Spin-wave interaction in low-dimensionality Heisenberg magnetic materials

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Logarithmic divergences of the fluctuational corrections to the spin-wave spectra are found by a microscopic approach. These are quantum-mechanical corrections for one-dimensional (1D) antiferromagnets and classical corrections for 2D ferromagnets and antiferromagnets. The temperature corrections to the spectrum of a 3D antiferromagnet is shown to behave $\propto T^4 \ln T$.

We wish to discuss two questions: 1) To what extent does the interaction between quantum fluctuations (zero-point vibrations of the spin) affect the structure of the ground state of a quantum-mechanical spin system? 2) Can quantum-mechanical effects alter the temperature dependence of the magnetic characteristics of ferro- or antiferromagnets?

1. We begin with a study of the structure of the ground state. We know that at $T = 0$ quantum-mechanical effects play a fundamental role in a one-dimensional (1D) space, where they lead to a smearing of the long-range magnetic order for all systems which have a seed ($S = \infty$) linear Goldstone spectrum (e.g., for the XY model or for an antiferromagnet).[1)] This fact, however, does not lead to an unambiguous prediction of the behavior of correlation functions: It does not tell us whether spin waves exist in the system at all distance scales. For 1D magnetic materials with $S = 1/2$, the answer to this question is known from the exact solutions[1,2]: The correlation functions fall off by a power law, and at all wavelengths there are spin waves, whose velocities differ from the corresponding classical values only by numerical factors.

For a long time it was assumed that this result should also apply to all other values of the spin. On the other hand, among the 1D quantum-mechanical systems with a seed Goldstone spectrum, there is one special one, in which the quantum-mechanical fluctuations are most pronounced. This is a 1D antiferromagnet whose seed spectrum $\epsilon_k = sJS|\sin k|$ contains two Goldstone modes,[1)] $k = 0$ and $k = \pm\pi$. Haldane[3] recently attempted to determine the correspondence between a 1D quantum-mechanical antiferromagnet and the 2D classical $O(3)$ σ model by a semiclassical approach. In this case, the incorporation of fluctuations leads to an exponential decay of the correlation functions and to the absence of spin waves at small wave vectors.[4,5] According to Haldane's hypothesis, a power-law decay of the correlation functions, which clearly prevails at $S = 1/2$, is characteristic of half-integer values of the spin, while for integer values S we should expect the correlation radius to remain finite, and we should expect a "paramagnetic" behavior.[2)] Despite the fact that Haldane's results have been disputed by several authors,[6] they did stimulate a rapid increase in the number of numerical simulations of the structure of the ground state of a 1D antiferromagnet (see the extensive bibliography in Ref. 7). The data from the numerical simulations demonstrate a qualitative difference between the behavior of systems with $S = 1/2$ and that of systems with $S = 1$ (the first explicit indication of this difference came in Ref. 8).

Let us consider the *microscopic* spin Hamiltonian of an antiferromagnet, $\mathscr{H} = J\Sigma_l S_l S_{l+1}$, and explicitly calculate the quantum-mechanical corrections to the spin-wave spectrum, retaining terms proportional to S^{-2}. The procedure for finding these corrections is standard, including (1) a diagonalization of a quadratic form in the Bose Hamiltonian of the antiferromagnet by means of a "generalized" UV transformation and (2) incorporation of anharmonic effects in second-order perturbation theory. The Bose Hamiltonian and a description of the procedure of the generalized UV transformation are given in Ref. 9, among other places. The diagrams which should be taken into account in the second step are of the type (we recall that the number of anharmonicities increases after a UV transformation):

In part, the contribution from these diagrams goes to cancel the "parasitic" divergences that appear after the UV transformation. The remainder leads to a logarithmically increasing correction to the magnon spectrum for wave vectors k near 0 or $\pm\pi$. Near $k = 0$ we thus have

$$\epsilon_k = 2JSk\left[1 + \frac{\pi - 2}{2\pi S} + \frac{\text{const}}{S^2} + \frac{|\ln k|}{\pi^2 S^2}\left(1 + O\left(\frac{|\ln k|}{\pi S}\right)\right)\right] \quad ; \; k \equiv |\mathbf{k}|. \qquad (1)$$

A logarithmic renormalization arises only from regions in which the wave vector of the one of the virtual magnons is close to 0, while those of the two others are close to $\pm\pi$; in other words, the renormalization is due *entirely* to the presence of a second Goldstone mode in the classical spectrum of elementary excitations. According to expression (1), the quantum-mechanical fluctuations grow with increasing distance scale; in other words, the effective spin decreases

$$\left(\frac{1}{\tilde{S}} - \frac{1}{S} \sim \frac{|\ln k|}{\pi S^2}\right),$$

and a perturbation theory in the reciprocal of the spin (which serves as a coupling constant[3]) breaks down at $k \lesssim k_0 = e^{-\pi S}$ [the expansion parameter $|\ln k|/\pi S$ in (1) reaches a value on the order of unity]. When a perturbation-theory approach is taken, of course, it is not possible to predict the behavior of the system for small vectors or, especially, to determine the difference between integer and half-integer spins. It nevertheless appears that the presence of corrections, which grow logarithmically with increasing scale [as is characteristic of the 2D $O(3)$ σ model[4]], indicates that there is the possibility of a qualitative difference between the structure of the ground state of a 1D antiferromagnet and that of 1D systems with a single Goldstone mode in the seed spectrum (e.g., the XY model). Imposition of a magnetic field gives rise to a gap $\sim H$ for the mode with $k = \pm\pi$ in the elementary spectrum of the spin waves. Accordingly, if the theoretical predictions are correct, in fields $H \sim H_E e^{-\pi S}$ (H_E is the exchange field) there should be a phase transition to a "quasi-antiferromagnetic" state with a power-law decay of the correlation functions and a Goldstone spectrum. This transition can apparently be seen experimentally (e.g., in the antiferromagnet $CsNiCl_3$).

2. At $T\neq 0$ the basic temperature renormalization of the energy of a spin wave is determined by the diagram

(it is assumed that the quadratic form has already been put in diagonal form in the antiferromagnet). The hatched square is the total scattering amplitude. It differs from the bare amplitude in that, first, it contains quantum renormalizations (the corrections for $T=0$) and, second, it contains temperature effects. Let us consider ferro- and antiferromagnets separately.

2a. For *ferromagnets* the situation in 3D space is quite well known: The temperature renormalization of the amplitude is unimportant, while the quantum-mechanical renormalization simply adds a factor, which depends explicitly on the magnitude of the spin, to the semiclassical result.[10] In 2D space this situation is different. According to our calculations, incorporating the renormalization of the amplitude gives rise to a factor which depends logarithmically on the wave vector:

$$\epsilon_k = JSk^2\left[1-\alpha\left(\frac{T}{JS^2}\right)^2 |\ln k| \left(1+O\left(\frac{T}{JS^2}|\ln k|\right)\right) - O\left(\frac{T}{JS}\right)^2\right], \qquad (2)$$

where

$$\alpha = \begin{cases} \zeta(2)\cdot(4\cdot(2\pi)^2)^{-1} = 1/96, & k \gg (T/JS)^{1/2}; \\ (2\pi)^{-2}, & k \ll (T/JS)^{1/2}. \end{cases} \qquad (3)$$

At $k\gg(T/JS)^{1/2}$, the logarithmic correction comes from the quantum-mechanical renormalization of the scattering amplitude, while at $k\ll(T/JS)^{1/2}$ it comes from incorporating the temperature dependence of the amplitude. The perturbation theory used to derive (2) breaks down at $k\sim e^{-JS^2/T}$ (the expansion parameter $(T/JS^2)|\ln k|$ reaches values on the order of unity); this is a natural reflection of the properties of the 2D $O(3)$ σ model, which describes a 2D Heisenberg ferromagnet at the macroscopic level.[4] The corresponding temperature dependence of the spin-wave energy for $k\ll(T/JS)^{1/2}$ was found by a macroscopic approach in Ref. 11. Expressions (2) and (3) have been derived without any assumption that the spin is large. There is a physical explanation for the absence of a complex dependence of the logarithmic correction on the value of S. A complex dependence on S could arise only from integrals whose values are determined by the structural details at distances on the order of interatomic distances. The coefficient of the logarithm, on the other hand, determines the correlation radius, which should depend on only the macroscopic properties of the system by virtue of the renormalizability of the σ model.

2b. For *antiferromagnets* at $T\neq 0$, a new result is found even in 3D space: Incorporating the *quantum-mechanical* renormalization of the amplitude leads to a temperature dependence of the spectrum of low-frequency spin waves which is different from the result $\Delta\epsilon_k \propto (T/JS)^4$, found in the semiclassical approximation.[12] For $k \ll (T/JS)^3$ we have

$$\epsilon_k = 2\sqrt{3}JSk \left\{1 - \frac{\pi^2}{2160\sqrt{3}S}\left(\frac{T}{JS}\right)^4 \left[1 + \frac{10\sqrt{3}}{3\pi^2 S}\left|\ln\frac{T}{JS}\right|\right]\right\}. \quad (4)$$

Expression (4) was derived under the assumption $S \gg 1$. Analysis shows that the corrections from higher-order perturbation theory, which stem from the temperature renormalization of the amplitude, are $\propto (T/JS)^4$ and do not contain a logarithmic factor. Consequently, at $(T/JS) \ll 1$ expression (4) describes the *main* temperature correction to the spectrum of 3D antiferromagnets. We wish to emphasize that the presence of a logarithm is, as in the case of $T=0$ (see Sec. 1), a direct consequence of the existence of two Goldstone modes in the spectrum of elementary excitations of the antiferromagnet.

It is not possible to derive an explicit result for the temperature renormalization of the spectrum in 2D space. According to estimates, at $k \ll T/JS$ the temperature dependence of the amplitude plays the leading role, giving rise to the same logarithmic renormalization of the spectrum as in a 2D ferromagnet (actually, the presence of two linear Goldstone modes in an antiferromagnet is in this case equivalent to a single quadratic mode in a ferromagnet). Taking the quantum renormalization of the amplitude into account may be important at $k \gg T/JS$, but we have not been able to find reliable estimates here.

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[1)]What is involved here is a description of the properties of an antiferromagnet without breaking it up into two sublattices. In the opposite case, we should speak in terms of two Goldstone branches in the spectrum.

[2)]For half-integer spins, the Lieb-Shults-Mattis theorem,[1] which has been proved for $S = 1/2$, holds. This theorem deals with the degeneracy of the ground state of an antiferromagnet, i.e., the Goldstone nature of its spectrum.[13]

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