES

I will start with the phase boundary $\gamma_2(\delta)$ ending at the integrable point $\gamma=7\pi/4$, where a triplet of $M=1$ excitations undergo softening at $k=0$. Since, from the technical point of view, it is simpler not to deal with the particles-bosons but with the quasiparticles, I will begin with a diagonalization of the quadratic form. As usual, this procedure forces one to restrict only with the vertices on resonance.

After a Bogoliubov transformation, the quadratic part of the Hamiltonian takes the form

$$H=J\sum_k \tilde{\varepsilon}_k^{(1)}(p_k^\dagger p_k+r_k^\dagger r_k+m_k^\dagger m_k)\ , \tag{14}$$

where $J=\cos\gamma(1-3\tan\gamma)/\sqrt{2}$ and the spin-wave spectrum

$$\tilde{\varepsilon}_k^{(1)}=\sqrt{2}(1-\nu_k)^{1/2} \tag{15}$$

is linear in k at small momenta.

The new boson operators of quasiparticles are linked with the initial ones by the canonical transformation

$$\begin{aligned} a_k&=l_k(p_k+x_k r_{-k}^\dagger)\ ,\\ b_k&=l_k(r_k+x_k p_{-k}^\dagger)\ ,\\ c_k&=l_k(m_k+x_k m_{-k}^\dagger) \end{aligned} \tag{16}$$

where

$$l_k=[1+(1-\nu_k)^{1/2}](1-\nu_k)^{-1/4}/2\ ,$$

$$x_k=\frac{\nu_k}{|\nu_k|}\left[\frac{2-\nu_k-2\sqrt{1-\nu_k}}{2-\nu_k+2\sqrt{1-\nu_k}}\right]^{1/2}\ .$$

In principle, the square root in (5) generates an infinite number of anharmonic terms. Nevertheless, I believe that the qualitatively correct critical behavior can be obtained if one proposes that the density of quasiparticles is small and restricts with the lowest-order anharmonic terms. Namely, I will show that the competition between cubic and quartic anharmonisms produces a fixed point in the one-loop approximation.

The cubic anharmonisms H_3 come from the $\mathbf{L}_l\cdot\mathbf{M}_{l+1}$ interaction. When rewritten in terms of the operators of quasiparticles and in the limit of small momenta, H_3 reads ($1\equiv k_1$, etc., $k_i\equiv 2k_i a$)

$$\begin{aligned} H_3=iJ/4\sum_{k_i}&\frac{g}{(|k_1k_2k_3|)^{1/2}}\\ &\times[(r_3^\dagger m_2^\dagger p_1^\dagger+r_1^\dagger m_2 p_3^\dagger)(f_{31}-f_{12}-f_{23})\\ &+(r_1^\dagger m_2^\dagger r_3+p_3^\dagger m_2 p_1)\\ &\times(f_{12}-f_{23}-f_{31})]+\text{H.c.}\ , \end{aligned} \tag{17}$$

where

$$f_{ij}=|k_i|k_j-|k_j|k_i\ ,$$

and the bare value of the coupling constant g^0 is $g^0=(\frac{3}{8}2\sqrt{2})^{1/2}$ (the normalization was chosen to obtain a correct one-loop β function). One can see that the anharmonic terms of H_3 fit the Adler principle and thus do not shift the "spin-wave" critical line $\gamma_2(\delta)$. Note also that the bare coupling g^0 remains unchanged along the phase boundary.

As it is obvious for isotropic systems in one dimension, the coupling constant grows logarithmically in passing to larger scales. In a one-loop approximation, the renormalization of g is given by the diagrams of Fig. 3. The result is

$$(\dot{g}^2)=\frac{dg^2}{d\ln(1/k)}=g^4/2\pi\ . \tag{18}$$

If this was the only contribution to the one-loop β function, then fluctuations would generate a mass dynamically and, hence, destroy the phase boundary. However, the bosonic Hamiltonian contains fourfold anharmonisms which are also quadratic in gradients. I will propose (and

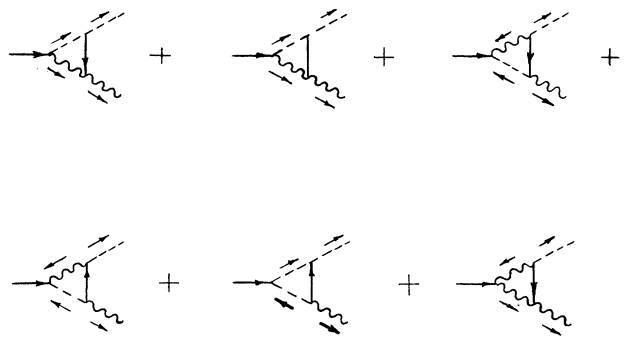

FIG. 3. The on-loop coupling constant g renormalization due to cubic anharmonisms. Solid, dashed, and wavy lines represent m, p, are r bosons, correspondingly.

then will confirm by calculations) that the most important parts of the fourfold vertices are those containing the scalar products of two momenta. Consider first the case of a purely bilinear interaction, $\gamma=0$ (i.e., $\delta=\frac{3}{8}$). One can make sure that, after a transformation to quasiparticles, the contributions of interest coming from different particle-particle interaction terms cancel each other. However, this turns out to be a property of a bare theory only. A way to see this is to consider one of the fourfold terms, say $m_1^\dagger m_2^\dagger r_3 p_4$, and to insert two different coupling constants, g_1 and g_2, for positive and negative contributions with the scalar products. Namely,

$$H_4 \Longrightarrow \frac{-1}{\sqrt{2}}\left[\frac{\sqrt{2}}{16N}\right]\sum_{k_i}\frac{1}{(|k_1k_2k_3k_4|)^{1/2}} \times[g_1(|k_1||k_2|-k_1k_2) +g_2(|k_3||k_4|+k_1k_2)] \times m_1^\dagger m_2^\dagger r_3 p_4 \ . \tag{19}$$

In a bare theory, $g_1^0=g_2^0=\frac{3}{8}$ and the scalar product disappears from (19). Meanwhile, in the one-loop renormalization, when only two fourfold terms are involved, g_1 does not change while g_2 diminishes according to $\dot{g}_2=-g_2^2\sqrt{8\pi}$ just as the current-current interaction term in the field-theoretical approach to the problem.[20] It is thus natural to assume that, at large scales, $g_2\Longrightarrow 0$ and to focus only on the first term in (19). To the lowest order in the coupling constant, the renormalization of this term comes from the interaction with cubic anharmonisms. The diagrams are presented in Fig. 4, and the result is

$$\dot{g}_1=\frac{3}{4\pi}g^2g_1 \ . \tag{20}$$

Comparing this expression with Eq. (18) for g, I conclude that $g_1=\lambda g^3$. The coefficient is fixed by the boundary condition $\lambda(g^0)^3=\frac{3}{8}$ and does not undergo any renormalization.

The next step is to find contribution fourfold terms make to the β function (18), but in order to convince one that they produce a fixed point, it is easier to calculate the corrections to the Green function of quasiparticles, $G=Z/(\Omega-|k|)$, which determines linear in T specific heat and, in contrast to the Green function or particles, has no amomalous dimension and, hence, no logarithmical contributions at the fixed point. The corresponding diagrams are presented in Fig. 5. The cubic terms give a negative contribution to self-energy while the fourfold terms are known from previous calculations for Heisenberg antiferromagnets[41] to give a positive contribution. The calculation of diagrams gives

$$\left[\frac{i}{Z}\right]=\frac{3}{8\pi}g^2\left[1-\frac{\lambda^2}{12\pi}g^4\right] \ . \tag{21}$$

As is seen from (21), the competition between cubic and quartic terms actually produces a fixed point

$$g_c^2=\frac{\sqrt{12\pi}}{\lambda} \ . \tag{22}$$

For nonzero γ, the number of fourfold terms increases and new coupling constants enter into the bare theory, but since there are absolutely no reasons to expect the point $\gamma=0$, $\delta=\frac{3}{8}$ to be an exceptional member of the boundary line, it is natural to assume the additional coupling constants to flow to zero at large distances. Meanwhile, the bare value of g_1, $g_1^0=\frac{3}{8}$, remains *unchanged* along all the critical line [only the total coefficient $1/\sqrt{2}$ in (19) is replaced by J], that is, the renormalization-group equations and, hence, the critical theory seem to be universal along all the phase boundary $\gamma=\gamma_2(\delta)$.

The last point is to consider the role of the $M=2$ excitations. I have checked that, in the random-phase approximation (i.e., when all the pair products of $M=2$ bosons are replaced by their expectation values), they do not influence the renormalization-group equations but simply renormalize the spin-wave velocity. This result is believed to also be true when higher-order corrections are included.

Note that the coefficient $\sqrt{8/3}$, which enters into the

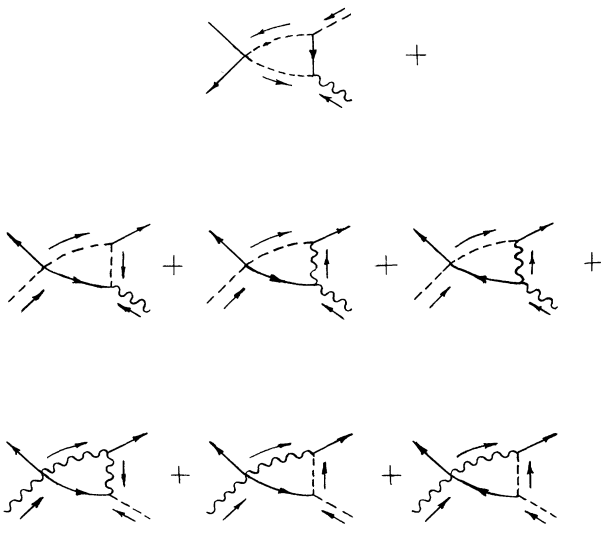

FIG. 4. Diagrams for the fourfold vertex renormalization in the leading order in the coupling constant. One-half of the diagrams is presented. The other one-half results from a replacement of the internal wave lines to the dashed ones and vice versa with a simultaneous replacement of the directions of all internal arrows.

FIG. 5. Diagrams for the renormalization of the Green function of quasiparticles. The contributions coming from qubic and quartic terms are opposite in sign. One-half of the diagrams is presented. The others are organized in the same way as in Fig. 4.

expression (5) linking the vector of antiferromagnetism with bosons and defines the bare values of g and g_1 (and, hence, g_c), is simply a properly normalized sum of the Clebsh-Gordan coefficients for total spin $M=1$ multiplied by the current Z projections of $S=1$. For arbitrary S, $\sqrt{8/3}$ is substituted by $R=2\sqrt{S(S+1)/3}$ (for $S=\frac{1}{2}$, $R=1$). Assuming, as in Ref. 20, that all the SU(2) integrable "antiferromagnetic" models belong to the boundaries of the spontaneously dimerized phases, where the $M=1$ excitations are soft, one has $(g^0)^2=2\sqrt{2}R^{-2}$, $g_1^0=R^{-2}$, that is, for large S, $g_c^2\propto 1/S$. Calculation of an exact proportionality coefficient as well as the critical exponents are out of the limits of the present approach since I have neglected all short-range corrections and restricted only with the vertices on resonance.

The general critical theory for the SU(2) integrable models with arbitrary S was developed in Refs. 20 and 27 and shown to be the same as for the $k=2S$ SU(2) Wess-Zumino-Witten (WZW) model. The critical coupling g_c was proved[26] to be exactly

$$g_c^2=4\pi/k=2\pi/S \ . \tag{23}$$

The present results qualitatively agree with the field-theoretical predictions: the σ model behavior is realized on cubic terms while fourfold anharmonisms mimic the role of the Wess-Zumino term. Note that, in the limit of large S, $g_c^2\propto 1/S$, as in (23). Also in agreement with Ref. 20, the shifting from the critical line freezes longitudinal fluctuations (i.e., produces a one-particle condensate of m bosons) and generates the phase factors in the vertices representing the interaction between initially soft r and p bosons that were shown[11] to produce the ϑ term in the long-wavelength action. The theory developed in Ref. 20 also predicts that the $k=2$ WZW model is a correct critical theory only for a translationally invariant $S=1$ Hamiltonian while, along a whole transition line, a critical theory is given by a σ model with $\vartheta=\pi$, which, in turn, was predicted[20] to be equivalent to the $k=1$ WZW model. In the frameworks of the present approach this would mean that only transverse fluctuations (described by r and p bosons) undergo softening on a transition line while the longitudinal fluctuations (described by m bosons) are frozen in the presence of the imposed staggered interaction.

The present analysis does not show any difference between the ending point and the rest of the transition line, $\gamma_2(\delta)$, which seems, to some extent, natural since the one-particle condensate of m-type bosons definitely does not exist within the dimerized phase.

I thus tentatively conclude that the critical theory on the whole boundary line $\gamma_2(\delta)$ is the same as it its ending point, i.e., is given by the $k=2$ WZW model.

Now I turn to the second phase boundary $\gamma=\gamma_1(\delta)$, where the dimer phase merges the 1D spin nematic state. A simple analysis shows that, in contrast to the previous case, anharmonic terms at $\gamma=\gamma_1(\delta)$ do not fit the Adler principle. So, first, the spin-wave critical line ceases to be an exact one and, secondly, the degeneracy of the spectrum removes when anharmonic corrections are taken into account. The finiteness of the spin nematic phase width in the "spin-wave" approximation makes it very unlikely that the whole region of this phase will disappear when anharmonic corrections are taken into account. I will thus presume that $M_z=\pm 2$ excitations (favoring ferromagnetic ordering) will retain a finite gap at the boundary of the dimerized state. As to the remaining three would be massless excitations, the absence of doubling in the spin nematic phase points that transverse fluctuations—the vibrations of the "on-site" order parameter—and longitudinal fluctuations involving the pairs of neighboring spins are completely decoupled. Thus, at the transition line $\tilde{\gamma}_1(\delta)$, which differs from $\gamma_1(\delta)$ due to finite anharmonic corrections, only longitudinal fluctuations (evidently created by an f boson which generates excitations with $M=2$ and $M_z=0$) will undergo softening while transvers ones will retain a dynamically generated mass. This seems rather natural since the remaining symmetry in the spin nematic phase is $SO(2)\times Z_2$ (the order-parameter space is isomorphic to P_Z). The interactions between two would be Goldstone modes in one dimension tend to restore the whole S_2 symmetry, they favor the Ising-like transition into the state where the "additional" Z_2 symmetry is frozen, which clearly means a dimerized state.

V. CONCLUSION

I will summarize briefly the main results of the work.

(i) The new transformation linking the spin operators of $S=1$ with bosons is presented. The state with no bosons corresponds to the dimer configuration. The analogous transformation can easily be written for arbitrary S.

(ii) The semiclassical phase boundaries of the dimerized phase in the generalized $S=1$ spin chain are obtained as functions of the strength of the staggered interaction. For the translationally invariant Hamiltonian, one of the boundaries is exactly an SU(2) integrable point.

(iii) The dimerized and ferromagnetic phases are separated by a disordered phase—a 1D version of the spin nematic state. The loss of a dimer long-range order occurs via an Ising-like transition.

(iv) Another critical line $\gamma_2(\delta)$ coming out of $\gamma=\tan^{-1}\frac{1}{3}$ and approaching the Bethe ansatz solvable point $\gamma=-\pi/4$, as δ moves to unity, is predicted to be in the same universality class of $k=2S=2$ Wess-Zumino-Witten model as its ending point $\gamma=-\pi/4$. The one-loop perturbation theory is developed which produces a fixed point due to competition between threefold and fourfold anharmonic terms. The latter were shown to mimic the role of the Wess-Zumino term in the field-theoretical treatment of the problem.

The result that the whole critical line $\gamma_2(\delta)$ is in the same universality class as its ending Bethe ansatz solvable point contradicts the prediction made in Ref. 20 (see also Ref. 42) and evidently means that, even in presence of the imposed staggered interactions, the transition to dimerization is governed by the softening of the longitudinal fluctuations of the SU(2) matrix. This, in turn, allows one to predict that, out of all Heisenberg antiferromagnets

with half-integer spins only, the $S=1/2$ system, which belongs to a family of SU(2) integrable models and has three massless bosons in a bare theory, becomes dimerized for an arbitrary small staggered interaction (in agreement with the exact result[43]), while for higher spins the imposed alternation does not produce long-range dimer order. This question needs further investigation.

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