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Unusual states in the Heisenberg model with competing interactions

A V Chubukov
Institute for Physical Problems, USSR Academy of Sciences, 117334 Moscow, ul. Kosygina 2, USSR

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Abstract. A phase diagram of the anisotropic Heisenberg model with competition between the nearest and the next-to-nearest neighbour exchange interactions is investigated by using the bosonisation scheme. An instability leading to a spontaneous dimerisation is found. The new 'superfluid' phases with both non-zero, though non-nominal, Z-magnetisation and broken symmetry in the XY-plane are detected in the anisotropic case.

1. Introduction

In the past few years there has been a considerable interest in the study of quantum fluctuations in spin chains. This interest was to a great extent initiated by the intriguing conjecture made by Haldane [1] that the ground-state properties of isotropic (collinear) Heisenberg antiferromagnets depend crucially on the parity of $2S$: for half-integer S the $T = 0$ behaviour was predicted to be critical and coincides with that in the integrable case of $S = \frac{1}{2}$, while for integer S quantum fluctuations were predicted to destroy not only long-range but also orientational order thus leading to a singlet ground state with a gap immediately above it. This conjecture was later confirmed by a large number of analytical [2–6] and numerical [7–11] calculations.

The subject of this paper is the role of quantum effects in one-dimensional versions of non-collinear magnets, that is in helical configurations arising as a result of a competition between the nearest and next-to-nearest neighbour exchange interactions. The possibility of obtaining new effects due to fluctuations in the case of non-collinear spin ordering follows from the particular features of the order parameter space which is isomorphic not to a two-dimensional (2D) sphere S_2, as in the collinear case, but to the projective space P_3 or, equivalently, to the surface of a three-dimensional sphere with diametrically opposite points identified. In the 2D case the importance of this difference was clarified by Kawamura and Miyashita [12]. They claimed that the existence of the non-zero first homotopy group for P_3 ($\pi_1(P_3) = Z_2$) leads to the possibility of a topological phase transition in isotropic two-dimensional systems in spite of the exponential decay of two-point correlation functions at any finite temperature. The low- and high-temperature phases differ in the structure of the vortex-like excitations and by analogy with the famous Kosterlitz–Thouless mechanism the transition may be regarded as a dissociation of bounded vortex pairs. Based on the usual analogy between temperature fluctuations in two dimensions and quantum fluctuations in one dimension, it is reasonable to propose the existence of an 'ordered' zero-temperature phase in the 1D version of non-collinear magnets, the two-valuedness of the Z_2 group implies that the order parameter, if it really exists, is of Ising type.

A further discussion demands a particular spin Hamiltonian to be chosen, which will be taken in the following form with a positive value of β:

$$H = \sum_l h_{l,l+1} + \beta h_{l,l+2} \tag{1}$$

where

$$h_{l,l+1} = S_l^x S_{l+1}^x + S_l^y S_{l+1}^y + \Delta S_l^z S_{l+1}^z.$$

We begin with the isotropic case ($\Delta = 1$). According to the classical description, the Néel state is stable for $\beta < \frac{1}{4}$, while for higher values of β the ground state is realised in helical the configuration with $\cos Q = -1/4\beta$.

In both cases classical excitations contain relativistic Goldstone modes at $K = 0$ and π in the antiferromagnetic phase, and at $K = 0$ and $\pm Q$ in the helical phase. The critical point $\beta = \frac{1}{4}$ is characterised by an additional softening: the spectrum

$$\varepsilon_k = 2S\{[1 - \beta(1 - \nu_{2k})]^2 - \nu_k^2\}^{1/2} \qquad \nu_k \equiv \cos k$$

contains two soft modes, both quadratic in k.

A calculation of quantum fluctuations changes this simple picture. In addition to the usual smearing of the site magnetisation which is peculiar to any 1D system with a continuous symmetry and holds for all β, it was proved in a number of papers [1–6] that quantum fluctuations also lead to a logarithmic renormalisation of the coupling constant g in the antiferromagnetic phase and generate the inner scale $R_c \sim e^{-2\pi/g}$ below which perturbation theory is invalid. A low-energy theory is given by the O(3) σ-model with coupling $g = 2/s(1 - 4\beta)^{1/2}$ and topological θ-term with $\theta = 2\pi S$. The last term is responsible for the above-mentioned difference between integer and half-integer S.

One rigorous result is also known for $\beta > \frac{1}{4}$: in the case when $\beta = \frac{1}{2}$ the exact ground state of the $S = \frac{1}{2}$ model was proved to be twofold degenerate and to consist of non-interacting dimers, that is the ground-state wavefunctions for a ring with an even number of spins are $\psi_1 = [12]\,[34]\,[56]\ldots$ and $\psi_2 = [23]\,[45]\ldots$ where [12] is a singlet configuration of nearest neighbours:

$$[12] = (\uparrow\downarrow - \downarrow\uparrow)\sqrt{2}. \tag{2}$$

This ground state corresponds to a broken translational symmetry. The fundamental excitations are $S = \frac{1}{2}$ solitons and soliton–antisoliton bound states [14, 15]. Affleck *et al* [16] have proved that all the excitations have a finite energy gap.

The situation for arbitrary $\beta > \frac{1}{4}$ (or, better, for $\beta > \beta_c$) since the fluctuations shift the critical point) was first considered by Haldane for a model with $S = \frac{1}{2}$ [15]. He pointed out the mechanism leading to dimerisation and obtained the renormalisation group equations favouring the realisation of the dimer state for all $\beta > \beta_c$. This result was later repeated in [17].

One of the aims of the present paper is to confirm Haldane's proposal by using an independent bosonisation scheme. This is done in section 2. We have found that for arbitrary S the instability against helical ordering is accompanied by an instability against spontaneous dimerisation and only the dimer configuration is stable below the critical point.

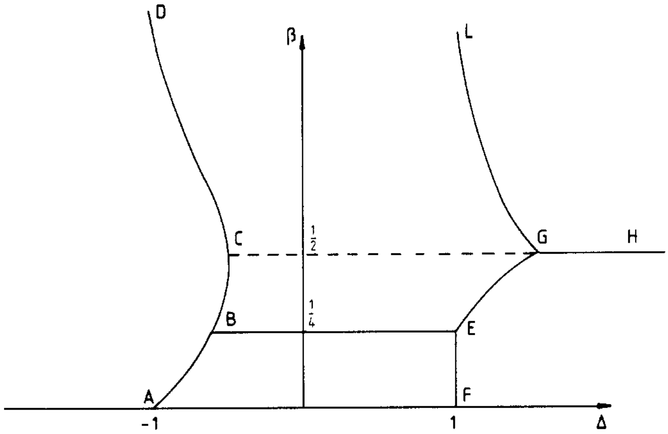


Figure 1. The classical phase diagram of the spin Hamiltonian (1) on the (β, Δ) plane. The ground state can be realised in five different phases: the Ising-like ferromagnet, to the left of the line AD; the helical state, between the lines BCD and EGL; the *XY*-like antiferromagnet, between the lines AF and BE; an Ising antiferromagnet, to the right of the line GEF; and the phase with the up–up–down–down spin configuration, to the right of the line LGH. The location of the line ACD is given by (17), the locations of the lines LG and EG are $\Delta_c = (1 + 8\beta^2)/8\beta^2$ and $\Delta_c = (1 + 8\beta^2)/8\beta(1 - \beta)$, respectively. The first-order transition line GH corresponds to $\beta = \frac{1}{2}$.

The general phase diagram of (1) in the (β, Δ) plane is also of considerable interest since the order parameter symmetry in a planar helical configuration again differs from that in the usual *XY*-antiferromagnet now due to the presence of the additional Z_2-degree of freedom, chirality. This distinguishes left- and right-twisted helicoids. The classical phase diagram is presented in figure 1 and consists of five phases: the Ising-like ferromagnetic state, to the left of line AD; the helicoidal state, between the lines BCD and EGL; the XY-like antiferromagnetic state, between the lines AF and BE; the Ising-like antiferromagnetic state, below the line EGH; and at least, the phase with the up–up–down–down spin configuration, to the right of the line LGH. One can expect the phase diagram to be seriously affected by fluctuations only in the vicinity of $\Delta = 1$, since fluctuations in anisotropic systems are believed not to be too strong and, in particular, not to wash away orientational ordering in *XY*-type systems. However, the analysis given below in section 3 shows that in one dimension the classical phase diagram changes considerably in the presence of quantum fluctuations not only in the vicinity of the $\Delta = 1$ line, but also for all $\Delta > -1$: the dimer phase stretches up to $\Delta = -\frac{1}{2}$ for $\Delta < 0$ and up to infinity for $\Delta > 0$, and, in addition, new phases which we call 'superfluid' ferromagnetic appear for arbitrary S, at least in the vicinity of the line AD. These phases arise due to the decoupling of the set of ordered states for planar helical or *XY* antiferromagnetic configurations and have non-zero, though non-nominal, Z-magnetisation together with the broken symmetry in the *XY*-plane. Moreover, these phases are not only one-dimensional phenomena, they definitely exist even in three dimensions.

The organisation of this paper is as follows: section 2 is devoted to the 1D isotropic model (1). By applying the bosonisation scheme at $\beta = \beta_c$ it will be proved, firstly, that this point is a critical one independent of the parity of $2S$ and, secondly, that $\beta = \beta_c$ is also a lability point against spontaneous dimerisation. The application of this scheme below the critical point allows a demonstration that the dimer state is the only stable state for $\beta > \beta_c$. The anisotropic $S = \frac{1}{2}$ model in one dimension is discussed in section 3. The new 'superfluid' ferromagnetic phases are identified and proposals are made about the general form of a phase diagram in the (β, Δ) plane.

An extension of the above analysis to $S > \frac{1}{2}$ and to higher spatial dimensions is presented in sections 4 and 5, respectively. The main results of the paper are summarised in section 6. Some technical aspects are transferred to appendices 1–3.

2. The isotropic case ($\Delta = 1$)

According to the classical picture the isotropic model (1) can be realised in two different phases: for $\beta < \frac{1}{4}$ the ground state is antiferromagnetic while for $\beta > \frac{1}{4}$ the competition between nearest and next-to-nearest neighbours leads to helical ordering with the helix wavevector Q: $\cos Q = -1/4\beta$. Our purpose is to investigate the role of quantum fluctuations for $\beta \geqslant \frac{1}{4}$ in one dimension. We start with the transition point. One can expect the fluctuation effects at $\beta = \frac{1}{4}$ to be stronger than those inside the antiferromagnetic phase due to additional softening of the one-particle spectrum, and one can also expect power law divergences of quantum corrections to arise. A simple way to check this is to apply a bosonisation scheme [5, 6, 18] via the Dyson–Maleev transformation. The Hamiltonian becomes

$$
\begin{aligned}
\frac{H}{2S} = \sum_k (a_k^\dagger a_k + b_k^\dagger b_k)[1 - (1 - \tilde{\gamma}_k)/4] + (a_k^\dagger b_{-k}^\dagger + a_k b_{-k})\gamma_k \\
- \frac{1}{2SN} \sum_{k_i} [2a_1^\dagger b_2^\dagger a_3 b_4 \gamma_{1-3} + (b_1^\dagger b_2 a_3 b_4 + a_1^\dagger a_2^\dagger b_3^\dagger a_4)\gamma_3 \\
- \tfrac{1}{8} a_1^\dagger a_2^\dagger a_3 a_4 (\tilde{\gamma}_{1-3} + \tilde{\gamma}_{2-3} - \tilde{\gamma}_3 - \tilde{\gamma}_4) \\
- \tfrac{1}{8} b_1^\dagger b_2^\dagger b_3 b_4 (\tilde{\gamma}_{1-3} + \tilde{\gamma}_{2-3} - \tilde{\gamma}_1 - \tilde{\gamma}_2)]
\end{aligned}
\tag{3}
$$

where $\tilde{\gamma}_k \equiv \nu_{2k}$. Two-boson fields appear as a reflection of antiferromagnetic short-range ordering: the neighbouring spins on even and odd sites are linked by different types of bosons. The formal non-Hermitity of (3) does not introduce problems since later we shall be interested only in the vertex renormalisation on resonance. The effective long-wavelength version of (3) is obtaining by diagonalising the quadratic form via a unitary transformation and passing to the low-energy limit in fourfold vertices. The result is

$$
\begin{aligned}
\frac{H}{2S} = \sum_k \varepsilon_k (c_k^\dagger c_k + d_k^\dagger d_k) - \frac{1}{4SN} \sum [\Phi_1 (c_1^\dagger c_2^\dagger d_3^\dagger d_4^\dagger + d_1 d_2 c_3 c_4 \\
+ c_1^\dagger c_2^\dagger c_3 c_4 + d_1 d_2 d_3^\dagger d_4^\dagger) + 2\Phi_2 (c_1^\dagger c_2^\dagger d_3^\dagger c_4 + d_1 d_2 c_3 d_4^\dagger) \\
\times 2\Phi_3 (c_1^\dagger d_2 c_3 c_4 + d_1 c_2^\dagger d_3^\dagger d_4^\dagger) + 4\Phi (c_1^\dagger d_2 c_3 d_4^\dagger)].
\end{aligned}
\tag{4}
$$

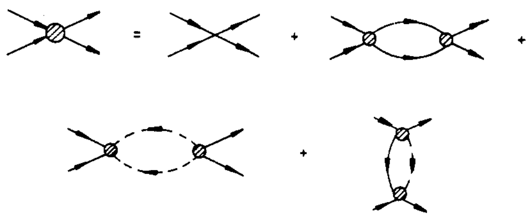


Figure 2. Diagrams representing the vertex renormalisation at the critical point. Full and broken lines represent propagators of the a- and b-type bosons, respectively.

Here $\varepsilon_k = (\sin^2 k)/2$ and

$$\begin{aligned}\Phi_1 &= k_1 k_2 (k_3^2 + k_4^2 - k_1 k_2 - k_3 k_4)/Q \\ \Phi_2 &= -k_1 k_2 (k_3^2 + k_4^2 - k_1 k_2 + k_3 k_4)/Q \\ \Phi_3 &= k_1 k_2 (k_3^2 + k_4^2 - k_3 k_4)/Q \\ \Phi_4 &= -k_1 k_2 (k_3^2 + k_4^2 + k_3 k_4)/Q\end{aligned} \tag{5}$$

where

$$Q = |k_1 k_2 k_3 k_4|.$$

The second-order correction to one of the vertices is presented graphically in figure 2. The corresponding analytical calculations lead to the following result: all the divergent terms in the 'horizontal' and 'vertical' diagrams cancel each other thus leading only to finite (small for $S \gg 1$) corrections. Mathematically, this happens because the difference between the divergent terms in 'horizontal' and 'vertical' channels, opposite in sign, is proportional to

$$\fint \frac{\mathrm{d}p}{p^2 - k^2},$$

which is finite for $k \to 0$, in contrast to the situation in two dimensions when this integral (with an additional factor of p in numerator) is logarithmically divergent (see section 5). We believe this result to be correct for all spin values independently of the parity of $2S$, since, formally, $\beta = \frac{1}{4}$ corresponds to the infinite coupling constant $g = 2S^{-1}(1 - 4\beta)^{-1/2}$ in the O(3) σ-model and the topological θ-term turns out not to be essential. Thus, the gapless critical behaviour at $\beta = \frac{1}{4}$ with the low-temperature specific heat $C \sim T^{1/2}$ survives in the presence of fluctuations. When reaching this point from the antiferromagnetic phase, the dynamically generated mass gap for integer S: $\Delta \sim g^{-1} \mathrm{e}^{-2\pi/g}$ disappears due to the pre-exponential factor.

The next step is to find the instabilities developing below the critical point. First of all the one-particle (magnon) spectrum is decreasing below zero at $\beta > \frac{1}{4}$, indicating the transition into the helical ground state. The classical excitation spectrum above it,

$$\varepsilon_k^2 = \frac{2S^2}{\beta}\left(\frac{1 + 8\beta^2}{4\beta} + 2\nu_k + 2\beta\nu_{2k}\right)\left(1 - \nu_k - \frac{1 - 8\beta^2}{2}(1 - \nu_{2k})\right) \tag{6}$$

contains three Goldstone modes—at $k = \pm Q$, the ordering wavevector, and $k = 0$.

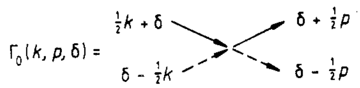
Another possible candidate to occur among the instabilities is that leading to a spontaneous dimerisation. According to Haldane [15], the dimer order parameter for $S=\frac{1}{2}$ is expressed via spin variables as

$$\langle S_n^+ S_{n+1}^- - S_{n-1}^+ S_n^- \rangle = (-1)^n |g|. \tag{7}$$

In terms of bosonic variables the appearance of $|g|$ means the condensation of a two-particle bound state leading to the appearance of an anomalous average in the form $\langle a_k^\dagger b_{-k}^\dagger \rangle = -\mathrm{i}\lambda_k \sin k$ with $\lambda_k = \lambda_{-k}$. We can take

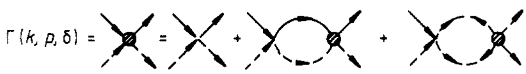
$$|g| \sim 2 \sum_k \lambda_k \sin^2 k. \tag{8}$$

In order to check whether this instability actually occurs one needs to solve these equations for the corresponding two-particle Green functions demanding the bare vertices to be odd in the wavevectors. There is only one vertex in (3) fitting this requirement



$$= -\frac{1}{S} \sin k \sin p.$$

The corresponding Dyson equations are of the ladder type and involve in addition to the 'normal' full vertex $\Gamma(k, p, \delta)$ also the anomalous one



(9)

(10)

The full and broken lines denote Green functions for the a and b magnons, respectively.

The solution of (9) and (10) gives the two branches of the two-particle collective excitations. For $\beta > \frac{1}{4}$ both solutions have a gap and a finite decay width, while at the critical point one of them turns out to be real and gapless near $\delta = 0$:

$$E \approx \frac{S\delta^2}{2}\left(1 - \frac{\delta^2}{4S^2}\right). \tag{11}$$

For $\beta > \frac{1}{4}$, E becomes negative at $\delta = 0$ initiating the development of the instability. We have checked that $\Gamma = -\tilde{\Gamma}$ for the solution (11) and $\Gamma \sim \sin k \sin p$. This implies that $\langle a_k^\dagger b_{-k}^\dagger \rangle \sim \sin k$ and $\langle a_k^\dagger b_{-k}^\dagger \rangle = -\langle a_k b_{-k} \rangle$, or, equivalently $\langle a_k^\dagger b_{-k}^\dagger \rangle = -\mathrm{i}\lambda_k \sin k$ with $\lambda_k = \lambda_{-k}$. Thus we have shown that $\beta = \frac{1}{4}$ is also a critical point with respect to a spontaneous dimerisation.

Our next aim is to prove that in the presence of zero-point vibrations the helical state ceases to be a local minima and shifts to a dimer state which turns out to be the only stable ground state for $\beta > \frac{1}{4}$. Basically, the helical ordering implies the breaking of

SO(3) symmetry, that is the order parameter space is doubly connected. The above analysis shows that the discrete Z_2 symmetry is also broken for $\beta > \frac{1}{4}$. By making the Z_2 degree of freedom 'frozen' we come to a simply-connected order parameter space S_3 coinciding with that in the O(4) σ-model where it is widely believed that fluctuations completely restore the symmetry. Supposing that this restoration really occurs, we are thus left with only a discrete broken symmetry, that is with a dimer state.

The instability of helical configuration can be ascertained also by direct calculations without appeal to the analogy with the σ-model. To do this we start with the classical helical configuration and use the bosonisation procedure based on the Dyson–Maleev transformation. The low-energy theory which arises describes three interacting massless bosons and contains two different types of anharmonic terms. Those linking the excitations with the momentum near 0 and near $\pm Q$, the helical ordering wavevector, are of the same form as in spin nematics with integer S [18] and the corresponding coupling constant undergoes a logarithmic renormalisation, while those for excitations with the momentum only near 0 or only near $\pm Q$ contain additional small factors (in complete analogy with the situation in the XY-model) and can be omitted in the low-energy limit. This situation differs from that in spin nematics with half-integer S [18] where the bare excitations are also three massless bosons, but where the renormalisation group equations are organised in such a way that one boson field decouples from the other two, thus leading to a critical (gapless) behaviour.

Denoting the bosonic variables near 0 as c_k and those near $\pm Q$ as d_k, the effective low-energy Hamiltonian can be written in the following form:

$$
\begin{aligned}
H/c = \sum_k \varepsilon_k(c_k^\dagger c_k + d_k^\dagger d_k) - \frac{2}{N}\sum [\Phi(c_1^\dagger c_2^\dagger d_3^\dagger d_4^\dagger + d_1 d_2 c_3 c_4 \\
+ c_1^\dagger c_2^\dagger d_3 d_4 + d_1^\dagger d_2^\dagger c_3 c_4 - 2\Phi(c_1^\dagger c_2^\dagger d_3^\dagger d_4 + d_1 d_2 c_3^\dagger c_4 - c_1^\dagger c_2 d_3^\dagger d_4^\dagger \\
- d_1 d_2 c_3^\dagger c_4) + 4\Phi c_1^\dagger c_2 d_3^\dagger d_4] \qquad (12)
\end{aligned}
$$

where $\varepsilon_k = |k|$, $c = [(1+4\beta)/4\beta](16\beta^2-1)^{1/2}$ and

$$
\Phi = \frac{k_1 k_2 g}{16(|k_1||k_2||k_3||k_4|)^{1/2}} \qquad g = \frac{1}{S}\left(\frac{4\beta+1}{4\beta-1}\right)^{1/2}. \qquad (13)
$$

The one-loop renormalisation group equation is obtained immediately

$$
\frac{\mathrm{d}g}{\mathrm{d}\ln 1/k} = 2\frac{g^2}{2\pi}. \qquad (14)
$$

As expected, it coincides with that in the O(4) σ-model.

3. The anisotropic case

The classical phase diagram of (1) for arbitrary Δ was discussed in the introduction. Our aim is to show that new phases appear on this diagram when quantum effects are taken into account. In this section the $S = \frac{1}{2}$ model in one dimension will be considered. We start with the lability line of the ferromagnetic phase. To the left of this line the ground state is being realised in an Ising-like ferromagnet. The bosonic version of the spin Hamiltonian (1) is obtained immediately via the Dyson–Maleev transformation:

$$H = E_0 + \sum_k a_k^\dagger a_k[|\Delta|(1+\beta) + \nu_k + \beta\tilde{\nu}_k] - \frac{1}{2N}\sum_k a_1^\dagger a_2^\dagger a_3 a_4 \times \{|\Delta|[\nu_{1-3} + \nu_{2-3} + \beta(\tilde{\nu}_{1-3} + \tilde{\nu}_{2-3})] + \nu_3 + \nu_4 + \beta(\tilde{\nu}_3 + \tilde{\nu}_4)\}. \tag{15}$$

The one-particle excitations soften at $\Delta = \Delta_c$, where

$$\Delta_c = \begin{cases} -\dfrac{8\beta^2+1}{8\beta(1+\beta)} & \beta \geqslant \frac{1}{4} \\ -\dfrac{1-\beta}{1+\beta} & 0 < \beta < \frac{1}{4}. \end{cases} \tag{16}$$

For $\beta = \frac{1}{2}$ softening first occurs at $k = \pi$, while for $\beta > \frac{1}{4}$ this happens at $k = Q$, the helix vector: $\cos Q = -1/4\beta$. At $\beta = 0$ the critical point $\Delta = -1$ reinforces the isotropic ferromagnet and the vertex functions satisfy the Adler principle, that is they tend to zero in the limit of zero momentum. Hence, all the bound states with an arbitrary number of magnons also soften only at the critical point, thus leading to a first-order (but without hysteresis) transition from the Ising-type ferromagnet to the XY antiferromagnet. The situation changes when we switch to the next-to-nearest neighbour exchange. Now the critical value Δ_c reinforces the anisotropic system and the attractive interaction between magnons survives in the limit of zero momentum. As a result the bound states soften before the critical value Δ_c is achieved. For $S = \frac{1}{2}$ only two-particle excitations act on the physical subspace and only two-particle bound states are believed to be relevant.

The two-particle bound-state spectrum was obtained in a standard manner as a pole of the two-particle Green function. As expected, it softens earlier than the one-particle instability comes for all β except $\beta = \frac{1}{2}$ where we run into 'hidden' symmetry. The peculiarity of the $S = \frac{1}{2}$ problem is that for all β between 0 and $\frac{1}{2}$ the two-particle instability occurs first at the total momentum $k = 2\pi$, while for $\beta > \frac{1}{2}$ this first happens at $k = \pm 2Q$ (reminding the reader that $\cos Q = -1/4\beta$, that is $Q = 2\pi/3$ at $\beta = \frac{1}{2}$). The exact expression for the critical value of Δ: $\Delta = \Delta_c^{(2)}$ is sufficiently complicated that we restrict ourselves only with the limiting cases

$$\Delta_c^{(2)} = \begin{cases} \Delta_c - 8\beta^4 & \beta \ll 1, k = 2\pi \\ \Delta_c - 2(\frac{1}{2} - \beta)^2 & \beta \leqslant \frac{1}{2}, k = 2\pi \\ \Delta_c - \dfrac{8}{9}\left(\dfrac{3\sqrt{3}-5}{2-\sqrt{3}}\right)^2 (\beta - 1/2)^4 & \beta \geqslant \frac{1}{2}, k = 2Q. \end{cases} \tag{17}$$

We believe that for $S = \frac{1}{2}$ the two-particle instability is not accompanied by instabilities of higher order, that is the transition is continuous and small condensates, $g_k = \langle a_k^\dagger a_{-k+2\pi}^\dagger \rangle \equiv \langle a_k^\dagger a_{-k}^\dagger \rangle$ or $\tilde{g}_k = \langle a_k^\dagger a_{-k+2Q}^\dagger \rangle$, with g real arise while crossing the critical line $\Delta_c^{(2)}(\beta)$ for $\beta < \frac{1}{2}$ or $\beta > \frac{1}{2}$, respectively. Some calculations favouring this proposal are presented in appendix 1.

The appearance of a non-zero anomalous condensate signifies the breaking of a continuous symmetry with respect to rotations in the XY-plane, since, for example,

$$\frac{1}{N}\sum_k g_k \nu_k = \langle S_l^x S_{l+1}^x - S_l^y S_{l+1}^y \rangle. \tag{18}$$

For $\beta < \frac{1}{2}$ the order parameter space is isomorphic to

$$V = Z_2 \otimes T_1 \tag{19}$$

where T_1 is a projective line, or equivalently, a circle with opposite points identified. The latter restriction is connected with the 'nematic'-type ordering in the XY-plane: $\langle S_x \rangle = \langle S_y \rangle = 0$.

For $\beta > \frac{1}{2}$ the order parameter space in the 'superfluid' phase is a little more complicated. In addition to the $Z_2 \otimes T_1$ degree of freedom an additional twofold discrete degeneracy connected with the 'freezing' of a chiral degree of freedom appears. The order parameter space is now isomorphic to

$$V_1 = Z_2 \otimes Z_2 \otimes T_1. \tag{20}$$

From the formal point of view the appearance of the new phases may be regarded as the splitting $S_1 \Rightarrow Z_2 \otimes T_1$ of the broken degrees of freedom in the XY antiferromagnetic and helical states.

Obviously long-range nematic ordering in the XY plane is impossible in one dimension due to Coleman's theorem. However, orientational ordering and, hence, a massless branch of excitations survives in the presence of quantum fluctuations.

The appearance of a condensate also initiates the density of particles $f_k = \langle a_k^\dagger a_k \rangle$ to be non-zero. The total density does not diverge since one-particle excitations do have a finite gap. Hence, while crossing the critical line $\Delta_c^{(2)}(\beta)$ the magnetisation changes continuously:

$$S_z = \tfrac{1}{2} - \frac{1}{N}\sum_k f_k = \tfrac{1}{2} - O(\Delta - \Delta_c^{(2)}).$$

This justifies the notation of 'superfluid' ferromagnetic for the new phases.

The case $\beta = \frac{1}{2}$ needs a separate discussion. This value of β is singled out since the Hamiltonian (1) can obviously be rewritten as $H = \frac{1}{2}\Sigma_l H_l$, where each H_l describes a triad of equivalently interacting spins:

$$H_l = h_{l-1,l} + h_{l,l+1} + h_{l-1,l+1}. \tag{21}$$

For $S = \frac{1}{2}$ H_l, in turn, can be rewritten in terms of a total spin $\tilde{S}$ of a triad and its Z-projection:

$$H_l = -\tfrac{3}{8}(2 + \Delta) + \tfrac{1}{2}[\tilde{S}(\tilde{S} + 1) + (\Delta - 1)\tilde{S}_z^2]. \tag{22}$$

One can immediately make sure that the ferromagnetic state ($\tilde{S} = \frac{3}{2}$, $\tilde{S}_z = \pm\frac{3}{2}$) minimises H_l for $\Delta < -\frac{1}{2}$, while for $\Delta > \frac{1}{2}$ the dimer state (2) constructed from non-interacting singlets ($\tilde{S} = \frac{1}{2}$, $\tilde{S}_z = \pm\frac{1}{2}$) appears to be the ground state. Thus the intermediate 'superfluid' phase does not realise at $\beta = \frac{1}{2}$. This is also seen from equation (17). The first-order type of the transition makes it unreasonable to expect to detect the dimerisation by looking for an instability which could be revealed in the appearance of a small-dimer condensate, as it was in the isotropic case. On the other hand, the appearance of the two independent gapless collective excitations at the critical points at $k = 2\pi$ and $4\pi/3$, can

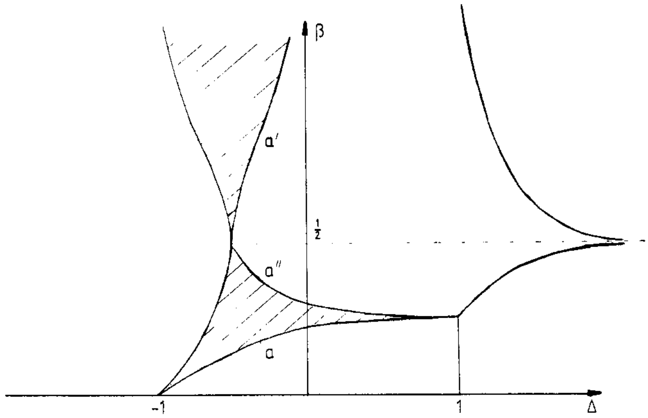


Figure 3. The proposed $T = 0$ phase diagram for the $S = \frac{1}{2}$ model (1) in one dimension. The regions of 'superfluid' phases are shown hatched.

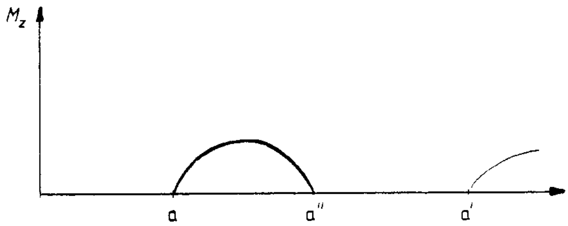


Figure 4. The Z-magnetisation along the line a′a in figure 3.

be regarded as a manifestation of an additional 'hidden' symmetry at $\beta = 1/2$. I believe, though cannot prove by direct calculations, that the massless excitations will interact with each other at $\Delta > -\frac{1}{2}$ inducing a smearing of the 120° triangular plane ordering even in the anisotropic case, that is the dimer state appears to be the only stable ground state for all $\Delta > -\frac{1}{2}$.

Analytical calculations are available only in the vicinity of the line ACD in figure 1. The locations of the other boundaries of the new phases are not known exactly. We believe that in one dimension the entire line BE is split, and the 'superfluid' ferromagnetic states exist for all $|\Delta| < 1$, even in the vicinity of the isotropic model.

The proposed phase diagram for $S = \frac{1}{2}$ is presented in figure 3. Some remarks concerning the line AE are made in appendix 2. This phase diagram differs significantly from the classical one: the helical state completely disappears when quantum fluctuations are included. Instead, two 'superfluid' ferromagnetic states appear, with the dimer state between them. The dimer state also serves as an intermediate state between the Ising-like antiferromagnet and the up–up–down–down spin configuration. The proposed behaviour of the magnetisation M_z along the arbitrarily chosen line aa′ is presented in figure 4.

4. Other spin values

In this section some arguments will be presented, both qualitative and quantitative, favouring the proposal that the main conclusions of the two previous sections, such as dimerisation and the appearance of 'superfluid' phases, remain unchanged for $S > \frac{1}{2}$. However, instead of two-particle instabilities driving the situation in the case of $S = \frac{1}{2}$, the higher-order instabilities connected with the condensation of 4S particle bound states will lead to dimer and superfluid phases in the spin-S model (1). The simplest way to understand this is to take the Ising limit $\Delta \to \infty$. One can immediately make sure that at the classical first-order transition point $\beta = \frac{1}{2}$ a set of dimerised states with $\psi = [12]_s[34]_s$, where

$$[12]_s = (|S\rangle|-S\rangle + e^{i\varphi}|-S\rangle|S\rangle)/\sqrt{2} \tag{23}$$

and φ is arbitrary, satisfy the ground state in addition to the Néel and up–up–down–down spin configurations. The dimer order parameter can be written in the following manner:

$$\langle (S_n^+)^{2s}(S_{n+1}^-)^{2s} - (S_{n-1}^+)^{2s}(S_n^-)^{2s}\rangle \sim (-1)^n g. \tag{24}$$

Clearly, the instability leading to dimerisation is connected with the condensation of the 4S particle bound states.

Another confirmation is given by the analytical calculations performed in the neighbourhood of the point C in figure 1 for a model with $S = 1$. We have shown (the calculations are presented in appendix 3) that an attractive interaction between the two-particle bound states appears at the deviation from the $\beta = \frac{1}{2}$ transition point, resulting in the four-particle bound-state condensation with total momentum $k = 0$ for $\beta < \frac{1}{2}$ and $k = 4Q$ for $\beta > \frac{1}{2}$. The transition is again continuous, and 'superfluid' phases do have a non-zero, though non-nominal, net magnetisation in the z-direction.

Unfortunately, in contrast to the $S = \frac{1}{2}$ case we have failed to find an exact ground-state wavefunction anywhere inside the dimer phase. The suggested ground state for $\beta = \frac{1}{2}$—the state constructed purely from the singlet configurations for nearest neighbours, that is with $\psi = [\overline{12}]\,[\overline{34}]\,[\overline{56}]\ldots$, where

$$[12] = (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle - |00\rangle)/\sqrt{3} \tag{25}$$

(the notation is obvious)—appears to be an eigenstate of (1) only for isotropic model. However, this state does not minimise H_l and we thus cannot prove that non-interacting singlets form a true ground state even in the isotropic case. An attempt was made to construct a simple dimer ground state at the critical point C ($\beta = \frac{1}{2}$, $\Delta = -\frac{1}{2}$), but the only state minimising all the H_l on a circle containing four spins appeared to be the ferromagnetic one. Hence, the dimer ground state at this first-order transition point cannot be constructed from non-interacting dimers, in contrast to the $S = \frac{1}{2}$ case.

5. Higher spatial dimensions

One generally expects antiferromagnets in dimensions of two and more to possess long-range order in the ground state, at least for sufficiently large S. Ioffe and Larkin pointed out that this is not necessarily so for the isotropic model (1) in two dimensions [19]. In reality, the additional softness of the magnon excitations at the critical point $\beta = \beta_c$ ($\beta_c = \frac{1}{4}$ in the quasiclassical consideration) leads to a logarithmically divergent perturbation theory for the coupling constant in the 2D case (see section 2). This being the case it is natural to propose that fluctuations completely restore the continuous symmetry in the neighbourhood of the critical point for arbitrary S. At the same time zero-point vibrations are believed to be small outside the critical region and not to wash away the planar helical ordering. The dimerisation, therefore, turns out to be a purely one-dimensional phenomena for the model considered†. In contrast, 'superfluid' states exist in higher dimensions as well. In reality, these phases appear in the one-dimensional phase diagram as a result of the attractive interaction between the massless bosons. Evidently, this interaction also ensures the condensation of bound states in two dimensions. The only difference is that the 2D critical line $\Delta_c^{(2)}(\beta)$, apart from the one-particle instability line $\Delta_c(\beta)$ only up to exponentially small terms. For $S = \frac{1}{2}$

$$\Delta_c^{(2)} = \begin{cases} \Delta_c - \frac{1}{4}\exp(-\pi/16\beta^2) & \beta \ll 1 \\ \Delta_c - \frac{1}{4}\exp[-\pi/8(\frac{1}{2} - \beta)] & \beta \lesssim \frac{1}{2} \\ \Delta_c - \frac{1}{4}\exp\left(-\frac{3\pi}{16(\beta-\frac{1}{2})^2}\frac{2-\sqrt{3}}{3\sqrt{3}-5}\right) & \beta \gtrsim \frac{1}{2}. \end{cases} \tag{26}$$

In the 3D case the possibility of forming a bound-state condensate depends on the strength of the interaction potential. Nevertheless, the 'superfluid' phase definitely arises in the neighbourhood of the point B ($\beta = \frac{1}{4}$, $\Delta = -\frac{3}{5}$) in figure 1 since the one-particle spectrum demonstrates here an additional softness:

$$\varepsilon_k = \tfrac{1}{2}(1 + \nu_k)^2 \sim k^4. \tag{27}$$

This ensures the bound-state condensation prior to the one-particle instability and, hence, a continuous transition with the intermediate 'superfluid' phase even in three dimensions.

6. Summary

The present paper was devoted to the study of how the quantum fluctuations influence the ground state of antiferromagnets with competing interactions. The main results of this work are the following:

(i) The collinear and non-collinear phases in the 1D isotropic model (1) ($\Delta = 1$) are separated by the critical point $\beta = \beta_c$ ($\beta_c = \frac{1}{4}$ in the quasiclassical case). The excitation spectrum at this point contains two gapless branches (both quadratic in k) which are not seriously affected by fluctuations.

(ii) The critical point $\beta = \beta_c$ simultaneously appears to be the point of instability against spontaneous dimerisation. For $\beta > \beta_c$ quantum fluctuations smear out the classical helical ordering and the dimer state turns out to be the only stable ground state.

(iii) The new phases which we call 'superfluid' ferromagnetic appear in the general phase diagram of (1) in one or two dimensions for any non-zero β except $\beta = \frac{1}{2}$. These phases are characterised by both the non-zero, though non-nominal, Z-magnetisation and the nematic-type ordering in the XY-plane. In the 1D case zero-point vibrations smear out the long-range nematic ordering but orientational ordering survives. In three dimensions the 'superfluid' phase definitely exists in the neighbourhood of the point B in figure 1.

A spontaneous dimerisation in one-dimensional systems with a sufficiently strong antiferromagnetic next-to-nearest neighbour interaction was first predicted by Haldane [15]. He considered the model with an anisotropic ($\Delta \neq 1$) interaction for nearest

† In principle, dimerisation can arise inside the phase with unbroken continuous symmetry.

neighbours and an isotropic interaction for next-to-nearest ones. This model differs from (1) in the anisotropic case. We examined the lability line of the ferromagnetic phase for the Haldane model and found that for $\beta < \frac{1}{4}$ that one-particle instability occurs at the isotropic line $\Delta = -1$. Hence, a preliminary two-particle instability is not realised and, as a consequence, no 'superfluid' phase appears for $\beta < \frac{1}{4}$. In contrast, for $\beta > \frac{1}{4}$ magnon instability occurs at the anisotropic points $\Delta_c = -[1 + (4\beta)^2]/8\beta$ and the solution of the two-particle problem for $S = \frac{1}{2}$ immediately points out the instability against the formation of the anomalous condensate to occur first. For β close to $\frac{1}{4}$ this happens at

$$\Delta_c^{(2)} = \Delta_c - 144(4\beta - 1)^3 \tag{28}$$

and the condensate has the total momentum $2k_c$, where $\cos k_c = -1/4\beta$. Thus, only one type of 'superfluid' state is realised in the Haldane model.

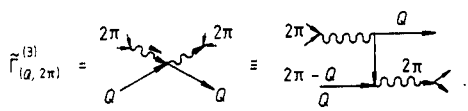
The dimerisation transition in the $S = \frac{1}{2}$ isotropic model was detected in a numerical experiment [20]. The situation in the anisotropic case is less clear. Quite recently Tonegawa and Harada reported [21] their numerical investigations of (1) for $0 < \Delta < 1$. They did not detect any intermediate phase between *XY* and the dimer ones. Though it has been proved in this paper that the 'superfluid' phases definitely exist only in the vicinity of the two-particle instability line and the other boundaries of these phases are not known exactly, I, nevertheless, believe in the phase diagram of figure 3 and hope that further numerical results will clarify the situation.

Acknowledgments

It is a pleasure to thank Professor M I Kaganov and Dr D V Khveschenko for useful discussions.

Appendix 1

Some calculations are presented here favouring the proposal that for $S = \frac{1}{2}$ the two-particle instability is not accompanied by instabilities of higher order. Namely, we shall check the possibility for a preliminary instability due to the interaction between one-particle and collective modes to occur. To do this one must calculate the corresponding bare vertex. The case for $\beta \leq \frac{1}{2}$ will be considered. The diagram of interest is that representing the interaction between a magnon with $k = Q$, the one-particle instability wavevector (full line), and the collective mode with the total momentum 2π (wavy line):



(A1.1)

For zero total frequency $\Gamma^{(3)}_{Q,2\pi}$ is given by the following expression:

$$\Gamma^{(3)}_{Q,2\pi} = \Phi^{(2)}_{Q,2\pi-Q} / \varepsilon_{2\pi-Q} \tag{A1.2}$$

where $\Phi^{(2)}_{Q,2\pi-Q}$ stands for the numerator in the total two-particle vertex function

$\Gamma^{(2)}_{q,2\pi-Q} = -\Phi^{(2)}_{Q,2\pi-Q}/\Omega$ (Ω is the total frequency of two magnons) and $\varepsilon_{2\pi-Q} = \varepsilon_Q \simeq \frac{3}{2}(\Delta_c - \Delta)$ is the magnon excitation energy for $k = Q$. The calculation of Φ demands a solution of the integral equation for the total two-particle vertex function. The result is

$$\Phi^{(2)}_{Q,2\pi-Q} = -9(\tfrac{1}{2} - \beta)^3 \tag{A1.3}$$

that is

$$\Gamma^{(3)}_{q,2\pi-Q} = -6\frac{(\frac{1}{2} - \beta)^3}{\Delta_c - \Delta}. \tag{A1.4}$$

Solving then the integral equation for the total vertex $\tilde{\Gamma}^{(3)}_{Q+2\pi}$ we obtain the condition for the three-particle instability to occur. It is

$$1 = \frac{6(\frac{1}{2} - \beta)^3}{\Delta_c - \Delta}\frac{1}{N}\sum_q I_q^{-1} \tag{A1.5}$$

where

$$I_q = \tfrac{3}{2}(\Delta_c - \Delta) + \left(\cos q + \frac{1}{4\beta}\right)^2 + E_{Q-q} \tag{A1.6}$$

and E_k is the two-particle bound-state energy. By comparing this result with that leading to equation (17) we may be certain that the preliminary three-particle instability does not occur since $\Delta_c^{(2)}$ given by (17) is the solution of the equation identical to (A1.5) but without E_{Q-q} term in (A1.6).

Appendix 2

A qualitative explanation is presented here of how the transition occurs on the line AE on the general $S = \frac{1}{2}$ 1D phase diagram. The aim is to ascertain the grounds for the appearance of non-zero value of S_z if one starts from the XY-phase. The fermionic language will be useful in this context. By applying the Jordan–Wigner transformation [22] one can rewrite the spin Hamiltonian in terms of fermionic variables. To the right of the line ACD the one-particle energy $\varepsilon_k = -\Delta(1 + \beta) + \nu_k + \beta\nu_{2k}$ is negative for k close to π and the density of fermions is non-zero. The Mermin–Wagner theorem demands that

$$\frac{1}{N}\sum_k \langle c_k^\dagger c_k \rangle = \tfrac{1}{2}$$

or, equivalently, that $p_F = \frac{1}{2}\pi$. This is achieved owing to the increase in the Green function numerator while approaching the Fermi level [23]†. The excitation spectrum can be divided into two parts: excitations in the vicinity of the Fermi level which form the Luttinger liquid, and the remaining part which is usually omitted in the macroscopic treatment. It is well known that, in spite of the attractive interaction between 1D massless fermions at the Fermi level, the bound state does not appear since the initial bare interaction experiences an effective logarithmic screening in the zero-sound

† It will be recalled that anywhere in the XY-phase, except for the point $\Delta = \beta = 0$, that the excitations are free bosons but not free fermions [24].

channel [23]. In contrast, the attractive interaction between excitations outside the Luttinger liquid region does not experience a zero-sound-type renormalisation and exactly these excitations ensure that the superfluid transition occurs, since while approaching the critical lines AB or BC the spin wave velocity goes to zero and, hence, the applicability region of the Luttinger liquid theory diminishes. The two-particle condensation changes the spectrum 'far' from the Fermi level. The continuity condition then demands a simultaneous change in the Fermi momentum, which, in turn, leads to the violation of the condition

$$\frac{1}{N}\sum_k c_k^\dagger c_k = \tfrac{1}{2}$$

and to the appearance of non-zero Z-magnetisation.

Appendix 3

In this appendix it will be shown that at the deviation from $\beta = \frac{1}{2}$ an attraction between two-particle bound states appears for $S = 1$, leading to a formation of a four-particle anomalous condensate. The first step to do this is to introduce an additional bosonic field connected with the collective mode. This procedure was discussed in detail in [18]. For the purpose discussed it is convenient to link spin operators with a pair of bosons via the following transformation:

$$\begin{aligned} S_z &= 1 - b^\dagger b - 2a^\dagger a \\ S_+ &= \sqrt{2}(b^\dagger a + Ub) \\ S_- &= \sqrt{2}(a^\dagger b + b^\dagger U). \end{aligned} \tag{A3.1}$$

At $T = 0$ this transformation is exact for the same reasons as the Holstein–Primakoff one: it fits the commutation relations and obeys the constraint $\hat{S}^2 = S(S+1)$ on the physical subspace (formed by the vacuum state and the states with one excited boson of type a or b), in addition, matrix elements between physical and non-physical states are equal to zero. The b-type excitations change S_z to unity and thus correspond to simple spin waves, while a-type excitations overturn single spins and, hence represent two-particle collective excitations.

The determation of the a-type boson Green function demands a solution of a ladder-type integral equation now due to the presence of cubic anharmonicities. In contrast to the case $S = \frac{1}{2}$, two-particle excitations first soften in the vicinity of $\beta = \frac{1}{2}$ only at $k_c = 2\pi - 2Q$ (note that the total momentum value is shifted by 2π in this approach). The instability is realised at

$$\Delta_c^{(2)} = \Delta_c - 2\left(\frac{3\sqrt{3}-5}{7-3\sqrt{3}}\right)^2 (\beta - \tfrac{1}{2})^4.$$

Near its pole the a-type boson Green function is as follows:

$$G_a = \frac{Z}{-E_\delta + \Omega} \tag{A3.2}$$

where $E_\delta = \frac{3}{4}(\delta - k_c)^2$ and $Z \sim (\beta - \frac{1}{2})^2$.

The next step is to construct the vertex function describing the interaction between gapless collective modes. This problem is rather complicated because of the presence of odd anharmonicities. Nevertheless I am convinced by direct calculations that at least near $\beta = \frac{1}{2}$ this interaction is of attractive type: for $\beta > \frac{1}{2}$ the attraction leads to the instability against bound-state condensation with the total momentum $2k_c$ the difference $|\Delta_c^{(4)}| - |\Delta_c^{(2)}|$ is of the order of $Z^4(\beta - \frac{1}{2})^4$, while for $\beta < \frac{1}{2}$ the earliest instability is due to the four-particle bound-state condensation with $k = 0$, the difference $|\Delta_c^{(4)}| - |\Delta_c^{(2)}|$ is now proportional to $Z^4(\beta - \frac{1}{2})^2$.

One can see that if Z-factors are not taken into account, then the situation for $S = 1$ repeats that for $S = \frac{1}{2}$ with the only difference being that the role of one-particle excitations is now played by the two-particle collective modes.

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