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Dynamics of a spin nematic with $S = 3/2$ on a triangular lattice

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The behavior of the spectra of elementary excitations of a spin nematic with a magnetic ion spin of 3/2 on a triangular lattice in collinear spin states is studied. It is shown that the lattice geometry does not change the dispersion laws in collinear phases. The study of the dependence of the excitation energy on the value of the wave vector showed a weak dependence on the direction of the wave vector

Keywords: spin nematic, triangular lattice, multipole order parameters, excitation spectra.

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1. Introduction

Interest in searching new magnetic states of a substance has been increasing recently [1–10]. Study of models at low temperatures, when the quantum nature of magnetism is revealed, is of particular interest. Magnetic lattice configuration frequently plays a significant role. Thus, compounds with a honeycombed superlattice of magnetic layers interlaid with non-magnetic alkali metal atoms are quasi-two-dimensional systems [11]. Due to the synthesis of such objects, interest in studying the quantum behavior in real systems not exposed to boundary conditions has grown. Thus, frustration occurs in the honeycombed crystal lattice due to the competition of exchange interactions that ultimately defines the spin state of a system [12–14]. Thus, dynamic and static properties of non-Heisenberg magnetic materials with $S = 1$ having a triangular lattice, i. e. a three-sublattice magnetic material, are described in [7–10,15–18]. These states certainly have specific features associated with the features of a lattice, but generally retain the dipole and tensor phase properties [7].

Similar states for the highest spins $S > 1$ are underexplored, but qualitatively new effects, that were not available for the case of $S = 1$, have been identified for them. Thus, for $S = 3/2$, nematic states were found on the square lattice, i. e. phases with $\langle S \rangle = 0$for which time reflection symmetry was impaired due to nontrivial properties of multipole (three-spin) mean values [7,8,19–22]. Due to this, for $S = 3/2$ on the square lattice, antinematic phase may exist, where director-vector is antiparallel in two sublattices [20].

Thus, the studies of the simplest spin nematic model suggest that systems of this kind have several unusual properties. States of this kind were studied extensively in crystal magnets [7–9,15,16,23–24], including low-dimensional systems [8,25,26]. Currently, additional interest in such states has appeared and is associated with the study of properties of ultracold Fermi gases, examples of which include the ^{132}Cs, ^{9}Be, ^{135}Ba gases with $S = 3/2$ in optical lattices with one atom per cell [27–30]. It is also significant that strong non-Heisenberg interaction of magnetic ions is typical of such systems, which is necessary for the existence of nematic states [31].

Study [32] investigates phase states of the spin nematic with the magnetic ion spin of 3/2 on a triangular lattice, including all potential exchange invariants. It is shown that both dipole(ferro-/antiferromagnetic) and tensor (nematic and intinematic) phases might be implemented in the system. This study is devoted to the investigation of behaviors of elementary excitation spectra of the spin nematic with the magnetic ion spin of 3/2 on a triangular lattice in collinear (ferromagnetic and nematic) phases.

2. Model

Let's consider an isotropic magnet with the magnetic ion spin $S = 3/2$ that has a triangular lattice. Hamiltonian of such system, including all admissible spin invariants, is written as:

$$H = -\frac{1}{2}\sum_{n \neq n'}\Big[J(\mathbf{S}_n\mathbf{S}_{n'}) + K(\mathbf{S}_n\mathbf{S}_{n'})^2 + L(\mathbf{S}_n\mathbf{S}_{n'})^3\Big], \qquad (1)$$

where $\mathbf{S}_n$ is the spin operator in the n-th site, J, K and L are exchange integrals, summing in (1) is conducted by all pairs of the nearest neighbors on the triangular lattice. The system will be examined for the low temperature ($T \to 0^0$ K) case because this is the case when quantum properties of the system are most pronounced.

It is more convenient to conduct further calculations in terms of the Stevens operators [33] because a full set of S^i, O_2^l and O_3^l operators is the unitary transformation generator of group $SU(4)$, and unique mean operators are the magnet order parameters. In this case, Hamiltonian (1)

will be written as:

$$H = -\frac{1}{2}\sum_{n\neq n'}\left\{\tilde{J}(\mathbf{S}_n\mathbf{S}_{n'}) + \tilde{K}O^m_{2n}O^m_{2n'} + LO^l_{3n}O^l_{3n'}\right\}, \quad (2)$$

where $\tilde{J} = J - \frac{K}{2} + \frac{587}{80}L$, $\tilde{K} = \frac{K}{2} - L$, are the combinations of exchange integrals and the interconnection between the Stevens operators and spin operators for the system of interest is described in [32]

We restrict ourselves only to the case of positive values of J, K and L, i. e. we will discuss the properties of three-sublattice collinear states with various relations of exchange integrals.

As shown in [32], when $J-K/2+103L/16>0$, then a state with system order parameters equal to $\langle S^z\rangle = 3/2$, $q^0_2 = 3$, $q^0_3 = 3/2$, $q^3_3 = 0$ is advantageous, which corresponds to the ferromagnetic (FM) phase with the maximum possible magnetic moment on a site equal to 3/2. In case of $J - K/2 + 103L/16 < 0$, we have $\langle S^z\rangle = 0$, $q^0_3 = 0$, $q^0_2 = 3$, $q^3_3 = 3$, i. e. nontrivial mean values $\langle (S^+)^3\rangle$ and $\langle (S^-)^3\rangle$ occur and q^3_3 is non-zero. Thus, with such relation of constitutive parameters, nematic state (SN) is implemented with mean magnetic moment on site equal to zero. Note that this nematic state actually differs from that of the spin nematic with $S = 1$. Accordingly, vanishing of $J - L/2 + 103L/16 = 0$ defines the phase transition line of the FM−SN phases.

In mean field approximation, quadrupole mean values in the FM phase are calculated as follows:

$$\langle (S^z)^2\rangle = \frac{9}{4}, \quad \langle (S^x)^2\rangle = \langle (S^y)^2\rangle = \frac{3}{4}. \quad (3)$$

Nontrivial octupole mean value q^3_3 is equal to zero and q^0_3 is a trivial constant that doesn't affect the system behavior. Therefore, quadrupole mean value symmetry is completely defined by the magnetic moment symmetry. Consideration of multipole moments is not exhibited in the ground state symmetry of the FM phase.

quadrupole mean values in the M phase are geometrically represented by a spheroid in spin space. Symmetry of this ellipsoid is defined by the magnetic moment direction that coincides with the major axis of this ellipsoid.

The shape of this quadrupole ellipsoid in SN state is the same as that in the FM phase and is calculated by expression (3). However, the symmetry of SN state actually doesn't contain the C_∞ axes (as the symmetry of lattice cell); it is lower than the symmetry defined by the quadrupole ellipsoid. Actually, unlike the FM state, the following cubic mean values are non-zero in the SN phase:

$$\langle (S^x\cos\chi + S^y\sin\chi)^3\rangle = \frac{3}{4}\cos 3\chi, \quad (4)$$

where the angle χ defines rotation of the spin system about the OZ axis. Mean value is $\langle (S^z)^3\rangle = 0$. Actually, non-zero mean cubic values define the triad axis.

3. Dynamic properties

Let's consider the dynamic properties of the studied system. Elementary excitation spectrum in the obtained phases may be obtained from the Green's function pole analysis [34]. Matsubara Green's functions are defined as follows [22]:

$$G^{\lambda\lambda'}(n,\tau';n',\tau') = -\langle \hat{T}\tilde{X}^\lambda_n(\tau)\tilde{X}^{\lambda'}_{n'}(\tau')\rangle. \quad (5)$$

Calculation was conducted by the diagram technique for Hubbard operators [35]. Dispersion equation defining the elementary excitation spectra is derived and dispersion equation for magnet with $S = 3/2$ is solved considering all possible spin invariants in [20,36]. Dispersion equation was derived using zero-order inverse interaction radius approximation, i. e. only loopless diagrams ($\Sigma^{\alpha\beta}(k,\omega_n) \sim G^{\alpha\beta}_0(k,\omega_n)$, where $G^{\alpha\beta}_0(k,\omega_n)$ is zero Green's function [35]) were taken into account among all irreducible Larkin diagrams.

In low-temperature approximation, three magnon excitation branches will exist, whose spectra are written as:

$$\varepsilon_1(k) = \frac{3}{4}z\left[J - J_k + \frac{3}{2}(K - K_k) + \frac{63}{16}(L - L_k)\right],$$

$$\varepsilon_2(k) = \frac{3}{2}z\left[K - K_k - \frac{5}{4}(L - L_k) + J - \frac{1}{2}K + \frac{103}{16}L\right],$$

$$\varepsilon_3(k) = \frac{9}{4}z\left[(L - L_k) + J - \frac{K}{2} + \frac{103}{16}L\right]. \quad (6)$$

J_k, K_k, L_k are the Fourier components of the corresponding exchange integrals, k is the dimensionless wave vector. When looking at the triangular lattice in the XOY plane, it can be seen that the coordination number is equal to $z = 6$. Assuming the interionic distance $\Delta = 1$, the form of Fourier components of exchange integrals may be found. For example, for bilinear exchange:

$$J_K = \frac{1}{z}\sum_{\bar{\Delta}} J_{n,n+\Delta}e^{i\bar{k}\bar{\Delta}}$$

$$= \frac{J}{3}\left(\cos k_x + 2\cos\left(\frac{k_x}{2}\right)\cos\left(\frac{\sqrt{3}k_y}{2}\right)\right). \quad (7)$$

Figure 1 shows the dependence of the magnon spectra of the studied system on the wave vector in the FM phase. Far from the phase transition line, the spectrum branches ε_i are shown as solid heavy lines. Near the line $J - K/2 + 103L/16 = 0$, the excitation spectrum branches are shown as dashed lines.

The first excitation branch (6) ε_1 is a zero-gap Goldstone mode with the parabolic dispersion law in the long-wavelength limit $k \to 0$, which is typical of the isotropic ferromagnetic material. The analysis shows that the „transverse" spin density oscillations are associated with rotations of the major axis of the quadrupole ellipsoid.

We now discuss the behavior of other excitation modes (6) ε_2 and ε_3. Note that, when the bicubic

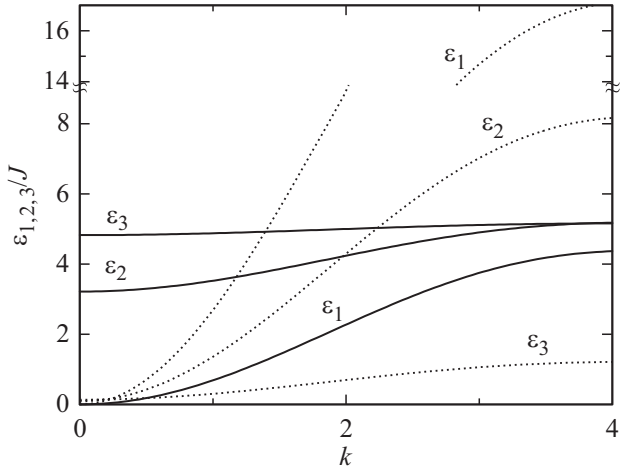

Figure 1. Elementary excitation spectra in the FM phase are shown schematically. Solid lines describe the spectrum behavior in the center of the phase, dashed lines describe the spectrum behavior on the phase transition line to the SN phase ($K = J$ and $L = J/10$ are selected). The first branch is separated for clarity.

exchange interaction constant is equal to zero $L = 0$, only two excitation branches are well defined — ε_1 and ε_2, and the frequency ε_3 becomes a purely local state at $L \to 0$. Note that for a magnet with $S = 1$ at $K = 0$ [37], the non-Heisenberg magnet's specifics disappears: nematic phase is not implemented, and one the modes in the M phase becomes a purely local state. In the limiting case $L = 0$, ε_1 and ε_2 are written in the same way as two collective modes of the spectrum for a magnet with $S = 1$. All this suggests that the physical significance of ε_2 is the same as for the ferromagnetic material with $S = 1$, i.e. the mode with ε_2 describes the „longitudinal" spin behavior [37]. This mode includes longitudinal oscillations of the absolute magnetization vector, which remains parallel to the major axis of the quadrupole moment ellipsoid, and deformation of the other ellipsoid axes without rotation of the major axes. On the other side, ε_3 is defined by the specifics of magnet behavior with $S = 3/2$ which is caused by nontrivial octupole means values.

We consider now the stability of the ferromagnetic phase with respect to arbitrary elementary disturbances that correspond to spectra (6). As is easily seen from the elementary excitation spectra in the ferromagnetic phase, at $k \to 0$ (Figure 1), the magnon branches ε_2 and ε_3 have an energy gap proportional to $J - K/2 + 103L/16$. Hence it appears that condition of stability against uniform disturbances is written as $J - K/2 + 103L/16 > 0$. The same result was obtained above from the free energy analysis (4). Thus, $J - K/2 + 103L/16 = 0$ is the phase transition line between the ferromagnetic and nematic phases.

Near the phase transition line to the SN phase, the gap in the spectrum of ε_2 and ε_3 in the long-wavelength limit $k \to 0$ vanishes (Figure 1).

Analysis of the excitation spectra in the FM phase depending on the wave vector orientation (Figure 2, three directions are shown: OM, OP, ON) has shown that behavior of the excitation branches is almost independent on the spin wave propagation direction.

We next review the excitation spectra in the SN phase. However, note that two excited energy levels of the magnetic ion coincide in this phase, i.e. the system becomes „quasi two-level". This leads to coincidence of two excitation branches. Thus, the excitation spectra in the SN phase are written as:

$$\varepsilon_{1,2}(k) = \frac{3z}{2\sqrt{2}}\sqrt{\left[K - K_k - \tfrac{5}{4}(L - L_k)\right] \times \left[K - \tfrac{5}{4}L - \tfrac{1}{2}\left(J_k + \tfrac{3K_k}{2} + \tfrac{63}{16}L_k\right)\right]},$$

$$\varepsilon_3(k) = \frac{9z}{4}\sqrt{(L - L_k)\left(L - J_K + \frac{K_k}{2} - \frac{119}{16}L_k\right)}. \quad (8)$$

Dispersion patterns of the first two modes coincide, their frequencies remain finite at $L = 0$. From (8), it follows that at $L = 0$ the „octupole" branch frequency $\varepsilon_3 = 0$, and for $\varepsilon_{1,2}$ in the limit $L \to 0$ we have

$$\varepsilon_{1,2}(k) = \frac{3z}{4}\sqrt{(K - K_k)\left(2K - \left(J_k + \frac{3K_k}{2}\right)\right)}, \quad (9)$$

i.e. their spectrum is similar to the elementary excitation spectrum in the nematic phase of the magnet with $S = 1$ [37]. Therefore, $\varepsilon_{1,2}$ describe the quadrupole ellipsoid oscillations, which defines the double degeneracy of these modes. Thus, the main specifics of the system with $S = 3/2$ is defined by ε_3 that is associated with the exchange integral L and caused by the behavior of octupole parameters q_3^3, and represents rotation of the „octupole triangle" about the OZ axis.

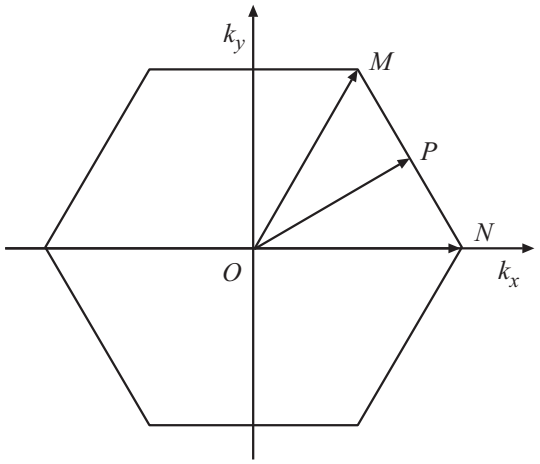

Figure 2. The first hexagonal Brillouin zone. Coordinates of points in the center $O(0, 0)$ and at the boundary $M(2\pi/3, 2\pi/\sqrt{3})$, $P(\pi, \pi/\sqrt{3})$, $N(4\pi/3, 0)$.

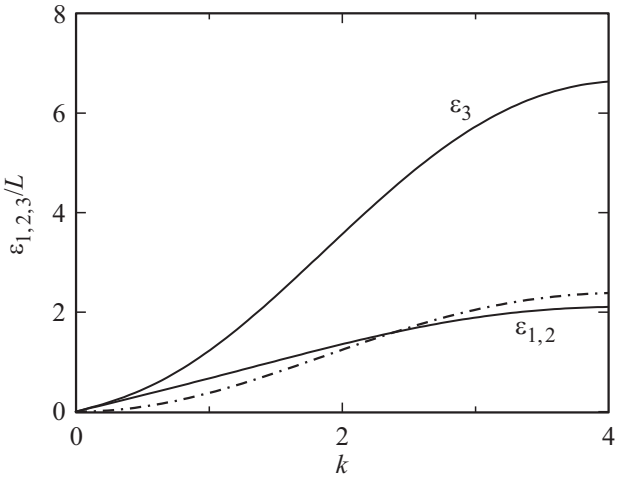

Figure 3. Elementary excitation spectra in the SN phase. Dashed line shows the spectrum of $\varepsilon_{1,2}$ in the vicinity of the phase transition to the FM phase.

Figure 3 shows the behavior of elementary excitation spectra $\varepsilon_{1,2}$ and ε_3 in the nematic phase (equation (8)). For ease of comparison with [20], dependence of the spectra on the wave vector is plotted in terms of L, and recall that this phase is only stable at $L > 0$ [20,32,36]. For plotting $\varepsilon_i(k)$ $(i = 1, 2, 3)$, $K = 2L$, $J/10 = K$ was chosen for clarity as in [20]. Analysis of the dependence of excitation energy on the wave vector shows weak dependence on the wave vector direction (Figure 2). Elementary excitation spectrum also weakly depends on whether far from the phase transition line in FM or on the line $J - K/2 + 103L/16 = 0$.

4. Conclusion

Note first that the mean field approximation used in this work prevents from complete study of the state of the frustrated system, in particular, in a spin-glass phase. However, the goal was to study dynamic properties of collinear states such as ferromagnetic and nematic, for study of which the mean field approximation is quite sufficient (at low temperatures). Investigations of dynamic properties conducted in this work show that the lattice configuration affects the dispersion patterns in collinear ferromagnetic and nematic phases. The number of excitation branches and their behavior throughout the wave vector in the corresponding phases for the triangular lattice is equivalent to a simple square lattice [20,36]. In addition, for adequate comparison of the excitation spectra on the triangular and square lattices, the same exchange integrals were used as in [20]. All exchange integrals both in the ferromagnetic and nematic phases are assumed to be positive. Difference in the coordination number z for the square and triangular lattices was also considered. In [20], the coordination number was taken equal to $z = 2$ for simplicity of calculations, in our case $z = 6$. Differences in the coordination number for various types of lattices make quantitative comparison a little more complicated, but nevertheless such comparison was made. There is a quantitative difference in spectral behavior of the square and triangular lattices. Thus, for the triangular lattice, the „octupole“ excitation branch ε_3 in the ferromagnetic phase (at $L = K$, $L = J/10$ as in [20]) is almost zero-dispersion (Figure 1), while, for the square lattice, this branch has a pronounced dispersion (Figure 1 in [20]). Moreover, the energy of this excitation branch in the triangular lattice is significantly lower than the energy of the same branch for the square lattice. In the nematic phase (at $K = 2L$, as in [20]) , such significant quantitative difference in the excitation spectra for the square and triangular lattices is not available, which is probably due to the fact that the mean magnetic moment in this phase is equal to zero. The absence of qualitative difference in the excitation spectrum behavior for lattices with various configurations is presumably associated with the simple symmetry of collinear phases studied in this work. It is suggested that the study of dynamic properties in the antiferromagnetic and antinematic states of the magnet with $S = 3/2$ on the triangular lattice taking into account all allowable spin invariant system symmetries will make it possible to identify new features in the excitation spectrum behavior.

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Conflict of interest

The authors declare no conflict of interest.

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