

Fluctuation corrections to the spectra of one- and two-dimensional Heisenberg magnets

Yu. A. Kosevich and A. V. Chubukov

Institute of Physical Problems, Academy of Sciences of the USSR, Moscow

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The logarithmically diverging temperature corrections to the spin-wave spectra of isotropic 2D Heisenberg ferromagnets and antiferromagnets and the quantum correction to the Green's function of the isotropic 1D antiferromagnet are computed by means of a microscopic approach. In each case the series of principal logarithmically diverging diagrams is summed, and the region of applicability of the spin-wave description is found. It is shown that, on the scales where perturbation theory is valid, the 1D antiferromagnet is equivalent to the $O(3)$ σ model. The effect of the anisotropy, a magnetic field, and the exchange between the spin chains (or layers) on the critical properties of Heisenberg magnets is discussed. It is also shown that the temperature renormalization of the spectrum of a 3D antiferromagnet is $\sim T^4 |\ln T|$.

§1. INTRODUCTION

Recently both experimenters and theorists have become very interested in the study of magnetic systems that, because of the strong exchange-interaction anisotropy, can with a high degree of accuracy be classified with the quasi-one-dimensional (1D) and quasi-two-dimensional (2D) magnetic substances. This interest is due mainly to the fact that the role of the fluctuations is often much more important in the low-dimensional magnetic materials than in the corresponding three-dimensional (3D) systems. Especially noticeable is the enhancement of the fluctuation effects when we go over to the low-dimensional analogs of three-dimensional spin systems with n -component vector order parameters. The simplest examples here are the easy plane ($n = 2$) and isotropic ($n = 3$) ferromagnets and antiferromagnets.

Let us recall some well known results pertaining to the behavior of systems with vector order parameters in low-dimensional spaces.

1. At any finite temperature the long-range order in 2D and 1D spaces is destroyed by thermal (classical) fluctuations (the Mermin-Wagner theorem¹).

2. In 1D space the long-range magnetic order is destroyed even at $T = 0$ as a result of the quantum fluctuations, the zero point spin oscillations (if, of course, they occur).^{2,3}

3. The 2D magnetic materials with $n = 2$ and those with $n = 3$ possess essentially different low-temperature properties in spite of the fact that long-range order cannot exist in 2D space for any $T \neq 0$. For $n = 2$ there exists a critical temperature T_c (the Berezinskii-Kosterlitz-Thouless transition temperature)^{4,5} below which the spin system behaves as if it has been frozen at the phase transition point, i.e., the correlation length at all temperatures below T_c is equal to infinity, while the correlation functions of the order-parameter components decrease at large distances according to a power law: $G(R) \sim R^{-\eta}$. The situation is different in the $n = 3$ case: no phase transition occurs right down to $T = 0$, so that the system is in the paramagnetic phase at any finite temperature, and the correlation functions decrease exponen-

tially (like $e^{-R/\xi}$) with distance. The assertion that no phase transition occurs at $T \neq 0$ in isotropic 2D ferromagnets and antiferromagnets (systems with $n = 3$) follows from the results of the exact solution of the problem of the spectrum of the one-dimensional nonlinear $O(3)$ σ model of relativistic field theory.^{6,7} This model is equivalent to the isotropic-2D-magnet models (see, for example, Ref. 8).

4. No phase transition occurs in 1D space right down to $T = 0$ for any value of n . Differences in behavior of magnets with two- and three-component order parameters could be expected here at $T = 0$, since allowance for the quantum fluctuations in 1D space leads to the same logarithmically diverging corrections to the order parameter as allowance for the classical fluctuations in 2D space. But in the quantum case the question of the existence of such differences is for the present open. On the one hand, in the classical treatment the Lagrangian of the simplest 1D system with $n = 3$ —the 1D antiferromagnet—coincides with the Lagrangian for the 1D $O(3)$ σ model. On the other hand, it is known from the exact solution⁹ that the structure of the correlation functions at large scales in a 1D antiferromagnet with spin $S = 1/2$ is the same as the structure of the corresponding functions in magnets with a two-component order parameter¹⁰: these functions decrease in a power-law fashion, i.e., the correlation length is infinite at $T = 0$. It has been rigorously proved^{9,11} that this is valid for all antiferromagnets with half-integral spin.¹¹

It was for a long time believed that the divergence of the correlation length at $T = 0$ was a general property of all exchange magnetic materials. Recently, however, Haldane, on the basis of the analogy between the classical Lagrangians of an antiferromagnet and the σ model, put forward the hypothesis that there is a qualitative difference between the structures of the ground states of 1D antiferromagnets with integral and half-integral spins.¹³ According to his hypothesis, for all half-integral values of S the correlators decrease in a power-law fashion (more exactly, like $1/R$), while for integral values of S a 1D antiferromagnet exhibits all the properties of the $O(3)$ σ model, i.e., because of the strong quantum

fluctuations, the correlation length is finite, and the antiferromagnet remains in the paramagnetic phase even at $T = 0$. In spite of the fact that Haldane's predictions called in question the results of a number of other authors,^{14,15} they stimulated a rapid growth of the number of papers on the numerical modeling of the ground-state structure of 1D antiferromagnets.^{11,16-18} The data obtained in the numerical experiments support the hypothesis that systems with $S = 1/2$ and 1 have different ground-state structures.

In the present paper we study the fluctuation effects in low-dimensional magnetic materials within the framework of standard low-temperature perturbation theory. Specifically, we compute the dominant fluctuation corrections to the Green's functions of low-dimensional isotropic ferromagnets and antiferromagnets both at finite temperatures and at $T = 0$. This formulation of the problem presupposes two aims: first, the determination of the dominant temperature corrections to the spin-wave spectra and, second, the verification through direct computations of Haldane's conjecture that an isotropic 1D antiferromagnet can remain in the paramagnetic phase even at $T = 0$. The Green's function is a convenient characteristic for such a verification, since in systems without long-range order (which are studied below) the structure of the fluctuation corrections to it depends on the laws of decrease of the correlations. In the case of the power law of decrease the spin waves exist on all scales of distances, and therefore the fluctuation corrections to the Green's function are finite. On the other hand, if the correlation length is finite (the correlations fall off exponentially), then the fluctuation corrections increase with increasing wavelength, and, ultimately, at distances greater than the correlation length the perturbation theory becomes inapplicable.

The paper is organized as follows. In §2 we compute the dominant temperature corrections to the spin-wave spectrum of a 2D ferromagnet with arbitrary spin in different temperature ranges. In §3 we compute the temperature corrections to the spectra of isotropic 2D and 3D antiferromagnets with large spin. We also compute in this section the quantum corrections to the Green's function of the 1D antiferromagnet. Section 4 is devoted to a discussion of the results obtained. There we also consider how a magnetic field, anisotropy, and the exchange between the spin chains affect the ground-state structure of quasi-one-dimensional antiferromagnets with integral spin. Some of the results obtained have been published in a short communication.¹⁹

§2. THE TWO-DIMENSIONAL FERROMAGNET

The Hamiltonian of an isotropic ferromagnet can be written as:

$$\mathcal{H} = -\frac{J}{2} \sum_{i,\Delta} S_i S_{i+\Delta}. \quad (1)$$

Here J is the exchange integral between the nearest atoms located in the XY plane at a distance Δ from each other. The magnitude of the spin S is assumed to be arbitrary. Using the Dyson-Maleev transformation,²⁰ we rewrite the Hamiltonian (1) in terms of the Bose operators. Then going over to the Fourier transforms of the operators a^+ and a , we obtain

$$\mathcal{H} = -\frac{J(0)NS^2}{2} + J(0)S \left[\sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} a_{\mathbf{k}}^+ a_{\mathbf{k}} + \frac{1}{N} \sum_{1,2,3,4} \Psi_{12^{34}} a_1^+ a_2^+ a_3 a_4 \delta(1+2-3-4) \right]. \quad (2)$$

The subscripts 1, 2, 3, ... correspond to $\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \dots$

The interaction between the magnons is described by the amplitude

$$\Psi_{12^{34}} = -\frac{1}{4S} [v_{1-3} + v_{2-3} - v_1 - v_2]. \quad (3)$$

Above we used the following notation:

$$\varepsilon_{\mathbf{k}} = 1 - v_{\mathbf{k}}, \quad v_{\mathbf{k}} = J(\mathbf{k})/J(0), \quad J(\mathbf{k}) = J \sum_{\Delta} e^{i\mathbf{k}\Delta}. \quad (4)$$

The dominant temperature renormalization of the spin-wave spectrum

$$\Delta \varepsilon_{\mathbf{k}} = \Delta \varepsilon_{\mathbf{k}}^{(1)} + \Delta \varepsilon_{\mathbf{k}}^{(2)},$$

is given by the following diagrams:

$$\Delta \varepsilon_{\mathbf{k}}^{(1)} = \text{diagram 1}, \quad \Delta \varepsilon_{\mathbf{k}}^{(2)} = \text{diagram 2}. \quad (5)$$

The hatched vertices are the total scattering amplitudes taken at resonance at $T = 0$. Their deviation from the bare vertices lies in their exchange renormalization, which occurs as a result of the finiteness of the magnitude of the spin S . For an arbitrary value of S this renormalization is by no means weak. Let us, in order to avoid any misunderstanding, emphasize that all the purely quantum corrections are included in the renormalization of the vertices. Therefore, in the formula (5) the quantity $\Delta \varepsilon_{\mathbf{k}}^{(2)}$ is determined by that part of the diagram which contains the product of two Bose functions [see Eq. (7) below]. In analytic form, Eq. (5) can be written as:

$$\Delta \varepsilon_{\mathbf{k}}^{(1)} = \frac{4}{N} \sum_{\mathbf{p}} n_{\mathbf{p}} \Gamma_{\mathbf{p}\mathbf{k}}^{\mathbf{p}\mathbf{k}}, \quad (6)$$

$$\Delta \varepsilon_{\mathbf{k}}^{(2)} = -\frac{8}{N^2} \sum_{\mathbf{q}, \mathbf{l}, \mathbf{p}} \frac{n_{\mathbf{p}}(n_{\mathbf{q}} + n_{\mathbf{l}}) - n_{\mathbf{q}} n_{\mathbf{l}}}{\varepsilon_{\mathbf{q}} + \varepsilon_{\mathbf{l}} - \varepsilon_{\mathbf{p}} - \varepsilon_{\mathbf{k}}} \Gamma_{\mathbf{p}\mathbf{k}}^{\mathbf{q}\mathbf{l}} \Gamma_{\mathbf{q}\mathbf{l}}^{\mathbf{p}\mathbf{k}}. \quad (7)$$

Here the Γ_{\dots} are the total vertices. Their determination requires summation over all the virtual two-particle processes, which at $T = 0$ amounts to summation of the series of ladder diagrams. The corresponding Dyson equations can be written down and solved in the usual manner. The answers in the present case are as follows. The total zero-angle scattering amplitude $\Gamma_{\mathbf{k}\mathbf{p}}^{\mathbf{k}\mathbf{p}}$ has the form

$$\Gamma_{\mathbf{k}\mathbf{p}}^{\mathbf{k}\mathbf{p}} = -\mathbf{k}\mathbf{p}/8S + \lambda k_i^2 p_i^2, \quad (8)$$

where, to within logarithmic terms,

$$\lambda = -(32\pi S^2)^{-1} |\ln \{\max k, p\}|. \quad (9)$$

It is sufficient to know the amplitudes $\Gamma_{\mathbf{k}\mathbf{p}}^{\mathbf{q}\mathbf{l}}$ and $\Gamma_{\mathbf{q}\mathbf{l}}^{\mathbf{k}\mathbf{p}}$ only in the leading, bilinear—in the wave vectors—order. In this approximation there is no difference between the bare and total amplitudes:

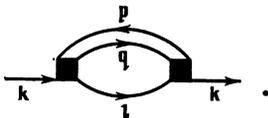
$$\Gamma_{kp}^{q1} = -q1/8S, \quad \Gamma_{q1}^{kp} = -kp/8S. \quad (10)$$

Knowledge of the expressions for the total vertices enables us to compute with the aid of the formulas (6) and (7) the temperature corrections to the spin-wave spectrum. To within logarithmic terms, we have

$$\Delta \varepsilon_k^{(1)} = -(\varepsilon_k/12S^2) (T/J(0)S)^2 |\ln\{\max(T/J(0)S, k^2)\}|, \quad (11)$$

$$\Delta \varepsilon_k^{(2)} = -\frac{2\varepsilon_k}{\pi^2 S^2} \left(\frac{T}{J(0)S}\right)^2 \times \begin{cases} |\ln(k^2 J(0)S/T)|, & k^2 \ll T/J(0)S, \\ 0(1), & k^2 \gg T/J(0)S. \end{cases} \quad (12)$$

It can be seen from these expressions that, for small wave vectors, the dominant temperature renormalization of the spin-wave spectrum is always proportional to $T^2 |\ln k|$, but that the coefficient of proportionality depends on the relation between k^2 and $T/J(0)S$: for $k^2 \gg T/J(0)S$ the dominant renormalization of the spectrum comes from $\Delta \varepsilon_k^{(1)}$, i.e., is determined by the quantum effects (the deviation of the total amplitude Γ_{kp}^{q1} from the bare amplitude at $T=0$), while for $k^2 \ll T/J(0)S$ the renormalization of the energy is largely due to $\Delta \varepsilon_k^{(2)}$, i.e., is determined by the classical (temperature) fluctuations. In the latter case the correction to the spin-wave energy for exponentially small wave vectors is comparable in magnitude to the bare-energy value, thus making the temperature perturbation theory inapplicable. The determination of the characteristic scale at which this occurs requires the summation of the series of dominant logarithmically diverging diagrams. By separating out, as usual, in each diagram the cross section in which the integration momentum is smallest, we can represent the sum of such diagrams in the form



The black squares are the total vertices with allowance for the temperature renormalization [below they are denoted by $\Gamma_{\dots}(T)$]. The problem of finding these vertices amounts to that of summing the "parquet" diagrams (see Ref. 21),²⁾ e.g.,

$$(13)$$

In each diagram we have separated out that two-particle cross section in which the integration momentum is smallest. The total vertex in the "parquet" approximation has been computed by many authors.²³ We shall need $\Gamma_{kp}^{q1}(T)$ and $\Gamma_{q1}^{kp}(T)$ in the case when the three momenta q , l , and p are of the same order of magnitude. Taking account of the fact that, to within logarithmic corrections, the dependence

of the amplitude on the external momenta is determined by the limits of the integration over the internal momenta, and going over to logarithmic variables, we obtain ($L = |\ln q|$)

$$\Gamma_{q1}^{kp}(T) = -\frac{kp}{8S} g(T, L), \quad \Gamma_{kp}^{q1}(T) = -\frac{lq}{8S} g(T, L), \quad (14)$$

where

$$g(T, L) = 1 + \frac{2T}{\pi J(0)S^2} \int_0^L du g^2(T, u), \quad g(T, 0) = 1. \quad (14a)$$

The solution of Eq. (14a) is elementary:

$$g(T, L) = \{1 - [2T/\pi J(0)S^2]L\}^{-1}. \quad (15)$$

Knowledge of $\Gamma_{kp}^{q1}(T)$ and $\Gamma_{q1}^{kp}(T)$ allows us to refine the formula (12) in the region $k^2 \ll T/J(0)S$:

$$\Delta \varepsilon_k^{(2)} = -\varepsilon_k \frac{(2T/\pi J(0)S^2)^2 |\ln k|}{1 - (2T/\pi J(0)S^2) |\ln k|}. \quad (16)$$

This formula was obtained earlier through a macroscopic treatment by Pokrovskii and Feigel'man²⁴ and Lebedev.²⁵

It can be seen from Eqs. (15) and (16) that perturbation theory ceases to be applicable at scales

$$R_c \sim 1/k_c \approx \exp[\pi J(0)S^2/2T].$$

Accordingly, R_c , the greatest distance over which spin waves still exist, is the correlation length in a 2D ferromagnet. Of course this assertion is, to a certain extent, based on the results of the exact σ -model solution,⁶ since it is implied that the fluctuations do also grow outside the region controlled by the perturbation theory.

Let us point out that the spin-wave energy correction $\Delta \varepsilon_k^{(2)}$ is negative (cf. §3). For the temperature fluctuations this is natural, since a decrease in the energy of a magnon with a definite k must be associated with an increase in the equilibrium number of quasiparticles with a given momentum, i.e., enhancement of the fluctuation effects. Let us also note that, although the spin-wave damping constant²⁴

$$\gamma_k \sim \varepsilon_k (T/J(0)S^2)^2$$

grows logarithmically with decreasing wave vector,²⁵ it remains everywhere in the region of applicability of the perturbation theory smaller than the temperature renormalization of the spin-wave energy, since the latter contains an additional logarithmic factor. The real and imaginary parts of the spin-wave energy are comparable at the scale $R \approx R_c$, when the temperature correction is practically equal to the bare value ε_k ($|\Delta \varepsilon_k^{(2)}| \approx \varepsilon_k$). At distances much greater than the correlation length the spectrum is purely diffusive (as in a normal paramagnet), $\varepsilon_k \sim iDk^2$ (D is the diffusion coefficient).

Let us, in concluding this section, briefly discuss the question of the renormalization of the spectrum when allowance is made for the weak interplanar exchange. The corresponding correction to the Hamiltonian has the form

$$\mathcal{H}_1 = -\delta \sum_{1, \Delta_2} S_1 S_{1+\Delta_2}. \quad (17)$$

Allowance for the exchange interaction along the third axis changes the temperature correction to the spectrum of the spin waves with $\mathbf{k} = (k_x, k_y)$ in the region of the very low temperatures, where $\delta \gg T/J(0)S$ and the quasi-two-dimen-

Here the continuous and dashed lines denote the bare magnon Green's functions for the various sublattices.

In analytic form the formula (25) can be written as:

$$\Sigma(\mathbf{k}, \omega) = \frac{1}{32N^2S^2} \frac{1}{\varepsilon_{\mathbf{k}}} \sum_{\mathbf{p}, \mathbf{q}, \mathbf{l}} \left\{ \frac{(n_{\mathbf{p}}+1)(n_{\mathbf{q}}+1)(n_{\mathbf{l}}+1) - n_{\mathbf{p}}n_{\mathbf{q}}n_{\mathbf{l}}}{\varepsilon_{\mathbf{p}}\varepsilon_{\mathbf{q}}\varepsilon_{\mathbf{l}}} \times \left[\frac{f_{\mathbf{k}-\mathbf{p}}f_{\mathbf{q}+1}^*}{\varepsilon_{\mathbf{p}}+\varepsilon_{\mathbf{q}}+\varepsilon_{\mathbf{l}}-i\omega} + \frac{f_{\mathbf{k}+\mathbf{p}}^*f_{\mathbf{q}+1}}{\varepsilon_{\mathbf{p}}+\varepsilon_{\mathbf{q}}+\varepsilon_{\mathbf{l}}+i\omega} \right] + \frac{n_{\mathbf{p}}(n_{\mathbf{q}}+n_{\mathbf{l}}+1) - n_{\mathbf{q}}n_{\mathbf{l}}}{\varepsilon_{\mathbf{p}}\varepsilon_{\mathbf{q}}\varepsilon_{\mathbf{l}}} \left[\frac{f_{\mathbf{k}-\mathbf{q}}f_{\mathbf{p}-1}+f_{\mathbf{k}-1}f_{\mathbf{p}-\mathbf{q}}+f_{\mathbf{k}+\mathbf{p}}^*f_{\mathbf{q}+1}}{\varepsilon_{\mathbf{q}}+\varepsilon_{\mathbf{l}}-\varepsilon_{\mathbf{p}}-i\omega} + \frac{f_{\mathbf{k}+\mathbf{q}}^*f_{\mathbf{p}-1}+f_{\mathbf{k}+1}^*f_{\mathbf{p}-\mathbf{q}}+f_{\mathbf{k}-\mathbf{p}}f_{\mathbf{q}+1}}{\varepsilon_{\mathbf{q}}+\varepsilon_{\mathbf{l}}-\varepsilon_{\mathbf{p}}+i\omega} \right] \right\}. \quad (26)$$

It is implied that the momentum conservation law is obeyed in each process.

Let us note that, since \mathcal{H}_{int} contains terms with different numbers of boson creation and annihilation operators, in the construction of the perturbation theory, besides the normal self-energy functions, the anomalous functions $\Sigma^{++}(\mathbf{k}, \omega)$ and $\Sigma^{--}(\mathbf{k}, \omega)$ will appear. Accordingly, the structure of the total (normal) Green's function will be the same as in the case of a Bose-gas of particles in the presence of a condensate:

$$G(\mathbf{k}, \omega) = \frac{i\omega + \varepsilon_{\mathbf{k}} - \Sigma(-\mathbf{k}, -\omega)}{(\omega - i\Sigma^A)^2 + (\varepsilon - \Sigma^S)^2 - \Sigma^{++}(\mathbf{k}, \omega)\Sigma^{--}(\mathbf{k}, \omega)} \sim \frac{1}{\omega^2 + \varepsilon^2}, \quad (27)$$

where

$$\Sigma^{S,A} = \frac{1}{2} (\Sigma(\mathbf{k}, \omega) - \Sigma(-\mathbf{k}, -\omega)), \quad (28)$$

while $\tilde{\varepsilon}_{\mathbf{k}}$ is the renormalized spin-wave energy. The quantity $\Sigma^{++}(\mathbf{k}, \omega)\Sigma^{--}(\mathbf{k}, \omega)$ is of higher order in $1/S$ ($O(1/S^4)$), and therefore to the specified accuracy ($O(1/S^2)$) the structure of the Green's function does not change:

$$\tilde{G}^{-1}(\mathbf{k}, \omega) \approx \varepsilon_{\mathbf{k}} - i\omega - \Sigma(\mathbf{k}, \omega) \quad (29)$$

[$\tilde{G}(\mathbf{k}, \omega)$ is the total Green's function to within $O(1/S^2)$]. Nevertheless, the presence of the anomalous self-energy parts is important for the interpretation of the results obtained for the 1D antiferromagnet at $T=0$ (see below).

Let us now consider separately the quantum and classical corrections to the Green's function. Let us start with the temperature-dependent corrections. At $T \neq 0$ we shall be interested in the temperature renormalization of the spin-wave spectrum $\varepsilon_{\mathbf{k}} \rightarrow \varepsilon_{\mathbf{k}}(T)$. To calculate it the value of $\Sigma(\mathbf{k}, \omega)$ must be taken at resonance ($i\omega \equiv \varepsilon_{\mathbf{k}}$). The most interesting temperature dependence of the spectrum is the one for 2D space. Calculations with Eq. (26) show that, here at small wave-vector values $k \ll T/J(0)S$, the dominant contribution to the renormalization of the energy is made by the terms containing two Bose functions:

$$\Delta \varepsilon_{\mathbf{k}}(T) = -\frac{1}{2} \varepsilon_{\mathbf{k}} (2T/\pi J(0)S^2)^2 \ln^2 k. \quad (30)$$

Notice that the quadratic—in the logarithm—correction is entirely due to the parts $f_{\mathbf{a}-\mathbf{b}}$ and $f_{\mathbf{a}+\mathbf{b}}^*$ ($\mathbf{a}, \mathbf{b} = \mathbf{k}, \mathbf{p}, \mathbf{q}, \mathbf{l}$),

which are proportional to the scalar products of the corresponding wave vectors [see Eq. (24)].

The presence of fluctuation corrections that increase logarithmically with decreasing wave vector value means that, as in a 2D ferromagnet, the spin-wave description is inapplicable at long wavelengths. The determination of the characteristic scale at which it becomes impossible to consider the 2D antiferromagnet as an ordered system requires finding the total temperature renormalizations of all the amplitudes. Let us, as an example, consider the renormalization of the amplitude $\Phi_{q|pk}^{(4)}$ ($\Phi^{(4)} \rightarrow \Phi^{(4)}(T)$). In the "parquet" approximation the equation for $\Phi^{(4)}(T)$ can be diagrammatically represented as:

$$(31)$$

The black squares are the total vertices $\Phi^{(i)}(T)$. In each diagram we have chosen the two-particle cross section in which the integration momentum is smallest. Similar equations can be written for the other total vertices.

Of importance to us will be the renormalization of that part of the expression for $\Phi_{q|pk}^{(4)}$ which is proportional to the scalar product of the vectors \mathbf{k} and \mathbf{p} , since it is this part that produces the quadratic—in the logarithm—correction to the spectrum in second order perturbation theory.

As in §2, it is necessary to know the amplitude $\Phi_{q|pk}^{(4)}(T)$ in the case when the momenta \mathbf{q} , \mathbf{l} , and \mathbf{p} are of the same order of magnitude:

$$\Phi_{q|pk}^{(4)}(T) \rightarrow \mathbf{p}\mathbf{k}\tilde{g}(T, L). \quad (32)$$

This applies to the remaining amplitudes $\Phi^{(i)}(T)$. Equation (31), written as an equation for $\tilde{g}(T, L)$, coincides exactly with Eq. (14). Accordingly, the static renormalization of the vertex has, as in the case of a ferromagnet, the form

$$\tilde{g}(T, L) = (1 - 2TL/\pi J(0)S^2)^{-1}. \quad (33)$$

It therefore follows that the spin-wave description in antiferromagnets becomes inapplicable at the same scales $R_c \sim \exp[\pi J(0)S^2/2T]$ at which the corresponding description in ferromagnets becomes applicable.

Let us note, however, that in the case of an antiferromagnet we cannot refine Eq. (20) in the region $[2T/\pi J(0)S^2]L \sim 1$ by substituting into it the renormalized values of the vertices (as was done in the case of the ferromagnet). This is due to the fact that in the present case the line renormalizations determined by the perturbation theory series in the parameter $\{[2T/\pi J(0)S^2]L\}^2$ also become important as we approach the critical region. In a ferromagnet the analogous parameter, which is equal to $[2T/$

$\pi J(0)S^2]L$, is small on all the scales under consideration. Thus, the expressions obtained within the framework of perturbation theory [including Eq. (33)] are applicable to an antiferromagnet under conditions that are more stringent than in the case of a ferromagnet: it is required that the quantity $[2T/\pi J(0)S^2]L$ be much smaller than unity. Let us note further that, according to estimates, the damping constant for a spin wave with $k \ll T/J(0)S$ is proportional to $\gamma_k \sim \varepsilon_k T^2$, and is small compared to the temperature correction to the energy of the wave in the entire region of applicability of the perturbation theory.

In the wave-vector region $1 \gg k \gg T/J(0)S$ it is impossible to obtain the answer for the spectrum renormalization in its explicit form. Most probably the dominant contribution to $\Delta \varepsilon_k$ in this region is made by the terms containing one Bose function [see Eq. (26)], i.e., as in a 2D ferromagnet, the spectrum renormalization will be determined largely by the quantum effects. According to the estimates, for $1 \gg k \gg T/J(0)S$

$$\Delta \varepsilon_k \propto \varepsilon_k [T/J(0)S]^2, \quad (34)$$

but the coefficient of proportionality may vanish.

Let us now turn to the case of 3D space. It is well known that, to first order in $1/S$, the temperature renormalization of the spin-wave energy in a 3D antiferromagnet [see Eq. (21)] is the same as in the models with easy plane anisotropy^{26,33}: $\Delta \varepsilon_k \propto \varepsilon_k T^4$. Corrections to this result can arise from both the quantum and temperature renormalizations of the two-particle zero-angle scattering amplitude [corresponding to them in Eq. (26) are the terms containing respectively one and two Bose functions]. Analysis of such corrections in 3D ferromagnets, where $\Delta \varepsilon_k \propto \varepsilon_k T^{5/2}$ in first order in $1/S$, has been carried out by Dyson.³⁴ The result is well known: the temperature renormalization of the amplitude is not important, and the quantum renormalization attaches to the semiclassical result only a factor $Q(S)$ that is explicitly dependent on the magnitude of the spin. In 3D antiferromagnets the situation is, as follows from Eq. (26), different: allowance for the quantum renormalization of the amplitude in first order in $1/S$ causes an additional factor to appear that is a logarithmic function of the wave vectors. Consequently, the formula for the correction to the spectrum has the form

$$\Delta \varepsilon_k = -\varepsilon_k \frac{\pi^2 Z^{1/2}}{5S} \left(\frac{T}{J(0)S} \right)^4 \times \left[1 + \frac{10(2/Z)^{1/2}}{\pi^2 S} |\ln\{\max k, T/J(0)S\}| \right], \quad (35)$$

i.e., at small wave vectors $\Delta \varepsilon_k \propto \varepsilon_k T^4 |\ln T|$. The calculation shows that the corrections due to the temperature renormalization of the amplitude are proportional to T^4 , and do not play a noticeable role.

Let us emphasize that the presence of a renormalization that is a logarithmic function of the temperature is a direct consequence of the existence of two Goldstone modes in the elementary-excitation spectrum of an antiferromagnet. In magnetic materials with easy-plane anisotropy, such a renormalization does not occur in zero magnetic field. Let us note, though, that the logarithmic—in the temperature—

renormalization of the amplitude arises in easy-plane magnetic materials in $H \neq 0$ fields as a result of the three-particle anharmonicities.^{32,35,36} This is a general property of all Bose liquids with a Goldstone spectrum.³⁷

Expression (35) was derived under the assumption that $S \gg 1$. Higher powers of the logarithm do not arise in the subsequent orders in $1/S$, since all the amplitudes in an antiferromagnet are of zero order in the energies. Furthermore, we can, on the basis of the analogy with the 2D ferromagnet, in which allowance for the quantum renormalization of the amplitude also leads to a logarithmic correction [see Eq. (9)], assume that in this case a complicated spin dependence in the coefficient attached to the logarithm does not also arise. We cannot, however, prove this rigorously.

To conclude the discussion of the fluctuation effects at finite temperatures, let us note that, in 1D space, the temperature corrections to the spectrum increase in a power-law fashion as the wave vector decreases. In this case the spin-wave description is already inapplicable at scales proportional to the reciprocal temperature.

Let us now consider the situation at $T = 0$, when the renormalizations are entirely due to the quantum effects.

As was indicated in the Introduction, the quantum effects in antiferromagnets are strongest in 1D space, where allowance for them leads to the destruction of the long-range order in the ground state. Calculations with expression (26) lead in this case to the following result: the renormalization of the spin-wave energy is finite,⁴⁾ but there appears a logarithmically increasing correction to the bare Green's function:

$$\bar{G}(k, \omega) = \left(1 + \frac{L}{2\pi^2 S^2} \right) \frac{1}{\varepsilon_k - i\omega}, \quad (36)$$

where

$$L = |\ln \max(|\omega|, \varepsilon_k)|. \quad (37)$$

Let us now take account of the fact that, because of the presence of the anomalous self-energy parts, the total Green's function is "phonon-like" [see the formula (27)]. It is not difficult to verify that the logarithmic terms in the normal and anomalous self-energy parts are identical. Accordingly, the expression for the total Green's function with allowance for the quantum renormalization is

$$G(k, \omega) \sim Z_L / (\omega^2 + \varepsilon_k^2), \quad (38)$$

where

$$Z_L = 1 + L/\pi^2 S^2, \quad (39)$$

i.e., as in 2D space at $T \neq 0$, the presence of two Goldstone branches in the spectrum leads to the appearance of fluctuation corrections that increase logarithmically with increasing scale. The summation of the principal logarithmically diverging diagrams is carried out in the same way as in the case of a 2D antiferromagnet. Of the "parquet" diagrams at $T = 0$ only those in which the arrows on the internal lines point in the same direction survive. Let us denote the result of the renormalization by $\Phi^{(i)}(1/S)$, and introduce, as before, the function $g_{\text{quas}}(1/S, L)$: $\Phi^{(i)}(1/S) = \Phi^{(i)} g_{\text{quas}}(1/$

S, L). In analytic form Eq. (31), written as an equation for $g_{\text{quas}}(1/S, L)$, looks like:

$$g_{\text{quas}}(1/S, L) = 1 + \frac{1}{\pi S} \int_0^L du g_{\text{quas}}^2(1/S, u), \quad g_{\text{quas}}(1/S, 0) = 1, \quad (40)$$

whence

$$g_{\text{quas}}(1/S, L) = \left(1 - \frac{L}{\pi S}\right)^{-1}. \quad (41)$$

In first order in $1/S$, the logarithmic renormalization of the amplitude is found in Ref. 29 (the value of the coefficient is determined more accurately in Ref. 39).

Knowledge of the renormalization of the amplitude allows us (as in the case of the $2D$ ferromagnet) to refine the expression (39):

$$Z_L = 1 + \frac{L}{\pi^2 S^2} \left(1 - \frac{L}{\pi S}\right). \quad (42)$$

This can be done, since allowance for the renormalization of the amplitude leads to greater corrections to Z_L than allowance for the renormalizations of the virtual-magnon Green's functions. It can be seen from Eq. (42) that there also exists in the $1D$ antiferromagnet a characteristic scale $R_c \sim e^{\pi S}$ beyond which the standard spin-wave description is inapplicable.

It is convenient to represent Eqs. (41) and (42) as the results of the solution of the differential equations

$$\frac{dZ_L}{dL} = \left(\frac{1}{2\pi}\right)^2 g_L^2, \quad \frac{dg_L}{dL} = \left(\frac{1}{2\pi}\right) g_L^2, \quad (43)$$

in which $g_L = (2/S)g_{\text{quas}}(1/S, L)$ is the "effective reciprocal spin" (coupling constant) $g_0 = 2/S$. The first equation relates the renormalization of the Green's function to the coupling constant, while the second determines the renormalization of the coupling constant itself. Both equations are approximate: we have discarded in them the terms of higher orders in g_L , terms which from the beginning have an additional power of $1/S$ and therefore do not fall into the category of the principal logarithms, and have ignored the renormalization of the virtual-magnon Green's functions. The discarded terms are of the order of those considered at the same scales $R_c \sim e^{\pi S}$ where the effective reciprocal spin attains the value of unity. On large scales the formulas (43) need to be refined. It can be seen at the same time that, for $R \ll R_c$, the equations for g_L and Z_L in the $1D$ case are exactly the same as the equations for the coupling constant $4T_L/J(0)S$ and the effective mass in a $2D$ ferromagnet [see the formulas (15) and (16)]. In fact the Matsubara frequency plays the role of a second coordinate. Since the $2D$ ferromagnet is, in turn, equivalent to the $O(3)$ σ -model, for which the exact solution is known,⁶ these analogies allow us to expect that the fluctuation corrections in a $1D$ antiferromagnet will continue to grow outside the region where the perturbation theory is applicable, so that as a result the spectrum $\omega(k)$ will contain a finite (though for $S \gg 1$ exponentially small) gap:

$$\omega^2(k) = \bar{\varepsilon}_k^2 + \Delta^2, \quad \Delta \sim e^{-\pi S}, \quad \bar{\varepsilon}_k \sim k. \quad (44)$$

Two circumstances are important for the interpretation of

this formula. First, an elementary excitation in an antiferromagnet at $T = 0$ has an infinite lifetime, since the decay of a magnon is forbidden by the conservation laws.²⁷ For this reason the values of $\omega(k)$ essentially determine the energy levels of the system. Secondly, the excitation energy is measured from the true ground state, which differs from the classical ground state on account of the same quantum renormalization. The finiteness of $\omega(0)$ means in this case that the ground state is a singlet. Accordingly, the spin-spin correlation functions fall off exponentially at $T = 0$.

§4. DISCUSSION OF THE RESULTS

Let us enumerate the main results obtained in the present paper.

1. We have found logarithmically increasing temperature corrections to the spin-wave spectra of isotropic $2D$ ferromagnets and antiferromagnets ($\Delta\varepsilon_k \propto \varepsilon_k T^2 |\ln k|$ for ferromagnets and $\Delta\varepsilon_k \propto \varepsilon_k T^2 \ln^2 k$ for antiferromagnets), and have established the limits of applicability of the spin-wave description. It has been shown that, in an antiferromagnet, the logarithmic renormalizations are due to the presence in its spectrum of two linear Goldstone modes.

2. We have found the dominant temperature renormalization of the spectrum of $3D$ antiferromagnets. $\Delta\varepsilon_k \propto \varepsilon_k T^4 |\ln T|$.

3. It has been shown that the quantum corrections to the Green's function in a $1D$ antiferromagnet at $T = 0$ also increase logarithmically as the wave vector decreases ($\Delta G(k, \omega) \propto GS^{-2} |\ln k|$). The characteristic scale beyond which the perturbation theory is, in the general case, inapplicable has been determined.

The results pertaining to $2D$ space are quite natural, since it has been rigorously proved^{6,7} that isotropic $2D$ ferromagnets and antiferromagnets remain in the paramagnetic phase right down to $T = 0$. Less obvious are the result pertaining to $1D$ space. Let us discuss them in greater detail. In the main, what we have been able to do is to confirm through direct calculations Haldane's hypothesis¹³ concerning the existence in a $1D$ antiferromagnet with a large spin of a "natural" scale of distances $R_c \sim e^{\pi S}$ at which the semiclassical spin-wave description becomes inapplicable. Further, Haldane formulated his hypothesis on the basis of the equivalence of the classical Lagrangians of the antiferromagnet and the $O(3)$ σ -model. As can be seen from the formula (43), this equivalence remains when allowance is made for the quantum fluctuations within the framework of perturbation theory. On the other hand, it has been rigorously proved^{9,11} that, for all half-integral spin values, the spectrum does not contain any gap. Thus, we have a contradiction between the predictions of perturbation theory and the rigorous results. Haldane¹³ has suggested that the cases of half-integral S values are special, and that the perturbation theory predictions for integral S are correct. Standard perturbation theory does not allow us to prove this, just as it does not allow us to elucidate the cause of the specific behavior of $1D$ antiferromagnets with half-integral spins.

The difference between the cases of integral and half-integral S values can be explained by assuming that, at the

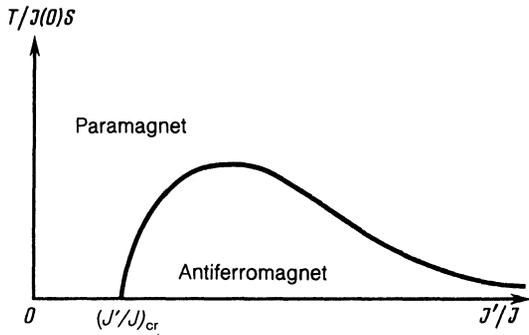


FIG. 1. Proposed dependence of the paramagnetic-antiferromagnetic phase transition temperature on the ratio of the intrachain (J) and interchain (J') exchange integrals. The spin S is integral. The spin space is magnetic-field and anisotropy free (i.e., $H = 0$ and $\alpha = 0$). The vanishing of T_N at a finite value of the ratio J'/J ($(J'/J)_{cr} \sim e^{-\pi S}$ for $S \gg 1$) is due to the quantum-fluctuation-governed anomalies. The decrease of T_N in the region $J'/J \gg 1$ is a reflection of the quasi-two-dimensional character of the antiferromagnet in this limit. The phase diagram for the case of half-integral spin values is different in the region $J'/J \ll 1$, since in this case $(J'/J)_{cr} = 0$.

macroscopic level, an antiferromagnet is described by the σ model with an additional topological θ term that, for half-integral S , assumes the value⁴⁰ π . It is assumed⁴¹ that the properties of the σ model with a θ term differ, when $\theta = \pi$, from the normal properties: in particular, a gap is not produced. An approximate construction of a σ model with a θ term that corresponds to an antiferromagnet is carried out in Ref. 42. In this model θ is indeed equal to π for half-integral S .

The existence of an energy gap in the spectrum of isotropic 1D antiferromagnets with integral S values is confirmed also by the results of numerical experiments for systems with $S = 1$ (Refs. 11, 16, and 18). Let us assume that there is indeed a gap in the isotropic case (S is integral), and let us investigate the situation in the presence of a magnetic field H , anisotropy α , and exchange J' between the spin chains. Each of the additional terms in the Hamiltonian contributes to the weakening of the quantum fluctuations, since the system either becomes weakly three-dimensional ($J' \neq 0$), or acquires the characteristics of an XY magnet ($H \neq 0$ or $\alpha \neq 0$, $\alpha > 0$) or an Ising magnet ($\alpha \neq 0$, $\alpha < 0$). If even one of the parameters H , α , and J' is comparable in magnitude to the intrachain exchange J , then the correlation length is certainly infinite, and the spectrum contains no gap.⁵ In this case there exists long-range order in the ground state (when $J' \sim J$ or $\alpha \sim J$, $\alpha < 0$), or the spin-spin correlation functions decrease in power-law fashion (when $H \sim J$ or $\alpha \sim J$, $\alpha > 0$). But the correlation length cannot go to infinity abruptly. Therefore, when any additional interaction is switched on, the transition from the "paramagnetic" phase into the state with infinite correlation length will occur only when this interaction becomes appreciable at characteristic scales of the order of $e^{\pi S}$ (S is assumed to be large). Consequently, the critical parameter values (those at which the transition occurs) are finite, and are, in order of magnitude, equal to

$$\Delta \sim JS e^{-\pi S}, \quad \Delta = \mu H, \quad |\alpha| S, \quad J' S. \quad (45)$$

Essentially the situation here is the same as the situation that obtains in the anisotropic σ model,⁴⁴ except that the role of temperature is played by the quantity $2/S$.

It should be noted that, although the arguments adduced above seem to us to be fairly natural, they are not rigorous. Therefore, it is possible that switching on any of the interactions will cause long-range order to develop at once, but not as a result of a phase transition. This seems to us to be highly improbable.

The finiteness of the critical value J' means that the "paramagnetic" ground state is realized not only in purely one-dimensional, but also in real three-dimensional Heisenberg antiferromagnets with strong exchange-interaction anisotropy in coordinate space. Figure 1 shows the phase diagram of antiferromagnets in the plane of the variables $T/J(0)S$ and J'/J .

It is convenient to use for the experimental verification of the effects discussed here the fact that a magnetic field suppresses the critical fluctuations in low-dimensional antiferromagnets, since there appears a gap for one of the modes and the order parameter becomes a two-component one (this is pointed out in Ref. 45 too).

In quasi-two-dimensional antiferromagnets (of the type K_2NiF_4) the transition temperature in zero field is, in order of magnitude, equal to $T_N \sim J/\ln(J/\tilde{J}) \ll J$ (\tilde{J} is the exchange integral between the spins in neighboring planes: $\tilde{J} \ll J$). On the other hand, in the quasi-two-dimensional XY model, the properties of which are acquired by the antiferromagnet after the field has been switched on, the transition occurs at a temperature $T \sim J$ even in the $\tilde{J} = 0$ case.^{4,5} Therefore, if in ordinary 3D systems the value of T_N falls as the field intensity increases, in the present case, in fields that are weak compared to the exchange interaction, the Néel temperature should increase with increasing field intensity. Estimates show that, for $H \ll J(0)S$,

$$T_N \sim J/\ln \left[\frac{J(0)S}{J(0)S+H} \right].$$

From the quasi-one-dimensional antiferromagnets with integral spin, let us choose the crystal $CsNiCl_3$ [J'/J lies in the range from 0.007 (Ref. 46) to 0.017 (Ref. 47)]. This material possesses the lowest, though finite, 3D-transition temperature [$T_N = 4.85$ °K (Ref. 46)]. It seems to us that the anomalies produced by the quantum fluctuations can be indirectly observed in it through the dependences $\chi_{\perp}(H)$, $\chi_{\parallel}(H)$, and $\epsilon_0(H)$ ($CsNiCl_3$ is an easy-axis antiferromagnet with anisotropy⁴⁷ $\alpha/J(0) = 0.019$). Indeed, in zero field, because of the smallness of the anisotropy and the weakness of the exchange interaction between the chains, the quantum effect should still manifest themselves quite distinctly, i.e., the values of both susceptibilities at $H = 0$ should be greater than the classical values, but the ϵ_0 value should, on account of the zero-point vibrations, be lower. The application of a magnetic field results in the suppression of the quantum fluctuations, a fact which should be manifested in the field dependences of the susceptibilities and the uniform-precession frequency; the susceptibilities should tend to their classical values, while $\epsilon_0(H)$ should deviate from the linear dependence in the manner shown in Fig. 2. It

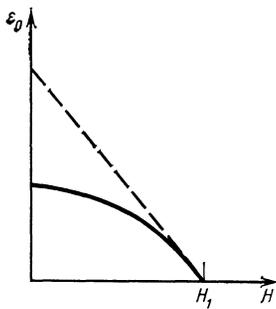


FIG. 2. Proposed magnetic-field dependence of the uniform precession frequency ε_0 in CsNiCl_3 . The dashed line is a plot of the classical dependence $\varepsilon_0(H)$ (for the same spin-flip-transition field H_1).

is, moreover, possible that the experimentally observed⁴⁶ growth of the function $T_N(H)$ in CsNiCl_3 and RbNiCl_3 is also explained by the suppression of the quantum fluctuations in a magnetic field, although here it is difficult to determine which fluctuations (the quantum or classical) are more important.⁶⁾ Let us further note that, recently, using the neutron-scattering method, Buyers *et al.*⁴⁷ found in the spectrum of CsNiCl_3 at temperatures higher than T_N a gap, which was explained as owing its origin to the quantum fluctuations. This conclusion seems doubtful to us, since the existence of a finite transition temperature indicates that the quantum fluctuations “do not suffice” for the production of a gap.

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¹⁾Notice that, as follows from the exact solution, the same ground-state structure arises in the “polynomial” antiferromagnetic model with arbitrary spin. The corresponding Hamiltonian is written in the form of a polynomial of degree $2S$ in $S_i S_{i+1}$ with completely determined coefficients.¹²

²⁾We can, on the basis of the analogy with the σ model, write down the result of the summation at once, since in the classical theory there corresponds to each vertex a temperature, and its renormalization in the σ model is known.²² It, however, seems to us that it will be useful to derive the formula for the temperature renormalization of the vertex without recourse to the σ model.

³⁾Alternatively, we can work with the normal and anomalous Green’s functions (see, for example, Ref. 32), but in the present case the uv transformation is more convenient.

⁴⁾The result we obtained earlier [formula (1) in Ref. 19] is incorrect. We apologize to readers. The error was caused by an incorrect extraction of the logarithmic terms from background of parasitic divergences, which arise in calculations based on the Holstein-Primakoff formalism.³⁸ The computational method used in the present paper does not contain divergences.

⁵⁾Let us note that, for large positive values of the single-ion anisotropy constant (i.e., for $\alpha \gg J$), the ground-state structures of Heisenberg magnets with integral and half-integral spins are also different.⁴³ This effect is due to the spin-orbit interaction, and does not bear a direct relation to what is considered in the present paper.

⁶⁾The classical fluctuations may also be important for the determination of the field dependence of T_N in a quasi-one-dimensional antiferromagnet, since the $3D$ transition in the quasi-one dimensional XY model has a higher critical temperature.⁴⁵

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