Journal of Magnetism and Magnetic Materials 325 (2013) 125–129

Contents lists available at SciVerse ScienceDirect

Journal of Magnetism and Magnetic Materials

journal homepage: www.elsevier.com/locate/jmmm

Spin nematic and orthogonal nematic states in $S=1$ non-Heisenberg magnet

Yu.A. Fridman [a,*], O.A. Kosmachev [a], Ph.N. Klevets [a,b]

[a] V.I. Vernadsky Taurida national university, Academician Vernadsky ave., 4, 95007 Simferopol, Ukraine
[b] Institut für Physik, Universität Augsburg, Universitätsstraße 1, 86159 Augsburg, Germany

ARTICLE INFO

Article history:
Received 8 May 2012
Received in revised form
13 August 2012
Available online 27 August 2012

Keywords:
Nematic
Orthogonal nematic
Magnon spectrum
Phase transition

ABSTRACT

Phases of $S=1$ non-Heisenberg magnet at various relationships between the exchange integrals are studied in the mean-field limit at zero temperature. It is shown that four phases can be realized in the system under consideration: the ferromagnetic, antiferromagnetic, nematic, and the orthogonal nematic states. The phase diagram is constructed. It is shown that the phase transitions between the ferromagnetic phase and the orthogonal nematic phase and between the antiferromagnetic phase and the orthogonal nematic phase are the degenerated first-order transitions. For the first time the spectra of elementary excitations in all phases are obtained within the mean-field limit.

1. Introduction

Quantum spin systems are excellent objects for searching of the unusual phases. The whole set of the exotic states has been found in them, and the most prominent example is the famous Haldane phase in the integer-spin antiferromagnetic chains [1,2]. Recently, another exotic state – the spin nematic – has been probably discovered in the one-dimensional $LiCuVO_4$ [3,4]. A spin nematic state has zero dipolar order parameter, $\langle \mathbf{S} \rangle = 0$; but the rotational symmetry is spontaneously broken because of the non-zero quadrupolar order parameters $\langle S_\alpha S_\beta + S_\beta S_\alpha \rangle - \frac{2}{3} S(S+1)\delta_{\alpha\beta}$, α, $\beta = x, y\ z$. Generally, the spin-S system can be characterized by the multipolar order parameters $\langle S_{\alpha_1} S_{\alpha_2} \ldots S_{\alpha_n} \rangle$ where $n=1$ corresponds to the dipolar order parameter, $n=2$ – to the quadrupolar order parameter, $n=3$ – to the octupolar, and so on [5]. The states with zero magnetization per site but with the finite multipolar order parameters are a purely quantum phenomenon. For the last twenty years such states have been being actively studied in the crystal magnets [6–9] including the low-dimensional systems [10–12]. This interest is related mainly with the investigation of multicomponent Bose–Einstein condensates of the integer-spin atoms [13–15]. The quadrupolar tensor is uniaxial for spin-1 systems, but the spin nematic states with non-axial symmetry are possible in the systems with higher integer-spin values [16].

The aim of the present work is to build the phase diagram of a completely isotropic spin-1 Hamiltonian and to discuss the interesting properties of the phases with unusual ordering (the spin nematic and the orthogonal nematic). We show that the phase diagram contains the spin nematic and orthonematic states in addition to standard ferro- and antiferromagnetic states within the frameworks of the mean-field approximation. Such an analysis of the phases in non-Heisenberg magnet can be applied to both the two-dimensional and three-dimensional systems. Also, up to our best knowledge, we for the first time obtain the spectra of elementary excitations in all phases.

In the present work we consider the three-dimensional system. In one-dimensional systems the quantum fluctuations destroy the long-range magnetic order in all possible phases except the ferromagnetic phase (where the order parameter is conserved due to its commutation with the Hamiltonian); moreover, the Lieb–Schulz–Mattis theorem requires the ground state to be critical or to have broken translational invariance (is dimerized, trimerized, etc.).

The Hamiltonian that allows to investigate the phases of the non-Heisenberg spin-1 magnet has a very simple form

$$\mathcal{H} = -\frac{1}{2}\sum_{n \neq n'} J(n-n')(\vec{S}_n \vec{S}_{n'}) + K(n-n')(\vec{S}_n \vec{S}_{n'})^2 \qquad (1)$$

where $J(n-n')$, $K(n-n')$ are the constants of the Heisenberg and the biquadratic exchange coupling, respectively; S_n^i is the ith component of the spin operator at the site n.

Let us consider the phases of the system described by the Hamiltonian (1) with respect to the ratio of between the exchange integrals. Besides, we suppose that the magnet is at low-temperature, i.e., the temperature is far below the temperature of magnetic ordering. Previously, the models similar to (1) have been investigated rather extensively [10,17–24]; however, the dynamical properties of spin nematics at various ratios between

* Corresponding author. Tel.: +38 0652 480433.
E-mail address: frid@tnu.crimea.edu (Yu.A. Fridman).

0304-8853/$ - see front matter
http://dx.doi.org/10.1016/j.jmmm.2012.08.027

the exchange integrals are studied insufficiently because of certain mathematical difficulties related with the calculation of the dispersion equation of elementary excitations in two-sublattice non-Heisenberg magnet. We are going to take the advantage of the Hubbard operators' technique [25] to describe the dynamical properties of the model (1). Implementation of the diagram technique for the Hubbard operators allows to develop the regular procedure for calculation of the thermodynamical and dynamical characteristics of the magnet. As it was noted in Ref. [25], all the systems with pair interaction have the same representation in the Hubbard operators' representation which is, without doubts, very convenient while developing the general formalism.

2. Free energy density analysis

The further calculations will be carried out in the representation of irreducible tensor operators. Then the Hamiltonian (1) can be re-written as follows:

$$\mathcal{H} = -\frac{1}{4}\sum_{n\neq n'}[2J(n-n')-K(n-n')](\vec{S}_n\vec{S}_{n'})+K(n-n')O_{2n}O_{2n'} \quad (2)$$

where $O_{2n}O_{2n'} = \frac{1}{3}O_{2n}^0O_{2n'}^0 + O_{2n}^1O_{2n'}^1 + \tilde{O}_{2n}^1\tilde{O}_{2n'}^1 + O_{2n}^2O_{2n'}^2 + \tilde{O}_{2n}^2\tilde{O}_{2n'}^2$; $O_2^0 = 2(S^z)^2 - S(S+1)$; $O_2^1 = \frac{1}{2}[S^z,(S^+ + S^-)]_+$; $O_2^2 = \frac{1}{2}\left[(S^+)^2 + (S^-)^2\right]$; $\tilde{O}_2^1 = \frac{1}{2i}[S^z,(S^+ - S^-)]_+$; $\tilde{O}_2^2 = \frac{1}{2i}\left[(S^+)^2 - (S^-)^2\right]$, and plus sign in subscript denotes anticommutator ($[\ldots,\ldots]_+$). Separating the mean-field values, related with the ordering of the magnetic moment and the quadrupolar moments, in the Hamiltonian (2), one obtains the single-site Hamiltonian

$$\mathcal{H}_0(n) = \Delta - \overline{H}S_n^z - B_2^0O_{2n}^0 - B_2^2O_{2n}^2 \quad (3)$$

where $\overline{H} = \left(J_0 - \frac{K_0}{2}\right)\langle S^z\rangle$; $B_2^0 = \frac{K_0}{6}q_2^0$; $B_2^2 = \frac{K_0}{2}q_2^2$; $\Delta = \frac{1}{2}\left(J_0 - \frac{K_0}{2}\right)\langle S^z\rangle^2 + \frac{K_0}{4}\left[\frac{(q_2^0)^2}{3} + (q_2^2)^2\right]$; $q_2^0 = \langle O_{2n}^0\rangle$; $q_2^2 = \langle O_{2n}^2\rangle$; $J_0 = \sum_{n'}J(n-n')$; and $K_0 = \sum_{n'}K(n-n')$. While deriving Eq. (3), we have taken into account that the non-diagonal quadrupolar averages q_2^i $(i=xy,yz,zx)$ equal zero. Because our main goal is to investigate the ground state at zero temperature when the dimensionality of space is 2 or higher, the mean-field approximation is quite adequate.

Solving the Schrödinger equation with the Hamiltonian (3), one obtains the energy levels of a magnetic ion

$$E_1 = \Delta - B_2^0 - \overline{H}\cos 2\alpha - B_2^2\sin 2\alpha, \quad E_0 = \Delta + 2B_2^0,$$
$$E_{-1} = \Delta - B_2^0 + \overline{H}\cos 2\alpha + B_2^2\sin 2\alpha \quad (4)$$

and the eigenvectors of the Hamiltonian (3)

$$|\psi(1)\rangle = \cos\alpha|1\rangle + \sin\alpha|-1\rangle, \quad |\psi(0)\rangle = |0\rangle,$$
$$|\psi(-1)\rangle = -\sin\alpha|1\rangle + \cos\alpha|-1\rangle \quad (5)$$

Parameter α, introduced in Eqs. (4) and (5), is the parameter of generalized u–v transform and is determined by

$$\tan 2\alpha = B_2^2/\overline{H} \quad (6)$$

We construct the Hubbard operators on the basis of eigenvectors of the Hamiltonian (3), $X^{M'M} = |\psi(M')\rangle\langle\psi(M)|$, related with the spin operators as follows:

$$S^z = \cos 2\alpha(H^1 - H^{-1}) - \sin 2\alpha(X^{1-1} - X^{-11});$$
$$S^+ = \sqrt{2}[\cos\alpha(X^{10} + X^{0-1}) + \sin\alpha(X^{01} + X^{-10})]; S^- = (S^+)^\dagger \quad (7)$$

The Hamiltonian (3) is diagonal in Hubbard operators' representation, $\mathcal{H}_0 = \sum_{M=-1,0,1}E_MH_n^M$ where H^M are the diagonal Hubbard operators.

We will consider two cases:

1. $J(n-n') > 0$, when the single-lattice magnetic structure is realized in the system;
2. $J(n-n') < 0$, when the two-sublattice magnetic structure is realized in the system.

2.1. Phase in single-lattice non-Heisenberg magnet

Let us consider the single-lattice magnetic with $J(n-n') > 0$. As it follows from Eq. (4), in this case, the lowest energy level is E_1, and the order parameters (at $T\to 0$), as it follows from Eq. (7), are given by

$$\langle S^z\rangle = \cos 2\alpha, \quad q_2^0 = 1, \quad q_2^2 = \sin 2\alpha \quad (8)$$

Taking into account the relationships (8) and that the lowest energy level is E_1, the free energy density (per site) can be presented in the low-temperature limit as

$$F = -\frac{J_0 - K_0}{2}\cos^2 2\alpha \quad (9)$$

It should be noted that in the low-temperature limit the free energy density coincides with the average internal energy. Only the terms depending on the parameter α were taken into account while deriving Eq. (9). By minimizing the internal energy (9) with respect to the parameter α, one can find the spin states that are realized in the single-lattice magnet.

1. At $\alpha=0$ and $J_0 > K_0$ we obtain that $\langle S^z\rangle = 1$, $q_2^0 = 1$, $q_2^2 = 0$. Obviously, such values of the order parameters correspond to the ferromagnetic (FM) ordering. The wave-function of the ground state is $|\psi(1)\rangle = |1\rangle$.
2. At $\alpha=\pi/4$ and $J_0 < K_0$ we obtain the following order parameters: $\langle S^z\rangle = 0$, $q_2^0 = 0$, and $q_2^2 = 1$. As we know [19], such an ordering is of the tensor type, and the nematic (N) phase is realized in the system. In this case, the wave-function of the ground state is $|\psi(1)\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |-1\rangle)$.

2.2. Phases in two-sublattice non-Heisenberg magnet

Consider now the two-sublattice system which is realized at $J(n-n') < 0$. First of all, let us consider the case $|J| > |K|$. If we choose the quantization axis along the Z-axis, then the average spin value of the first sublattice (per site) is parallel to the Z-axis, and the average spin value of the second sublattice is antiparallel to this axis. It is reasonable to turn the quantization axis for second sublattice so that the directions of the quantization axes coincide for both sublattices. This simplifies mathematical calculations and allows to consider the two-sublattice magnetic as the single-sublattice system. The unitary rotation $U(\theta) = \prod_n \exp(i\theta S_n^y)$ at angle $\theta = \pi$ transforms the components of the spin operator in the second sublattice to $S_n^x \to -S_n^x$, $S_n^y \to S_n^y$, $S_n^z \to -S_n^z$ (at this, the standard commutation relationships are conserved). The single-site Hamiltonian looks as

$$\mathcal{H}_0(n) = \tilde{\Delta} + \overline{H}S_n^z - B_2^0O_{2n}^0 - B_2^2O_{2n}^2 \quad (10)$$

where $\tilde{\Delta} = -\frac{1}{2}\left(J_0 - \frac{K_0}{2}\right)\langle S^z\rangle^2 + \frac{K_0}{4}\left(\frac{(q_2^0)^2}{3} + (q_2^2)^2\right)$

Solution of the Schrödinger equation with the Hamiltonian (10) yields the energy levels and the eigenvectors coinciding with (3) and (4) with the account of the following substitutions: $\overline{H} \to -\overline{H}$ and $\Delta \to \tilde{\Delta}$. In this case, the free energy density is given by

$$F = \frac{J_0}{2}\cos^2 2\alpha$$