Properties of one-dimensional antiferromagnets with integer and half-integer spins

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The properties of the ground state and low-lying excited states of one-dimensional antiferromagnets with large spin S are studied. For Heisenberg antiferromagnets, the hypothesis of Haldane concerning the difference between systems with integer and half-integer spins is confirmed. It is shown that in generalized magnets there are regions in which the behavior is different from that in Heisenberg models.

1. INTRODUCTION

In recent years interest in the study of the properties of the ground state and low-lying excited states of a one-dimensional antiferromagnet (AFM) with an arbitrary value of the site spin has increased again. One reason for this has been the hypothesis, put forward by Haldane in 1982, that there is a critical difference in the behavior of antiferromagnets with integer and half-integer spins.[1] According to his hypothesis, the low-energy properties of all isotropic Heisenberg AFM[1)] with half-integer spin are similar to the properties of the $S=\frac{1}{2}$ model solved exactly by Bethe[2]: There is no long-range order in the ground state, but the correlation length is infinite, i.e., the correlators decay by a power law. On the other hand, for integer spins, according to Haldane's prediction, the correlation length in the ground state is finite, i.e., at $T=0$ an AFM with integer spin is in a "spin liquid" state. A considerable number of papers, which have included not only theoretical investigations[3–9] but also numerical calculations[10–16] and a real experiment,[17] have been devoted to checking Haldanes prediction. Although the results of the numerical experiments enable us now to speak with confidence of the existence of a qualitative difference in the structure of the ground states of one-dimensional AFM with $S=1/2$ and $S=1$, a complete theoretical description of the effect does not yet exist.

In an earlier paper of one of the authors[7] it was shown that the standard spin-wave perturbation theory constructed on the classical (Néel) ground state of the AFM is logarithmic, and the quantum correction to the Green function, calculated for $S\gg 1$, is comparable in order of magnitude to the bare value of the Green function in the region of wave vectors $k_{\text{char}}\sim\Delta^{-1}Se^{-\pi S}$ (Δ is the interatomic spacing). Over large scales the spin-wave description becomes inapplicable and to establish the structure of the spectrum one must construct an effective long-wavelength Hamiltonian.

One of the aims of the present paper is to establish the dependence of the structure of the spectrum of a Heisenberg AFM on the parity of the doubled spin $2S$ and to determine the type of critical behavior for half-integer spins. Another aim is to find the boundaries of the universality class of the Heisenberg model and to elucidate the possibilities of the existence of other types of critical behavior.

The structure of the article is as follows. In Sec. 2 we construct the effective long-wavelength Hamiltonian of a Heisenberg AFM with a large but finite spin, and convince ourselves that it is equivalent to the Hamiltonian of a σ-model containing a topological θ-term (a θ-model) with coefficient $\theta=2\pi S$. The Haldane hypothesis is thereby confirmed, since, depending on the parity of $2S$, the model realized is either the ordinary σ-model ($2S$ is even), in which, as is well known from the exact solution,[18] dynamical generation of mass occurs, or the σ-model with $\theta=\pi$ ($2S$ is odd), in which one assumes the presence of a critical point, and, consequently, the power-law decay of the correlators[19,20] that is characteristic for integrable models. In Sec. 3 we study the consequences of adding to the Hamiltonian a term $\sim\gamma(S_l\cdot S_{l+1})^2$ that is quadratic in the scalar product of the spins, and show that within the phase characterized by the presence of short-wavelength antiferromagnetic order there is a narrow (for $S\gg 1$) region of values of $\gamma(\Delta\gamma\sim S^2e^{-2\pi S})$ in which the θ-model description is inapplicable. In Sec. 4 we consider the consequences of taking two-ion and single-ion anisotropy into account. In Sec. 5 we summarize the principal results of the paper and compare our approach with the approaches of other authors. Finally, in Sec. 6 we discuss the available experimental data.

2. HEISENBERG ANTIFERROMAGNET

We start from a Heisenberg AFM described by the Hamiltonian

$$H=J\sum_l \mathbf{S}_l\mathbf{S}_{l+1}. \tag{1}$$

The standard way of investigating this for $S\gg 1$ is to choose the axes of quantization of the spins in correspondence with the Néel ground state, in which the AFM is considered as a system of two interlocking ferromagnetic sublattices A and B, and to go over from the spin operators to bosons—one type for each of the sublattices. The latter is implemented most conveniently by means of a Dyson-Maleev transformation[22]:

$$\begin{aligned}
&S^z_{n,A}=S-a_n^+a_n,\qquad S^z_{n,B}=-S+b_n^+b_n,\\
&S^+_{n,A}=(2S)^{1/2}(1-a_n^+a_n/2S)\,a_n,\\
&S^+_{n,B}=(2S)^{1/2}b_n^+(1-b_n^+b_n/2S),\\
&S^-_{n,A}=(2S)^{1/2}a_n^+,\qquad S^-_{n,B}=(2S)^{1/2}b_n,
\end{aligned}\tag{2}$$

where the integer n labels successive sites in the sublattices A and B, and the distance between neighboring sites in each of the sublattices is equal to 2Δ. The sublattices introduced must be completely equivalent, and therefore, in particular,

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the Fourier components of the Bose operators a_n and b_n should transform in the same way upon change of the wave vector k by a reciprocal-lattice period $2\pi/2\Delta$. To satisfy this requirement, the coordinate origins in the two sublattices must be chosen to be the same, or, in other words, we must assign to neighboring spins in the chain the same site label in the doubled cell (the description in Ref. 3 was constructed in a similar manner).

After a number of standard procedures (transformation to the Fourier representation, diagonalization of the quadratic form, and normal ordering of the Bose operators), the Hamiltonian of the AFM acquires the form

$$H=2JSV\Big\{\sum_k \varepsilon_k(c_k^+c_k+d_k^+d_k)+H_4\Big\}, \qquad (3)$$

where $V=1+(\pi-2)/2\pi S$, $\varepsilon_k=|\sin k\Delta|$, and the term H_4 contains nine different fourth-order anharmonic terms:

$$H_4=\sum_{1,2,3,4}\{\Phi_1c_1^+c_2^+c_3c_4+\bar{\Phi}_1d_3^+d_4^+d_1d_2+2\Phi_2c_1^+c_2^+d_3^+c_4$$
$$+2\bar{\Phi}_2d_1d_2c_3d_4^+ +2\Phi_3c_1^+d_2c_3c_4+2\bar{\Phi}_3d_3^+d_4^+c_2^+d_1+4\Phi_4c_1^+d_2c_3d_4^+$$
$$+\Phi_5c_1^+c_2^+d_3^+d_4^+ +\bar{\Phi}_5c_3c_4d_1d_2\}. \qquad (4)$$

It is assumed that each process in (4) has its own momentum-conservation law. The amplitudes Φ_i and $\bar{\Phi}_i$ differ from the corresponding expressions in Ref. 23 by the phase factors that arise when the same site label is used for a pair of neighboring spins: With each operator d_k we associate a factor $e^{ik\Delta}$, and with each d_k^+ we associate a factor $e^{-ik\Delta}$. For non-Umklapp processes the amplitudes Φ_i and $\bar{\Phi}_i$ coincide. For small wave vectors of the quasiparticles the explicit forms of the amplitudes are

$$\Phi_1=\bar{\Phi}_1=\Phi,\quad \Phi_2=\bar{\Phi}_2=\Phi\exp(-ik_3\Delta),$$
$$\Phi_3=\bar{\Phi}_3=-\Phi\exp(ik_2\Delta), \qquad (5)$$
$$\Phi_4=-\Phi\exp(i(k_2-k_4)\Delta),\quad \Phi_5=\bar{\Phi}_5=\Phi\exp(-i(k_3+k_4)\Delta),$$

where

$$\Phi=\frac{1}{8SV}\cdot\frac{|k_1k_2|-k_1k_2}{|k_1k_2k_3k_4|^{1/2}}.$$

To construct the effective Hamiltonian we must renormalize the Hamiltonian (3) by integrating over momentum scales from $\pi/2\Delta$ to $\pi\Lambda/2\Delta$, where $\Lambda\ll 1$. We have calculated the renormalization of the four-point amplitude for zero total momentum of the scattered particles in the two-loop approximation. The corresponding diagrams are depicted in Fig. 1. The fact that the total momentum is equal to zero enabled us to avoid the need to ensure the cancellation of the "parasitic" corrections[2)] (containing the combination $|k_1k_2|+k_1k_2$) to the vertices. The renormalization leads to an identical change of the coefficients of all the four-point amplitudes, and this proves both renormalizability and the presence in the problem of only one coupling constant g. The bare value g_0 for the long-wavelength theory is formed by nonlogarithmic corrections built up over short distances. A contribution to g_0 is made both by intrinsic corrections to the vertex and by corrections to the Z-factor of the Green function and to the velocity of the spin waves. To terms of order $1/S^2$ the value of g_0 is

$$g_0=\frac{2}{SV}\left[1+\frac{1}{(\pi S)^2}\left(3-\frac{7\pi^2}{12}\right)\right]. \qquad (6)$$

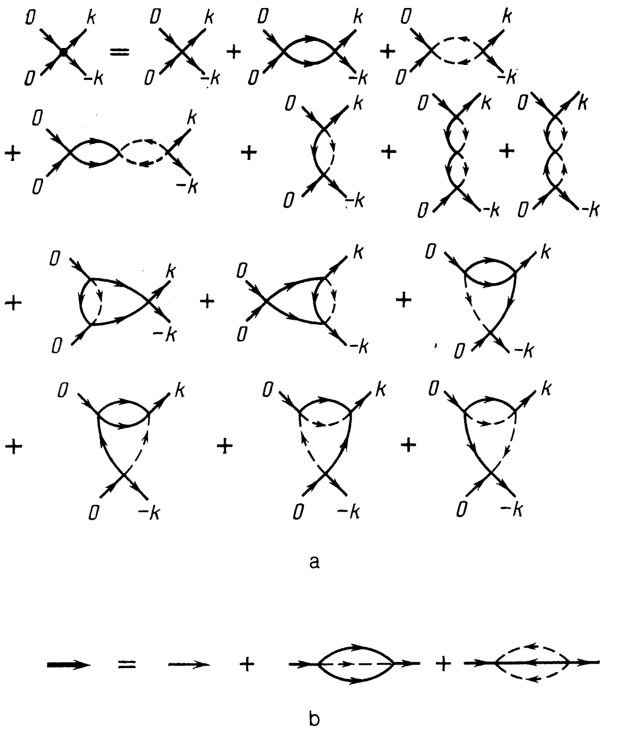

FIG. 1. The diagrams that must be taken into account in order to find the renormalization of the Hamiltonian (2) in the two-loop approximation. The solid and dashed lines denote the Green functions of the magnons of the two branches of the spectrum. a) The diagrams making a contribution to the renormalization of the four-point amplitude Φ_1 for zero total momentum of the quasiparticles. Half of the diagrams are written out; the other half are obtained by replacing all the internal solid lines by dashed lines (and vice versa) with a simultaneous change of direction of the arrows in each of the diagrams given. b) The diagrams determining the renormalization of the magnon Green function (the thick line is the exact Green function).

Inclusion of the logarithmic corrections in the two-loop approximation leads to an equation for the coupling constant that coincides with the equation for the invariant charge in the σ-model[24]:

$$\frac{dg}{dL}=\frac{g^2}{2\pi}+\frac{g^3}{4\pi^2},\qquad g=g(L),\quad g(0)=g_0,\qquad L=\ln\frac{1}{k\Delta}. \qquad (7)$$

The next step is to establish the equivalence of the effective long-wavelength Bose Hamiltonian to a Hamiltonian of the σ-model type (with the same cutoff parameter Λ):

$$H_\sigma=A\int dx\left[\left(\mathbf{l}-\frac{\lambda S}{2}\nabla\mathbf{n}\right)^2+\frac{1}{\beta^2}(\nabla\mathbf{n})^2\right], \qquad (8)$$

expressed in terms of a unit vector field $\mathbf{n}$ and the generator $\mathbf{l}$ of rotations, the commutator of which with an arbitrary vector $\mathbf{q}$ is equal to

$$\left[\frac{1}{\Lambda}l_i(x_1)q_j(x_2)\right]=i\varepsilon_{ijk}q_k(x_1)\delta(x_1-x_2). \qquad (9)$$

The normalization of the argument of the δ-function is chosen so that the quantity $\delta_{ij}/2\Delta$ goes over into $\delta(x_i-x_j)$ in the continuum limit.

We shall parametrize the continuous variables $\mathbf{n}(x)$ and $\mathbf{l}(x)$ in terms of the pair of Bose operators $a(x)$ and $b(x)$ as follows:

$$n_z=1-\frac{1}{2S}(a^+a+b^+b), \qquad 2\Delta l_z=b^+b-a^+a,$$

$$n^+=\frac{1}{(2S)^{1/2}}\left(a-b^+-\frac{a^+aa}{2S}+\frac{b^+b^+b}{2S}\right),$$

$$2\Delta l^-=(2S)^{1/2}(a^++b), \tag{10}$$

$$n^-=\frac{1}{(2S)^{1/2}}(a^+-b),$$

$$2\Delta l^+=(2S)^{1/2}\left(a+b^+-\frac{a^+aa}{2S}-\frac{b^+b^+b}{2S}\right).$$

The normalization of the commutators

$$[a(x_1)a^+(x_2)]=[b(x_1)b^+(x_2)]=2\Delta\Lambda\delta(x_1-x_2)$$

corresponds to the fact that $a(x)$ and $b(x)$ contain only Fourier components with $|k|<\pi\Lambda/2\Delta$. The commutation relations between l_i and l_j, and also between l_i and n_j, are fulfilled identically. In addition,

$$\mathbf{n}^2=1+O\left(\frac{\Lambda}{S}\right),$$

$$[n_i(x_1)n_j(x_2)]=i\varepsilon_{ijk}\left(\frac{l_k(x_1)}{\Lambda}\right)\left(\frac{\Lambda}{S}\right)^2\Delta^2\delta(x_1-x_2),$$

i.e., for $\Lambda\to 0$, $\mathbf{n}$ turns out to be a unit vector with commuting components. The parametrization thereby preserves the geometrical structure of the σ-model.

Using the representation (10), we have obtained from (8) a Bose Hamiltonian expressed in terms of the continuum fields a and b. After the transformation to the operators c and d that diagonalize the quadratic form this Hamiltonian acquires the same operator form as the original Hamiltonian (see the formulas (3) and (4)).

Choosing the coefficient A in (8) from the condition that the quadratic forms coincide, we obtain the following expressions for the coefficients φ_i and $\bar{\varphi}_i$-the analogs of Φ_i and $\bar{\Phi}_i$ in (5):

$$\varphi_1=\bar{\varphi}_1=\varphi, \quad \varphi_2=\bar{\varphi}_2=\varphi\exp(-i\lambda k_3\Delta),$$

$$\varphi_3=\bar{\varphi}_3=-\varphi\exp(i\lambda k_2\Delta), \quad \varphi_4=-\varphi\exp[i\lambda(k_2-k_4)\Delta],$$

$$\varphi_5=\bar{\varphi}_5=\varphi\exp[-i\lambda(k_3+k_4)\Delta], \tag{11}$$

$$\varphi=\frac{\beta}{16}\frac{|k_1k_2|-[(2\beta-\lambda)/(2\beta-\lambda^2)]k_1k_2}{|k_1k_2k_3k_4|^{1/2}}.$$

The values of the coefficients λ and β are determined by the equality $\Phi=\varphi$ and by the condition that the phase factors in (5) and (11) coincide. The first condition leads to a simple equation for λ: $\lambda(\lambda-1)=0$. The value of λ is fixed uniquely by comparing the phase factors: The presence of such a factor in (5) gives $\lambda=1$. The value of β is determined from the condition that the common coefficients of the four-point vertices be equal. As expected, β coincides with g_0.

We emphasize that, for finite spin, comparison of the Bose Hamiltonian with the continuum σ-model is justified only after the short-wavelength renormalization has been carried out and the cutoff parameter Λ has been established.

The Hamiltonian (8) is none other than the Hamiltonian of the σ-model with a topological θ-term, the coefficient of which is equal to $\theta=2\pi\lambda S=2\pi S$. Since the properties of the θ-model are substantially different for $\theta=2\pi n$ and $\theta=2\pi(n+1/2)$ (see the Introduction), Haldane's hypothesis concerning the dependence of the structure of the ground state on the parity of $2S$ is thereby confirmed. Moreover, it can be stated that the long-wavelength dynamics of Heisenberg antiferromagnets with different (at least large) spins is described by one and the same θ-model. If we assume that this description also remains valid for small S, including $S=1/2$, then, on the basis of the phase diagram of the θ-model with a single critical point,[19,20] it is possible to establish the nature of this critical point by starting from the exact solution for $S=1/2$. The value of the central charge c of the corresponding conformal theory turns out to be equal to unity in this case.

Arguments in favor of the equivalence of the behavior of all one-dimensional Heisenberg antiferromagnets with half-integer spins to the behavior of a chain with spin $S=1/2$ were put forward by Haldane. Certain arguments in favor of this assertion were also given in Ref. 6.

3. THE GENERALIZED MODEL

We turn to the generalized model, by adding to the Hamiltonian the term

$$J\gamma\sum_l(\mathbf{S}_l\mathbf{S}_{l+1}+S(S+1))^2.$$

As before, we shall assume that $S\gg 1$ and set $\tilde{\gamma}=\gamma S\sim 1$. After the standard transformations that led earlier to the formula (3), we arrive at a Bose Hamiltonian in which not only the common coefficients in the fourth-order anharmonic terms, but also the dependences of the corresponding amplitudes on the wave vectors, are changed: Besides the terms that were contained in the Heisenberg Hamiltonian, other terms, having a different dependence on the momenta in the short-wavelength region, also appear. In addition, of course, anharmonic terms of higher orders will also arise.

We illustrate the change of the structure of the four-point amplitudes using the example of the amplitude Φ_1: Its analog Φ_1' in the generalized model has the form

$$\Phi_1'=\Phi_{1,2}'^{3,4}=\Phi_1Q_1+\Psi_1Q_1',$$

where

$$\Phi_1=\left[-\frac{1}{4S}\prod_{i=1}^{4}\left(\frac{1+\varepsilon_i}{2\varepsilon_i}\right)^{1/2}\right]$$

$$\times(\nu_{1-3}x_1x_3+\nu_{2-3}x_2x_3+\nu_{1-4}x_1x_4+\nu_{2-4}x_2x_4$$

$$-\nu_3x_3-\nu_4x_4-\nu_{1+2-4}x_1x_2x_4-\nu_{1+2-3}x_1x_2x_3), \tag{12}$$

$$\Psi_1=\frac{1}{4S}\prod_{i=1}^{4}\left(\frac{1+\varepsilon_i}{2\varepsilon_i}\right)^{1/2}(1+\nu_{1+2-3-4}x_1x_2x_3x_4-\nu_1x_1-\nu_2x_2$$

$$+\nu_{1+2}x_1x_2+\nu_{3+4}x_3x_4-\nu_{3+4-1}x_1x_3x_4-\nu_{3+4-2}x_2x_3x_4),$$

with

$$x_i=\left(\frac{1-\varepsilon_i}{1+\varepsilon_i}\right)^{1/2}, \qquad \nu_i=\cos k_i\Delta,$$

$$Q_1=\left[1-4\tilde{\gamma}S+4\tilde{\gamma}\left(\frac{6}{\pi}-1\right)+O\left(\frac{1}{S}\right)\right]\Big/\left(1+\frac{8}{\pi}\tilde{\gamma}\right), \tag{13}$$

$$Q_1'=4\tilde{\gamma}S\left[1+\left(1-\frac{3}{\pi}\right)\frac{1}{S}+O\left(\frac{1}{S^2}\right)\right]\Big/\left(1+\frac{8}{\pi}\tilde{\gamma}\right).$$

In the region of small wave vectors the momentum dependence of Ψ_1, like that of Φ_1, is determined by formula (5), so that the bare (including the effect of the normal ordering but not of the renormalizations) coefficient of the four-point vertex,

$$g_0=\frac{2}{S}\frac{1+12\tilde{\gamma}/\pi}{1+8\tilde{\gamma}/\pi}, \tag{14}$$

turns out to be a function of $\tilde{\gamma}$. The coefficients of the other four-point vertices vary in an analogous manner.

In the given case, however, the four-point anharmonic terms do not have a term in $1/S$ and this leads to a substantial renormalization of the four-point vertex. We emphasize that we are referring to the nonlogarithmic renormalizations that give corrections to g_0 in zeroth order in $1/S$. The logarithmic corrections contain powers of $1/S$ and in the given approximation are not taken into account. In the long-wavelength limit the renormalization of g_0 is determined by the ladder sequence of diagrams represented graphically in Fig. 2a. The diagrams that are of zeroth order in $1/S$ but do not appear in the ladder sequence are depicted in Fig. 2b. The first two of these are direct corrections to the vertex on account of the four-point and six-point anharmonic terms, and the last diagram is a correction to the Z-factor of the Green function. In the first nonvanishing order in $\tilde{\gamma}$ these diagrams cancel each other. The diagrams of Fig. 2b have the same Internal structure; this permits us to hope that the cancellation will still occur when the bare vertices in the diagrams are replaced by exact vertices.

For zero total momentum of the magnons, summation of the ladder sequence depicted in Fig. 2a leads to the following result (for imaginary frequencies):

$$\Phi_{k,-k}^{p,-p}=\frac{1}{4S}\frac{k^2}{|kp|}\frac{1+12\tilde{\gamma}/\pi+O(\tilde{\gamma}(p\Delta)^2)}{1+12\tilde{\gamma}/\pi+\frac{1}{\pi}(\tilde{\gamma}\omega^2\ln(1/|\omega|))}, \tag{15}$$

where ω is the total frequency of the magnons being scattered ($|\omega|\ll 1$). It can be seen from (15) that if $\tilde{\gamma}$ lies outside the neighborhood of $\tilde{\gamma}_0=-\pi/12$, there is no real renormalization of the vertex in zeroth order in $1/S$. However, if $|\tilde{\gamma}-\tilde{\gamma}_0|\lesssim S^3e^{-2\pi S}$, then for the characteristic wave vectors $k_{\text{char}}\sim\Delta^{-1}Se^{-\pi S}$ the four-point vertex does not have the form dictated by the Hamiltonian (7). In this region the θ-model description is found to be inapplicable and there arises the possibility of the onset of new behavior.

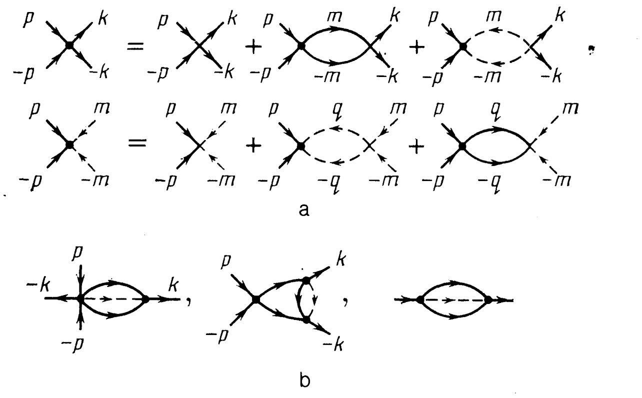

FIG. 2. The diagrams determining the renormalization of the four-point vertex in the generalized AFM in zeroth order in $1/S$. a) The ladder sequence of diagrams that leads, when summed, to formula (15). b) Diagrams that are of zeroth order in $1/S$ but do not appear in the ladder sequence. The first two diagrams are the direct corrections to the vertex on account of the fourth-order and sixth-order anharmonic terms, and the last diagram is a correction to the Z-factor of the Green function. According to the calculation, in the first nonvanishing order in $\tilde{\gamma}$ (to which corresponds the use of the bare values of the amplitudes) the total contribution from these diagrams is equal to zero.

It is natural to suppose that when terms of higher order in $(S_l\cdot S_{l+1}+S(S+1))$ are added to the Hamiltonian a loss of stability by way of the formation of bound pairs of magnons with $\omega^2<0$ will occur on entire surfaces in the space of the parameters of the Hamiltonian, and near these surfaces the four-point vertex loses the form dictated by the gradient expansion and the θ-model description becomes inapplicable. In addition, loss of stability on account of condensation of bound states of a large number of magnons is possible. These conjectures are based on an exact analysis of one-dimensional ferromagnets,[25,26] in which an analogous mechanism of loss of stability of the ferromagnetic state is realized, and near the stability boundaries the gradient structure of the vertices is also lost.[26]

At the same time, within the phase characterized by short-range antiferromagnetic order, regions in which the behavior of the antiferromagnet differs from the θ-model behavior are, in principle, possible. For the general model of spin S these could be phases characterized by the critical behavior inherent to integrable spin-σ ($1\leqslant\sigma\leqslant S$) models.[21] This conjecture is also based on an analysis of one-dimensional ferromagnets,[26] for which, in certain regions of the space of the parameters of spin-S Hamiltonians, the properties of the integrable spin-σ models ($1\leqslant\sigma\leqslant S$) are preserved. In particular, for the model with bilinear and biquadratic terms investigated in this section we may expect that in the neighborhood of a certain point $\tilde{\gamma}^*(S)$ a phase with critical behavior inherent to an integrable model with spin $S=1$ will be realized. It appears to us that everywhere outside a small (for $S\gg 1$) neighborhood of $\tilde{\gamma}^*$ the θ-model description will remain valid for so long as the antiferromagnetic state is stable over short length scales (the possible loss of stability of the antiferromagnetic state is related to the vanishing of the spin-wave velocity).

The conclusion that the θ-model behavior is valid everywhere outside a neighborhood of $\tilde{\gamma}^*$ is confirmed by the results of recent numerical experiments for $S=1$ (Ref. 15): The gap in the spectrum vanishes only in the neighborhood of the integrable model. However, the numerical results obtained have been questioned, and therefore require further verification.

4. THE ROLE OF ANISOTROPY

As a rule, in real antiferromagnets both two-ion and single-ion anisotropy are present. The corresponding terms in the spin Hamiltonian have the following form:

$$H_a=J\alpha\sum_l S_l^zS_{l+1}^z+D\sum_l(S_l^z)^2. \tag{16}$$

For definiteness we confine ourselves to the case $D=0$. Allowance for the anisotropy leads to two effects. The first is connected with the fact that the AFM is converted from an isotropic AFM to either an easy-plane or an easy-axis AFM, and therefore the logarithmic growth of the fluctuation corrections to the vertex ceases at a scale $k_{\text{an}}\sim\Delta^{-1}(D/J+|\alpha|)$

determined by the anisotropy. When the value of k_{an} turns out to be greater than $k_{char} \sim \Delta^{-1} S e^{-\pi S}$, the fluctuation effects inherent to isotropic antiferromagnets are not manifested, and the difference between integer and half-integer spins thereby disappears: In both case the ground state will be characterized either by long-range antiferromagnetic order of the Ising type or by a power-law decay of the correlators. We emphasize that this occurs irrespective of which of the types of anisotropy is causing the deviation from the isotropic situation.

The second effect is associated exclusively with the single-ion anisotropy: When the value of D is comparable to $JS(S+1)$ (this value is given by mean-field theory), for the case of integer site spin the orientational order is washed out at $T=0$ by quantum fluctuations. This effect has already been described repeatedly in the literature.[27] The breakdown of the orientational order occurs because, when the single-ion anisotropy is taken into account, the most favorable state for integer S is the ground state with zero z-component of each of the spins. This state is separated by a finite energy gap $\sim D$ from the first excited state, in which one of the spins has $S_l^z = \pm 1$. We emphasize that, despite the outward similarity to the situation in an isotropic AFM, the nature of the establishment of the spin-liquid state in the present case is entirely different and is connected exclusively with the influence of the anisotropy on the behavior of the isolated spin. Therefore, we cannot agree with the statements in the literature[6,8] that an AFM with integer spin is in a spin-liquid state for any value of D. For large integer S, at least, this is certainly not so: Orientational order is established for $D = D_1 \sim JSe^{-\pi S}$, and disappears for $D = D_2 \sim JS^2 \gg D_1$. The phase diagram of the anisotropic magnet with integer $S \gg 1$ described by the Hamiltonian (1), (16) is presented in Fig. 3a. For the reasons indicated above, it differs substantially from that given in Ref. 6. To the left of the line 1 and to the right of the line 2 there is long-range magnetic order (ferromagnetic in the first case, and antiferromagnetic in the second case) in the ground state. A phase characterized by orientational order lies in the center of the phase diagram. The regions in which the ground state is a singlet ("spin liquid") lie above the curve 3 and between the curves 2 and 4. In the first case the disorder arises as a consequence of the quantum nature of the individual spins, while in the second case it arises on account of fluctuations associated with the presence of two interacting Goldstone modes in the bare spectrum. At the intersection with curve 2 a transition of the Onsager type occurs, while at the intersections with curves 3 and 4 transitions of the Berezinskiĭ-Kosterlitz-Thouless type occur. In all cases, on the lines of the transitions the exponent η characterizing the law of decay of the correlations is equal to 1/4. The phase diagram for the anisotropic magnet with half-integer S differs from that given in Fig. 3a by the absence of the lines 3 and 4.

For small spins the phase diagram can be modified somewhat, since the lines 3 and 4 can intersect before either of them intersects with curve 2. The expected form of the phase diagram in this case is given in Fig. 3b. The dashed curve denotes the line of a transition between two different singlet phases. On this line the properties of the intermediate phase with XY symmetry at the critical point ($\eta = 1/4$) are preserved. Evidently, the phase diagram of an anisotropic magnet with $S=1$ has precisely this form. The basis for this

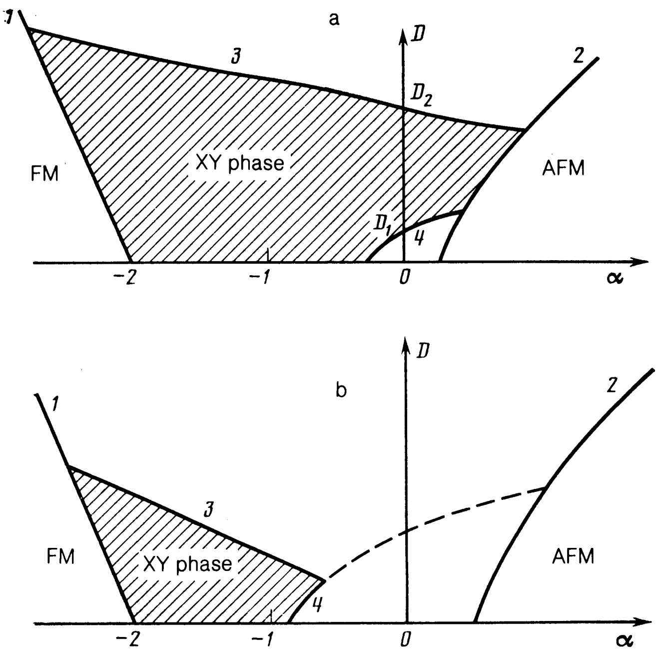

FIG. 3. The phase diagram of the ground state of an XXZ magnet with integer site spin, in the variables D and α (D is the single-ion anisotropy constant, and α is the two-ion anisotropy constant). To the left of the line 1 there is long-range ferromagnetic order, and to the right of the line 2 there is long-range antiferromagnetic order. The region of existence of orientational order is shaded. Above the curve 3 and between the curves 2 and 4 the ground state is a singlet state. The diagram for half-integer spins differs in the absence of the lines 3 and 4. a) The diagram for the case $S \gg 1$. b) The diagram for the case $S \sim 1$. The dashed line separates two different singlet phases.

is the fact that the values calculated from the quasiclassical formulas for the index η (Refs. 28, 29)] of D_2 for $\alpha = -1$ (the XY model) and of α_{cr} for $D=0$ are found to be

$$D_2 \approx 0.4J, \quad \alpha_{cr} \approx -0.85.$$

The smallness of $D_2/2J$ (for $\alpha = -1$) and $\alpha_{cr} + 1$ implies that the lines 3 and 4 should intersect in the immediate vicinity of the point $\alpha = -1$, $D_2 = 0$.

The phase diagram presented in Fig. 3b agrees well with the result of the numerical calculations of Refs. 10–16; not only is the general form of the diagram the same, but so too are the values of D_2 and α_{cr}, which in the numerical experiment are found to be equal to $0.4J$ and -0.9, respectively. The application of the quasiclassical formulas in the case $S=1$ is partly justified by the fact that for the XY model, the neighborhood of which is of interest to us in the present case, a calculation in the quasiclassical framework leads to an expression for η which, owing to the numerical smallness of the coefficients of the $1/S$-expansion, practically coincides with the first term of this expansion and agrees well (a point of particular importance) with the exact result for $S = 1/2$ (Refs. 28, 29).

5. CONCLUSIONS

We shall formulate the principal conclusions stemming from the analysis performed above. In the framework of the two-loop approximation we have established the equivalence of the Heisenberg antiferromagnet and the σ-model with a topological θ-term with coefficient $\theta = 2\pi S$. This equivalence makes it possible to confirm Haldane's hypothesis of a critical difference in the properties of one-dimensional antiferromagnets with integer and half-integer spins: For integer S there is a finite gap in the excitation spectrum, while for all (at least large) half-integer S at $T = \theta$ the same critical behavior obtains. If we conjecture that this is true also for $S = 1/2$, we can establish the type of critical behavior in the σ-model with $\theta = \pi$: It turns out to be the same as in the Gaussian theory with $c = 1$.

For a general model of spin S near the boundary of stability of the antiferromagnetic state the applicability of the θ-model description breaks down, since for the characteristic wave vectors the four-point vertex loses the form dictated by the gradient expansion. In the remainder of the region of values of the parameters for which short-range antiferromagnetic order exists the equivalence to the θ-model will be valid everywhere except for narrow (for $S \gg 1$) regions in which the type of critical behavior is supposedly the same as in the integrable spin-σ models ($1 \leqslant \sigma \leqslant S$).

We note that the first attempt to construct an effective Hamiltonian describing a one-dimensional antiferromagnet was undertaken by Affleck. In the limit $S \to \infty$ he obtained a θ-model Hamiltonian coinciding with (8). However, for finite S the value of the coefficient of the topological term was found to be equal to $\theta = 2\pi(S(S+1))^{1/2}$, which was a consequence of the fact that the change to the continuum model was made directly from the lattice Hamiltonian. In addition, in Affleck's approach the addition to the original lattice Hamiltonian of terms of higher orders in the scalar product of the spins had no effect on the structure of the effective long-wavelength Hamiltonian. In our opinion, a consistent derivation of the effective Hamiltonian should include the short-wavelength renormalization, which has been accomplished in the present paper. In later papers by Affleck,[4] it is stated that for any AFM with finite half-integer spin there is another universal critical behavior, which differs from the θ-model behavior, is describable by the Wess-Zumino model with $c = 3S/(S+1)$ and with central charge $k = 2S$ in the current algebra, and is inherent in exactly integrable models,[30] while the θ-model description is realized in the limit $S \to \infty$. The combination of statements made in Refs. 3 and 4 is in contradiction with a theorem of Zamolodchikov,[31] from which it follows that the value of the conformal anomaly in the theory describing the critical point in the σ-model with $\theta = \pi$ cannot exceed $c = 2$ (the number of free bosons describing the ultraviolet behavior of the θ-model).

6. COMPARISON WITH EXPERIMENT

From the preceding account it is clear that in order to check Haldane's predictions we need antiferromagents that best satisfy the requirements of one-dimensionality and isotropy. Of the presently known magnets with integer spin the compounds $CsNiCl_3$ and $RbNiCl_3$ ($S = 1$) meet to these conditions best. These compounds have been discussed in a previous paper by one of the authors. Below we shall discuss one-dimensional antiferromagnets with half-integer spins. With a good degree of accuracy, $CsVCl_3$ ($S = 3/2$) and TMMC ($S = 5/2$) belong to this group. In both compounds the ratio of the exchange integrals within a chain and between chains amounts to $\sim 10^{-4}$. The anisotropy in TMMC does not exceed 2% of the exchange, and for $CsVCl_3$ the corresponding data are not available. We have already said in the preceding section that according to the predictions of Affleck the type of critical behavior of an AFM with half-integer spin is different for each specific S. On the contrary, the results of the present paper are evidence that for practically all antiferromagnets with half-integer S (at least for $S \gg 1$) the critical behavior is the same, and, by hypothesis, coincides with the critical behavior of an AFM with $S = 1/2$.

To discuss the possibility of an experimental verification of one or other of the theoretical predictions it is necessary to indicate the temperature T_{qu} at which quantum effects are manifested. This temperature should necessarily exceed the temperature of the three-dimensional phase transition; otherwise, the quantum effects inherent to the one-dimensional magnets will not be observed. The value of T_{qu} corresponds to the energy of a quasiparticle with the characteristic wave vector k_{char}, and is given by relation

$$T_{qu} = BV_S \frac{2\pi}{g_0} \exp\left(-\frac{2\pi}{g_0}\right), \tag{17}$$

where g_0 is given by formula (6) and V_S is the velocity of the spin waves:

$$V_S = 2JS\left[1 + \frac{\pi - 2}{2\pi S} + \frac{\pi^2 - 10}{4\pi^2 S^2} + O\left(\frac{1}{S^3}\right)\right]. \tag{18}$$

The value of the proportionality coefficient B can be determined as follows : for integer S, T_{qu} is none other than the gap, formed by the quantum fluctuations, in the energy spectrum. According to the data of the numerical experiments, for $S = 1$ we have $\varepsilon_0 = 0.4J$ (Refs. 10–14), whence $B = 5.68$. A calculation with this value of B leads to the following results: For TMMC, $V_S = 70.7$ K, so that $T_{qu} \simeq 0.5$ K, which is smaller than the temperature $T_{3D} = 0.85$ K of the three-dimensional phase transition; for $CsVCl_3$, $V_S = 978$ K, so that $T_{qu} \simeq 77$ K, whereas $T_{3D} \simeq 13$ K. Therefore, the possibility of observing quantum effects is available only in $CsVCl_3$. Nevertheless, Affleck compared the results of his theory, generalized to the anisotropic case, with experimental data for TMMC and found good agreement between theory and experiment.[32] In our opinion, this agreement is due to the fact that for large S the results of Affleck practically coincide with the quasiclassical results. Indeed, for example, Affleck predicts for the index η the value 1/5 for $S = 5/2$. Experiments on inelastic neutron scattering give the similar value $\eta = 0.16$ (Ref. 33). However, this same value can be obtained by making use for $\alpha \ll 1$ of the quasiclassical formula[29]

$$\eta = \frac{1}{\pi S}\left(1 - \frac{1}{2S} + \frac{1}{2\pi S} \ln \frac{8}{|\alpha|}\right)$$

and taking into account that the anisotropy amounts to 2% of the exchange. For $S = 5/2$, η turns out to be equal to 0.15, which is in excellent agreement with experiment. In an analogous way, the behavior of the magnetic susceptibility can also be explained in the quasiclassical framework.

To avoid misunderstandings, we note that both the theory of Affleck and the theory presented in the present paper aim to describe the behavior of antiferromagnets over large scales, when the quasiclassical approximation is inapplicable.

Less certain is the situation in $CsVCl_3$ where the estimates predict the existence of a relatively broad "quantum region" of temperatures (from T_{qu} to T_{3D}). From the available experimental data of measurements of the susceptibility in a broad range of temperature (from 700 K to T_{3D}) we can determine $\chi(T=0)$ approximately by extrapolating the results obtained in the quantum region. This extrapolation gives $\chi(0)=3.3\cdot 10^{-4}\,K^{-1}$ For the susceptibility $\chi(0)$ the theory predicts the value $\chi(0)=k/2\pi V_S$, where $k=2S=3$ if the results of Affleck are correct, and $k=1$ if the behavior of all Heisenberg magnets with half-integer spin is the same. Comparison with the experimental data gives $k\simeq 2$ (Ref. 34), which does not make it possible to give preference to either of the theories discussed. The situation could be clarified by experiments to measure the specific heat. If we assume that the anisotropy in $CsVCl_3$ has the same order of smallness as the exchange between the chains, then in the temperature range from T_{3D} to T_{qu} the specific heat should follow a linear law[36]: $C=\pi Tc/3V_S$, with $c=3S/(S+1)=9/5$ in Affleck's theory, and $c=1$ if the critical behavior does not depend on the spin.

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[1)]By a Heisenberg AFM we understand an antiferromagnet describable by a Hamiltonian that is bilinear in the spin operators.

[2)]The cancellation of these corrections has been verified in the one-loop approximation.

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