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Fluctuations in spin nematics

A V Chubukov

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

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Abstract. Fluctuation effects in nematic-type phases in quantum systems of spin 1 and $\frac{3}{2}$ are examined. The analogue of the Mermin–Wagner theorem is formulated and the perturbation theory is shown to be logarithmically divergent under certain conditions. The low-energy excitations depend on the parity of 2S.

1. Introduction

Interest in fluctuation effects in isotropic magnetic systems has been greatly revived in the last few years. In recent literature there have been many investigations of quantum effects in 1D [1-5] and in some 2D [6] antiferromagnets. In particular, the ground state of the 1D Heisenberg antiferromagnets is believed to depend crucially on the parity of 2S; for integers S, quantum fluctuations destroy not only long-range but also orientational ordering, i.e. the antiferromagnet remains in the paramagnetic phase even at T = 0, while, for odd half-integers S the orientational ordering at T = 0 is retained and the critical theory is that of the Wess–Zumino model with topological coupling k = 1 (and the conformal anomaly C = 1) independently of the value of $S = n + \frac{1}{2}$.

It is the main aim of the present paper to investigate the role of fluctuations in magnetic systems with somewhat different types of ordering at T = 0 (in 2D and higher dimensions), when the averaged microscopic value of the site spin is equal to zero ($\langle S \rangle = 0$), but quadrupolar ordering is present, i.e. $\langle S_x^2 \rangle = \langle S_y^2 \rangle \neq \langle S_z^2 \rangle$. This structure, which was called an axially symmetrical spin nematic [7], appears to be the ground state in the intermediate region between ferromagnetic and antiferromagnetic phases in the so-called generalised quantum spin models described by the isotropic Hamiltonians containing besides the usual Heisenberg exchange interaction $S_1 \cdot S_{1+\delta}$ also monomials of higher order [8, 9]. We recall that the generic spin S exchange Hamiltonian is a polynomial

$$H = \sum_{l,\delta} \sum_{n=1}^{2S} J_n (\boldsymbol{S}_1 \cdot \boldsymbol{S}_{1+\delta})^n$$

and all exchange integrals J_n are generally of the same order of magnitude.

We start with the discussion of some principle fluctuation effects in nematic states on general grounds not appealing to any concrete model. The nematic structures arise as a result of spontaneous breakdown of continuous symmetry: the fixation of the selected axis for quadrupolar correlators. The corresponding order parameter is a real unit vector \mathbf{n} , and the states with \mathbf{n} and $-\mathbf{n}$ are equivalent (the order parameter space is the projective plane P_2). Accordingly, the bare excitation spectrum contains two identical Goldstone branches (two angles, fixing the position of the unit vector on half the sphere). This fact (and to be more exact, the existence of even a single Goldstone mode) enables us to formulate the analogues of the Mermin–Wagner theorem and its quantum version (the Coleman theorem): long-range quadrupolar ordering is impossible at $T \neq 0$ in 2D and 1D spaces and at T = 0 in the 1D case. However, this theorem does not tell us anything about how the correlations decay. It thus appears that this theorem does not allow us to answer the question of whether the correlation length is finite or not.

One might expect the existence of two interacting Goldstone modes in nematic structures to be revealed in a logarithmic increase in the coupling constant g under renormalisation as happens for the usual Heisenberg antiferromagnet [3, 4]. This increase, if also continued outside the region of applicability of perturbation theory, will lead to dynamic mass generation and, for a singlet ground state, to paramagnetism in the 2D and 1D systems at $T \neq 0$ and in 1D systems even in the ground state.

For integers S, this result, if correct, agrees with the Haldane conjecture for a Heisenberg antiferromagnet while, for odd half-integers S, a rigorous theorem exists maintaining that the ground state of the 1D chain either is degenerate or has a gapless spectrum [10]. Then it is reasonable to expect the difference between the ground states for the integer and the half-integer spin values. However, the nature of this difference has nothing to do with that in the Heisenberg antiferromagnet. In fact, in a 1D antiferromagnet the difference arises on doubling of the unit cell, i.e. at the transition from the description in terms of site spins to the description in terms of the unit vector of antiferromagnetism [2, 4]; as the total spin of each neighbouring pair is always an integer, for initially half-integers S the low-energy theory is given by the O(3) σ -model with an additional topological θ -term with $\theta = \pi \pmod{2\pi}$. For half-integers S this term stops the initial logarithmic increase in the coupling constant. In contrast, nematic ordering arises at each site and the topological θ -term does not appear. The ground-state dependence on the parity of 2S now turns out to be a direct consequence of the Kramers theorem. In fact, in the foregoing discussion about dynamic mass generation, we presumed that the order parameter is a *real* unit vector n and the states with n and -n are equivalent but, according to the Kramers theorem, this is possible only for integers S. The calculations given below in §2 for S = 1 confirm that the nematic structure is characterised by a single essential coupling constant, which increases on renormalisation.

Alternatively, for half-integers S the wavefunction of separate spin is the odd-orderrank spinor. Hence, it is impossible to have an invariance concerning time reversal, i.e. the order parameter cannot be a real variable; as well as the vector part, it is also obligatory for it to contain a complex scalar reflecting the fixation of the rotation angle about the selected axis. In spin language this means the appearance of anisotropy for odd-order correlators. This additional breaking of the continuous symmetry is revealed in the appearance of the third Goldstone mode. Correspondingly, the order parameter space is $P_2 \otimes S_1$. We stress that it differs from the projective plane P_3 —the order parameter space of non-collinear antiferromagnet. The calculations, given below in § 3 for a model with $S = \frac{3}{2}$, show that for the logarithmic perturbation theory, in passing to higher scales the interaction between equivalent Goldstone branches (associated with P_2) increases, thus leading to dynamic mass generation, while the interaction of additional Goldstone branch with the other two decreases, and the additional Goldstone mode decouples. Thus the low-energy sector contains an additional *massless* branch of excitations. A similar mechanism causes critical behaviour to develop for the other half-integers S. Note that the difference between integers and half-integers S exists not only in 1D chains at T = 0 but also in 2D systems at finite temperatures. In the latter case there is a finite temperature of the Kosterlitz-Thouless-type transition for half-integers S. The correlation functions are presented in § 3. It is clear that there are both exponentially and power-law decaying correlations.

Another question is whether the process of dynamical mass generation immediately above the ground state for integers S really leads to a singlet ground state as happens in a 1D antiferromagnet where the low-energy theory is given by the O(3) σ -model [1]. Strictly speaking, in the perturbative approach we work with a simply connected order parameter space, i.e. we substitute P_2 by S_2 . Meanwhile, the first homotopy group for P_2 is non-zero: $\pi_1(P_2) = Z_2$; so this substitution may be regarded as freezing of the Z_2 degree of freedom. Then it is reasonable to assume twofold degeneracy of the ground state which most probably corresponds to dimerisation. An example is the well known Majumdar-Ghosh ground state for $S = \frac{1}{2}$ [11]. We cannot definitely answer whether quantum fluctuations in 1D always transfer a nematic state into a dimerised state. In our opinion, both situations (singlet ground state and twofold degeneracy) are possible. This question is discussed in more detail in § 2.

The possibility of calculating the fluctuation effects demands, first of all, a concrete definition of the Hamiltonian, then knowledge of the procedure of bosonisation and, at least, weak non-ideality of the arising Bose gas. The ordinary transformations linking spin operators with a single boson are invalid since they assume dipole ordering. Meanwhile, the transition from ferromagnetic or antiferromagnetic phases to the nematic phase is connected with the condensation of 2*S*-magnon bound states [12].

Thus it is convenient to explore the transformations linking spin S with 2S bosons; roughly speaking, each boson describes the transition from the ground state of a separate spin to one of the excited states.

Below we shall explore the following transformations for S = 1 and $S = \frac{3}{2}$ (the index of the site is omitted):

$$S = 1: \qquad S_z = -i(a^+b - b^+a)$$

$$S_x = -i(b^+U - Ub)$$

$$S_y = -i(Ua - a^+U)$$
(1)

where

$$U = (1 - a^{+}a - b^{+}b)^{1/2}$$

and

$$S = \frac{3}{2}: \qquad S_{z} = -\frac{3}{2}(c^{+}U_{1} + U_{1}c) + \frac{1}{2}(b^{+}b - a^{+}a)$$

$$S_{+} = \sqrt{\frac{3}{2}}(a^{+}U_{1} + a^{+}c) + 2b^{+}a + \sqrt{\frac{3}{2}}(U_{1}b - c^{+}b) \qquad (2)$$

$$S_{-} = \sqrt{\frac{3}{2}}(b^{+}U_{1} - b^{+}c) + 2a^{+}b + \sqrt{\frac{3}{2}}(U_{1}a + c^{+}a)$$

where

$$U_1 = (1 - a^+a - b^+b - c^+c)^{1/2}$$

For S = 1 the transformation was first proposed in [9]. An analogous transformation although written in a slightly different manner was earlier developed in [13]. In both transformations (1) and (2) the physical states of a separate spin are represented by a vacuum state and the states with only one excited boson. The commutation relations together with the constraint $\hat{S}^2 = S(S + 1)$ are satisfied in a physical subspace. As the matrix elements between physical and non-physical states are equal to zero, the accuracy of both transformations (1) and (2) is the same as that of the well known Holstein– Primakoff transformation for $S = \frac{1}{2}$; they are *exact* at T = 0 and at non-zero temperatures the kinematic interaction will cause the appearance of irrelevant exponentially small corrections (see e.g. [14]), which we shall not take into account.

Moreover, for the simplification of calculations it is convenient to modify the form of the transformations, eliminating the radicals. This is done in complete analogy with the passage from the Holstein–Primakoff to the Dyson–Maleev transformation [15].

The averaging of (1) and (2) over the vacuum state gives, for S = 1,

$$\langle S_i \rangle = 0$$
 $\langle S_z^2 \rangle = 0$ $\langle S_x^2 \rangle = \langle S_y^2 \rangle = 1$ (3)

and, for $S = \frac{3}{2}$,

$$\langle S_i \rangle = 0 \qquad \langle S_z^2 \rangle = \frac{9}{4} \qquad \langle S_x^2 \rangle = \langle S_y^2 \rangle = \frac{3}{4} \langle S_x^3 \rangle = \frac{3}{4} \qquad \langle S_y^3 \rangle = 0 \qquad \langle S_z^3 \rangle = 0.$$

$$(4)$$

In both cases the averaged value of the site spin equals zero; the z axis singles out the anisotropy direction for the quadrupolar correlators but, also, for $S = \frac{3}{2}$ the cubic correlators are simultaneously anisotropic, and this causes the appearance of the additional Goldstone mode.

The weakness of non-ideality of the Bose gas here implies the density of particles to be small because the interaction between bosons is always strong. We shall see below that this condition is valid near the point (S = 1) or the line $(S = \frac{3}{2})$ of the first-order transition from the ferromagnetic to the nematic phase. Accordingly, the closeness to the critical point (or line) indicates the small parameter of the problem.

The organisation of the paper is as follows: § 2 is devoted to the generalised model for S = 1. The bosonic version of the spin Hamiltonian suitable for the nematic phase will be constructed and the fluctuation corrections to the excitation spectrum and quadrupolar components together with the renormalisation group equation for the coupling constant will be obtained. We shall also discuss the effect of the magnetic field and consider separately the renormalisation equations at the points where the nematic phase merges with the ferromagnetic or antiferromagnetic phase. At the end of this section we shall briefly discuss the role of fluctuations in the so-called 'orthogonal' nematic structure [8]—the other possible intermediate phase between the ferromagnetic and antiferromagnetic phases. The generalised model for $S = \frac{3}{2}$ will be considered in detail in § 3 and special attention will be given to the nematic state (4). We shall carry out bosonisation and obtain the renormalisation group equations which will allow us to justify the statements made in § 1 and to predict the behaviour of various correlation functions. The main results of the work are summarised in § 4.



Figure 1. T = 0 phase diagram of the generic S = 1 model (in 2D and higher dimensions). The ferromagnetic (FM) phase is stable at $5\pi/4 > \gamma > \pi/2$, the antiferromagnetic (AFM) phase at $\gamma_0 > \gamma > \gamma_1$, the collinear nematic phase at $5\pi/4 < \gamma < \gamma_1$ and the orthogonal nematic phase at $\gamma_0 < \gamma < \pi/2$. Without short-wavelength renormalisations, $\gamma_0 = \pi/4$ and $\gamma_1 = 3\pi/2$.

2. Spin nematic with S = 1

The most generic exchange Hamiltonian for S = 1 and short-range interaction can be parametrised by a single parameter γ [2, 9]:

$$H = J \cos \gamma \sum_{l,\delta} \mathbf{S}_l \cdot \mathbf{S}_{l+\delta} + J \sin \gamma \sum_{l,\delta} (\mathbf{S}_l \cdot \mathbf{S}_{l+\delta})^2$$
(5)

where $0 \le \gamma < 2\pi$. For $\gamma = 0$ or π , expression (5) reduces to the usual Heisenberg model. The stability regions of different phases at T = 0 (in 2D or higher dimensions) are presented in figure 1. The ferromagnetic phase is stable at $\pi/2 < \gamma < 5\pi/4$ [8, 9, 12]. The loss of stability may occur in two ways: at $\gamma = \pi/2$ the whole branch of magnon (one-particle) excitations $\varepsilon_k^{(1)}(\gamma) = -JZ \cos \gamma (1 - \nu_k)$ (Z is the coordination number) softens to zero, i.e. one-particle instability occurs for all k, while at $\gamma = 5\pi/4$ the instability is because of the softening of the two-particle bound state at $k = 2\pi$. At the critical point $\gamma = 5\pi/4$ the dispersion of the soft two-particle branch $\varepsilon_k^{(2)} = JZ(1 - \nu_k)/\sqrt{2}$ coincides with $\varepsilon_k^{(1)}$.

The stability region of the antiferromagnetic phase can be determined only approximately in that this phase contains strong zero-point vibrations. However, we again come across two different types of instability: one-particle instability, when the whole magnon branch softens to zero, and two-particle instability, when the two-particle bound state is lowered below the antiferromagnetic vacuum [4, 9]. The extrapolation of the results obtained in the quasi-classical approximation ($S \ge 1$) [4] to S = 1 determines the stability region of the antiferromagnetic phase as an interval $\gamma_0 < \gamma < \gamma_1$; at $\gamma = \gamma_0 = \tan^{-1}\{4[1 - \sum_k (1 - \nu^2)_k^{1/2}]\}^{-1}$, one-particle instability occurs, while $\gamma = \gamma_1 = \pi + \tan^{-1}\{4[1 - \frac{3}{2}\sum_k (1 - \nu_k^2)^{1/2}]\}^{-1}$ is a critical point for two-particle instability.

We focus our attention on the intermediate phases that are stable at $5\pi/4 > \gamma > \gamma_1$ and $\gamma_0 < \gamma < \pi/2$. We start with the first region. The elementary calculations show that at the lability point ($\gamma = 5\pi/4$) any symmetrised state with an arbitrary number of flipped spins ($S_i^z = -1$) relative to the ferromagnetic vacuum ($S_i^z = 1$) is an eigenstate with energy equal to that of the ferromagnetic state. In other words, the barrier between two ferromagnetic ground states disappears at the critical point. Hence, it is most likely that the state equally moved away from both ferromagnetic states (i.e. nematic state (3) in the redefined axes) to be the ground state below the critical point. We call this state a collinear nematic state. The bosonic version of the spin Hamiltonian is obtained by using the modified variant of the transformation (1). The result is $(1 = k_1, 2 = k_2, \text{etc})$

$$\frac{H}{(-JZ\cos\gamma)} = (1 - \nu_{k} + \delta)(a_{k}^{+}a_{k} + b_{k}^{+}b_{k}) - \frac{1}{2}\delta\nu_{k}(a_{k}^{+}a_{-}^{+} + a_{k}a_{-k} + b_{k}^{+}b_{-k}^{+} + b_{k}b_{-k})$$

$$- \frac{1}{2}\sum_{k_{i}} (a_{1}^{+}a_{2}^{+}a_{3}a_{4} + b_{1}^{+}b_{2}^{+}b_{3}b_{4} + 2a_{1}^{+}b_{2}^{+}a_{3}b_{4})$$

$$\times (\nu_{1-3} + \nu_{2-3} - \nu_{3} - \nu_{4}) + \frac{1}{2}\delta\sum_{k_{i}} \{(b_{1}^{+}b_{2}^{+}a_{3}^{+}a_{4} + a_{1}^{+}a_{2}^{+}b_{3}^{+}b_{4})$$

$$\times (\nu_{1} + \nu_{2}) + \frac{2}{3}(a_{1}^{+}a_{2}^{+}a_{3}^{+}a_{4} + b_{1}^{+}b_{2}^{+}b_{3}^{+}b_{4})(\nu_{1} + \nu_{2} + \nu_{3})$$

$$- [a_{1}^{+}a_{2}^{+}a_{3}a_{4} + b_{1}^{+}b_{2}^{+}b_{3}b_{4} + \frac{1}{2}(b_{1}^{+}b_{2}^{+}a_{3}a_{4} + a_{1}^{+}a_{2}^{+}b_{3}b_{4})]$$

$$\times (\nu_{1-3} + \nu_{2-3}) - 2a_{1}^{+}b_{2}^{+}a_{3}b_{4}\nu_{2-4}\}.$$
(6)

The conversion of momentum is presumed. $\delta = \tan \gamma - 1$ is the non-ideality parameter. At $\delta = +0$, i.e. at the transition point, the Hamiltonian evidently describes the system of two interacting ferromagnets with $S = \frac{1}{2}$; zero-point vibrations are absent and (3) is an exact ground state. On passing into the nematic phase, zero-point vibrations arise and it becomes necessary to diagonalise the quadratic form.

When this is done without anharmonic corrections, the resulting spectrum consists of two coinciding branches linear at small k:

$$\varepsilon_k^{(0)} = (-JZ\cos\gamma)(1+\delta)^{1/2}\{(1-\nu_k)[1-\nu_k+\delta(1+\nu_k)]\}^{1/2}.$$
 (7)

At $\gamma_1^{(0)} = 3\pi/2$, both branches undergo softening at the edge of Brillouin zone, leading to the transition into the antiferromagnetic state. Anharmonic effects shift the critical value of $\gamma_1^{(0)} \rightarrow \gamma_1$.

The anharmonic corrections to the spin-wave velocity were calculated at $\delta \leq 1$ using ordinary methods [16, 17]. The corresponding diagrams are presented in figure 2. Strong exchange interaction forces summarise the ladder sequence of diagrams that become virtually revealed in the renormalisation of non-diagonal terms in the quadratic form

$$\delta \nu_k \Rightarrow B_k = \delta [1 - W(1 - \nu_k)] \tag{8}$$

where

$$W = \sum_{k} \frac{-ZJ\cos\gamma}{\varepsilon_{k}^{(0)}}$$

and coincide with the Watson integral [15] at the critical point. Other total vertices

Figure 2. Diagrams for the selfenergies which take part in the spinwave velocity renormalisation in the leading order in δ . coincide with the bare vertices in the leading order in δ . The final answer is the following:

$$\varepsilon_k = Ck \qquad C = (-ZJ\cos\gamma)(2\delta/Z)^{1/2}[1+\varphi(\delta,T)]^{1/2} \tag{9}$$

where

$$\varphi(\delta, T) = \frac{5}{2} \sum_{k} \left(\frac{B_{k} \nu_{k} - (A_{k} - \tilde{\varepsilon}_{k})}{\tilde{\varepsilon}_{k}} - 2 \frac{A_{k} - B_{0}}{\tilde{\varepsilon}_{k}} n_{k} \right).$$
(10)

Here $A_k = 1 - \nu_k + \delta$, $\tilde{\varepsilon}_k = \varepsilon_k/(-ZJ\cos\gamma)$. An explicit expression for $\varphi(\delta, T)$ will be given below.

Zero temperature and thermal fluctuations are responsible also for the renormalisation of quadrupolar components. The corrections are fully expressed in terms of a number of particles above the condensate:

$$N = \sum_{k} \langle a_{k}^{+} a_{k} \rangle = \sum_{k} \langle b_{k}^{+} b_{k} \rangle \simeq \sum_{k} \frac{A_{k} - \tilde{\varepsilon}_{k}}{2\tilde{\varepsilon}_{k}} + \frac{A_{k}}{\tilde{\varepsilon}_{k}} n_{k}$$

$$\langle S_{x}^{2} \rangle = \langle S_{y}^{2} \rangle = 1 - N \qquad \langle S_{z}^{2} \rangle = 2N.$$

$$(11)$$

An explicit dependence of $N(\delta, T) = N_1(\delta, 0) + N_2(\delta, \tilde{T})$ on δ and $\tilde{T} = T/(-JZ \cos \gamma)$ is as follows:

$$N_{1}(\delta, 0) = \begin{cases} (\sqrt{2}/12\pi^{2})(Z\delta)^{3/2} & 3D\\ Z\delta/8\pi & 2D \end{cases}$$
(12)

$$N_{2}(\delta, T) = \begin{cases} (\sqrt{3}/4)\tilde{T}^{2}\delta^{-1/2} & 1 \ge \delta \ge \tilde{T} \\ (3/2\pi)^{3/2}\tilde{T}^{3/2}\zeta(\frac{3}{2}) & 1 \ge \tilde{T} \ge \delta \end{cases} \quad (13)$$

logarithmically divergent $2D$
divergent $1D$

The divergence of N at finite temperatures in the 2D and 1D cases and at T = 0 in the 1D case is the obvious reflection of the Mermin–Wagner theorem and its quantum version when applied to the nematic state. In contrast, the leading corrections to the spin-wave velocity are finite:

$$\varphi(\delta, T) = \varphi_{1}(\delta, 0) + \varphi_{2}(\delta, T)$$

$$\varphi_{1}(\delta, 0) = \begin{cases} \delta[(5W - 3)/2] & 3D \\ (5Z/8\pi)\delta \ln(1/\delta) & 2D \\ (5/\pi)\delta^{1/2} & 1D \end{cases}$$

$$\varphi_{2}(\delta, T) = \begin{cases} -(9\sqrt{3}\pi^{2}/4)(\tilde{T})^{4}\delta^{-5/2} & 1 \ge \delta \ge \tilde{T} \\ -5(3/2\pi)^{3/2}(\tilde{T})^{3/2}\zeta(\frac{3}{2}) & 1 \ge \tilde{T} \ge \delta \\ -5[\zeta(3)/\pi](\tilde{T})^{3}\delta^{-2} & 1 \ge \delta \ge \tilde{T} \\ -(5/\pi)\tilde{T}\ln(\tilde{T}/\delta) & 1 \ge \tilde{T} \ge \delta \\ -(5/2\pi)\tilde{T}^{2}\delta^{-3/2} & 1 \ge \delta \ge \tilde{T} \\ -5\sqrt{2}\tilde{T}\delta^{-1/2} & 1 \ge \tilde{T} \ge \delta \end{cases}$$

$$1D$$

$$(15)$$

Nevertheless, as we shall see below, the next to the leading order corrections will be logarithmically divergent sometimes. Before passing to the discussion of this question, we shall briefly discuss the effect of magnetic field. First, the transition point will be shifted into the region of higher tan γ since the magnetic field stabilises the ferromagnetic state; the two-magnon instability will occur at

$$\tan \gamma_{\rm c} = 1 + H^* [[1 - \{ [2H^* + (H^*)^2]^{1/2} - 3H^*/2 \} / (4 - 5H^*/2)]]$$
(16)

where $H^* = H/(-JZ \cos \gamma)$. Another effect is that the transition will now be continuous since switching of the magnetic field singles out one of the ferromagnetic vacuum states. The calculation of the longitudinal magnetisation and excitation spectrum requires knowledge of the single-particle condensate $\langle b_{k=0} \rangle = (\mathcal{N})^{1/2}(i\psi), \langle b_{k=0}^+ \rangle = (\mathcal{N})^{1/2}(-i\psi)$ from the Hamiltonian (7) with an additional term $-H\Sigma_l S_l^x$. The value of ψ and, hence, $\langle S_l^x \rangle = 2\psi$ can be determined by minimising the energy or, equivalently, by demanding all the diagrams with a single outer end to be equal to zero. At $H^* \ll \delta$, we obtain $\psi = H^*/2\delta$. After this has been done, two branches of excitations arise as a result of a simple diagonalisation of quadratic form and in agreement with the general idea the result at $k \ll 1$ is

$$\varepsilon_{k}^{(1)} = \varepsilon_{k} [1 - (H/H_{c})^{2}]^{1/2}$$

$$\varepsilon_{k=0}^{(2)} = H.$$
(17)

Now we return to the purely nematic phase (H = 0) to discuss the coupling constant renormalisation. The first step is to transfer from the initial operators a and b to the new operators c and d diagonalising the quadratic form in (7) and to take the low-energy limit in the expansions of the vertex functions. When this is done, we obtain the following effective Hamiltonian:

$$\frac{H}{C} = \sum_{k} \varepsilon_{k}^{*} (c_{k}^{+}c_{k} + d_{k}^{+}d_{k}) + \Phi(c_{1}^{+}c_{2}^{+}d_{3}^{+}d_{4}^{+} + d_{1}d_{2}c_{3}c_{4} + c_{1}^{+}c_{2}^{+}d_{3}d_{4} + d_{1}^{+}d_{2}^{+}c_{3}c_{4}) + 2\Phi(c_{1}^{+}c_{2}^{+}d_{3}^{+}d_{4} + d_{1}d_{2}c_{3}^{+}c_{4} - c_{1}^{+}d_{3}^{+}d_{4}^{+}c_{2} - c_{3}^{+}c_{4}d_{1}d_{2}) - 4\Phi c_{1}^{+}d_{3}^{+}c_{2}d_{4}$$
(18)

where

$$\Phi = \left[\frac{\delta^{1/2} (Z/2)^{1/2} / 8(|k_1||k_2||k_3||k_4|)^{1/2} \right] (-|k_1||k_2| + k_1 k_2)$$

$$\varepsilon_k^* = |k| \qquad C = -J(2\delta Z)^{1/2} \cos \gamma.$$
(19)

Diagrams which are responsible for the renormalisation are presented graphically in figure 3. As usual we shall be interested in temperature renormalisation in 2D and in quantum renormalisation in 1D, when the perturbation theory is logarithmically



Figure 3. Diagrams for the coupling constant renormalisation: ——, Green functions for c-type bosons; – – –, Green functions for d-type bosons. Note that 'horizontal' diagrams are absent.

divergent. Direct calculations show that the general structure of the effective Hamiltonian survives after renormalisation but the interaction between two Goldstone bosons increases in passing to the low-energy limit; in the one-loop approximation the coupling constant (i.e. the coefficient g in the front of k_1k_2 in (19)) increases as

$$g = \begin{cases} (1 - TL/2\pi \tilde{J})^{-1} & \tilde{J} = J |\cos \gamma| \approx J/\sqrt{2} & D = 2\\ 1 - L/\pi \tilde{S} & \tilde{S} = \delta^{-1/2} & D = 1 & T = 0 \end{cases}$$
(20)

where $L = \ln(\Delta/k)$ (Δ is the inter-atomic spacing) and, as a result, fluctuations generate the inner scale

$$R_{\rm c} \sim \begin{cases} \Delta \exp(\pi \tilde{J}Z/2T) & \text{2D} \\ \Delta \exp(\pi \tilde{S}) & \text{1D} \end{cases}$$
(21)

below which the perturbation theory is invalid. Note that the next to leading corrections to the spin-wave velocity in the 2D case and to the Z-factor of the Green function in the 1D case also contain logarithmically divergent (as $\ln k$) terms. The corrections are the same as in the Heisenberg antiferromagnet [3, 18]. There are no reasons to expect the increase in g to stop outside the limits of perturbation theory; the scale R_c most probably determines the correlation length in the system and, hence, the mass gap immediately above the ground state. It thus appears that the continuous symmetry is completely restored by fluctuations. The open question is whether the same happens for discrete symmetries; in other words, is the ground state a singlet or is it twofold degenerate (i.e. dimerised)? Now it has been almost established by field-theory arguments [5], numerical calculations [19, 20] and a recently published exact solution of the purely biguadratic model [21] that at least in the region $3\pi/2 \le \gamma < 7\pi/4$ the ground state is dimerised. On the other hand we did not find any trials of instability which might lead to spontaneous dimerisation in the vicinity of the ferromagnetic lability point. The first-order transition from the ferromagnetic to the highly dimerised state also remains undecided since we cannot detect any dimerised state exactly at the critical point. We thus believe that the dimerised and ferromagnetic phases may be separated by the paramagnetic phase with a unique ground state, although this is a subject for further investigations.

Now we discuss the fluctuation effects at the transition points $\gamma = 5\pi/4$ and $\gamma = \gamma_1$ when the nematic phase merges with the ferromagnetic and antiferromagnetic phases. We shall not be interested in short-wavelength renormalisation, i.e. we shall assume that $\gamma_1 = 3\pi/2$. The possibility of another type of behaviour at these points is connected with the increasing number of Goldstone modes; at $\gamma = 5\pi/4$ the excitation spectrum consists of two branches, both quadratic in k (there is only one such branch inside the ferromagnetic phase), and at $\gamma = \gamma_1$ both branches soften at the edge of Brillouin zone and the number of Goldstone modes in the bare spectrum increases from two (inside the nematic and antiferromagnetic phases) to four. We start with $\gamma = 5\pi/4$ ($\delta = 0$), when the Hamiltonian describes the system of two interacting ferromagnets with $S = \frac{1}{2}$. The temperature renormalisation of the vertex is shown in figure 4 and the result is

$$g = (1 - 3TL/2\pi \tilde{J})^{-1}$$
 $\tilde{J} = J|\cos\gamma| = J/\sqrt{2}.$ (22)

The coefficient in front of L is three times greater than in equation (20) and 1.5 times greater than for non-interacting $S = \frac{1}{2}$ ferromagnets. Hence the correlation length is

⁺ The conjecture that the gap exists on both side of the integrable point $\gamma = 7\pi/4$ [22, 23] was first made in [2] and later confirmed by a number of numerical calculations [24].



Figure 4. Diagrams for the temperature renormalisation of the coupling constant at the transition point between the ferromagnetic and nematic phases. The designations are the same as in figure 3.

smaller than inside ferromagnetic and nematic phases:

$$R_{\rm c} \sim \Delta \exp(2\pi J/3T).$$

Now we turn to $\gamma = 3\pi/2$. In order to obtain the effective Hamiltonian we must transfer to the two-sublattice structure that demands the introduction of four types of bosons. The effective Hamiltonian now describes the system of two interacting antiferromagnets with $S = \frac{1}{2}$. When the phase factors are not taken into account (see [4]) the result is

$$H_{0} = JZ(H_{1} + H_{2} + H_{int})$$

$$H_{1} = \sum_{k} (a_{k}^{+}a_{k} + c_{k}^{+}c_{k}) - \nu_{k}(a_{k}c_{-k} + a_{k}^{+}c_{-k}^{+})$$

$$+ 2\sum_{k} (c_{1}^{+}c_{2}^{+}a_{3}^{+}c_{4} + a_{1}^{+}a_{2}^{+}c_{3}^{+}a_{4})\nu_{3} - 2\sum_{k} a_{1}^{+}c_{2}^{+}a_{3}c_{4}\nu_{2-4}$$
(23)
$$(23)$$

$$H_{2} = \sum_{k} (b_{k}^{+}b_{k} + d_{k}^{+}d_{k}) - \nu_{k}(b_{k}^{+}d_{-k}^{+} + b_{k}d_{-k}) + 2\sum_{k_{i}} (b_{1}^{+}b_{2}^{+}d_{3}^{+}b_{4} + d_{1}^{+}d_{2}^{+}b_{3}^{+}d_{4})\nu_{3} - 2\sum_{k_{i}} b_{1}^{+}d_{2}^{+}b_{3}d_{4}\nu_{2-4}$$
(23b)

$$H_{\text{int}} = 2\sum (a_1^+ b_2^+ d_3^+ a_4 + c_1^+ d_2^+ b_3^+ c_4 + b_1^+ a_2^+ c_3^+ b_4 + d_1^+ c_2^+ a_3^+ d_4)\nu_3 - 2\sum_{k_i} (a_1^+ d_2^+ a_3 d_4 + b_1^+ c_2^+ b_3 c_4 + b_1^+ d_2^+ a_3 c_4 + a_1^+ c_2^+ b_3 d_4)\nu_{2-4}.$$
 (23c)

The one-loop renormalisation of the coupling constant is the following:

$$g = \begin{cases} (1 - 3TL/2\pi J)^{-1} & \text{2D} \\ (1 - 3L/\pi)^{-1} & \text{1D} & T = 0. \end{cases}$$
(24)

In both cases the coefficient in front of L is three times greater than inside the nematic or antiferromagnetic phases and 1.5 times greater than for non-interacting antiferromagnets with $S = \frac{1}{2}$.

The answer in the 1D case demands caution, because the doubling of the unit cell leads to the appearance of topological terms in the long-wavelength action. For the present we did not investigate their role in detail.

At the end of this section we shall briefly discuss the situation at $\gamma = \pi/2$ when the whole branch of one-particle excitations becomes zero. One can check immediately that the ground-state wavefunction ψ at $\gamma = \pi/2$ is again a multiplication of the wavefunctions of separate spins ψ_l and any state with $\psi_l = |S_l^z = 0\rangle$, for even l and $\psi_l = (|S_l^z = 1\rangle + \alpha |S_l^z = -1\rangle)/\sqrt{1 + \alpha^2}$ for odd l with arbitrary α is an eigenstate with energy equal to that of the ferromagnetic state. The structure arising below the critical point is a nematic state with a right angle between the selected axes for the nearest neighbours. This ground state was called an 'orthogonal' quadrupolar structure [8]. It is characterised by the existence of a whole branch of excitations with zero energy since the system is invariant with respect to rotation of a selected axis for a separate spin about the direction of this axis for its neighbour. The bosonic version of the spin Hamiltonian is now as follows ($\cos \gamma > 0$):

$$\frac{H}{JZ\sin\gamma} = \sum_{k} (1 - \nu_{k} + \tilde{\delta}\nu_{k})a_{k}^{+}a_{k} - \frac{1}{2}\tilde{\delta}\nu_{k}(a_{k}a_{-k} + a_{k}^{+}a_{-k}^{+}) - \frac{1}{2}\sum_{k_{i}} (a_{1}^{+}a_{2}^{+}a_{3}a_{4} - \frac{1}{2}b_{1}^{+}b_{2}^{+}b_{3}b_{4})(\nu_{1-3} + \nu_{2-3}) - \sum_{k_{i}} a_{1}^{+}b_{2}^{+}a_{3}b_{4}(\nu_{2-4}) + \left(\frac{1}{2}\sum_{k_{i}} b_{1}^{+}b_{2}^{+}a_{3}(\tilde{\nu}_{1} + \tilde{\nu}_{2}) + \mathrm{HC}\right)$$
(25)

where $\tilde{\delta} = \cot \gamma$ and $\tilde{\nu}_k = (2i/Z)\Sigma_{\Delta} \sin(k\Delta)$. For simplicity, we put $\tilde{\delta} = 0$ in the anharmonic terms. As follows from (25), besides the branch with zero energy for all wavevectors ($\varepsilon_k^b \equiv 0$), the bare spectrum also contains the Goldstone mode $\varepsilon_k^{(a,0)} \simeq \delta^{1/2}k$. In particular, at the transition point $\varepsilon_k^{(a,0)} = JZ(1 - \nu_k)$. However, the cubic terms, which describe non-resonance transformation of an *a*-type boson into two excitations with zero energy, lead to strong renormalisation of the bare spectrum since in the limit of low frequency of the *a*-type boson the perturbation corrections diverge. The calculation of the *a*-boson dispersion relation requires us to solve the Dyson equation $G_a^{-1} = G_{a,0}^{-1} - \Sigma(k, \Omega)$ with Σ given by the following sequence of ladder type diagrams $(---- \rightarrow = G_b^{-1} = -1/\Omega)$

$$\Sigma \rightarrow \longrightarrow \rightarrow \longrightarrow + \rightarrow \longrightarrow (26)$$

The substitution of the solution of (26) into the equation for G_a^{-1} gives

$$G_a^{-1} = JZ(1 - \nu_k) - \Omega + (J^2 Z)(1 - \nu_k)/(\Omega - J)$$

= $[2\Omega/(\Omega - J)] \{ JZ[(Z + 1)/Z - \nu] - \Omega \}$ (27)

i.e. when the cubic terms are taken into account the second branch of the spectrum acquires the gap $\varepsilon_k^{(a)} = JZ[(Z+1)/Z - \nu]$. In the 1D case this result coincides with the expression for the two-particle bound-state spectrum in the ferromagnetic phase at $\gamma \Rightarrow \pi/2 + 0$ [11]. At $\gamma = \gamma_0^{(0)} = \pi/4$ (this value was obtained without short-wavelength corrections) the orthogonal nematic structure merges with the antiferromagnetic structure. Detailed calculations of the fluctuation properties of this phase were not carried out.

3. The model for $S = \frac{3}{2}$

The generic exchange Hamiltonian for $S = \frac{3}{2}$ is the following:

$$H = -J \sum_{l,\Delta} [\mathbf{S}_l \cdot \mathbf{S}_{l+\Delta} + \beta (\mathbf{S}_l \cdot \mathbf{S}_{l+\Delta})^2 + \gamma (\mathbf{S}_l \cdot \mathbf{S}_{l+\Delta})^3].$$
(28)

The phase diagram in the $\beta - \gamma$ plane is much more diverse than for S = 1. Bearing in mind that we wish to show the difference between the integers and half-integers S, we shall focus our attention on the region near the boundary between the ferromagnetic phase and the nematic phase (4) at small γ and positive β , γ and J. The calculation of the excitations above the ferromagnetic ground state [11] shows that the two-magnon bound state at $k = 2\pi$ softens on the line

$$1 - \beta/2 + 103\gamma/16 = 0. \tag{29}$$

The peculiarity of $S = \frac{3}{2}$ is that the three-particle instability and, hence, the transition to the nematic phase (4) occur on the same line. In fact, one can easily make sure by direct calculations that any symmetrised state with an arbitrary number of flipped spins $(S_l^z = -\frac{3}{2})$ relative to the ferromagnetic vacuum $(S_l^z = \frac{3}{2})$ is an eigenstate on the critical line with energy equal to that of the ferromagnetic state. Evidently the nematic phase (4) will be the ground state below the critical line. In 3D this structure will be only slightly destroyed by temperature and quantum fluctuations. The corrections differ from those for S = 1 only by numerical factors. Below we shall discuss only the principal effects due to fluctuations, i.e. we shall consider the role of temperature fluctuations in the 2D case and that of quantum effects in 1D chains.

The bosonic version of (28) is obtained by use of the modified version of transformation (3). The quadratic form in Bose operators is described by the expression

$$H_{2} = J_{1}Z\{(1 - \nu_{k} + \delta^{*})(a_{k}^{+}a_{k} + b_{k}^{+}b_{k}) + \delta^{*}\nu_{k}(a_{k}^{+}b_{-k}^{+} + a_{k}b_{-k}) + [\lambda(1 - \nu_{k}) + 3\delta^{*}\nu_{k}]c_{k}^{+}c_{k} + 3\delta^{*}\nu_{k}/2(c_{k}^{+}c_{-k}^{+} + c_{k}c_{-k})\}$$
(30)

where, at $\gamma \ll 1$ and in the vicinity of the critical line $J_1 \simeq 6J$, $\delta^* \simeq (\beta/2 - 1)/8$, $\lambda \simeq 3\gamma/4$. After the diagonalisation one obtains three Goldstone branches reflecting the spontaneous symmetry breaking: two branches with equal spin-wave velocities $C_{1,2} = J_1(2Z\delta^*)^{1/2}$ arise as a result of fixation of the anisotropy axis for quadrupolar correlations while the third Goldstone mode with $C_3 = C_{1,2}(3\lambda)^{1/2}$ arises because of the fixation of the angle of rotations about this axis (the anisotropy of cubic correlators). To simplify the expressions for anharmonic vertices, we shall omit the terms which give zero acting on physical states, and also cubic terms which only renormalise the coefficients. After doing this, we obtain the following expression:

$$H_{\text{int}} = -\frac{1}{2} \sum_{k_i} (a_1^+ a_2^+ a_3 a_4 + b_1^+ b_2^+ b_3 b_4) (1 + \frac{5}{6} \delta^*) (\nu_{1-3} + \nu_{2-3}) - \frac{1}{2} \lambda \sum_{k_i} c_1^+ c_2^+ c_3 c_4 (\nu_{1-3} + \nu_{2-3}) - \sum_{k_i} (a_1^+ c_2^+ a_3 c_4 + b_1^+ c_2^+ b_3 c_4) \nu_{1-4} - 2 \sum_{k_i} (a_1^+ b_2^+ a_3 b_4) (\nu_{1-3} (1 + \frac{7}{6} \delta^*) - \frac{4}{3} \delta^* \nu_{1-4}) - \frac{1}{2} \delta^* \sum_{k_i} (a_1^+ b_2^+ c_3 c_4 + c_3^+ c_4^+ b_2 a_1) (\nu_{1-4} + \nu_{2-4})$$

$$+ \sqrt{\frac{2}{3}} \delta^* \sum_{k_i} (a_1^+ a_2^+ c_3 b_4 + b_1^+ b_2^+ c_3 a_4 + c_3^+ b_4^+ a_1 a_2 + c_3^+ a_4^+ b_1 b_2) (\nu_{2-3} + \nu_{2-4}).$$
(31)

The correct structure of each vertex (which is dictated by symmetry considerations) is restored when short-wavelength renormalisation is taken into account. In particular, we made sure that on the critical line the restoration of the form of vertices to that dictated by the Adler principle occurs in exactly the same way as for the bosonic version of Heisenberg ferromagnet with $S = \frac{1}{2}$ obtained via the Holstein-Primakoff transformation with non-physical terms omitted [25]. However, below, we shall be interested only in coupling constant renormalisation. As the corresponding terms in the fourfold vertices are completely determined by the 'physical' part of interaction, the expression for the effective Hamiltonian can be obtained directly from (31):

$$H = H_2 + H_{\text{int}}^{(1)} + H_{\text{int}}^{(2)} + H_{\text{int}}^{(3)}$$
(32)

where

$$H_{2} = J_{1}(2\delta^{*}Z)^{1/2} \left(\sum_{k} \varepsilon_{k}^{*} (p_{k}^{+}p_{k} + q_{k}^{+}q_{k}) + (3\lambda)^{1/2} \sum_{k} \varepsilon_{k}^{*} t_{k}^{+} t_{k} \right)$$
(32a)

$$H_{\text{int}}^{(1)} = J_1 (2\delta^* Z)^{1/2} \left(\sum_{k_i} \Phi[p_1^+ p_2^+ p_3 p_4 + q_3^+ q_4^+ q_2 q_1 + p_1^+ p_2^+ q_3^+ q_4^+ + q_1 q_2 p_3 p_4 + 2(p_1^+ q_2 p_3 p_4 + q_3^+ q_4^+ p_2^+ q_1 - p_1^+ p_2^+ q_3^+ p_4 - q_1 q_2 p_3 q_4^+) - 4p_1^+ q_2 p_3 q_4^+ \right)$$
(32b)

$$H_{\text{int}}^{(2)} = J_1 (2\delta^* Z)^{1/2} \sum_{k_i} \{ \bar{\Phi}[-2(p_1^+ p_2 t_3^+ t_4 + q_1^+ q_2 t_3^+ t_4 + p_1 q_2 t_3^+ t_4 + p_1^+ q_2^+ t_3^+ t_4) \\ + (p_1^+ p_2 t_3^+ t_4^+ + q_1^+ q_2 t_3^+ t_4^+ + p_1^+ p_2^+ t_3^+ t_4 + q_1^+ q_2^+ t_3^+ t_4 \\ + p_1 q_2 t_3^+ t_4^+ + p_1 q_2 t_3 t_4 + q_1^+ p_2^+ t_3^+ t_4^+ + q_1^+ p_2^+ t_3^+ t_4] \}.$$
(32c)

Here $\varepsilon_k^* = |k|$ and

$$\Phi = -(Z\delta^*/2)^{1/2}g_0(k_1k_2 - |k_1||k_2|)/2(|k_1||k_2||k_3||k_4|)^{1/2}$$

$$\tilde{\Phi} = -(3Z\delta^*/2\lambda)^{1/2}\tilde{g}_0(k_1k_2/2(|k_1||k_2||k_3||k_4|)^{1/2}.$$
(33)

The bare values of the coupling constants g and \tilde{g} are equal to unity.

The anharmonic terms with only *t*-type operators which form $H_{int}^{(3)}$ are exactly the same as in the $S = \frac{1}{2}XXZ$ model after bosonisation. The corresponding order parameter is a complex scalar and, hence, the logarithmic renormalisation of *t*-type vertices is absent when only $H_{int}^{(3)}$ is taken into account. On the contrary, $H_{int}^{(1)}$ serves as an anharmonic part of a system whose order parameter is a spin vector and, thus, on passing to the low-energy limit the interaction between *p* and *q* excitations increases (the diagrams are presented in figure 5). In the one-loop approximation,

$$g = \begin{cases} (1 - TL/\pi J_1)^{-1} & \text{2D} \\ [1 - 2L(\delta^*)^{+1/2}/\pi]^{-1} & \text{1D} & T = 0 \end{cases}$$
(34)

i.e. it is reasonable to expect dynamic mass generation.



Figure 5. Diagrams for the coupling constants g(a) and $\tilde{g}(b)$ renormalisations in generic model for $S = \frac{3}{2}$. —, Green functions for *p*-type bosons; ---, Green functions for *q*-type bosons; $\sim \sim$, Green functions for *t*-type bosons.

After all, $H_{int}^{(2)}$ describes the interaction between the vector and scalar parts of the order parameter. All the diagrams in figure 5(b) have the same sign and lead to zero-charge behaviour of \hat{g} :

$$\tilde{g} = \begin{cases} [1 + (4\sqrt{3}/\pi)(\delta^*/\lambda)^{1/2}L]^{-1} & \text{1D} \quad T = 0\\ (1 + TL/\pi J\lambda)^{-1} & \text{2D} \end{cases}$$
(35)

i.e. on passing to large scales the *t*-mode decouples from *p*- and *q*-type bosons.

As a result the low-energy excitations are completely determined by the scalar part of the order parameter. The critical behaviour is the same as in the $S = \frac{1}{2}XXZ$ model with

$$H = -J_1 \sum_{l,\Delta} (\mathbf{S}_l \cdot \mathbf{S}_{l+\Delta} - \sigma S_l^z S_{l+\Delta}^z),$$

where the role of σ is played by $6\delta^*/\lambda$. In particular, in the 1D case the correlation functions of S^3 and S_z decrease by a power law with the same η as transverse and longitudinal correlations in the XXZ model correspondingly. All the other correlations decay exponentially. The distinction between these two correlation functions is preserved in the 2D case but now $\eta \sim T$ and the correlation length for other spin components contains T in the exponent.

4. Summary and discussion

We summarise briefly the main results of this work.

(i) The ground state of the generic S = 1 exchange magnet may be realised in two nematic phases: collinear and orthogonal phases with different types of low-energy excitations.

(ii) The perturbation theory is developed in the vicinity of the transition point from the ferromagnetic to the collinear nematic phase. The closeness to the critical point serves as a small parameter of the problem. The bosonisation was done using the transformation combining spin operators with 2S bosons.

(iii) The analogues of the Mermin–Wagner and Coleman theorems are formulated: long-range quadrupolar (nematic) ordering is destroyed by fluctuations in 2D at finite temperatures and in 1D even at T = 0.

(iv) For S = 1 the perturbation theory in the 2D case at $T \neq 0$ and in the 1D case at T = 0 is logarithmically divergent; the fluctuations generate an inner scale below which perturbation theory ceases to work. It is reasonable to propose that fluctuations continue to increase outside the limits of validity of perturbation theory, thus leading to dynamic mass generation.

(v) The ferromagnetic lability point $\gamma = \pi/2$ is specified by the existence of a whole branch of excitations with zero energy. All the other excitations have a gap.

(vi) For $S = \frac{3}{2}$ (and for all other half-integers S) the quadrupolar phase is characterised by an additional symmetry breaking concerning the rotations about the selected axis for quadrupolar correlators. This follows from the Kramers theorem which demands that the states for half-integers S be antisymmetrical with respect to time reversal. Hence, the number of Goldstone modes in the bare spectrum is equal to three. In the 2D case at $T \neq 0$ and in the 1D case at T = 0 the perturbation theory for the coupling constant is logarithmically divergent and as a result of calculations the low-energy behaviour is completely described by gapless excitations connected with the scalar part of the ordered parameter. Note that for $S \ge \frac{3}{2}$ we expect the other phases with more complex order parameter (e.g. of the type considered in [26]) to appear in generic phase diagrams in the spaces of 2S - 1 parameters. We also mention that in some sense the nematic structures serve in connection with fluctuations as an intermediate between Heisenberg antiferromagnets and the systems with large single-ion anisotropy; the logarithmic increase in the coupling constant is supported by the vector part of the order parameter (as happens in antiferromagnets) while the difference between the integer and halfinteger spins is due to the difference in the structure of states for a separate spin in agreement with what happens in systems with large single-ion anisotropy (see e.g. [22]).

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